20th Israel Materials Engineering Conference (IMEC20)

February 25–26, 2025

International Convention Center in Jerusalem

Dear Colleagues,

On behalf of the Local Organizing Committee, it is my great pleasure to welcome you to the 20th Israel Materials Engineering Conference (IMEC20), which is held at the International Convention Center in Jerusalem on February 25–26, 2025. This internationally recognized conference is part of an ongoing series that begun in 1981. It is the central conference for the materials community in Israel, combining fundamental and applied research. The persistent growth in the number of IMEC attendees over the years reflects an increased prominence of materials-related research in the Israeli academic landscape. IMEC brings together academia, research institutes, industry, investors, non-government organizations, and government representatives to exchange information, consolidate joint research programs, and discuss commercial endeavors and future opportunities.

The conference will cover both classical Materials Engineering topics and recent breakthroughs in the field, including nanomaterials, quantum materials, two-dimensional materials, materials for energy storage and conversion, materials-related issues in additive manufacturing, materials for theranostics in medicine, among others.

The wide range of materials-related topics covered by the conference attracts a broad interdisciplinary audience, including engineers, chemists and physicists, professionals in life sciences and medicine, archeologists, and more. This event will provide a suitable platform for disseminating research results and facilitating the synergistic exchange of ideas. The plenary and invited talks will be given by internationally renowned scholars. A special symposium on Physical Metallurgy, honoring the late Prof. Elazar Gutmanas will feature invited lectures from his colleagues and former students.

The commercial exhibition will showcase the latest equipment, materials, and services available in Israel.

We hope you will enjoy your time at IMEC20!

Sincerely yours,
Eugen Rabkin, Chairman
Alejandro Sosnik and Elad Koren, Local Organizing Committee

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The Materials Research Center
Department of Materials Science and Engineering
Technion - Israel Institute of Technology

Timetable at a Glance

	Tuesday, February 25, 2025				
	Registration Area, Foyer, Exhibition Area				
8:00-9:00	**Registration, Coffee Break, Poster Mounting**				
	Hall A				
9:00-9:10	**Opening Ceremony**				
	Hall A				
9:10-9:55	**Plenary 1** **Grain Growth is Not Curvature Flow: Why? Consequences?**				
9:55-10:40	**Plenary 2** **Magnesium Technologies for Aviation and Aerospace Applications**				
	Foyer, Exhibition Area				
10:40-11:10	**Coffee Break, Poster Viewing**				
	Hall A	Hall B	Hall C	Hall D	Hall E
11:10-13:10	**Nanomaterials**	**Polymers & Colloids**	**2D Materials**	**Materials in Archeology**	**E. Gutmanas Symposium**
	Foyer, Exhibition Area				
13:10-14:40	**Lunch Break & Poster Session**				
					Hall E
13:30-14:30					**How to Start Writing and Get Your Research Paper Done**
	Hall A	Hall B	Hall C	Hall D	Hall E
14:40-16:40	**Materials for Energy** *(14:40-16:55)*	**Bio- & Soft Materials I** *(14:40-16:30)*	**Ceramics and Composites**	**Quantum Materials**	**Mechanical Properties & Failure**
	Foyer, Exhibition Area				
16:40-18:10	**Welcome Reception & Posters**				

	Wednesday, February 26, 2025					
	Registration Area, Foyer, Exhibition Area					
8:00-9:00	**Registration, Coffee Break, Poster Mounting**					
	Hall A					
9:00-9:45	**Unveiling the Art of Self-Assembly in the Creation of Diverse Biomaterials**					
9:45-10:30	**Materials Science Challenges in Developing High Energy, Safe and Durable Rechargeable Batteries**					
	Poster Area, Exhibition Area					
10:30-11:00	**Coffee Break, Poster Viewing**					
	Hall A	Hall B	Hall C	Hall D	Hall E	Hall F
11:00-13:00	**Computational MS I**	**Surfaces & Interfaces**	**Additive Manufacturing I**	**Functional Materials**	**Physical Metallurgy**	**Bio- and Soft Materials II** *(11:00-12:55)*
	Foyer, Exhibition Area					
13:00-14:30	**Lunch Break & Poster Session**					
	Hall A	Hall B	Hall C	Hall D	Hall E	Hall F
14:30-16:30	**Computational MS II**	**Materials for Extreme Conditions**	**Materials Physics** *(14:30-16:35)*	**Materials Characterization**	**Corrosion & Electrochemistry**	**Additive Manufacturing II**
	Foyer, Exhibition Area					
16:30-17:00	**Coffee Break, Poster Viewing**					
	Hall A					
17:00-17:45	**Archaeometallurgy and Underwater Technologies for Cultural Heritage in the Eastern Mediterranean: Data Capture, Curation, Analyses and Dissemination**					
	Hall A					
17:45-18:15	**Best Poster Prize Announcement & Closing Remarks**					

General Information

VENUE
1 Shazar Blvd.
Jerusalem
Jerusalem
Tel: +972-2-6558558

PARKING
ICC guests may use the roofed or open-air parking spaces, both easily accessible for everyone, including people with disabilities. Select on Waze Binyaney Hauma Teddy Parking lot.
Rate: NIS 70 per day.

REGISTRATION & HOSPITALITY DESK
Registration and distribution of the Conference material will take place throughout the Conference, from 08:00 until the end of the last session.

BADGES
All participants and exhibitors are required to wear their badges throughout the congress.

GUEST ATTENDANCE POLICY
All event activities (including educational sessions, meal functions, exhibition area, etc.) are exclusively reserved for registered attendees. Badges provided at registration are required for entrance into all functions and will be strictly enforced.

REFRESHMENTS
Refreshment will be served in the exhibition and poster area at the time indicated in the program.

INTERNET
Free WI-FI will be available at all conference areas.

WEAPONS
Please note that no weapons of any kind are allowed at the ICC and no option to deposit weapons is available on-site.

IMEC20 SECRETARIAT
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Conventions Department
Tel: +972(0)73-3945279

Information for Speakers

PREPARATION

Presentation must be prepared in Microsoft-PowerPoint(*pptx) and compatible with Windows 11.
Presentation slides must be prepared with 16:9 format (landscape orientation).
All presentations will be delivered in English.
Please use a USB memory stick and name the file with time of Presentation, your Surname, presentation day and session Hall name (e.g. “830_Doe_Tue_Oren 1.pptx”).

ONSITE

Lecture halls are equipped with a set of screen/projector/laptop computer/wireless PowerPoint advancer and a set of loudspeakers/Audio mixer/microphone and Audio PC connection at the lectern.
The use of the provided laptops is mandatory.
The resolution of the projector is 1920 x 1200 pixels.
Technicians will be at the session halls throughout the Conference days.
Presenters are asked to hand the electronic file(s) of their presentation to the technicians at their session hall at least one hour prior to the beginning of their respective session.

IMPORTANT

It is required that your presentation strictly adheres to the given presentation talk time, as stated in the program.
Please find below the length of various presentation formats:

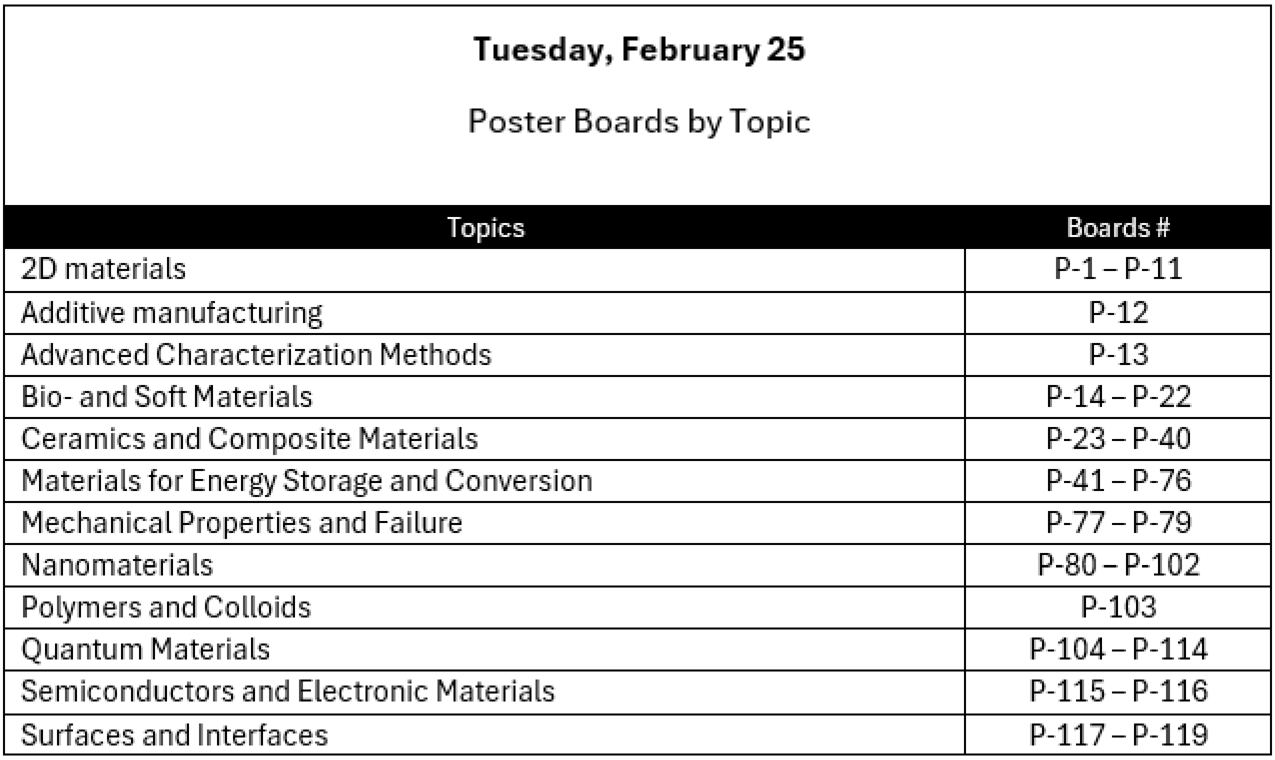
- Plenary talk: 45 minutes (42 minutes presentation + 3 minutes Q&A)
- E. Gutmanas Symposium – please make sure to check your invitation letter
    - Invited speaker: 25 minutes (23 minutes presentation + 2 minutes Q&A), or
    - Feature speaker: 15 minutes (14 minutes presentation + 1 minute Q&A)
- Parallel talk: 25 minutes (23 minutes presentation + 2 minutes Q&A)
- Oral abstract presentation: 15 minutes (13 minutes presentation + 2 minutes Q&A)

Information for Poster Presenters

PRESENTATION DAY 1

Tuesday, February 25

Poster Session 1: 13:10-14:40 on Tuesday, February 25
Poster Mounting Time 1: 8:00 on Tuesday, February 25
Poster Removal Time 1: 18:10 on Tuesday, February 25



Tuesday, February 25

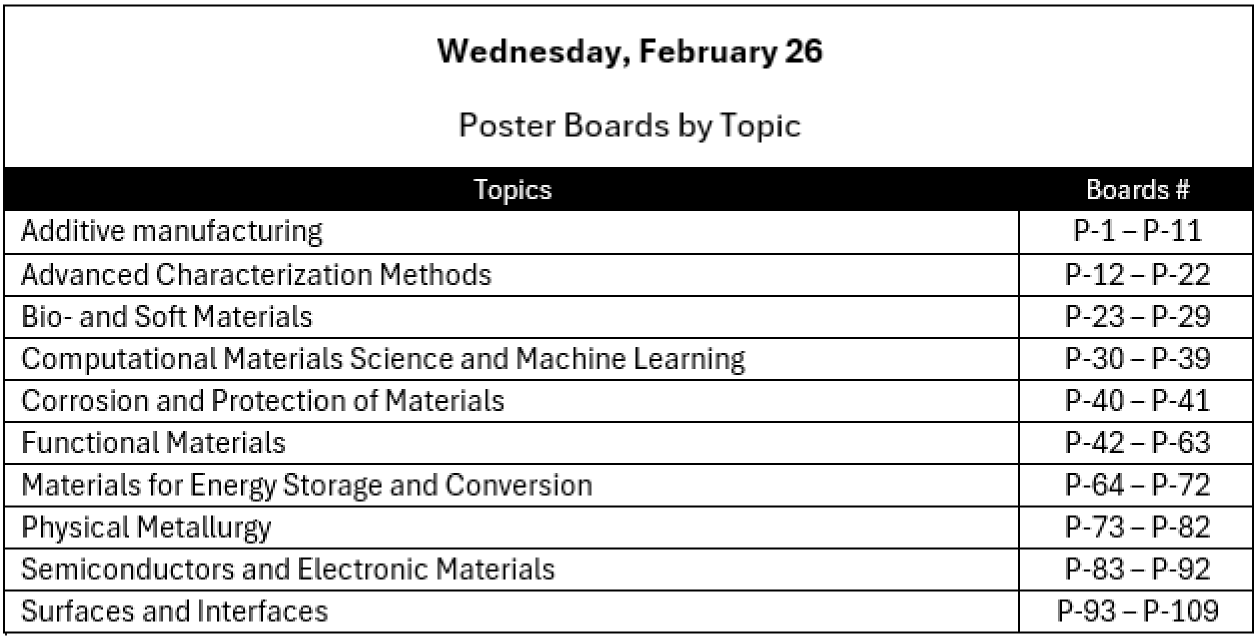
Poster Boards by Topic

Topics	Boards #
2D materials	P-1 – P-11
Additive manufacturing	P-12
Advanced Characterization Methods	P-13
Bio- and Soft Materials	P-14 – P-22
Ceramics and Composite Materials	P-23 – P-40
Materials for Energy Storage and Conversion	P-41 – P-76
Mechanical Properties and Failure	P-77 – P-79
Nanomaterials	P-80 – P-102
Polymers and Colloids	P-103
Quantum Materials	P-104 – P-114
Semiconductors and Electronic Materials	P-115 – P-116
Surfaces and Interfaces	P-117 – P-119

PRESENTATION DAY 2

Wednesday, February 26

Poster Session 2: 13:00-14:30 on Wednesday, February 26
Poster Mounting Time 2: 8:00 on Wednesday, February 26
Poster Removal Time 2: 18:15 on Wednesday, February 26



Wednesday, February 26

Poster Boards by Topic

Topics	Boards #
Additive manufacturing	P-1 – P-11
Advanced Characterization Methods	P-12 – P-22
Bio- and Soft Materials	P-23 – P-29
Computational Materials Science and Machine Learning	P-30 – P-39
Corrosion and Protection of Materials	P-40 – P-41
Functional Materials	P-42 – P-63
Materials for Energy Storage and Conversion	P-64 – P-72
Physical Metallurgy	P-73 – P-82
Semiconductors and Electronic Materials	P-83 – P-92
Surfaces and Interfaces	P-93 – P-109

Paper Posters will be displayed in the Poster Area, signage on site will guide you to the corresponding Poster Placements indicated via your poster board number.

Please refer to the Final Program for the poster board number assigned to you. Please use the board with the same number.

Please refer to the Final Program for your presentation day.

To promote your work, it is recommended that you also stand by your paper poster to answer any upcoming questions from interested delegates during break times.

Please strictly adhere to the mounting and removal times.

If the paper poster has not been removed by the removal time, it will be disposed of by Conference staff.

Please note the Conference organizer cannot be held responsible for posters displayed or left in the Poster area or in the venue.

INSTRUCTIONS FOR PAPER POSTERS

All Posters are in Portrait format.
Format: Max 100 cm wide x 150 cm high
Recommended: 90 cm wide x 120 cm high
The heading should include the title of the paper, authors, institutions and location of institutions.
Letters should be at least 35 mm.
The title should be emphasized by the use of a bold type face.

This writing should be easily readable at a distance of 2 meters
The text can be broken up by the inclusion of drawings, charts and photos.
Lettering for text and illustrations must be at least 10 mm.
Letters should be bold enough to enable viewers to read the poster from a distance of 2 meters (6 feet).
Tacks and technical equipment will be available for the hanging of posters.

RECOMMENDED STRUCTURE

Background – to include 3-5 telegraphic sentences outlining information necessary to understand the study and why it was done.

Aim – the aim of the study

Methods – outline methods used

Results – should be presented as graphs or charts. Provide a legend to explain symbols or other details.

Conclusions – should be stated in large type. Many viewers read this first, hence it should be easy to understand.

General Program

Tuesday, February 25, 2025

08:00 - 09:00 Registration, Coffee Break, Poster Mounting,

Registration Area, Foyer, Exhibition Area

09:00 - 09:10 Opening Ceremony

Hall A

09:10 - 09:55 Grain Growth is Not Curvature Flow: Why? Consequences?

Hall A

Chair: Eugen Rabkin, *Technion - Israel Institute of Technology, Israel*

09:10 - 09:55 Grain Growth is Not Curvature Flow: Why? Consequences?

Plenary Talk

David Srolovitz[1], Caihao Qiu[2], Jian Han[2], Gregory Rohrer[3], Marco Salvalaglio[4]
[1]*Mechanical Engineering, The University of Hong Kong, Hong Kong*
[2]*Materials Science and Engineering, City University of Hong Kong, Hong Kong*
[3]*Materials Science and Engineering, Carnegie Mellon University, USA*
[4]*Dresden Center for Computational Materials Science, TU Dresden, Germany*

09:55 - 10:40 Plenary Talk: Magnesium Technologies for Aviation and Aerospace Applications

Hall A

Chair: Eugen Rabkin, *Technion - Israel Institute of Technology, Israel*

09:55 - 10:40 Magnesium Technologies for Aviation and Aerospace Applications

Plenary Talk

Dan Shechtman
Technion - Israel Institute of Technology, Israel

10:40 - 11:10 Coffee Break, Poster Viewing

Foyer, Exhibition Area

11:10 - 13:10 Nanomaterials

Hall A

Chair: Gitti Frey, *Technion - Israel Institute of Technology, Israel*

11:10 - 11:35 When Nature Meets Nanotechnology: Bio-assisted Synthesis of Nanomaterials Using Renewable Resources

Invited Talk

Shachar Richter
Tel Aviv University, Israel

11:35 - 12:00 New Approach for "Dry" Colloidal Lithography, and its Applications in Advanced Optics and Nanomedicine

Invited Talk

Mark Schvartzman
Ben-Gurion University of the Negev, Israel

12:00 - 12:25 Oxygen Reduction Reaction Activity and Stability of Shaped Metal-doped PtNi Electrocatalysts: from Rotating Disk Electrode to Membrane Electrode Assembly

Invited Talk

Shlomi Polani
Department of Chemical Engineering, Ariel University, Israel

12:25 - 12:40 Formation of FePt L1 0 Epitaxial Nanoparticles via Physical Vapor Deposition

Contributing Talk

Julia Unangst, Eylül Suadiye, **Gunther Richter**[1]
Max Planck Institute for Intelligent Systems

12:40 - 12:55 Self-Assembled Superstructures of Metal-Organic Frameworks

Contributing Talk

Elad Gaver[1], Ifat Kaplan-Ashiri[2], Anna Eden Kossoy[2], Tatyana Bendikov[2], Ryuichi Shimogawa[3], Anatoly Frenkel[3], Maria Chiara di Gregorio[4], Michal Lahav[1], Milko van der Boom[1]
[1]*Department of Molecular Chemistry and Materials Science, The Weizmann Institute of Science, Israel*
[2]*Chemical Research Support, The Weizmann Institute of Science, Israel*
[3]*Department of Materials Science and Chemical Engineering, Stony Brook University, USA*
[4]*Department of Chemistry, Sapienza University of Rome, Italy*

12:55 - 13:10 Investigation of the Formation of ZIF-8-Derived ZnS@MoS_2 Core-Shell Composites for Energy Applications

Contributing Talk

Alen Sam Thomas[1], Lena Yadgarov
Department of Chemical Engineering, Ariel University, Israel

11:10 - 13:10 Polymers & Colloids

Hall B

Chair: Rakefet Ofek Almog, *Azrieli College of Engineering, Israel*

11:10 - 11:35 Monitoring the Kinetics of Crystal Growth for Self-Healing and Structural Control of Anisotropic Theophylline Crystals

Invited Talk

Angelica Elkan, Huan-Jui Lee, Sima Mafi, Irit Rosenhek-Goldian, Marcos Penedo, Georg E. Fantner, Anna Kossoy, Yael Diskin-Posner, Dan Oron, Peter Vekilov

11:35 - 12:00 Space Durable 3D Printed High-Performance PolymersBased on Cyanate Ester/Extended-Bismaleimide

Invited Talk

Yuval Vidavsky[1], Nurit Atar[1], Asaf Bolker[1], Brian E. Riggs[2], Timothy K. Minton[2], Irina Gouzman[1], Eitan Grossman[3]
[1]*Space Environment Department, Soreq NRC, Israel*
[2]*Department of Aerospace Engineering Sciences, University of Colorado at Boulder, USA*
[3]*NOGA 3D Innovations, Israel*

12:00 - 12:25 Multi-Stimuli Responsivity of Single-Layer Magnetic Polymer

Invited Talk

Amos Bardea[1], Fernando Patolsky[2]
[1]*Engineering, Holon Institute of Technology- HIT, Israel*
[2]*The Jan Koum Center for Nanoscience and Nanotechnology, Tel Aviv University, Israel*

12:25 - 12:40 A Novel, Fully Recyclable, Multipurpose, Photocurable Adhesive with Wide-Spectral Curing

Contributing Talk

Natanel Jarach[1,2], Michal Cohen[1], Rivka Gitt[1], Hanna Dodiuk[2], Shlomo Magdassi[1]
[1]*The Institue of Chemistry, The Hebrew University, Jerusalem, Israel*
[2]*Polymeric Materials Engineering, Shenkar - Engineering. Desiegn. Art, Ramat-Gan, Israel*

12:40 - 12:55 Additive Manufacturing of Flexible Sensors Based on Polymer Nanocomposites

Contributing Talk

Shani Ligati Schleifer[1], Oren Regev[1,2]
[1]*Chemical Engineering, The Ben Gurion University of the Negev, Israel*
[2]*Ilse Katz Institute for Nanoscale Science and Technology, The Ben Gurion University of the Negev, Israel*

12:55 - 13:10 Additive Manufacturing Process for Production of Complex and Oscillating POSS-based 4D Structures

Contributing Talk

Nicole Gorohovsky[1], Ronen Verker[1,2], Noa Lachman[1]
[1]*Department of Material Science and Engineering, Tel Aviv University, Israel*
[2]*Department of Space Environment, Soreq Nuclear Research Center, Israel*

11:10 - 13:10 2D Materials

Hall C

Chair: Sigal Ben-Zvi, *Intel Corporation, Israel*

11:10 - 11:35 Exploring Nonlinear Phenomena in the Photoconductivity of Two-Dimensional Semiconductors

Invited Talk

Doron Naveh
Bar-Ilan University, Israel

11:35 - 12:00 Layered Ferroelectricity: From Geometric Measures to First-Principles Calculations

Invited Talk

Oded Hod
School of Chemistry, Tel Aviv University, Tel Aviv, Israel

12:00 - 12:25 Controlled Growth of 2D Materials and Their Heterostructures

Invited Talk

Ariel Ismach
Department of Materials Science and Engineering, Tel Aviv University, Israel

12:25 - 12:40 New Family of All-Metal-Core Two-Dimensional Materials

Contributing Talk

Tamir Forsht[1], Anand Roy[1], Shiyi Gao[1], Joon Young Park[2], Kierstin Torres[2], Roni Gofman[3], Yuval Nitzav[3], Shahar Simon[4], Ayelet Zalic[4], Einav Grynszpan[4], Nag Pranab Kumar[5], Linda Wagner[6], Ifat Kaplan-Ashiri[6], Katya Rechav[6], Lothar Houben[6], Irit Goldian[6], Sidney Cohen[6], Hagai Cohen[6], Takashi Taniguchi[7], Kenji Watanabe[7], Haim Beidenkopf[5], BInghay Yan[5], Hadar Steinberg[4], Amit Kanigel[3], Philip Kim[2], Ernesto Joselevich[1]
[1]*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*
[2]*Department of Physics, Harvard University, Massachusetts, United States*
[3]*Physics Department, Technion-Israel Institute of Technology, Israel*
[4]*The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel*
[5]*Department of Condensed Matter Physics, Weizmann Institute of Science, Israel*
[6]*Chemical Research Support, Weizmann Institute of Science, Israel*
[7]*National Institute for Materials Science (NIMS),, Ibaraki, Japan*

12:40 - 12:55 The Chemistry of $Ti_3C_2T_x$ MXenes in Halide Perovskite Solutions

Contributing Talk

Kirill Sobolev[1], Omer Bartov[1], Adi Yakir[1], Sharon Hazan[2], Mariela J. Pavan[2], Vladimir Ezersky[2], Yevgeny Rakita[1,2]
[1]*Department of Materials Engineering, Ben Gurion University of the Negev, Israel*
[2]*Ilse Katz Institute for Nanoscale Science and Technology, Ben Gurion University of the Negev, Israel*

12:55 - 13:10 Integration of Single-Layer Graphene on IDA Gold Electrodes and Electrochemical Characterization

Contributing Talk

Nirit Sitbon[1], Yosi Shacham-Diamand[2], Ariel Ismach[1], Rakefet Ofek-Almog[3]
[1]*Tel Aviv university, Israel*
[2]*Reichmann University, Israel*
[3]*Azrieli College, Israel*

11:10 - 13:10 Materials in Archeology

Hall D

Chair: Tzilla Eshel, *University of Haifa, Israel*

11:10 - 11:30 On Ingots and Men: East Mediterranean Copper Trade during the Bronze and Iron Ages

Invited Talk

Naama Yahalom-Mack
Hebrew University of Jerusalem, Israel

11:30 - 11:50 Archaeometallurgical Approaches to The Analysis of Iron Mining Tools from Nahal ‘Amram, Israel

Invited Talk

Adi Eliyahu-Behar
Ariel University, Israel

11:50 - 12:10 The Nature of the Pumiceous Ash and Tuff used for the Construction of the Sebastos Harbor

Invited Talk

Yotam Asscher
University of Haifa, Israel

12:10 - 12:25 The Process of Natural Aging of Pb-Sn Solid Solution in Lead Inclusions in Tin-Leaded Bronzes

Contributing Talk

Sana Shilstein, Yishay Feldman, Sariel Shalev

Weizmann Institute of Science, Israel

12:25 - 12:40 Field Multi-focal Metallography as a Non-destructive Method in Archaeometallurgical Characterization: The Akko Tower Shipwreck as a Test Case

Contributing Talk

Noam Iddan, Dana Ashkenazi, Deborah Cvikel

University of Haifa, Israel

12:40 - 12:55 Crusader Military Activities on the Carmel Coast: the Typology, Imaging, and Metallography of Three Swords

Contributing Talk

Sara Lantos[1], Yoav Bornstein[1,2], Rabei Khamisy[1,2], Tzilla Eshel[1,2]
[1]*School of Archaeology and Maritime Cultures, University of Haifa, Israel*
[2]*Zinman Institute of Archaeology, University of Haifa, Israel*

12:55 - 13:10 Science and Archaeology: Win-Win

Contributing Talk

Tzilla Eshel
University of Haifa, Israel

11:10 - 13:10 E. Gutmanas Symposium

Hall E

Chair: Itamar Gutman, *RAFAEL, Israel*

11:10 - 11:35 Manipulating the Growth and Form of Biogenic Glass

Invited Talk

Igor Zlotnikov
Dresden University of Technology, Germany

11:35 - 12:00 Reactive Synthesis of Ceramic-Metal Composites

Invited Talk

Nahum Travitzky
Department of Materials Science, Glass and Ceramics, University of Erlangen-Nuremberg, Germany

12:00 - 12:25 Advancing the Knowledge of Dislocation Dynamics: A Simulation Perspective

Invited Talk

Dan Mordehai
Faculty of Mechanical Engineering, Technion, Israel

12:25 - 12:40 Cold Sintering Processes: A Historical Perspective on Biomaterials Applications

Featured Talk

Aliya Sharipova
Bio- and Medical Technology, Fraunhofer Institute for Ceramic Technologies and Systems IKTS, Germany

12:40 - 12:55 Reactive Infiltration Synthesis of Additively Manufactured Metal/Ceramic Composites

Featured Talk

Alexander Katz-Demyanetz
Israel Institute of Materials Manufacturing Technologies, Technion Research and Development Foundation, Israel

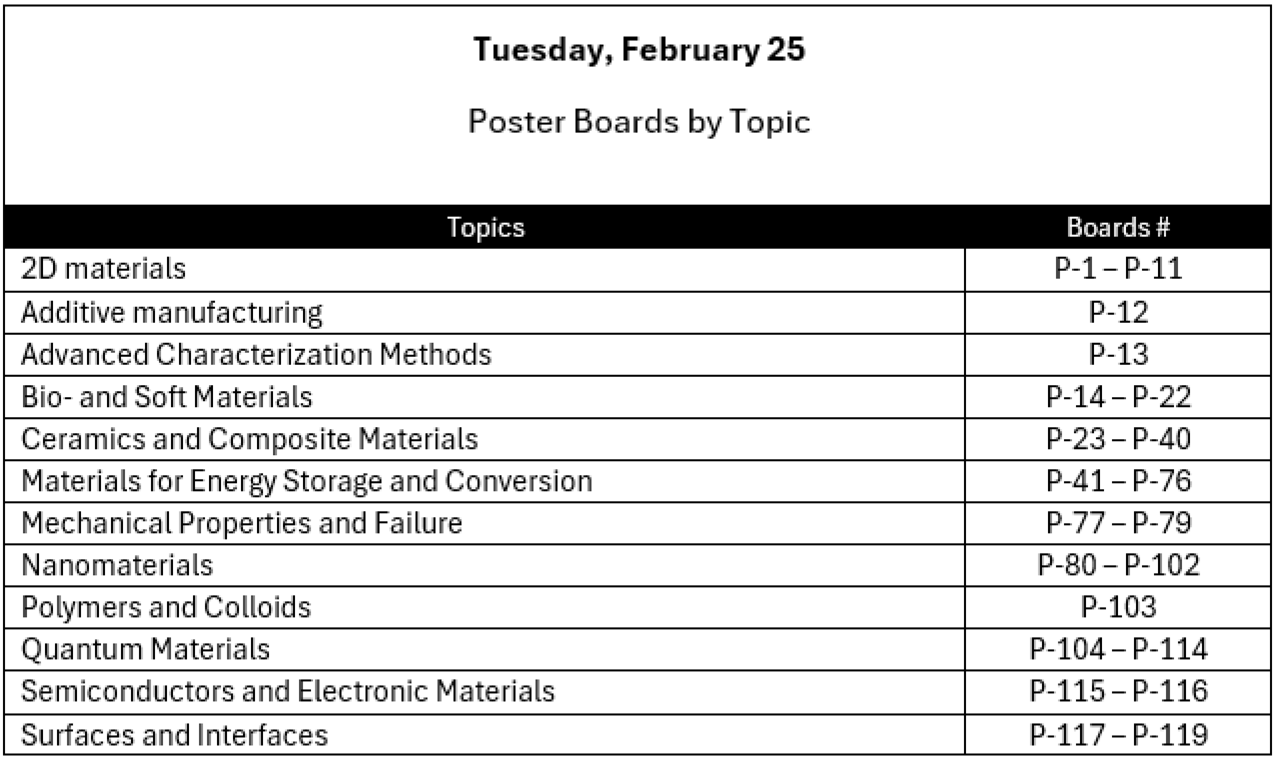
12:55 - 13:10 Some Reflections on a Promising Trend in Design of Architectured Materials and Engineering Structures

Featured Talk

Yuri Estrin
Department of Materials Science and Engineering, Monash University, Australia

13:10 - 14:40 Lunch Break & Poster Session

Foyer, Exhibition Area



Tuesday, February 25

Poster Boards by Topic

Topics	Boards #
2D materials	P-1 – P-11
Additive manufacturing	P-12
Advanced Characterization Methods	P-13
Bio- and Soft Materials	P-14 – P-22
Ceramics and Composite Materials	P-23 – P-40
Materials for Energy Storage and Conversion	P-41 – P-76
Mechanical Properties and Failure	P-77 – P-79
Nanomaterials	P-80 – P-102
Polymers and Colloids	P-103
Quantum Materials	P-104 – P-114
Semiconductors and Electronic Materials	P-115 – P-116
Surfaces and Interfaces	P-117 – P-119

13:30 - 14:30 How to Start Writing and Get Your Research Paper Done

Hall E

Workshop by Olga Degtyareva, PhD
Productivity for Scientists Ltd, UK

14:40 - 16:55 Materials for Energy

Hall A

Chairs: David Ehre, *Weizmann Institute of Science, Israel* &
Malachi Noked, *Bar-Ilan University, Israel*

14:40 - 15:05 Porosity and Energy: from Fuel Cells to Fracking

Invited Talk

David Eisenberg
Schulich Faculty of Chemistry, the Grand Technion Energy Program, and the Resnick Sustainability Center for Catalysis, Technion - Israel Institute of Technology, Israel

15:05 - 15:30 High Entropy Oxides as Materials for Energy Storage and Conversion

Invited Talk

Ronen Gottesman
The Institute of Chemistry, Casali Center of Applied Chemistry, and The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

15:30 - 15:55 Mixed Conductivity in the TiO2-SrF2 and LaOxFy Systems for Energy Applications

Invited Talk

Yatir Sadia[1,2,3], Stephen Skinner[3]
[1]*Material Engineering, Ben Gurion University, Israel*
[2]*Nuclear Research center of the Negev, Israel*
[3]*Material Engineering, Imperial College of London, United Kingdom*

15:55 - 16:10 Stabilization of Ti-based MXene Single Flakes Above the Reversible Hydrogen Potential

Contributing Talk

Brian Rosen[1,3], Sukanta Chakrabartty[1], Haridas Parse[1], Danielle Sviri[1], Mathias Kramer[2], Baptiste Gault[2], Dierk Raabe[2], Noam Eliaz[3], Amir Natan[4], Vipin Kumar[4], Maxim Sokol[3]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Israel*
[2]*Max Plank Institue for Renewable Materials, Germany*
[3]*Materials Science and Engineering, Tel Aviv University, Israel*
[4]*Physical Electronics, Tel Aviv University, Israel*

16:10 - 16:25 Minute-Scale High-Temperature Synthesis of Polymeric Carbon Nitride Photoanodes

Contributing Talk

Ayelet Tashakory[1], Sanjit Mondal[1], Venugopala Rao Battula[1], Gabriel Mark[1], Tirza Shmila[1], Michael Volokh[1], Menny Shalom[1]
Department of Chemistry, Ben-Gurion University of the Negev, Israel

16:25 - 16:40 Hydrogen Peroxide Formation Enables Efficient Oxygen Evolution in Near-Neutral Zn-Air Batteries

Contributing Talk

Roman Kapaev
Bar-Ilan University, Israel

16:40 - 16:55 Can Vacancy Defects in Graphene Underlayer Improve Hematite`s Catalytic Efficiency in Water Splitting? A First-principles Study

Contributing Talk

Labanya Bhattacharya[1], Avi Cohen[1], Maytal Caspary Toroker[1,2]
[1]*Department of Materials Science and Engineering, Technion-Israel Institute of Technology, Haifa-3200003, Israel*
[2]*The Nancy and Stephen Grand Technion Energy Program, Haifa-3200003, Israel*

14:40 - 16:30 Bio- & Soft Materials I

Hall B

Chair: Ulyana Shimanovich, *Weizmann Institute of Science, Israel*

14:40 - 15:05 Inorganic Condensates in Biomaterial Synthesis

Invited Talk

Assaf Gal
Weizmann Institute of Science, Israel

15:05 - 15:30 Amazing Alternative Caseins

Invited Talk

Dganit Danino
Technion - Israel Institute of Technology, Israel

15:30 - 15:45 Digital Light Processing 3D Printing of Stretchable and Compressible Porous Polymers for Soft Robotics

Contributing Talk

Ouriel Bliah[1], Seonggun Joe[2], Lucia Beccai[2], Shlomo Magdassi[1]
[1]*Casali Center for Applied Chemistry, Hebrew University of Jerusalem, Israel*
[2]*Soft Biorobotics Perception Lab, Istituto Italiano di Tecnologia, Italy*

15:45 - 16:00 The Mechanics of PEGDA Hydrogels: from Microstructure to Macroscopic Behavior

Contributing Talk

Michal Levin[1], Yongkui Tang[2,3], Claus Eisenbach[3,4], Megan Valentine[2,3], Noy Cohen[1]
[1]*Materials Science and Engineering, Technion, Israel*
[2]*Mechanical Engineering, University of California, Santa Barbara, Santa Barbara, CA, USA*
[3]*Materials Research Laboratory, University of California, Santa Barbara, Santa Barbara, CA, USA*
[4]*Institut for Polymerchemie, University of Stuttgart, Stuttgart, Germany*

16:00 - 16:15 Amino-Acid-Based Microstructures as Versatile Organic Photonic Platforms

Contributing Talk

Handelman Amir

Holon Institute of Technology, Israel

16:15 - 16:30 Characterization of Dolomite and Calcite Microcalcifications in Human Breast Tissue

Contributing Talk

Sahar Gal[1], Mariela J. Pavan[2], Netta Vidavsky[1,2]
[1]*Department of Chemical Engineering, Ben Gurion University of the Negev, Israel*
[2]*Ilse Katz Institute for Nanoscale Science & Technology, Ben Gurion University of the Negev, Israel*

14:40 - 16:40 Ceramics and Composites

Hall C

Chair: Maxim Sokol, *Tel Aviv University, Israel*

14:40 - 15:05 Self-compensation in Metal Oxides with Application on (Fast) Sintering of MgO

Invited Talk

Yoed Tsur
The Wolfson Department of Chemical Engineering, Technion, Israel

15:05 - 15:30 Challenges and Opportunities Utilizing Multilayer MXene as Precursors for Oriented TiC_x in Ceramic Composites

Invited Talk

Barak Ratzker[1,2], Or Messer[1], Maxim Sokol[1]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Israel*
[2]*Department of Microstructure Physics and Alloy Design, Max Planck Institute for Sustainable Materials, Germany*

15:30 - 15:55 Beyond Thin Films: ALD`s Role in Next-Generation Ceramic Materials

Invited Talk

Amnon Rothman
Department of Materials Engineering, Ben Gurion University, Israel

15:55 - 16:10 3D Printing of Alumina-based Ceramics through Photopolymerization and Sol-Gel Processes

Contributing Talk

May Yam Moshkovitz-Douvdevany[1], Shlomo Magdassi[1]
Institute of Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

16:10 - 16:25 Development of Ultra-High Temperature Ceramics by Ultra-Fast Sintering

Contributing Talk

Denis Zolotaryov
Israel Institute of Materials Manufacturing Technologies, TRDF, Technion, Israel

16:25 - 16:40 Impact-Induced Reactivity and Structural Transformations in Ti3SiC2 MAX Phases

Contributing Talk

Gil Goviazin[1], Dor Aaron Goldstein[2], Barak Ratzker[2], Or Messer[2], Maxim Sokol[2], Daniel Rittel[1]

[1]*Mechanical Engineering, Technion – Israel Institute of Technology, Israel*
[2]*Department of Materials Science and Engineering, Tel Aviv University, Israel*

14:40 - 16:40 Quantum Materials

Hall D

Chair: Tamar Goldzak, *Bar-Ilan University, Israel*

14:40 - 15:05 Exploring Fast and Ultrafast Dynamics of Matter with Electrons and Photons

Invited Talk

Michael Yannai, Matan Haller, Ron Ruimy, Alexey Gorlach, Nicholas rivera Rivera, Dmitri Basov, **Ido Kaminer**[1]
Technion - Israel Institute of Technology, Israel

15:05 - 15:30 Coherent Control of Phonon Anharmonicity

Invited Talk

Alon Ron
Tel Aviv University, Israel

15:30 - 15:55 Features of Uniform and Non-Uniform Strain in Transition-Metal Dichalcogenides Mono-layers

Invited Talk

Moshe Harats
Department of Materials Engineering, Ben Gurion University of the Negev, Israel

15:55 - 16:10 Collective Excitations in Perovskite Quantum Dot Superlattices and Heterostructures

Contributing Talk

Yehonadav Bekenstein[1], **Shai Levy**[1]
Materials Science and Engineering, Technion – Israel Institute of Technology, Israel

16:10 - 16:25 Intertwined Topological Phases in $TaAs_2$ Nanowires with Giant Magnetoresistance and Quantum Coherent Surface Transport

Contributing Talk

Anand Roy, Anna Eyal, Roni Majlin Skiff, Barun Barick, Samuel D. Escribano, Olga Brontvein, Katya Rechav, Ora Bitton, Roni Ilan, Ernesto Joselevich

16:25 - 16:40 Quantum Relativistic Materials

Contributing Talk

Asher Yahalom[1,2,3]
Department of Electrical & Electronic Engineering, Ariel University, Israel
Center for Astrophysics, Geophysics, and Space Sciences (AGASS), Ariel University, Ariel University
FEL User Facility, Ariel University, Ariel University

14:40 - 16:40 Mechanical Properties & Failure

Hall E

Chairs: Shmulik Osovski, *Technion - Israel Institute of Technology, Israel*
Roni Shneck, *Ben-Gurion University of the Negev, Israel*

14:40 - 15:05 The Fundamental Physics of the Onset of Frictional Motion: How Does Friction Start?

Invited Talk

Jay Fineberg[1], Shahar Gvirtzman[1]
The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

15:05 - 15:30 Dynamics of Deformation Twinning in Magnesium

Invited Talk

Eilon Faran[1], Doron Shilo[1]
Faculty of Mechanical Engineering, Technion, Israel

15:30 - 15:55 Structural Motifs in Soft Fibrous Tissues: Unraveling Structure-Mechanics Relationships to Inspire Biomimetic Material Design

Invited Talk

Mirit Sharabi
Mechanical Engineering, Ariel University, Israel

15:55 - 16:10 How Do Roses Build Failure-resistant Prickles?

Contributing Talk

Benny Bar-On, Liat Levavi
Ben-Gurion University of the Negev, Israel

16:10 - 16:25 A Critical Analysis on the Predictive Capabilities of Different Criteria for Ductile Failure Initiation in Metallic Materials

Contributing Talk

Elad Priel[1,2], Nitzan Rom[3], Jacob Bortman[4]
[1]*Mechanical Engineering, Shamoon College of Engineering, Israel*
[2]*Materials Engineering, NRCN, Israel*
[3]*Israel Atomic Energy Commission, Israel*
[4]*Mechanical Engineering, Ben Gurion University, Israel*

16:25 - 16:40 Strength of Precipitates in Ni-Al and Ni-Al-Fe Alloys

Contributing Talk

Igor Efremenkov, Michael Aizenshtein[1], Eugene Zaretsky[2], Shmuel Hayun[3]
[1]*Materials Department, NRC-Negev, Beer-Sheva, Israel*
[2]*Department of Mechanical Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel*
[3]*Department of Materials Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel*

16:40 - 18:10 Welcome Reception & Posters

Poster Area, Exhibition Area

Wednesday, February 26, 2025

08:00 - 09:00 Registration, Coffee Break, Poster Mounting

Registration Area, Foyer, Exhibition Area

09:00 - 09:45 Unveiling the Art of Self-Assembly in the Creation of Diverse Biomaterials

Hall A

Chair: Yuri Estrin, *Monash University, Australia*

09:00 - 09:45 Unveiling the Art of Self-Assembly in the Creation of Diverse Biomaterials

Plenary Talk

Ulyana Shimanovich
Weizmann Institute of Science, Israel

09:45 - 10:30 Materials Science Challenges in Developing High Energy, Safe and Durable Rechargeable Batteries

Hall A

Chair: Yuri Estrin, *Monash University, Australia*

09:45 - 10:30 Materials Science Challenges in Developing High Energy, Safe and Durable Rechargeable Batteries

Plenary Talk

Doron Aurbach
Department of Chemistry, BINA – BIU Institute of Nanotechnology and Advanced Materials, and INIES – Israel National Institute of Energy Storage, Bar Ilan university, Israel

10:30 - 11:00 Coffee Break, Poster Viewing

Foyer, Exhibition Area

11:00 - 13:00 Computational Materials Science I

Hall A

Chairs: Ilya Grinberg, *Bar-Ilan University, Israel*
David Srolovitz, *Hong Kong University, Hong Kong*

11:00 - 11:25 Thermodynamic Theory of Dislocation-Mediated Plasticity

Invited Talk

Alexander Umantsev
Department of Chemistry, Physics, and Materials Science, Fayetteville State University, United States

11:25 - 11:50 Predicting Two-Dimensional Semiconductors Using Conductivity Effective Mass

Invited Talk

Lee Burton
Tel Aviv University, Israel

11:50 - 12:15 Towards Fully Automated and Universal Metallographic Image Analysis Using AI Methods

Invited Talk

Ofer Beeri[1], Inbal Cohen[2], Matan Rusanovsky[1], Julien Robitaille[3], Francis Q. Lauzon[3], Shai Avidan[2], Gal Oren[4,5]
[1]*NRCN, Israel*
[2]*Tel Aviv University, Israel*
[3]*Clemex Technologies, Canada*
[4]*Stanford University, USA*
[5]*Technion, Israel*

12:15 - 12:30 Accurate Solid-State Electronic and Optical Excitations from Non-Empirical (Time-Dependent) Density Functional Theory

Contributing Talk

Guy Ohad[1], Stephen E. Gant[2,3], Dahvyd Wing[1], Michal Hartstein[1], Jonah B. Haber[2,3], María Camarasa-Gómez[1], Ayala V. Cohen[1], Francisca Sagredo[2,3], Marina R. Filip[4], Tim Gould[5], Jeffrey B. Neaton[2,3,6], Leeor Kronik[1]
[1]*Department of Molecular Chemistry and Materials Science, Weizmann institute of Science, Israel*
[2]*Department of Physics, University of California, Berkeley, CA, United States*
[3]*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States*
[4]*Department of Physics, University of Oxford, United Kingdom*
[5]*Queensland Micro- and Nanotechnology Centre, Griffith University, QLD, Australia*
[6]*Kavli Energy NanoSciences Institute at Berkeley, University of California, Berkeley, CA, United States*

12:30 - 12:45 Exploring the Optical Properties of Defects in Nanomaterials through Electronic Structure Calculations

Contributing Talk

Tamar Goldzak
Engineering, Bar Ilan University, Israel

12:45 - 13:00 Structure and Properties of Graphullerene: a Semiconducting Two-Dimensional C60 Crystal

Contributing Talk

Uri Argaman, Guy Makov

Ben-Gurion University of the Negev, Israel

11:00 - 13:00 Surfaces & Interfaces

Hall B

Chair: Igor Rahinov, *The Open University of Israel, Israel*

11:00 - 11:25 Quantitative Surface Optical Imaging and Spectroscopy

Invited Talk

Adi Salomon
Bar-Ilan University, Israel

11:25 - 11:50 High Purity Nanoporous Metallic Films: Direct Synthesis and Catalytic Applications

Invited Talk

Hannah-Noa Barad
Department of Chemistry, Institute of Nanotechnology & Advanced Materials, and Israel National Institute of Energy Storage (INIES), Bar-Ilan University, Israel

11:50 - 12:15 Surface Engineering on Gold: From Atomic Steps to Nanoporous Structures and Directed Nanowire Growth

Invited Talk

Lotan Portal, Rotem Zilberberg, Iryna Polishchuk, Maria Koifman Khristosov, Alexander Katsman, **Boaz Pokroy**[1]
Materials Science and Engineering, Technion Israel Institute of Technology, Israel

12:15 - 12:30 Electrofreezing of Super-Cooled Water as Induced by an Al Electrode

Contributing Talk

Shiri Dishon Ben Ami[1], Leah Fuhrman Javitt[1], Shakir Ali Siddiqui[2], Hagai Cohen[3], Kshatresh Dutta Dubey[2], Meir Lahav[1], Igor Lubomirsky[1]
[1]*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*
[2]*Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence, India*
[3]*Chemical Research Support, Weizmann Institute of Science, Israel*

12:30 - 12:45 Precursor and Bulk Dynamics of Thin Film Spreading

Contributing Talk

Haim Taitelbaum[1], Meital Harel[1]
Department of Physics, Bar Ilan University, Israel

12:45 - 13:00 Tailoring the Chemistry and Morphology of Vertically Aligned Carbon Nanotubes Forests, Implications for Smart Electrodes

Contributing Talk

Lev Rovinsky[1], Noa Lachman[1]
Materials Science and Engineering, Tel Aviv University, Israel

11:00 - 13:00 Additive Manufacturing I

Hall C

Chair: Alexander Katz-Demyanetz, *Israel Institute of Materials Manufacturing Technologies, Israel*

11:00 - 11:25 4D Bioprinting of Engineered Tissues

Invited Talk

Shulamit Levenberg
Biomedical Engineering, Technion - Israel Institute of Technology, Israel

11:25 - 11:50 Overview of Mechanical, Metallurgical, and Physical Properties of PBF Ti-6Al-4V

Invited Talk

Amnon Shirizly
Rafael, Israel

11:50 - 12:15 Soft 3D-printable Multifunctional Ionic Materials for Physical AI

Invited Talk

Aslan Miriyev
Department of Mechanical Engineering, Ben-Gurion University, Beer Sheva, Israel

12:15 - 12:30 Exploring New Pathways for Directed Assembly

Contributing Talk

Hagay Shpaisman[1]
Chemistry Department & Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel

12:30 - 12:45 Controlled Stretchable Lotus Leaf effect by Digital Light Processing

Contributing Talk

Noa Trink[1], Shlomo Magdassi
Institute of Chemistry, Casali Center, The Hebrew University of Jerusalem, Israel

12:45 - 13:00 3D-Printed Patient-specific Bone Reconstruction Implants Based on Poly Ether Ether Ketone (PEEK)

Contributing Talk

Itamar Tulpan[1], Sahar Halevy[1], Sivan Hazan[1], Galit Katarivas Levy[1]
Department of biomedical engineering, Ben Gurion University, Israel

11:00 - 13:00 Functional Materials

Hall D

Chair: Amit Kohn, *Tel Aviv University, Israel*

11:00 - 11:25 Pyrolytic Radical Polymerization of Molecular Covalent Crystals

Invited Talk

Elena Meirzadeh
Molecular chemistry and materials science, Weizmann Institute of Science, Israel

11:25 - 11:50 On the Role of Twinning in Phase Transitions of Ferroelectric Perovskites

Invited Talk

Semën Gorfman
Materials Science and Engineering, Tel Aviv University, Israel

11:50 - 12:15 Non-Ergodic-Induced Negative Differential Piezoresponse in Relaxor Ferroelectrics

Invited Talk

Cecile Saguy, Benjamin Kowalski, Alp Sehirlioglu, **Yachin Ivry**[1,4,5]
[1]*Solid-State Institute, Technion−Israel Institute of Technology, Israel*
[4]*Department of Materials Science and ENgineering, Technion−Israel Institute of Technology, Israel*
[5]*The Nancy and Stephen Grand Technion Energy Program (GTEP), Technion−Israel Institute of Technology, Israel*

12:15 - 12:30 Melt Alloying of Two-Dimensional Hybrid Perovskites: Composition-Dependence of Thermal and Optical Properties

Contributing Talk

Arad Lang[1], Celia Chen[1], Chumei Ye[1], Lauren N. McHugh[2], Xian Wei Chua[3], Samuel D. Stranks[3], Sian E. Dutton[4], Thomas D. Bennett[1]
[1]*Materials Science and Metallurgy, University of Cambridge, United Kingdom*
[2]*Department of Chemistry, University of Liverpool, United Kingdom*
[3]*Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom*
[4]*Cavendish Laboratory, University of Cambridge, United Kingdom*

12:30 - 12:45 Preparation and Core-electron Spectroscopy of Y- or Sc- Doped AlN Films

Contributing Talk

David Ehre[1], Asaf Cohen[1], Sergey Khodorov[1], Igor Lubomirsky[1], Ellen Wachtel[1], Hagai Cohen[2], Junying Li[3], Anatoly Frenkel[3]
[1]*Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*
[2]*Chemical Research Support, Weizmann Institute of Science, Israel*
[3]*Materials Science and*

Chemical Engineering, Stony Brook University, New York, United States

12:45 - 13:00 Synthesis and Nonlinear Optical Characterization of Para Red Azo Dye Crystals

Contributing Talk

Alon Krause[1], Tchiya Zar[1]
Chemistry, Bar Ilan University, Israel

11:00 - 13:00 Physical Metallurgy

Hall E

Chairs: Konstantin Borodianskiy, *Ariel University, Isreal*
Louisa Meshi, *Ben-Gurion University of the Negev, Israel*

11:00 - 11:25 Heusler Alloys for Spintronics and Magnetocaloric Applications: Understanding through the Lens of Diffraction Techniques

Invited Talk

Pnina Ari-Gur[1], Amila Madiligama[2], Sven Vogel[3], Viktor Koledov[4]
[1]*Mechanical & Aerospace Engineering, Western Michigan University, USA*
[2]*Physics, Penn State DuBois, USA*
[3]*Los Alamos National Laboratory, USA*
[4]*Russian Academy of Science, Moscow, Russia*

11:25 - 11:50 Local Electrical Properties of Grain Boundary Complexions in Alloys

Invited Talk

Hanna Bishara
Tel Aviv University, Israel

11:50 - 12:15 Structural Materials for Nuclear Fusion Energy: Knowledge Gaps and Opportunities in Metallic Materials Innovation

Invited Talk

Aleksandra Baron-Wiechec[1], Haishan Zhou[2], Yuping Xu[2]
[1]*Materials Science and Engineering, Guangdong Technion – Israel Institute of Technology, China*
[2]*Fusion Reactor Materials and Components Division, Institute of Plasma Physics,*

Chinese Academy of Sciences, China

12:15 - 12:30 Recovery and Recrystallization of Deformed Metal Nanoparticles

Contributing Talk

Jonathan Zimmerman[1], Eugen Rabkin[1]
Technion - Israel Institute of Technology, Israel

12:30 - 12:45 Dynamics of Martensitic Transformations

Contributing Talk

Nitzan Mizrahi[1], Roni Z. Shneck, Oleg Gendelman[2], Oliver Kastner[3]
[1]*Davidson Inst, Weissman Institute of Science, Israel*
[2]*Mechanical Engineering, Technion, Isreal*
[3]*Elastokalorik Ltd., Germany*

12:45 - 13:00 Stress Relaxation and Anisotropy in Zircaloy-4 Cladding: Insights from Uniaxial and Biaxial Testing under Pellet-Cladding Interaction Conditions

Contributing Talk

Shmuel Samuha[1], Malachi Nelson[2], David Kamerman[3], Peter Hosemann[4]
[1]*Materials Engineering, NRCN, Israel*
[2]*Nuclear Engineering, University of California, Berkeley, and Idaho National Laboratory, USA*
[3]*Fuel Development, Performance, and Qualification, Idaho National Laboratory, USA*
[4]*Nuclear Engineering, University of California, Berkeley, USA*

11:00 - 12:55 Bio- and Soft Materials II

Hall F

Chair: Amir Handelman, *Holon Institute of Technology, Israel*

11:00 - 11:25 Bioinspired Materials for Biomedical Applications

Invited Talk

Lihi Adler-Abramovich
Department of Oral Biology, The Goldschleger School of Dental Medicine, Faculty of Medical & Health Sciences, Tel Aviv University, Israel

11:25 - 11:40 Effect of Binary Mechanical Environment on T-cell Function

Contributing Talk

Jatin Jawhir Pandit[1], Abed Al-Kader Yassin[2], Carlos Ureña Martin[1], Guillaume Le Saux[1], Angel Porgador[2], Mark Schvartzman[1]
[1]*Department of Materials Engineering,Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Israel*
[2]*The Shraga Segal Department of Microbiology, Immunology, and Genetics Faculty of Health Sciences, Ben-Gurion University of the Negev, Israel*

11:40 - 11:55 Shaping Molecular Crystals: The Role of Polymers and Small Molecules

Contributing Talk

Dolev Brenman-Begin[1], Zohar Eyal[1], Rachael-Lynn Deis[1], Anna-Eden Kossoy[2], Iddo Pinkas[2], Tatyana Bendikov[2], Lyudmila Veikhman[2], Dvir Gur[1]
[1]*Department of Molecular Genetics, Weizmann Institute of Science, Israel*
[2]*Department of Chemical Research Support, Weizmann Institute of Science, Israel*

11:55 - 12:10 Enhanced Mechanophore Activation in Hydrogel Networks Driven by Pre-Tension

Contibuting Talk

Meytal Forer[1,2], Alessio Maselli[2,3], Yifan Liao[2], Josh Grolman[2]
[1]*Nano Science and Nano Technology, Technion - Israel Institute of Technology, Israel*
[2]*Materials Science and Engineering, Technion - Israel Institute of Technology, Israel*
[3]*University of Naples Federico II, Italy*

12:10 - 12:25 Study of the Active Site in Azurin Blue Copper(II) Protein with Cryogenic X-ray Photoelectron Spectroscopy

Contributing Talk

Tatyana Bendikov[1], Sudipta Bera[2], Katya Rechav[1], David Cahen[2]
[1]*Department of Chemical Research Support, Weizmann Institute of Science, Israel*
[2]*Department of Molecular Chemistry & Materials Science, Weizmann Institute of Science, Israel*

12:25 - 12:40 Memory in Bioinspired Capillary Networks and their Perspective Applications

Contributing Talk

Bat-El Pinchasik
School of Mechanical Engineering, Tel-Aviv University, Israel

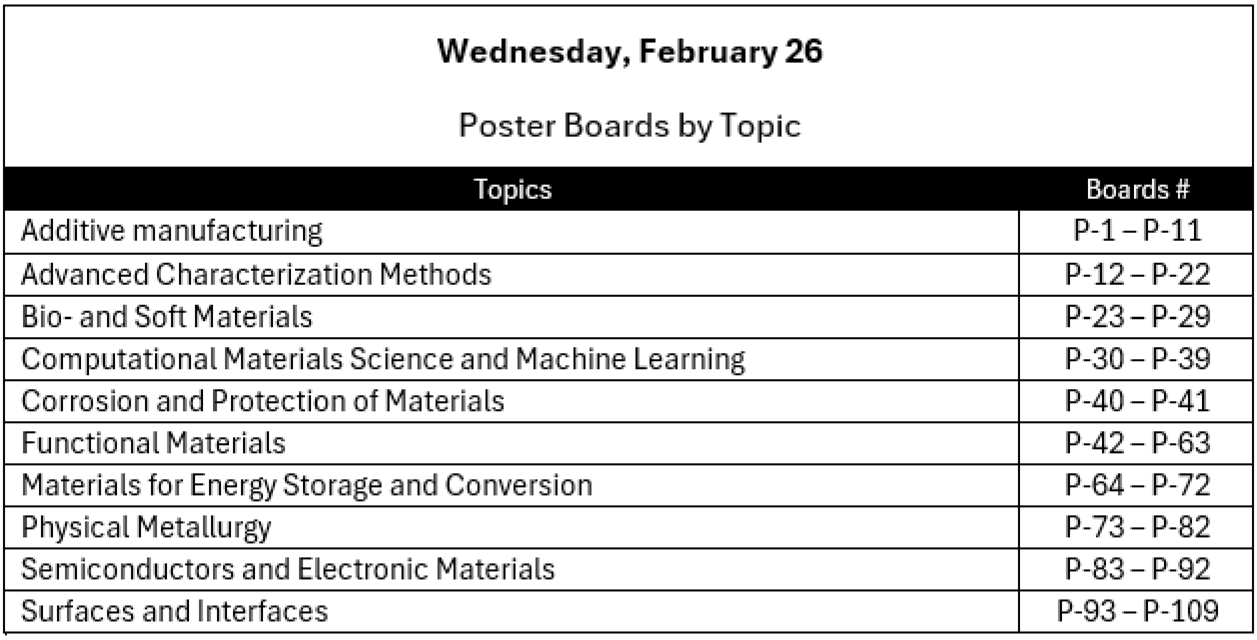
12:40 - 12:55 Short Peptides as Tools for Novel Bioink Formulation in Tissue Engineering

Contributing Talk

Francesca Netti[1,2,3], Moran Aviv[1,2,3,4], Yoav Dan[1,2,3], Safra Rudnick-Glick[1,2,3], Michal Halperin-Sternfeld[1,2,3], Lihi Adler-Abramovich[1,2,3]
[1]*Faculty of Medical & Health Sciences, Tel Aviv University, Israel*
[2]*Jan Koum Center for Nanoscience and Nanotechnology, Tel Aviv University, Israel*
[3]*The Center for the Physics and Chemistry of Living Systems, Tel Aviv University, Israel*
[4]*Afeka Tel Aviv Academic College of Engineering, School of Mechanical Engineering, Israel*

13:00 - 14:30 Lunch Break & Poster Session

Foyer, Exhibition Area



Wednesday, February 26

Poster Boards by Topic

Topics	Boards #
Additive manufacturing	P-1 – P-11
Advanced Characterization Methods	P-12 – P-22
Bio- and Soft Materials	P-23 – P-29
Computational Materials Science and Machine Learning	P-30 – P-39
Corrosion and Protection of Materials	P-40 – P-41
Functional Materials	P-42 – P-63
Materials for Energy Storage and Conversion	P-64 – P-72
Physical Metallurgy	P-73 – P-82
Semiconductors and Electronic Materials	P-83 – P-92
Surfaces and Interfaces	P-93 – P-109

14:30 - 16:30 Computational Materials Science II

Hall A

Chairs: Guy Makov, *Ben-Gurion University of the Negev, Israel*
Alex Umantsev, *North Carolina State University, USA*

14:30 - 14:55 Computational Thermodynamics: Principles and New Applications to Electrodeposition of Reactive Metals from Molten Salts

Invited Talk

Eli Brosh
Department of Materials, NRCN, Israel

14:55 - 15:20 Light-Matter Interaction Dynamics with Ab Initio Data-Driven Computations

Invited Talk

Sivan Refaely-Abramson
Weizmann Institute of Science, Israel

15:20 - 15:45 Charge Transport through Catalytic Materials

Invited Talk

Maytal Caspary Toroker
Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Israel

15:45 - 16:00 Surface Tension Calculations in Liquid Metals Using First Principles and Machine Learning

Contributing Talk

Netanela Cohen[1], Oswaldo Diéguez
Department of Materials Science and Engineering, Tel Aviv University, Israel

16:00 - 16:15 Predicting and Understanding Color Polymorphism in ROY from First Principles

Contributing Talk

Michal Hartstein[1], Guy Ohad[1], Leeor Kronik[1]
Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

16:15 - 16:30 Nonlinear Self-calibrated Spectrometer with Single GeSe-InSe Heterojunction Device

Contributing Talk

Rana Darweesh[1,2], Rajesh Kumar Yadav[1,2], Elior Adler[1,2], Michal Poplinger[1,2], Adi Levi[1,2], Jea-Jung Lee[3], Amir Leshem[1], Ashwin Ramasubramaniam[4,5], Fengnian Xia[3], Doron Naveh[1,2]
[1]*Faculty of Engineering, Bar-Ilan University, Israel*
[2]*Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel*
[3]*Department of Electrical Engineering, Yale University, USA*
[4]*Department of Mechanical and Industrial Engineering, University of Massachusetts, USA*
[5]*Materials Science and Engineering Graduate Program, University of Massachusetts, USA*

14:30 - 16:30 Materials for Extreme Conditions

Hall B

Chairs: Ehud Galun, *MAFAT, Israel*
Or Messer, *Tel Aviv University, Israel*

14:30 - 14:55 The Influence of Solutes and Fields on Anisotropic Grain Growth of Alumina

Invited Talk

Rachel Marder, **Wayne Kaplan**[1]
Department of Materials Science & Engineering, Technion - Israel Institute of Technology

14:55 - 15:20 Directed Energy Deposition (DED) of Refractory Ultrahigh Temperature Ceramics (UHTCs) for Extreme Environments

Invited Talk

Noam Eliaz[1,2], Shir Andreev Batat[1,2], Vladimir Popov[1,2]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Israel*
[2]*TAU Additive Manufacturing Center, Tel Aviv University, Israel*

15:20 - 15:45 Ceramic Matrix Composites – Challenges and Development Approach for Military Applications

Invited Talk

Amit Schleyer[1], Omri Diner[1], Matanel Zered[1], Ido Koresh[1], Maria Gandman[1], Boris Kositski[1], Eli Levin[1], Eyal Aharon[1], Shai Friedman[1], Anat Shenhar[1], Dvir Blumer[1]
Dep. of Advanced Materials, RAFAEL Advanced Defense Systems, Israel

15:45 - 16:00 $AlFeCoCrNi_x$ (with x=1.2, 2.1, 2.6) High Entropy Alloys: Microstructure, Properties and Heavy Ion Irradiation Resilience

Contributing Talk

Yuval Hodaya Malinker[1], Shai Salhov[2], Malki Pinkas[2], Daniel Primetzhofer[3], Louisa Meshi[1]
[1]*Department of Materials Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel*
[2]*Nuclear Research Center-Negev, P.O. Box 9001, Beer-Sheva 84100, Israel*
[3]*Tandem Laboratory, Uppsala University, Box 529, 751 21 Uppsala, Sweden*

16:00 - 16:15 Implementation of Time-domain Frequency-dependent Acoustic Drag to Model the Shock Attenuation Characteristics of Methyl Cellulose Hydrogel

Contributing Talk

Orel Guetta[1,2], Daniel Rittel[2]
[1]*IAEC, Israel*
[2]*Mechanical engineering, Technion, Israel*

16:15 - 16:30 Microstructure and Properties of Ultra High Temperature Ceramic Matrix Composite Produced by Infiltration of Eutectic Zr-Si into Carbon-Carbon Preform

Contributing Talk

Neta Kurz[1], Eugen Rabkin[2], Itamar Gutman[1]
[1]*Rafael, Israel*
[2]*Materials Science and Engineering, Technion, Israel*

14:30 - 16:35 Materials Physics

Hall C

Chair: Yoav Kalcheim, *Technion - Israel Institute of Technology, Israel*

14:30 - 14:55 Charge Transport in Calcium-Manganate Oxides for Thermoelectric Applications

Invited Talk

Yaron Amouyal
Technion - Israel Institute of Technology, Israel

14:55 - 15:20 Chalcogenides for Extreme Light-Matter Interactions

Invited Talk

Tomer Lewi
Faculty of Engineering, Bar-Ilan University, Israel

15:20 - 15:45 Designing Nickelates for High-temperature Superconductivity

Invited Talk

Muntaser Naamneh, Yoav Mairovich
Ben-Gurion University, Israel

15:45 - 16:10 Probing Phase Transitions and Stability within Molecular Ices by the Discharge of Weakly Bound Electrons and Ions

Invited Talk

Roey Sagi[1,2], Micha Asscher[2]
[1]*Nuclear Research Center- Negev, Beer Sheva, Israel*
[2]*Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel*

16:10 - 16:35 Metasurfaces: From Science to Applications

Invited Talk

Uriel Levy
Hebrew University of Jerusalem, Israel

14:30 - 16:30 Materials Characterization

Hall D

Chairs: Tatyana Bendikov, *Weizmann Institute of Science, Israel*
Yaron Kauffmann, *Technion - Israel Institute of Technology, Israel*

14:30 - 14:55 Discovering Order in Meta-Stable Materials with SNEM

Invited Talk

Yevgeny Rakita
Materials Engineering, Ben Gurion University of the Negev, Israel

14:55 - 15:20 Elucidating the Structure and Composition of Buried Interfaces with New Solid State NMR Methods

Invited Talk

Michal Leskes
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

15:20 - 15:45 Point Spread Function Engineering in Optical Microscopy - Why and How to Ruin a Perfectly Good Microscope

Invited Talk

Yoav Shechtman
Technion, Israel Institute of Technology, Israel

15:45 - 16:00 X-Ray Diffraction Analysis of Layered Compounds: from Regular Structures to Nanoparticles with Curved Turbostratic Layers

Contributing Talk

Yishay Feldman
Department of Chemical Research Support, Weizmann Institute of Science, Israel

16:00 - 16:15 Interplanar Spacing Metrology at 30 fm Uncertainty Using Scanning Transmission Electron Microscopy

Contributing Talk

Amram Azulay[1], Itai Silber[2], Yoram Dagan[2], Amit Kohn[1]
[1]*Department of Materials Science and Engineering, The Iby and Aladar Fleischman Faculty of Engineering, Tel Aviv University, Israel*
[2]*School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Israel*

16:15 - 16:30 Advanced and Future Logic Device Architecture: Challenges and Solutions in Materials Metrology

Contributing Talk

Yovav Kalifon
CTO group, Nova Ltd., Israel

14:30 - 16:30 Corrosion & Electrochemistry

Hall E

Chair: Brian Rosen, *Tel Aviv University, Israel*

14:30 - 14:55 Synthesis of Functional Coatings Using the Molten Salt Plasma Electrolytic Oxidation

Invited Talk

Konstantin Borodianskiy[1], Yuliy Yuferov[1]
Chemical Engineering, Ariel University, Israel

14:55 - 15:20 Enhancing the Efficiency and Stability of Reversible Zinc and Iron Electrodeposition in Mildly Acidic Electrolyte Solutions

Invited Talk

Daniel Sharon
Institute of Chemistry, The Hebrew University of Jerusalem, Israel

15:20 - 15:45 Corrosion Performance of Biomaterials in Physiological Environments

Invited Talk

Galit Katarivas Levy
Biomedical Engineering, Ben-Gurion University of the Negev, Israel

15:45 - 16:00 One-step Synthesis of Single Atom Catalysts (SACs) on Nanocarbons Using Thermal Delamination: A New Paradigm For High Performance, Binder-Free, Electrodes for Water Splitting

Contributing Talk

Daniel Nessim

Bar Ilan University, Israel

16:00 - 16:15 Sulfur Corrosion in Copper within Insulating Liquids

Contributing Talk

Grisaru Marius
Consulting Marius Grisaru, Israel

16:15 - 16:30 Performance of $LaFeO_3$ and $La_{0.8}Sr_{0.2}FeO_3$ perovskites in Reverse Water-Gas Shift

Contributing Talk

Gal Sror[1], Leonid Vradman[2], Miron Landau[1], Moti Herskowitz[1]
[1]*Chemical Engineering, Blechner Center for Industrial Catalysis and Process Development, Ben-Gurion University of the Negev, Be'er-Sheva, Israel*
[2]*Department of Chemistry, Nuclear Research Centre-Negev, Be'er-Sheva, Israel*

14:30 - 16:30 Additive Manufacturing II

Hall F

Chair: Bat-El Pinchasik, *Tel Aviv University, Israel*

14:30 - 14:45 Additive Manufacturing of Hypereutectic Al-Si Alloys

Contributing Talk

Dr. Tatiana Vompe
The Israel Institute of Materials Manufacturing Technologies, Technion Research and Development Foundation, Israel

14:45 - 15:00 Inconel 939 Superalloy - The Effect of Portevin-Le Chatelier on Additively Manufactured and Casted Alloy

Contributing Talk

Moshe Nahmany[1,2], Danny Moreno[1], Yohanan Nahmana[1], Matan Zakai[1], Ariel Yehuda Cohen[1], Moshe Shapira[1], Ronny Shneck[3]

[1]*Bet Shemesh Engines LTD, Bet Shemesh, ISRAEL*
[2]*Materials Department, Nuclear Research Center- Negev, Beer Sheva, ISRAEL*
[3]*Materials Engineering Department, Ben-Gurion University of the Negev, , Beer Sheva, ISRAEL*

15:00 - 15:15 Fabrication of Full Dense SiC-Si Composites using Directed Energy Deposition

Contributing Talk

Vladimir Popov[1], Shir Andreev Batat[1], Noam Eliaz[1]
Materials Science and Engineering, Tel Aviv University, Israel

15:15 - 15:30 “Writing” Crystal Phases in Amorphous Calcium Carbonate via Bio-Inspired Laser-Induced Patterned Transformations

Contributing Talk

Hadar Shaked, Iryna Polishchuk, Niv Ben-Arie, Daniela Dobrynin, Javier Gainza, Alexander Katsman, Boaz Pokroy

15:30 - 15:45 3D-printing of Functional, Mineral-Infused Substrates for Coral Settlement Enhancement

Contributing Talk

Almog Sulam, Iryna Polishchuk, Boaz Pokroy

Technion - Israel Institute of Technology, Israel

15:45 - 16:00 Degradation and Biocompatibility of 3D-Printed PLA Reinforced with WS_2 Nanotubes for Bone Scaffold Applications

Contributing Talk

Ofek Golan[1], Noa Granada[1], Lin Lemesh[1], Salome Azoulay-Ginsburg[2], Roey J. Amir[2], Francesca Netti[3], Lihi Adler-Abramovich[3], Noa Lachman[1]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Israel*
[2]*Department of Organic Chemistry, Tel Aviv University, Israel*
[3]*Department of Oral Biology, Tel Aviv University, Israel*

16:00 - 16:15 HfB2 Coating Fabrication Using Laser Powered Directed Energy Deposition

Contributing Talk

Shir Andreev Batat[1], Vladimir Popov[1], Zlatomir Apostolov[2], Noam Eliaz[1]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Tel Aviv, Israel*
[2]*Materials and Manufacturing Directorate, Air Force Research Laboratory, Ohio, USA*

16:15 - 16:30 Sustainable 3D-Printable Ionic Eutectogels for Multifunctional Sensing

Contributing Talk

Yuchen Wang[1], Sergey Nechausov[1], Yi Jiang[1], Aslan Miriyev[1]
Mechanical engineering, Ben Gurion University, Israel

16:30 - 17:00 Coffee Break, Poster Viewing

Foyer, Exhibition Area

17:00 - 17:45 Archaeometallurgy and Underwater Technologies for Cultural Heritage in the Eastern Mediterranean: Data Capture, Curation, Analyses and Dissemination

Hall A

Chairs: Eugen Rabkin, *Technion - Israel Institute of Technology, Israel*
Tzilla Eshel, *University of Haifa, Israel*

17:00 - 17:45 Archaeometallurgy and Underwater Technologies for Cultural Heritage in the Eastern Mediterranean: Data Capture, Curation, Analyses and Dissemination

Plenary Talk

Thomas Levy
Center for Cyber-Archaeology and Sustainability, University of California, San Diego, United States

17:45 - 18:15 Best Poster Prize Announcement & Closing Remarks

Hall A

Poster Presentations

Tuesday, February 25, 2025

P-1 Angular Emission Properties of Transition Metal Dichalcogenides under Uniaxial Strain

Lee Grimberg, Moshe Harats

P-2 Interlayer Excitons in Non-uniformly Strained 2-Dimensional Heterostructures

Svyatoslav Kostyukovets, Moshe G. Harats

P-3 Solubility of MoS_2 and Graphite in Molten Salt: Flowers, Faceted Crystals or Exfoliation?

Avia Lavi[1], Adi Lavi[1], Efrat Ruse[1], Oren Regev[2]
[1]*Nuclear Research Center-Negev*
[2]*Department of Chemical Engineering, Ben-Gurion University of the Negev*

P-4 Characterization of Piezoelectric Properties of 2D Perovskite Layes

Tal Medichi[1,2], Moria Lighthouse[3], Oded Milo[4], Lioz Etgar[3], Doron Azulay[4,5]
[1]*Department of Materials Engineering, Azrieli College of Engineering*
[2]*Chemistry Department, The Hebrew University*
[3]*Institute of Chemistry, Casali Center for Applied Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University*
[4]*Racah Institute of Physics, The Hebrew University*
[5]*Department of physics, Azrieli College of Engineering*

P-5 Enhancing Activated Carbon Adsorption for Advanced Wastewater Treatment and Effective Organic Pollutants Removal

Yaal Lester[1], Aya Mrar[1], Aki Sebastian Ruhl[2]
[1]*Civil Engineering, Azrieli College of Engineering Jerusalem*
[2]*Technische Univesitaet Berlin – TUB*

P-6 Chiral Photodoping in Hybrid Graphene-$Bi_2Se_{2.5}S_{0.5}$ Photodetectors

Michal Poplinger[1,2], Ilias Cheliotis[3], Adamantia Logotheti[3], Rajesh Kumar Yadav[1,2], Pilkhaz Nanikashvili[1,2], Adi Levi[1,2], Amaia Pesquera[4], Amaia Zurutuza[4], Ioanna Zergioti[3], Doron Naveh[1,2]
[1]*Faculty of Engineering, Bar-Ilan University*
[2]*Institute for Nanotechnology and Advanced Materials, Bar-Ilan University*
[3]*Department of Physics, School of Applied Mathematical and Physical Sciences, National Technical University of Athens*
[4]*Graphenea SA, Donostia-San Sebastian*

P-7 Reactive Intercalation: A Novel Approach for Atomically Thin Heterostructures for Electronic and Optoelectronic Applications

Anway Pradhan, Avinash Patsa, Pranab K. Mohapatra, Ariel Ismach[1]
Department of Materials science and engineering, Tel Aviv University

P-8 Investigating the Growth of 2D Ternary Compounds via Chemical Vapor Deposition

Nitin Shinde[1], Shavit Gideon[1], Anway Pradhan[1], Ariel Ismach[1]
Department of Materials Science and Engineering, Tel Aviv University,

Ramat Aviv, Tel Aviv 6997801,

P-9 Coupled Pyroelectric-photovoltaic Effect in 2D Ferroelectric α-In$_2$Se$_3$

Michael Uzhansky

P-10 Direct Determination of Torsion in Twisted Graphite and MoS2 Interfaces

Gautham Vijayan[1], Elad Koren[1]
Faculty of Materials Science and Engineering, Technion - Israel Institute of Technology

P-11 MXene-CNC Super Performing Composite Films for Flexible and Degradable Electronics

Daniel Voignac[1]
Applied physics and Plant science, Hebrew University of Jerusalem

P-12 Multiple Wavelength Printing in VAT Photopolymerization 3D Printing - Analyzing Solubility and Mechanical Properties of Printed Models

Yali Reuveni, Liron Ben Arush

P-13 Characterization of a Single Nano-cavity by Scanning Electrochemical Microscopy (SECM)

Iska Cohen[1,2], Daniel Mandler
[1]*Department of Materials Engineering, Azrieli College of Engineering*
[2]*Chemistry Department, The Hebrew University of Jerusalem*

P-14 Intrinsic Mechanics and Bundled Collagen fibers Microstructure of Fetal membranes in Preterm birth

Noa Ben-Moshe, Rachel Bitton, Meytal Forer, Alaa A. Arraf, Ron Beloosesky, Joshua M. Grolman

P-15 Robust and Facile Methodology to Fabricate Ligand Patterns for Ex-vivo Cell Interactions

Shaked Cohen[1], Brit Maman, Sivan Tzdaka, Guillaume Le Saux, Jatin Jawhir Pandit, Mark Schvartzman
Department of Materials Engineering, Ilse Katz Institute for the Nanoscale Science and Technology, Ben-Gurion University of the Negev

P-16 Aided Porous Medium Emulsification System: A Novel Method for Fabricating Microgels for Biomedical Applications

Tina Khairallah[1], Luai Khoury[1]
Materials Science and Engineering, Technion

P-17 Nanoscale Device for the Control Study of the Special Activation- Inhibitory Balance in T Cells

Brit Maman[1], Esti Toledo[1], Sivan Tzadka[1], Guilaume Le Saux[1], Mark Schvartzman[1]
Material Engineering, Ben Gurion University of the Negev

P-18 Soft Robotics Actuators Based on 2D Materials

Tal Navon[1], Daniel Mandler[2]
[1]*Department of Materials Engineering, Azrieli College of Engineering*
[2]*Chemistry Department, The Hebrew University of Jerusalem*

P-19 Effect of Electric Fields on Silk Proteins Self-Assembly

Felipe Ptak[1], Aleksei Solomonov[1], Ulyana Shimanovich[1]
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science

P-20 Accessible Nano Fabrication Process for Metallic Structures and Patterns for Advanced Applications

Tomer Sherf

P-21 Soft Printing of Gold Nanoislands on Flexible Polymeric Substrates

Aleksei Solomonov[1], Anna Kozell[1], Alexander B. Tesler[2], Iddo Pinkas[3], Seth Walensky[1], Ulyana Shimanovich[1]
[1]*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science*
[2]*Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg*
[3]*Department of Chemical Research Support, Weizmann Institute of Science*

P-22 Magnetically Drug Release Wafer for Glioblastoma

Ehud Zippin[1], Avia Lavon[1], Galit Katarivas Levy[1]
Department of Biomedical Engineering, Ben-Gurion University of the Negev, Beer-Sheva 84190, Israel

P-23 Thermal Behavior of Ablative Materials: A Study on Carbon Phenol Composites

Chen Assulin[1], Shmulik Hayun
Material Engineering Department, Ben Gurion University of the Negev

P-24 Thermal Management: High Thermal Conductivity Low Electrical Conductivity Coating Material for Electronic Devices

Noam Avtalion[1], Shani Ligati Schleifer, Lucas Luciano Cullari, Oren Regev
Department of Chemical Engineering, Ben Gurion University of the Negev

P-25 Ceramic Surface as a Detection Technique for Investigating Microbe-Mineral Interactions

Yair Farber[1], Yaniv Shlosberg[2], Robert Armon[3], Eyal Kurzbaum[4,5]
[1]*Kinneret Academic College*
[2]*Ben-Gurion University*
[3]*Technion*
[4]*Shamir Research Institute*
[5]*Tel-Hai College*

P-26 Without a Grain of Salt: Facile Micropatterning for Clean MXene Thin-Film Electronics

Bar Favelukis[1]
material engineering, Tel Aviv University

P-27 Effect of Tantalum Carbide Stoichiometry on Densification and Mechanical Properties

Svetlana Fink Ilyasafov

P-28 Three-Terminal Resistivity Switching Device Based On Reversible Oxygen Ion Migration at Room Temperature

Daniel Freidzon

P-29 Tungsten-Reinforced MAX Phase Composites for Structural Applications

Avia Greenberg[1]
Materials Science and Engineering, Tel Aviv University

P-30 Unlocking the Potential of $Y_2W_3O_{12}$ for High-Temperature Thermal Expansion Engineering

Hagay Hayun[1], Hadar Shpack[1], Yaniv Gelbstein[1]
Materials Engineering, Ben-Gurion University of the Negev

P-31 The Influence of Dopants and Fields on Microstructural Evolution of Alumina

Asaf Kazmirsky[1], Rachel Marder[1], Wayne D. Kaplan[1]
Department of Materials Science and Engineering, Technion - Israel Institute of Technology

P-32 One-pot Approach for Acoustic Directed Assembly of Metallic and Composite Microstructures by Metal Ion Reduction

Avraham Kenigsberg[1], Heli Peleg-Levy[1], Haim Sazan[1], Liron Kenigsberg[1], Silvia Piperno[1], Hagay Shpaisman[1]
Department of Chemistry and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University

P-33 Expanding MAX Phases: Discovery of a Double A-Layer Ti_2Bi_2C with Rhombohedral Symmetry

Yiftach Kushnir[1], Barak Ratzker, Maxim Sokol
Department of Materials Science and Engineering, Tel Aviv University

P-34 Immobilization of Cs-bearing Zeolites in Geopolymeric-zeolite Systems

Yarden Lior-Shain[1,2], Eyal Grinberg[1], Yaniv Gelbstein[2], Michal Arbel-Haddad[1]
[1]*Nuclear Research Center Negev*
[2]*Department of Materials Engineering, Ben-Gurion University of the Negev*

P-35 Ultra-fast High Temperature Sintering: Exploring Alumina

Rachel Marder

P-36 Using Electrical Conductivity for Structural Health Monitoring in Cement-Carbon Nanofiller Composites

Anat Menkin[1], Oren Regev, Assaf Ya'akobovitz, Yarden Jahn
Department of Chemical Engineering, Ben Gurion University of the Negev

P-37 Enhancing Oxidation Resistance in Ti3AlC2 MAX Phase With Refractory Elements Doping

Asaf Nitsan[1], Maxim Sokol
The Department of Materials Science and Engineering, The Faculty of Engineering, Tel Aviv University

P-38 Effect of Co-doping on Non-classical Electrostriction in Zr-doped Ceria

Tali Savich[1]
Weizmann Institute

P-39 The Effect of Hafnium and Tantalum on the Corrosion and Electro-Catalytic Properties of $Ti_3C_2T_z$

Danielle Sviri Belilty[1], Haridas Parse[1], Bar Favelukis[1], Maxim Sokol[1], Brian Rosen[1]
Material Science and Engineering, Tel Aviv University

P-40 Tuning the $LaFeO_3$ Particles size by Elucidating the Molten Salt Synthesis Mechanism

Yonatan Yevilevich[1,2], Leonid Vradman[2,3], Jonatan Zana[1], Hen Dahan[1], Moti Herskowitz[2]
[1]*Department of Chemistry, Nuclear Research Centre Negev*
[2]*Ben-Gurion University of the Negev*
[3]*Israel Atomic Energy Commission*

P-41 Ratchet Based Ion Pumps for Fine Tuning of Electrochemical Reactions

Dafna Amichay[1]
Electrical engineering, Tel Aviv university

P-42 Surface vs. Bulk: Exploring Alumina Coating`s Dual Role in High Energy Cathodes

Aliza Ashman[1], Shakked Schwartz, Ayan Maity, Michal Leskes
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science

P-43 Effect of Hydration on Electrical and Electromechanical Properties of Lanthanum-cerium Oxides

Or Ben Zion[1], Tahel Malka[1], David Ehre[1], Isaac Abrahams[2], Igor Lubomirsky[1]
[1]*Molecular Chemistry and Materials Science, Weizmann Institute of Science*
[2]*Department of Chemistry, Queen Mary University of London*

P-44 Energy Band Engineering of Charge Transfer Layers for Voltage Loses Optimization in Photovoltaic Application

Yael Bornstein[1,2], Ido Hadar[2]
[1]*Department of Material Engineering, Azrieli College of Engineering*
[2]*Chemistry Department, The Hebrew University of Jerusalem*

P-45 Structural and Electrical Properties of Metal-oxide Based Photoelectrodes for Water Splitting Devices

Neta Clyman-Antebi[1], Ronen Gottesman[2], Oded Millo[3], Doron Azulay[3,4]
[1]*Department of Materials Engineering, Azrieli College of Engineering*
[2]*Institute of Chemistry, The Hebrew University of Jerusalem*
[3]*Racah Institute of Physics, The Hebrew University of Jerusalem*
[4]*Department of physics, Azrieli College of Engineering*

P-46 Optimizing the Thermoelectric Properties of TiCoSb-based Half-Heusler Alloys

Noam Cohen[1], Yaniv Gelbstein[1], Yatir Sadia[1,2]
[1]*The Department of Materials Engineering, Ben Gurion University of the Negev*
[2]*Energy Research, Nuclear Research Center of the Negev*

P-47 Synthesis of Noble-metal-free Electrocatalysts as Free-standing Electrodes for Electrochemical Applications

Roni Cohen Vaza, Jonathan Tzadikov, Liel Abisdris, Menny Shalom

P-48 Influence of O_2 on Zinc Electrodeposition in Batteries with Near-Neutral Electrolytes

Shay Elmakies[1], Roman Kapaev[1], Malachi Noked[1]
BINA, Bar-Ilan University

P-49 Tailoring the Growth of Epitaxial Phase Pure Ilmenite Nitio3 Thin Film Photoanodes

Ron Fishov[1], Alexander Rashkovskiy[1], Daniel Grave[1]
Department of Materials Engineering, Ben-Gurion University of the Negev

P-50 Removal of Carbon Dioxide by Its Dissolution of Calcium Carbonate

Shiri Hadad[1], Jonathan Erez[2], David Avnir[3]
[1]*Materials Engineering, Azrieli College of Engineering Jerusalem*
[2]*Institute of Earth Sciences, The Hebrew University of Jerusalem*
[3]*Institute of Chemistry, The Hebrew University of Jerusalem*

P-51 Peptide Self-Assembly Evolution and its Effects on Proton Conductivity

Sachin Ishwarlal Jadhav[1], Hamody Maudi[1], Guillaume Le Saux[1]
Material engineering, Nurit Ashkenasy, Ben Gurion university of the negev, Beersheva

P-52 Investigation of Charge Carrier Dynamics in Spinel Ferrite Photoabsorbers by Time-Resolved Microwave Conductivity (TRMC)

Rohit Kumar Saini[1], Kumaraswamy Miriyala[1], Alexander Rashkovskiy[1], Daniel A Grave[1]
Department of Materials Engineering, Ben Gurion University of Negev, Beer-Sheva, Israel

P-53 Operando Optical Imaging and Processing for Nickel Hydroxide Electrodes

Aleksandr Kurilovich

P-54 Thermally Conductive Molten Salt for Thermal Energy Storage: Synergistic Effect of a Hybrid Graphite-Graphene Nanoplatelet Filler

Adi Lavi[1], Avia Ohayon-Lavi, Efrat Ruse, Oren Regev
NRCN

P-55 Analyzing Dendrite Formation and SEI Composition in All-Solid-State Lithium Metal Batteries under Varying Current Density using Overhauser Dynamic Nuclear Polarization (DNP)

Nadav Maimon[1], Ayan Maity, Michal Leskes
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science

P-56 Ionic Conductivity and Phase Stability in the SrF2- Bi2O3 System

Yossi Marciano[1,2], Pinhas Ben-Naim[1,2], Avi Aviv[1,2], Yatir Sadia[1,2,3], Yaniv Gelbstein[1]
[1]*The Department of Materials Engineering, Ben-Gurion University of the Negev*
[2]*Nuclear Research Center of the Negev*
[3]*Department of Materials, Imperial College of London*

P-57 Quantification of Mobile Charge Carrier Yield and Spatial Collection Efficiency in Ultrathin Film Light-trapping $ZnFe_2O_4$ Photoanode

Kumaraswamy Miriyala[1,2], Sa'ar Shor Peled[1,2], Dino Klotz[3], Daniel A. Grave[1,2]
[1]*Department of Materials Engineering, Ben-Gurion University of the Negev*
[2]*Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev*
[3]*International Institute for Carbon-Neutral Energy Research (I2CNER, Kyushu University*

P-58 Electrochemical Charging of MAX Phases and MXenes as Candidates for Hydrogen Storage Materials

Rebeca Miyar[1], Bar Favelukis[2]
[1]*Max Planck Institute for Sustainable Materials*
[2]*Tel-Aviv University*

P-59 The Effects of High Temperature Compression on the Physical and Mechanical Behavior of the Thermoelectric GeTe Alloy

Gilad Mordechai Guttmann[1,2], Shamuel Samuha[2], Reuven Gertner[2], Hila Haimov[1], Shlomo Haroush[1], Yaniv Gelbstein[1]
[1]*Department of Materials Engineering, Ben Gurion University of the Negev*
[2]*Department of Materials Engineering, Nuclear Research Center Negev*

P-60 Enhanced Proton Conduction in Zwitterionic Peptide Assemblies

Hamody Muadi[1], Sachin Ishwarlal Jadhav, Guillaume Le Saux, Nurit Ashkenasy*
Department of Material Engineering, Ben Gurion University

P-61 Possible Bond Character Effect on Self-healing Properties for Sustainable Energy Conversion

Yuval Mualem[1,2,3], David Cahen[4], Yevgeny Rakita[5], Hannah-Noa Barad[1,2,3]
[1]*Department of Chemistry, Bar-Ilan University*
[2]*Institute of Nanotechnology & Advanced Materials (BINA, Bar-Ilan University*
[3]*Israel National Institute of Energy Storage (INIES*
[4]*Department of Molecular Chemistry & Materials Science, Weizmann Institute of Science*
[5]*Department of Materials Engineering, Ben Gurion University of the Negev*

P-62 Towards Eco-Friendly Batteries: Using Advanced Natural Polymer-Based Binders for Carbonaceous Li-Ion Anodes

Maisam Nassar[1], Ekaterina Grishina[1], Yair Ein-Eli[1]
Department of Materials Science and Engineering, Technion – Israel Institute of Technology

P-63 The Stability and Performance of Bi2O2Te for Thermoelectric Applications

Noy Peretz[1], Yatir Sadia[1,2], Yaniv Gelbstein[1]
[1]*The Department of Materials Engineering, Ben-Gurion University of the Negev*
[2]*Nuclear Research Center of the Negev*

P-64 Solid-state Synthesis of High-entropy Oxides for Use as Electrochemical Catalysts in Electrochemical Cells

Jenan Rabayah[1,2], Ronen Gottesman[1], Ruth Sfez[2]
[1]*The Institute of Chemistry & The Center for Nanoscience and Nanotechnology, The Hebrew university of Jerusalem*
[2]*Department of Material Engineering, Azrieli Collage of Engineering*

P-65 Nickel-doping Strategy for Perovskite Anodes toward High-performance Ammonia-fueled Solid Oxide Fuel Cells

Or Rahumi[1], Konstantin Borodianskiy[1]
Department of Chemical Engineering, Ariel University

P-66 Hydrogen Release Kinetics in Thermolysis of Commercial Magnesium Hydride

Matan Rothberg[1], Ilan Pri-Bar[2], Yaniv Gelbstein[1,2]
[1]*Unit of Energy Engineering, Ben-Gurion university of the Negev, Beer-Sheva*
[2]*Department of Materials Engineering, Ben-Gurion university of the Negev, Beer-Sheva*

P-67 Biphasic Electrolytic Process for Generation of Green Hydrogen and Value-added Chemicals

Guilin Ruan[1,2], Avner Rothschild[1,2]
[1]*Department of Materials Science and Engineering, Technion - Israel Institute of Technology*
[2]*The Grand Technion Energy Program (GTEP, Technion - Israel Institute of Technology*

P-68 Mixed Phase TiO2 Nanowire Array Substrate to Enhance Hydrogen Evolution Activity of Ru Nanoparticles in Near-neutral Electrolyte

Matan Sananis[1], Elena Davydova, Avner Rothschild
Material Science and Engineering, Technion

P-69 Eletrochemical Bubble Release from Tunable Porous Carbons

Nicola Seraphim[1], Noa Soffer-Lugassy[1], David Eisenberg[1]
Technion

P-70 Cathode Composite Engineering for High-Energy Sulfide-Based All-Solid-State Lithium Batteries

Mamta Sham Lal[1], Arka Saha[1], Malachi Noked[1]
Bar-Ilan University

P-71 Pt Single-Atom Catalysis in Carbon Nanotubes as a Platform for Confinement Limited Electrocatalysis

Manoj Shanmugasundaram[1]
Chemistry, Bar-Ilan University

P-72 Influence of Doping on Mobile Charge Carrier Generation and Collection in Hematite Photoanodes for Solar Fuel Production

Saar Shor Peled[1], Daniel Grave[1]
Materials Engineering, Ben-Gurion University

P-73 Investigation of the Surface Processes and Kinetics of the First Hydrogenation of Pure Mg Chips

Daniel Shtuckmeyster[1], Matvey Bereznitsky[1,2], Lee Shelly[3], Nitzan Maman[3], Ezra Hanuka[4], Nir Moskovich[4], Roni Z. Shneck[1], Isaac Jacob[2]
[1]*Materials engineering, Ben Gurion University*
[2]*Unit of Nuclear Engineering, Ben Gurion University*
[3]*Ilse Katz Institute for Nanoscale Science and Technology, Ben Gurion University*
[4]*ICL*

P-74 Tuning the Physical Properties of Crystals via the Incorporation of Organic Molecules

Johanna Sklar[1], Boaz Pokroy[1], Iryna Polishchuk[1], Arad Lang[1], El'ad N. Caspi[2]
[1]*Department of Materials Science and Engineering, Technion – Israel Institute of Technology*
[2]*Physics Department, Nuclear Research Centre*

P-75 Design and Performance of Pt_3Ni and PtCu Nanocrystals as Electrocatalysts for Oxygen Reduction Reaction in Acidic Medium

Valeria Yarmiayev[1], Melina Zysler, David Zitoun
Department of Chemistry, Bar Ilan Institute of Technology and Advanced Materials (BINA), Bar Ilan University

P-76 Composition and Microstructure Effects on the Hydrogen Desorption Temperature and Storage Capacity of Ti_xZr_{1-x} Thin Films

Ido Zukerman[1,2], Meir Buzaglo[1], Chen Assulin[2], Shmuel Hayun[2]
[1]*Divison of Chemistry, NRC-Negev*
[2]*Materials Engineering, Ben Gurion University*

P-77 Enhancing Fatigue Resistance and Fatigue Limit of SLM PH 15-5 Stainless Steel Using Hot Isostatic Pressing Process

Rami Carmi[1], Igal Alon[1], Roni Shneck[2], Louisa Meshi[2], Shmuel Essel[3], Arie Bussiba[2]
[1]*Nuclear Research Center Negev*
[2]*Department of Materials Engineering, Ben Gurion University of the Negev*
[3]*Israel Aerospace Industries*

P-78 CoCrFeNiTi0.2 High Entropy Alloy (HEA) vs CoCrFeNi Medium Entropy Alloy (MEA): Microstructure, Mechanical Properties and Hydrogen Embrittlement

Ilan Prilutsky[1,2], Shlomo Levy[3], Shlomo Haroush[1], Noa Lulu-Bitton[3], Yoav Snir[3], Louisa Meshi[1]
[1]*Material Engineering Department, Ben Gurion University*
[2]*Material Engineering Department, Israeli Atomic Energy Commision*
[3]*Material Engineering Department, Nuclear Research Center Negev*

P-79 Failure Analysis of a Carabiner and Quench Cracking in 7xxx Aluminum Alloys

Idan Zvi Friedberg[1,2]
Mechanical Engineering Department, Ben Gurion University
Technology Division, IDF - Ground Forces

P-80 Insight Into the Complex Surface Chemistry of Inorganic Ligand Exchanged Nanocrystals from Solid-State NMR spectroscopy

Ran Eitan Abutbul[1], David J. Lewis[2], Daniel Lee[1]
[1]*Department of Chemical Engineering, The University of Manchester*
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P-81 Biocompatible Monodispersed Nanohydrogels for Drug Delivery

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P-82 Solvent-Driven Polymorphism and Growth Dynamics in Supramolecular Crystals

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P-83 Mechanistic Insights into the Nucleation and Growth of Bimetallic Gold Nano-Stars

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P-84 Achieving Polymer-like Quasi-elasticity in Gold Nanoparticles through Chemical Treatment

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P-85 The Strange Case of Ordering Transformation in FePd: A Nanomechanical Enigma

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P-86 Revealing the Nucleation and Growth Mechanism of Gold Nanoparticles within Mucin Glycoprotein

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P-87 Exploring Halide Perovskite Nanocrystal Decomposition: Insight by In-Situ Electron Paramagnetic Resonance Spectroscopy

Philip Immanuel, Anastasiya Sedova, Lena Yadgarov

P-88 Enantioselective Solid-State Synthesis of Guided Chiral Nanowires

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P-89 Order-Disorder Transition in Nickel-Platinum Nanoparticles

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P-90 Collective Interactions of Excitons in Halide Perovskite Nanocrystal Superlattices

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P-91 Periodic Edge-sharing/Corner-sharing Perovskite Heterostructures Nanocrystals

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P-92 Simple and Scalable Wet Chemical Synthesis of Nanomaterials: the Cases of High-Concentration Metal Oxide Nanocolloids and Two-Dimensional Chalcogenide-Hydroxide Materials

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P-93 Shuttle Peptide-Modified Doubly Self-Assembled Polymeric Nanoparticles for the Targeted Delivery of an Anticancer Antibody in Glioblastoma

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P-94 Electrochemical Reduction-Oxidation Processes for the Removal of Perfluoroalkyl Substances from Water

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P-95 Shuttle Peptide Modified Polymeric/Ceramic Hybrid Nanoparticles for Sonodynamic Therapy of Brain Cancer

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P-96 Phase Stability and Mechanical Properties of Cobalt Nanoparticles

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P-97 Parameter Optimization of High-energy Ball Milling Process for TiO_2 Powder using the Taguchi Method

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P-98 Mapping Stability and Efficiency for Anion Mixtures of Sodium Indium Double Perovskites Applying a High-Throughput Approach

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P-99 Synthesis of Copper Nanowires for Fabrication of Stretchable Electrodes

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P-100 Enhancing Water Treatment Efficiency: MXenes as an Energy-Efficient Catalyst

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P-101 Development of High Efficiency Nano-Structured Ratchets for Selective Ion Pumps

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P-102 Water Decontamination through Sulfate-Radical Oxidation in a Nano-Enabled Catalytic Filtration Process for Water Reuse

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P-103 Hydration Effects Driving Network Remodeling in Hydrogels During Cyclic Loading

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P-104 Magneto-optical and Transport Measurements of Magnetic Weyl Semimetals

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P-105 Metal-Insulator Transition Dynamics in Boron-Doped VO_2 Thin Films

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P-106 Effect of Ion Irradiation on the Resistive Switching properties of Mott Insulators

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P-107 High-Temperature Superconductor-Based Photon Detector

Ankit Kumar[1], Dmitry Panna[1], Shlomi Bouscher[1], Avi Koriat[1], Yuval Nitzav[2], Ronen Jacovi[1], Gabriel Natale[3], Vincent Plisson[3], Kenneth S. Burch[3], Amit Kanigel[2], Alex Hayat[1]
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P-108 Single Crystal Diamond Growth by Chemical Vapor Deposition for Nano-scale Sensing

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P-109 Observation of Three-Photon Cascaded Emission from Triexcitons in Giant $CsPbBr_3$ Quantum Dots at Room Temperature and Multiexciton Dependence on Blinking State

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P-110 Mechanisms Driving Defects–induced Resistive Switching in V2O3 Mott Insulator Thin Films

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P-111 Light-Matter Interactions and Trion Dynamics in WS_2 Nanotubes

Hila Shalom

P-112 Single Photon Emitter from Hexagonal Boron Nitride Nano-Bubbles

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P-113 Self-Induced Strain: A Tool for Modulating Phase Transitions in Mott insulators

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P-114 Unveiling the Structure of Electrons and Photons: a Lattice-based Theory for Quantum Materials

Roy Winter

P-115 Electrochromic Materials: P-Type Semiconductor Polymers Based on Furans for Smart Windows

Hila Friedlander

P-116 Validation of Integrated UV Filtering System for Treating Mikvas Water

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P-117 Enhancing Tribological Performance Through Nanoscale Coating and Interfacial Modification

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P-118 Impact of Coating Structure on Reaction Rates of Coupled Dissolution–Precipitation Reactions

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P-119 Investigation of the Growth Kinetics of Hydroxyapatite on CP-Ti and Ti65Zr Alloys Treated by Plasma Electrolytic Oxidation

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Wednesday, February 26, 2025

P-1 Novel Hydrothermal Surface Modification Process for Powder Manufacturing of Al.

Maria Atamna, Michael zingrad, alexander sobolev

P-2 The Effect of 3D Printing Process (PBF vs. DED) on Properties of 15-5 PH Stainless Steel

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P-3 The Influence of Hip and Heat Secondary Treatments on the Hydrogen Embrittlement, Microstructural and Mechanical Behavior of Electron Beam Melted (EBM) Ti–6Al–4V Alloy

Noa Bitton, Nissim Navi

P-4 Poly-Tungsten - 3D Printing

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P-5 Zirconium Oxide Coatings on TI-6AL-4V Alloy via Electrophoretic Deposition for Improved Orthopedic Implants

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P-6 3D-printed Patient-specific Metallic Lattice Bone Reconstruction Implants

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P-7 The Effect of Heat Treatments on the Microstructure, Properties, and Residual Stress in 3D Printed AlSi10Mg

Chen Erlich

P-8 The Effect of HIP on the Dynamic Properties of SS316L Made by EB-PBF

Gleb Gil Goviazin[1], Dor Braun, Eithan Tiferet, Shmuel Samuha, Shmuel Hayun, Amnon Shirizly, Daniel Rittel
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P-9 Additively Manufactured PEI-Based Patient-specific Bone Replacement Implants

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P-10 Novel Hybrid Patient-specific 3D-printed Garment for Hypertrophic and Keloid Scar Treatment

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P-11 3D-printed Silica-phosphate Glass

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P-12 Electrochemically Controlled X-Ray Spectroscopies of Solid-liquid Interfaces

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P-13 Structural Phase Transitions in $K(Ta_{1-x}Nb_x)O_3$: Insights from High-Resolution single crystal X-Ray Diffraction

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P-14 Chemical Tomography of Cancer Organoids and Proteo-genomic Development Stages through Chemical Communication Signals

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P-15 Quench Rate Effects on the Boson Peak in Orthoterphenyl

Shachar Keren, Omer Yaffe, Matan Menahem, Nimrod Benshalom

P-16 Nonlinear Orthotropic CMC Modelling with Abaqus

Eli Levin[1], Matanel Zered, Royi Padan
Rafael

P-17 Revisiting Asymmetric Raman Lineshapes in Silicon Using Green`s Function Analysis

Maya Levy Greenberg[1]
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P-18 Crystallographic Laws of Easy Polishing Directions in Diamond Single Crystals

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P-19 Interfacial Electric-Field Inhomogeneities in Hafnia-Film, Studied by 4D-STEM

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P-20 Qualitative and Quantitative Micro-CT Studies on Metal-Organic Framework (MOF) Single Crystals

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P-21 Characterization of the Structure of an $Al_{81}Fe_{10}Pt_{9}$ Phase Using 3D Electron Diffraction Method

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P-22 Optical Microscopy Based Prediction of Nanoparticle Height Distribution in Pt Nanogrates Using Artificial Intelligence

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P-23 Monodispersed Nanohydrogels for Drug Delivery

Gerardo Byk[1], Eswaran Lakshmanan[1], Sinyal Abu-Rabyah[1], Danit Zegal[1], Gila Kazimirsky[1], Nir Osherov[2], Yana Shadkhan[2], Maria Lujan Cuestas[3], Shaul Deniz Cemal[1]
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P-24 A Self-healing Multispectral Transparent Adhesive Peptide Glass

Gal Finkelstein-Zuta, Ehud Gazit

P-25 In-vitro Behavior of Zn-Nd Base Alloy as Structural Material for Biodegradable Implants

Efrat Hazan Paikin

P-26 Electrically Conductive Peptide/MXene Hydrogel Scaffold for Tissue Regeneration

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P-27 Innovative Lithographic Platform For Reference-free Traction Force Microscopy

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P-28 Artificial Silk Fibers with Tunable Mechanical Performance

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P-29 Copper Oxide Nanoparticle Embedded Super Absorbing Biopolymers to Enhance Nutrient Supply and Water Retention in Agriculture

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P-30 Monte Carlo Simulated Annealing and Machine Learning Interatomic Potentials for High-Entropy Materials Design

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P-31 Computational Studies of Liquid Potassium Under Pressure Using First Principles and Machine Learning Methods

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P-32 In-gap States and Carrier Recombination in Quasi-2D Perovskite Films

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P-33 Evaluation of Mn Doped Perovskite-type Oxides as Electrolyte Materials for Hydrogen Conversion

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P-34 The Effect of Oxygen Terminations on Charge Transport Across Mos_2 Monolayers

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P-35 Uniaxial Strain-Induced Multiferroicity in $EuTiO_3$ Membranes: Insights from DFT Simulations

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P-36 Adsorption and Intermediate Reactants Study of Nitrogen Reduction Reaction on Bi Surface Using Machine Learning Based on DFT Calculated Database

Sean Pachmanov Dvir, Maytal Caspary Toroker

P-37 First Principles Calculations of the Magnetic Structure of the RE-based -MAX Phases – a Family of Nanolaminated Magnetic Materials

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P-38 MD Calculations of High Pressure Pb-Sn Alloy

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P-39 Ab Initio Study Of Point Defects In Tungsten Metal

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P-40 The Effect of TiO2 Particles in Zinc Coating on Corrosion of Low Carbon Steel ST 37

Harel Cohen, Svetlana Lugovskoy, Alex Lugovskoy

P-41 Enhanced Corrosion Protection and Electrochemical Activity for Aluminum Fluoride Surface

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P-42 Experimental Apparatus for SMA Springs Analysis: Design and Results

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P-43 Material Coefficient Extraction Through Design and Modeling of Magnetoelectric Devices in Higher Bending Modes

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P-44 Conductive Peptide-Based MXene Hydrogel as a Piezoresistive Sensor

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P-45 Controlling Independently the Pyroelectricity and Piezoelectricity of Doped Mixed Crystals

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P-46 Bio-Inspired Core-Shell Crystalline Guanine Spherulites

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P-47 Nitridochromates as Potential Functional Materials

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P-48 Characterization of Electro-mechanical Performance of Soft Ionic Materials

Yi Jiang, Yuchen Wang, Sergey Nechausov, Aslan Miriyev

P-49 Development and Characterization of Bovine Serum Albumin-based Sponges for Efficient Removal of Perfluorooctane Sulfonate

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P-50 THZ-Raman Spectroscopy Probes Lattice Dynamics of Metal-Organic-Frameworks

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P-51 Studying the Involvement of Cells and the Interplay of Mineral and Silk Protein Gel in Mollusk Shell Formation

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P-52 Influence of SrTiO3(001) Substrate Temperature on the Structure and Magnetic Properties of FePd Films

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P-53 Porous Galfenol Films on Porous Silicon: Magnetic and Magnetostrictive Properties

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P-54 Post–Functional Integration of Mechanophores into Heterogeneous Biologically Derived Materials via “Dip–Conjugation”

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P-55 Trypsin-Induced BSA-PEGDA Hydrogel as an Extendable Soft Robotic Drug Carrier

Yuchen Liu

P-56 Unique Pathway of Metal to Halide Perovskites Conversion

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P-57 Dry Etched Periodic Nanopores in GaN and Their Effect on Electromechanical Properties

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P-58 Magnetron Sputtered Fe_3Si Full Heusler Compound Thin Films: the Effect of Microstructural Evolution on Physical Properties

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P-59 Tuning Electrochemical Doping and Charge Transport in OECTs by Controlling Microstructure through Blends

Efrat Reyn[1], Sasha Simotko[1,2], Moam Moscovich[1], Gitti L. Frey[1,2]
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P-60 Challenges in Synthesizing Tungsten-Based Refractory Multi-Principal Element Alloys

Tatiana Efremenkova[1], Shmuel Hayun[1]
Materials Engineering Department, Ben-Gurion University of the Negev

P-61 Ferroelasticity in Halide Perovskites Affects Electro-Optical Properties through Facet Stability

Noam Veber[1], Betty Shamaev[1], Yehonadav Bekenstein[1]
Materials Science and Engineering, Technion

P-62 Influence of Magnetic Field on Longitudinal and Transverse Wave Propagation in Magneto-active Polymers

Ankush Yadav, Pavel Galich[1]
Aerospace Engineering, Technion - Israel Institute of Technology

P-63 High Entropy Rare Earth Oxides

Sapir Yail

P-64 Pressure-dependent Phase Behavior of Metallic Alloys: Thermodynamic Modeling and Experimental Insights into Binary and Ternary Systems

Shir Ben Shalom[1], Moran Emuna[2], Peleg Lider[1], Yaron Greenberg[2], Eyal Yahel[2], Guy Makov[1]
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[2]*Physics Department, Nuclear Research Centre Negev*

P-65 Pressure Effect on Ternary Phase Diagrams: Bi-Sb-Pb as a Case Study

Shir Ben Shalom[1], Peleg Lider[1], Guy Makov[1]
Materials Engineering, Ben-Gurion University of the Negev

P-66 The Structure of Liquid Bismuth Along the Melting Curve

Shir Ben Shalom[1], Neta Ellert[1], Laura Henry[2], Moran Emuna[3], Yuri Kirshon[1], Pierre Piault[2], Andrew King[2], Nicolas Guignot[2], Yaron Greenberg[3], Eyal Yahel[3], Guy Makov[1]
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P-67 MeV Proton Irradiation Effect on Li Ion Anodes

Inbal Gavish Segev[1], Alexander Bychkov[2], Gaelle Gutierrez[3], Jongmin Lee[4], Markus Strobl[4], Guy Makov[5], Yair Ein Eli[2]
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P-68 Silver-Antimony-Telluride Compounds: Phase Content, Crystallography, Thermoelectric Performance, and High-Pressure Analysis

Sergei Grazhdannikov[1], Baihong Sun[1,2], Yansun Yao[3], Elissaios Stavrou[1,2], Yaron Amouyal[1]
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[3]*Department of Physics and Engineering Physics, University of Saskatchewan*

P-69 Electrochemical Properties and Pressure-Induced Phase Transformations of LiC_4N_3 and NaC_4N_3

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P-70 Mitigation of Irradiation-Assisted Stress Corrosion Cracking by Laser Annealing

Maayan Matmor[1], Jonathan Tatman[2], Mitch Hargadine[2], Mehdi Balooch[3], Shahin Tariqu Alaei[3], Chou Peter[2], Peter Hosemann[4]
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P-71 An Analysis of Modelling and Self-Consistent Calculations for Properties at High Pressure using DFT: For Rare-Earth Elements

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P-72 Ultra-low doping of Silver Thin Films with 228Th: Deposition and Radiative Emission Characterization

Michael Shandalov[1], Shachar Moskovich[2], Guy Heger[2], Lior Arazi[2], Eyal Yahel[1], Yuval Golan[2]
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P-73 Effects of Grain Boundary Types and Precipitates on the Electrical Properties of DED-printed Aluminum

Omer Coriat[1], Amram Azulay[1], Vladimir Popov[1], Hanna Bishara[1]
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P-74 Study of the Microstructural Changes of AlCoCrFeNi System as Function of Cr and Al Variation Applying Pseudo-binary Diffusion Couple Approach

Yuval Malinker[1], Guy Hillel[1], Louisa Meshi[1]
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P-75 Room-temperature Recrystallization of Mo Induced by Nanoindentation

Feitao Li[1], Eugen Rabkin[1]
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P-76 Spontaneous Formation of a Eutectic Au-Co Interface via a-Low Temperature Reduction Process

Inna Popov[1], Shay Avisar[2], Anat Shvets[2], Avi Bino[2]
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P-77 The Spinodal Decomposition Impact on Electrical Resistivity Stability of CuMn Alloys.

Saja Sarhan, Hanna Bishara[1], Amram Azulay
Materials Science and Engineering, Tel Aviv University

P-78 The Effect of the Elastic Energy on the Microstructure of Nano $TiNi_2Sn$ Precipitates in a Half-Heusler TiNiSn Matrix

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P-79 The Strong Effect of NiCr Adhesion Layers in Surface Micromachined MEMS Sensors

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P-80 Characterization of Microstructure, Surface Morphology and Electrical Properties of Si-Ti-Pt-Au Contacts

Ligal Tarrab-Mizrachi, **Tamar Tepper-Faran**[2], Shlomo Berger
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P-81 Towards Understanding the Effect of Increased Configurational Entropy on Structure and Stability of Quasicrystals and their Approximants

Avner White[1], Louisa Meshi[1]
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P-82 Mechanical Properties of Ni-NiO Core-Shell Nanoparticles Prepared by Solid-State Dewetting and Oxidation

Chunli Wu[1,2], Yuanshen Qi[1,2], Eugen Rabkin[1]
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P-83 Recombinaiton Dynamics in Chalcogenide-based Perovskite

Yarden Arad[1], Omer Yaffe, Matan Menahem, Guy Reuveni, Maya Levy Greenberg
Chemistry, Weizmann

P-84 Epitaxial MoS_2 Nanofin-Nanoribbon Hybrids for Electronic Devices

Yarden Daniel[1], Lothar Houben[2], Katya Rechav[2], Olga Brontvein[2], Ifat Kaplan-Ashiri[2], Iddo Pinkas[2], Ernesto Joselevich[1]
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P-85 All Optical Controlled Neuromorphic FET based on vdW Ferroelectric/Semiconductor Heterostructure

ANURAG GHOSH[1], ELAD KOREN[1]
Faculty of Materials Science and Engineering, Technion-Israel Institute of Technology

P-86 Ultrafast Dynamics of VO_2 Switching Devices for Neuromorphic Applications

Amir Gildor[1], Sariel Hodisan[2], Shahar Kvatinsky[2], Yoav Kalcheim[1]
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P-87 Influence of Kinetic Parameters and Effusion Cell Configuration on the Compositional Uniformity of InAsSb Films via Molecular Beam Epitaxy

Noam Hadari[1], Nechemya Yaron[1], Nir Cahana[1], Olga Klin[1], Yossi Cohen[1]
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P-88 Effects of Sb Alloying on the Microstructure and Thermoelectric Properties of 5 at. % In-doped Bi_2Te_3

Badie Jubran[1]
Department of Materials Science and Engineering, Technion – Israel Institute of Technology

P-89 Fully Balanced Ambipolar OECTs through Tunability of Blend Microstructure

Noam Moscovich[1], Sasha Simotko[1,2], Amit Hadar[1], Ido Zerachia[1], Gitti L. Frey[1,2]
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P-90 Stabilization of Cubic Phase of SnS using Cation Impurities

Susmita Paul[1], Neeraj Mishra[1], Yuval Golan[1], Guy Makov[1]
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P-91 Optimizing Thermoelectric Performance of $(GeTe)_{0.962}(Bi_2Te_3)_{0.038}$ Alloy Through Anisotropic Texturing

Hadar Shpack[1], Naor Madar, Yaniv Gelbstein
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P-92 A Blending Approach for Dual Surface and Bulk Functionality in Organic Transistors

Sasha Simotko[1,2], Yogesh Yadav[1], Gitti L. Frey[1,2]
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P-93 Order-Disorder Transitions in Cerium and Praseodymium Hydrides, Manifested in Temperature-Dependent Raman Scattering Spectroscopy

Shahar Aziza[1,2], Shmuel Hayun[2], Tsachi Livneh[1]
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P-94 The Influence of Time, Atmosphere and Surface Roughness on the Interface Strength and Microstructure of AA6061–AA1050
Diffusion Bonded Components

Michael Ben Haroush[1]
Material Processing, NRCN

P-95 Development of Bioinspired Fatty Acid-Based Coatings for Advancing Sustainable Agricultural Practices

Niv Ben-Arie[1], Iryna Polishchuk[1], Boaz Pokroy[1]
Department of Materials Science and Engineering, Technion Israel Institute of Technology

P-96 Effect of ZrO_2 Nanoparticles and Electrical Parameters on PEO Coatings for MRI 230D Magnesium Alloy

Ilia Bulatov[1], Alexander Sobolev[1]
Chemical Engineering, Ariel University

P-97 Determination of the Diffusion Coefficients of Silver in Selected Thermoelectric Chalcogenide Compounds

Muhamed Dawod[1], Yaron Amouyal[1]
Materials science and engineering, Technion

P-98 Effects of Grain Size and Misorientation on Thermoelectric Properties of Antimony Telluride-based Compounds

Guy Feldus[1], Yaron Amouyal[1], Zegeng Su[1], Muhamed-Khalid Dawod[1]
Department of Materials Science and Engineering, Technion

P-99 Design and Realization of a Hot Embossing Setup for Surface Engineering of Metal-plated PVDF

Basma Haj Yahya

P-100 Defining the Surface Properties of Aerogels by their Drying Media

Guy Lazovski[1], Murial E. Layani Tzadka[1], Adira Marcus[1], Shilat Ashush[1], Pechersky Savich[2], Galit Bar[1], Igor Lubomirsky[2]
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P-101 Quantitative Model for Low Temperature Sputter Deposition on Porous Substrates

Shaul Pagis-Sharon[1], Nivedita Lalitha Raveendran[1], Michal (Pellach) Leshem[2], Ester Segal[2], Yonatan Calahorra1[1]
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[2]*Department of Biotechnology and food engineering, Technion- Israel Institute of Technology*

P-102 Insights into the Oxidation Pathways of Nickel Nanoparticles Under Oxygen Evolution Reaction (OER) Conditions

Bat-Or Shalom, Miguel A. Andres, Ashley R. Head, Olga Brontvein, Alex S. Walton, Kacper Polus, Boruch Z. Epstein, Robert S. Weatherup, Baran Eren

P-103 Influence of the PEO Process Parameters on the Coating Microstructure of Ti Alloy

Gal Shitrit[1], Alexander Sobolev[1]
Chemical Engineering, Ariel University

P-104 Effect of Methylcellulose Concentration in PEO Process on Coating Properties for Titanium Dental Implants

Boris Shmukler[1], Alexander Sobolev[1]
Chemical Engineering, Ariel University

P-105 The Influence of Crystal Orientation and Thermal State of a Pure Cu on the Formation of Helium Blisters

Daniel Shtuckmeyster[1,2], Nitzan Maman[3], Moshe Vaknin[2], Gabriel Zamir[2], Victor Y. Zenou[1,2], Ulrich Kentsch[4], Itzchak Dahan[2], Roni Z. Shneck[1]
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P-106 Ceramic-Metal Interface: Relationships between Residual Stress, Microstructure, and Mechanical Properties of Brazed Alumina-aluminum Composite Joints

Stalin Sundara Dhas[1], Kalaichelvan K[1]
Department of Ceramic Technology, Anna University

P-107 Fabrication of Vertically Aligned Nanocolumns for Advance Electrolyte Applications

Yuliy Yuferov[1], Ilia Rozenblium[1], Konstantin Borodianskiy[1]
Department of Chemical Engineering, Ariel University

P-108 Development of Dispersion-Strengthened Coatings for Aluminum Powders via Hydrothermal Process

Karin Zaolinov[1], Michael Zinigrad[1], Alexander Sobolev[1]
Chemical Engineering, Ariel University

P-109 Pattern Formation through the Oriented Growth of Au-Si Thin Films on Si Single Crystals

Rotem Zilberberg[1], Iryna Polishchuk[1], Lotan Portal[1], Silvia Milita[2], Giuseppe Falini[3], Alexander Katsman[1], Boaz Pokroy[1]
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Program Abstracts

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Grain Growth is Not Curvature Flow: Why? Consequences? (Tuesday, February 25, 2025 09:10)

Invited Lecture

Physical Metallurgy

Grain Growth is Not Curvature Flow: Why? Consequences?

David Srolovitz[1], Caihao Qiu[2], Jian Han[2], Gregory Rohrer[3], Marco Salvalaglio[4]
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[3]*Materials Science and Engineering, Carnegie Mellon University, USA*
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Grain growth in polycrystals is traditionally considered a capillarity driven process, with grain boundaries (GBs) migrating toward their centers of curvature (i.e., mean curvature flow). Experimental and simulation evidence shows that this simplistic view is untrue. We demonstrate that the failure of the classical mean curvature flow description of grain growth originates from the shear deformation naturally coupled with GB motion (i.e., shear coupling). Our findings are built on large-scale microstructure evolution simulations incorporating the fundamental (crystallography-respecting) microscopic mechanism of GB migration. The nature of the deviations from curvature flow revealed in our simulations is consistent with observations in recent experimental studies on different materials. We demonstrate how to incorporate the mechanical effects that are essential to the accurate prediction of microstructure evolution.

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Magnesium Technologies for Aviation and Aerospace Applications (Tuesday, February 25, 2025 09:55)

Invited Lecture

Materials for Security and Defense

Magnesium Technologies for Aviation and Aerospace applications

Dan Shechtman[1]
Technion - Israel Institute of Technology, Israel

Magnesium alloys are increasingly used in aviation and aerospace due to their favorable properties, including low density and high strength-to-weight ratio. These alloys, primarily composed of magnesium and small amounts of other elements like aluminum, zinc and rare earth metals, help reduce aircraft and space craft weight, leading to improved fuel efficiency and performance. Their lightness contributes to increased payload capacity and enhanced maneuverability. Issues such as lower corrosion resistance and flammability compared to other materials are addressed by selected composition and surface treatments. Overall, magnesium alloys offer significant benefits for modern aviation and aerospace applications.

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Nanomaterials (Tuesday, February 25, 2025 11:10)

Invited Lecture

Nanomaterials

When Nature Meets Nanotechnology: Bio-assisted Synthesis of Nanomaterials Using Renewable Resources

Shachar Richter

Renewable resources are of great importance since they can be used for the benefit of humankind while helping to resolve ecological and environmental issues. In this respect, Protein-based materials from renewable resources are of particular interest since, from a material science point of view, proteins can serve as excellent building blocks for developing new structures, composites, and novel materials.

In this talk, I will demonstrate how we can leverage some of these materials to synthesize nanostructures that could be used for various applications, such as photothermal materials, smart-wound dressing, antibacterial coating, heavy-metal sorption materials, and more. The role of Jellyfish, an important renewable resource for many of our applications, will be discussed.

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Nanomaterials (Tuesday, February 25, 2025 11:10)

Invited Lecture

Nanomaterials

New Approach for "Dry" Colloidal Lithography, and its Applications in Advanced Optics and Nanomedicine

Mark Schvartzman

Colloidal lithography, based on the self-assembly of nanoscale building blocks, has long been considered an attractive alternative to top-down fabrication for producing nanoscale materials and functional systems. However, challenges such as scalability and the presence of structural defects—arising from the kinetic control of the self-assembly process—have hindered its transition from research laboratories to practical applications.

Traditionally, colloidal self-assembly is conducted at the liquid-air interface using techniques like dip coating, spin coating, or Langmuir-Blodgett troughs. Alternatively, assembly in dry environments, achieved through mechanical rubbing of nano-/microparticles between two surfaces, has demonstrated scalable self-assembly with closely packed particles and minimal defects, surpassing liquid-air methods. Specifically, rubbing between silicon-based elastomer surfaces has produced defect-free assemblies. However, this approach has been limited to fabricating structures on elastomer surfaces, significantly restricting its broader application.

To address this limitation, we developed a novel nanofabrication approach based on the mechanical transfer of rubbing-assembled nano-/microparticles from elastomer surfaces to diverse target substrates. Initially, this transfer was facilitated using a thin film of polyethyleneimine (PEI) molecular glue. To eliminate contamination issues associated with PEI, we introduced a cleaner method that employs frozen water as a transfer medium. After particle transfer, the water melts and evaporates, leaving the particles intact. The structural parameters of the formed 2D crystal, including Fast Fourier Transform and Voronoi tessellation analysis, revealed unprecedented order and quality in the assemblies.

This innovative approach has been successfully applied in two key areas. The first is the scalable engineering of subwavelength antireflective structures for precision optics. By implementing high-quality assemblies on materials such as silicon and sapphire, we achieved antireflective performance surpassing previous techniques. The second area involves nanostructures for studying and manipulating biophysical cues in T-cell stimulation—key lymphocytes in the immune system. This includes creating nanopatterns to explore how ligand arrangement regulates T-cell activation and inhibition. Additionally, this method has been applied to scalable fabrication of 3D priming nanostructures for controlled ex-vivo engineering of Chimeric Antigen Receptor (CAR) T cells for cancer immunotherapy. CAR T cells produced using these nanostructures demonstrated superior performance compared to standard protocols, showing improved proliferation, reduced exhaustion, enhanced CAR expression, and heightened antitumor activity.

In summary, this nanofabrication approach overcomes traditional challenges of colloidal lithography, enabling realistic applications in producing nanostructures. Its potential applications span various fields, including optics and nanomedicine, making it a transformative tool for advancing technology and healthcare.

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Nanomaterials (Tuesday, February 25, 2025 11:10)

Invited Lecture

Materials for Energy Storage and Conversion

Oxygen Reduction Reaction Activity and Stability of Shaped Metal-doped PtNi Electrocatalysts: from Rotating Disk Electrode to Membrane Electrode Assembly

Shlomi Polani[1]
Department of Chemical Engineering, Ariel University, Israel

The synthesis of platinum-based catalysts for the cathode of proton exchange membrane fuel cells (PEMFCs) is a particularly active area aimed at meeting the technological requirements for activity and stability. However, developments in this area are still insufficient for the various applications of PEMFCs in the transportation sector. To enable widespread commercialization of passenger cars, their high cost must be reduced to less than 0.125 g_{Pt} cm^{-2} by producing more active catalysts and lowering the high Pt loading at the cathode, which is required for the sluggish kinetics of the oxygen reduction reaction. In addition, an improvement in catalyst stability is also required for these applications.

The seminal work of Stamencovic et al. on the highly active 1 1 1 Pt_3Ni single crystal led to an increased interest in mainly small octahedral PtNi nanocatalysts, which showed increasing activity at the rotating disk electrode over the years. Nevertheless, these high activities could not be transferred to the desired membrane-electrode assembly single cell.

In this talk, I will present our recent developments of novel synthesis protocols and the use of applied measurement setups as well as their limitations in evaluating intrinsic activity in reliable potentials for this class of nanocatalysts.

We have prepared highly active and stable metal-doped octahedral PtNi catalysts at high and low current densities. Our catalysts showed significant improvements over the benchmark catalysts in various experimental electrochemical test setups used to evaluate their performance. We also used advanced microscopy techniques in-situ to monitor their morphological stability during heat treatment.

Our results serve as a guide for the rational development and testing of active and stable electrocatalysts for the next generation of transportation technologies.

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Nanomaterials (Tuesday, February 25, 2025 11:10)

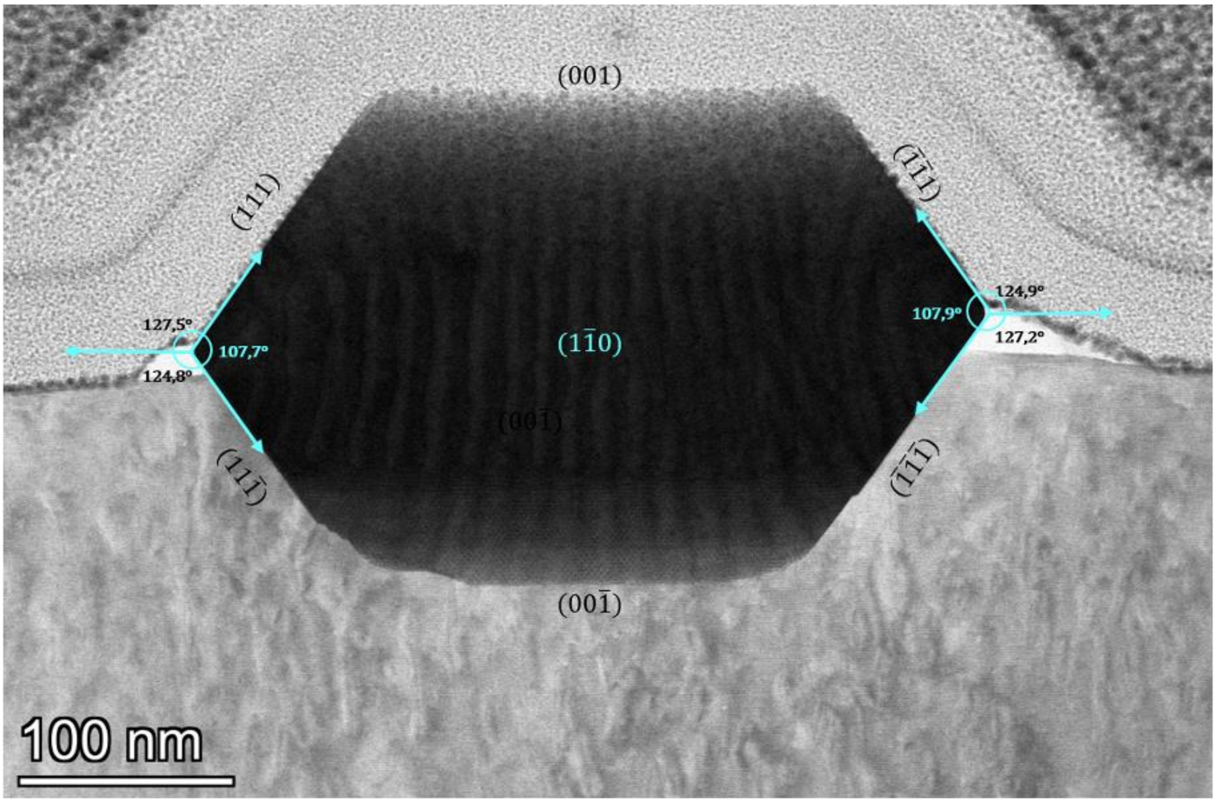
Oral Presentation

Nanomaterials

Formation of FePt $L1_0$ Epitaxial Nanoparticles via Physical Vapor Deposition

Julia Unangst, Eylül Suadiye, **Gunther Richter**[1]
Max Planck Institute for Intelligent Systems

Nanomaterials, defined by particles with at least one dimension under 100 nm, are characterized by an exceptionally high surface-to-volume ratio. This property gives them unique characteristics and enhanced reactivity, making them promising building blocks for novel materials with tailored properties. The L10 phase of Iron-Platinum (FePt) has garnered particular attention due to its remarkable properties. With a magneto crystalline anisotropy constant of in the ordered L10 phase, FePt offers one of the highest magnetic anisotropies among known materials
This study focuses on the development and characterization of FePt $L1_0$ thin films and epitaxial FePt $L1_0$ nanoparticles synthesized using physical vapor deposition. The core objective is to optimize fabrication processes to achieve the desired $L1_0$ ordering at the nanoscale. Two synthesis methods—nucleation growth and dewetting—are systematically explored. Special emphasis is placed on understanding the effects of key parameters, such as deposition rate and substrate temperature. By intentionally varying these parameters, the work provides valuable insights into the growth mechanisms and resulting material structures.
The formation of FePt $L1_0$ nanoparticles is described in the context of Wulff shape and Winterbottom concepts. The role of surface and interface diffusion plays in the microstructure formation is discussed in detail.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100 nm

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Nanomaterials (Tuesday, February 25, 2025 11:10)

Oral Presentation

Nanomaterials

Self-Assembled Superstructures of Metal-Organic Frameworks

Elad Gaver[1], Ifat Kaplan-Ashiri[2], Anna Eden Kossoy[2], Tatyana Bendikov[2], Ryuichi Shimogawa[3], Anatoly Frenkel[3], Maria Chiara di Gregorio[4], Michal Lahav[1], Milko van der Boom[1]
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[2]*Chemical Research Support, The Weizmann Institute of Science, Israel*
[3]*Department of Materials Science and Chemical Engineering, Stony Brook University, USA*
[4]*Department of Chemistry, Sapienza University of Rome, Italy*

We demonstrate sub-micron-sized metal-organic frameworks (MOFs) that can assemble in large structures. Their assembly properties are dependent on their size and morphology. Understanding the parameters that control the assembly of sub-micron particles into superstructures can result in the formation of crystal-from-crystals with usual properties. These new MOFs were prepared by the solvent diffusion method using bivalent cobalt and nickel salts. A tetrahedral ligand having four imidazole groups is used for coordination to first-row metals. The coordination chemistry of imidazole groups for the formation of MOFs has been less explored than the coordination chemistry of pyridine nor carboxylates.[1] The use of imidazole coordination chemistry resulted in stable crystals with a high level of uniformity in both size and shape.[2] Imidazole coordination is weaker than that of carboxylate1 and it is stronger than coordination of pyridine-derivatives to the same metal centers.[3] It is plausible that during the crystal growth ligand-metal dissociation occurs prior to the formation of the obtained structures, drop casting of the MOFs on silicon wafers resulted in homogeneous films that upon solvent evaporation formed the structures shown in Figure 1 below.

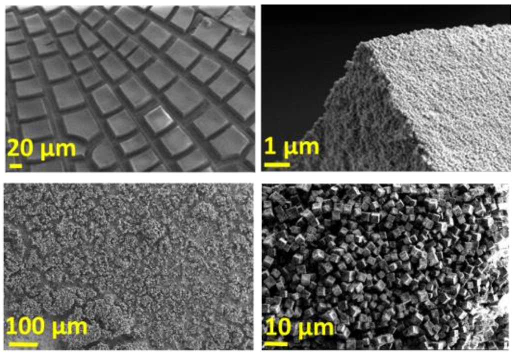

Figure 1. Scanning electron microscope (SEM) images of nickel (top) and cobalt (bottom) based metal-organic frameworks (MOFs) and their self-assembled superstructures.

[1] A. Nimmermark, L. Öhrström, J. Reedijk, Zeitschrift fur Krist. 2013, 288, 311–317.

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[3] A. Richaud, N. Barba-Behrens, F. Méndez, Org. Lett. 2011, 13, 972–975.

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Nanomaterials (Tuesday, February 25, 2025 11:10)

Oral Presentation

Nanomaterials

Investigation of the Formation of ZIF-8-Derived ZnS@MoS_2 Core-Shell Composites for Energy Applications

Alen Sam Thomas[1], Lena Yadgarov
Department of Chemical Engineering, Ariel University, Israel, Israel

Developing efficient photocatalysts is crucial for advancing sustainable energy solutions, particularly in photocatalysis and electrocatalysis applications like hydrogen evolution reaction (HER) and nitrate reduction. Combining MoS_2, a two-dimensional transition metal dichalcogenide, with ZIF-8-derived ZnS creates a unique ZnS@MoS_2 core-shell structure, which exhibits enhanced photocatalytic activity due to its unique structural and electronic synergy.1 MoS_2 offers visible solid light absorption, high chemical stability, and exceptional catalytic activity, especially at edge sites and sulfur vacancies.2 By pairing it with ZnS derived from highly porous ZIF-8, we introduce additional active sites and extend light absorption across UV and visible spectra, improving photocatalytic performance.

We successfully fabricated ZIF-8 derived ZnS@MoS_2 composite through a novel synthesis route, achieving effective control over synthesis parameters for the desired structure. We intensely studied the formation mechanism of the core-shell. Initial results are interesting, demonstrating enhanced activity in photocatalysis. With ongoing optimization to further increase efficiency in photocatalysis, this work highlights the potential of ZnS@MoS_2 core-shell structures in developing highly active, stable, and versatile photocatalysts for renewable energy applications.

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Polymers & Colloids (Tuesday, February 25, 2025 11:10)

Invited Lecture

Bio- and Soft Materials

Monitoring the Kinetics of Crystal Growth for Self-Healing and Structural Control of Anisotropic Theophylline Crystals

Angelica Elkan, Huan-Jui Lee, Sima Mafi, Irit Rosenhek-Goldian, Marcos Penedo,
Georg E. Fantner, Anna Kossoy, Yael Diskin-Posner, Dan Oron, Peter Vekilov

One of the major challenges in the field of organic crystalline materials is understanding the mechanisms of crystal nucleation and growth and applying this knowledge to design crystals with desired properties. As a model, we use the Theophylline crystal to demonstrate that driving crystallization into classical growth mode, in which the crystal grows molecule-by-molecule, allows for controlling the crystal`s structure, shape, and dimensions. Theophylline has multiple polymorphs as well as hydrated and anhydrous forms. By tailoring conditions, we were able to achieve structure specificity and navigate the crystal shape either to 1D needle-like or 2D crystalline sheets. Moreover, we show that crystals that grow by the classical mode of direct monomer incorporation have the potential to regrow and heal once a “defect” is introduced by mechanical cut, or by local thermal subliming of crystalline sections.

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Polymers & Colloids (Tuesday, February 25, 2025 11:10)

Invited Lecture

Polymers and Colloids

Space Durable 3D Printed High-Performance PolymersBased on Cyanate Ester/Extended-Bismaleimide

Yuval Vidavsky[1], Nurit Atar[1], Asaf Bolker[1], Brian E. Riggs[2], Timothy K. Minton[2],
Irina Gouzman[1], Eitan Grossman[3]
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[2]*Department of Aerospace Engineering Sciences, University of Colorado at Boulder, USA*
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To accomplish the potential of the New-Space emerging era and facilitate scientific and commercial space exploration, the development of versatile, customized, and affordable space technologies is essential. 3D printing is established as a disruptive technology, enabling the production of complex and lightweight structures with enhanced performance. However, the harsh conditions of the space environment, including atomic oxygen (AO), extreme temperatures, and ionizing radiation, pose significant challenges to the durability and longevity of additive manufacturing-produced polymers. Until now, there are no additive-manufacturing polymeric materials that are specifically developed and qualified to withstand space hazards. To address these challenges, presented in this work, novel materials for additive manufacturing, composed of cyanate ester and extended-bismaleimide that are engineered to withstand the extreme conditions in space. The developed materials demonstrate superior thermo-mechanical properties, enhanced durability to AO erosion, ionizing radiation (10 years in orbit), and thermal stability. Moreover, it is found that printing orientation governs the AO erosion, thus guiding optimal printing designs for enhanced durability to AO. The materials show improved performance, endurance, and reliability, thus contributing to the development of space-qualified components and enabling the advancement of additive manufacturing for future space missions.

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Polymers & Colloids (Tuesday, February 25, 2025 11:10)

Invited Lecture

Polymers and Colloids

Multi-Stimuli Responsivity of Single-Layer Magnetic Polymer

Amos Bardea[1], Fernando Patolsky[2]
[1]*Engineering, Holon Institute of Technology- HIT, Israel*
[2]*The Jan Koum Center for Nanoscience and Nanotechnology, Tel Aviv University, Israel*

Materials possessing multiple properties and functionalities that can be controlled or modulated by external stimuli are a central focus of current research in material sciences due to their potential to significantly enhance various future technological applications. Herein, we report a significant advancement in this field through the development of a smart multifunctional organomagnetic composite material. By utilizing a thin layer of polydimethylsiloxane (PDMS) and polypyrrole (PPy) precursors, doped with nickel nanoparticles (NiNPs), we have created an innovative organomagnetic, PDMS/PPy/NiNPs (PPN), single-layer composite film that displays multi-stimuli responsivity. The study presents the first demonstration of a multifunctional flexible, three-component film structure integrating the structural and flexible PDMS component, together with a conductive polymer component, and metal-based nanoparticles into a single-layer design, which displays enhanced and unprecedented responsivity properties against multiple different stimuli. Unlike typical stacked multi-layered structures that exhibit one or two functionalities at most, this novel configuration exhibits multiple functionalities, including magnetoresistance, mechanical stress response, piezoresistivity, and temperature sensitivity.

The significance of this novel multi-responsive composite material is underscored by the growing demand for advanced materials in biomedical devices, magnetic switches, sensors, e-skin, transistors, and organic spintronic devices. These promising organomagnetic self-standing layers, providing a robust platform for future technological innovations.

Reference:

Amos Bardea, Adam Cohen, Alexander Axelevitch, and Fernando Patolsky, A Flexible Organo-Magnetic Single-Layer Composite Film with Built-In Multistimuli Responsivity. ACS Applied Materials & Interfaces 2024 16 (44), 60686-60698 DOI: .1021/acsami.4c14857

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Polymers & Colloids (Tuesday, February 25, 2025 11:10)

Oral Presentation

Polymers and Colloids

A Novel, Fully Recyclable, Multipurpose, Photocurable Adhesive with Wide-Spectral Curing

Natanel Jarach[1,2], Michal Cohen[1], Rivka Gitt[1], Hanna Dodiuk[2], Shlomo Magdassi[1]
[1]*The Institue of Chemistry, The Hebrew University, Jerusalem, Israel*
[2]*Polymeric Materials Engineering, Shenkar - Engineering. Desiegn. Art, Ramat-Gan, Israel*

Polymers are one of today’s most used materials, and they can be found in almost all aspects of our lives. Among them are adhesives, utilized in applications spanning from daily uses like household items and DIY to sophisticated applications like electronics to biomedical products. Today, most polymeric adhesives are based on infusible and insoluble polymers known as thermosets, such as epoxies, polyurethanes, and silicones. Despite their high mechanical properties and significant resistance to chemicals and heat, recent years have shed light on their environmental impact. These polymeric adhesives cannot be easily removed or reused without damaging the underlying substrate, thus contributing to environmental problems.

One approach to address these challenges is incorporating dynamic or reversible bonds within the polymeric structure, obtaining a debonding-on-demand adhesive. By incorporating such bonds, effectively transforming the thermosets into a new class of polymers known as covalent adaptable networks (CANs) or vitrimers, a complete dissociation or softening can be achieved when exposed to specific stimuli, making these polymers unique materials for solving the challenges associated with traditional adhesives.

In this research, we developed a new solvent-free, photocurable adhesive containing disulfide linkages, which is fully recyclable, addressing some of the main challenges in this field, including the requirement of high-temperature treatment or adding solvents. Furthermore, this study demonstrates that this adhesive can be cured under different wavelengths using appropriate photoinitiators, effectively attached to a wide range of substrates.

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Polymers & Colloids (Tuesday, February 25, 2025 11:10)

Oral Presentation

Additive Manufacturing

Additive Manufacturing of Flexible Sensors Based on Polymer Nanocomposites

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Flexible sensors are usually lightweight and could be employed in various applications such as wearable devices, soft robotics, and biomedicine. Flexible strain sensors respond to mechanical deformation with a change in their electrical properties and are one of the main elements in soft intelligent devices. We produced such sensors by additive manufacturing, allowing accurate production with minimum waste and avoiding the use of expensive metals. We 3D-printed polymeric nanocomposites loaded with electrically conductive fillers, such as carbon nanotubes (CNT), known for their high electrical conductivity (EC). The preferred additive manufacturing technique was digital light processing (DLP), which requires the development of a stable polymer-filler dispersion. The electrical percolation threshold was measured at 0.15 wt% CNT for the 3D-printed composite. Simultaneously, with the application of stress, the electrical resistivity was measured at the percolation threshold, resulting in a 20% change compared to the resistivity without any applied stress. In addition, the 3D-printed composite restores its initial shape and mechanical properties after applying cyclic stress loading. The developed 3D-printed composite can be applied as a sensitive, flexible strain sensor that is easily produced, lightweight, and can be used for various applications.

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Polymers & Colloids (Tuesday, February 25, 2025 11:10)

Oral Presentation

Additive Manufacturing

Additive Manufacturing Process for Production of Complex and Oscillating POSS-based 4D Structures

Nicole Gorohovsky[1], Ronen Verker[1,2], Noa Lachman[1]
[1]*Department of Material Science and Engineering, Tel Aviv University, Israel*
[2]*Department of Space Environment, Soreq Nuclear Research Center, Israel*

Two-way shape memory polymers (2WSMPs) are a fascinating class of materials with the unique ability to revert between two distinct shapes in response to external stimuli. Upon exposure to a specific stimulus, such as heat or humidity, the polymer undergoes a reversible transition, enabling it to switch back and forth between the two shapes. This dynamic behavior of 2WSMPs opens up a wide range of potential applications in fields like medicine, aerospace, soft robotics, and smart textiles.

In this study, complex and high-performance 2WSMPs actuators were manufactured for the first time via direct ink writing (DIW) additive manufacturing (AM) technique of crosslinked poly Oligomeric Silsesquioxanes (PolyPOSS) thermoset applied on a Kapton film. For this purpose, a fused filament fabrication (FFF) 3D printer was converted into a DIW 3D printer.

Initially, physical parameters such as PolyPOSS gelation time at various temperatures, as well as its wetting ability on Kapton substrates were investigated. Then, PolyPOSS printing parameters were meticulously investigated, and ideal printing parameters were identified while establishing a unique printing protocol for thermoset polymers.

Parameters such as printing speed, volumetric flow rate, layer height, and layer width were investigated, and the results were confined and evaluated according to a single printing index developed uniquely for this purpose. A set of printing parameters that yields the lowest printing index, i.e., the most unified printed lines, was identified. The optimal line distance to print a uniform layer was then tested. After obtaining a satisfactory first layer, an additional set of printing parameters, this time for a second layer, was established.

Finally, various complex 2WSMP actuators were printed. The actuators' response to various temperatures, gripping abilities, and unique as well as oscillating shape memory behaviors was recorded.

We thus showed that using AM allows complex 2WSMP structures to be produced in a manner that would be nearly impossible with conventional casting manufacturing methods.

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2D Materials (Tuesday, February 25, 2025 11:10)

Invited Lecture

2D materials

Layered Ferroelectricity: From Geometric Measures to First-Principles Calculations

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The ability to locally switch confined electric polarization is vital in modern technologies, aiming to complement or replace traditional magnetic components toward storing, retrieving, and processing large volumes of information. Non-centrosymmetrically stacked layered materials have recently emerged as promising candidates for vertical polarization switching via lateral interlayer shifts – a mechanism known as Slidetronics.[1] In my talk, I will elucidate the microscopic origins of polarization in layered materials; demonstrate that it is dictated by interlayer registry;[2] explain its cumulative nature[3] and its saturation behavior;[4] show that it can emerge also in intrinsically non-polar systems, such as graphitic interfaces;[5] and extend the notion of slidetronics to the quasi-one-dimensional case of facetted nanotubes (see Fig. 1).[6]

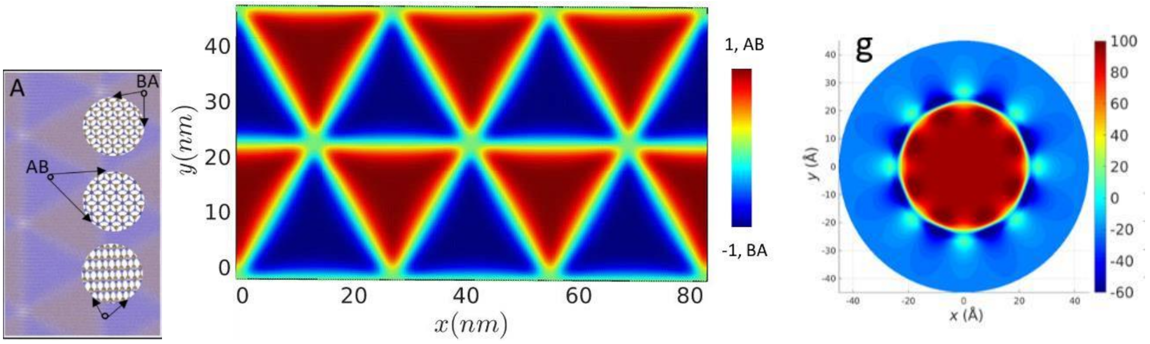

Figure 1: Polarization patterns in low-dimensional systems. Left: Surface reconstruction patterns in a marginally twisted *h*-BN bilayer. Middle: Local polarization registry index patterns in a marginally twisted *h*-BN bilayer.[2] Right: electrostatic potential difference map (in meV) calculated at the (001) cross section of a (55,0)@(63,0) double-walled boron nitride zigzag nanotube.[5]

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2D Materials (Tuesday, February 25, 2025 11:10)

Invited Lecture

2D materials

Controlled Growth of 2D Materials and Their Heterostructures

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The next generation of electronics and optoelectronics depend on new materials and methods that can be integrated with current technologies or reach beyond the capabilities of silicon based devices. Two-dimensional materials have emerged as promising candidates to achieve such goals. As is common for new materials, much of the early work has been focused on measuring and optimizing intrinsic properties on small samples (e.g., micromechanically exfoliated flakes). However, real-world devices and systems inevitably require large-area and highly-crystalline films that are integrated with other materials (e.g. dielectrics, other semiconductors and contacts). These requirements are particularly challenging due to the ultra-thin nature of 2D materials. In this talk I will describe our attempts to study the growth of transition metal dichalogenides (TMDs) via CVD-based (MOCVD, HCVD, etc.) methodologies. High crystallinity films might be obtained by controlling the nucleation density, and thus the domain size, or/and via epitaxial growth, which in 2D materials is referred as van der Waals (vdW)- (2D on 2D) or quasi-vdW epitaxy (2D on 3D). Our strategies to achieve both will be described. Finally, ongoing research in my lab related to non-conventional approaches for the growth of 2D materials and heterostructures will be discussed.

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2D Materials (Tuesday, February 25, 2025 11:10)

Oral Presentation

2D materials

New Family of All-Metal-Core Two-Dimensional Materials

Tamir Forsht[1], Anand Roy[1], Shiyi Gao[1], Joon Young Park[2], Kierstin Torres[2], Roni Gofman[3], Yuval Nitzav[3], Shahar Simon[4], Ayelet Zalic[4], Einav Grynszpan[4], Nag Pranab Kumar[5], Linda Wagner[6], Ifat Kaplan-Ashiri[6], Katya Rechav[6], Lothar Houben[6], Irit Goldian[6], Sidney Cohen[6], Hagai Cohen[6], Takashi Taniguchi[7], Kenji Watanabe[7], Haim Beidenkopf[5], BInghay Yan[5], Hadar Steinberg[4], Amit Kanigel[3], Philip Kim[2], Ernesto Joselevich[1]

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Since the discovery of graphene by Novoselov and Geim[1], many two-dimensional (2D) materials have been created and led to great scientific and technological developments. Finding more van-der-Waals (vdW) materials, and exfoliating them down to the 2D limit, are crucial steps towards even more exciting developments and finding new physical phenomena. However, the synthesis of an important class of 2D materials, composed of an extended network of metal-metal bonds, has been proven to be challenging due to the tendency of metal atoms to form a close-packed 3D structures [2,3].

Here, we present the synthesis of a family of vdW materials with an all-metal-core and extended metal-metal bonds with exceptionally high coordination, based on the work of the late Chemist John D. Corbett [4], and their exfoliation down to 2D materials. We studied the properties of these materials by SEM, TEM, AFM, STM, ARPES, transport measurements and SQUID. We show that different members of this family have a plethora of unique properties, as some of them are metallic, others are topological insulators, and some are ferromagnetic materials. Lastly, we show that these materials can be alloyed, marking the first steps in a new field of 2D metallurgy.

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2D Materials (Tuesday, February 25, 2025 11:10)

Oral Presentation

2D materials

The Chemistry of $Ti_3C_2T_x$ MXenes in Halide Perovskite Solutions

Kirill Sobolev[1], Omer Bartov[1], Adi Yakir[1], Sharon Hazan[2], Mariela J. Pavan[2],
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[2]*Ilse Katz Institute for Nanoscale Science and Technology, Ben Gurion University of the Negev, Israel*

MXenes are the novel family of 2D materials sharing the chemical formula $M_{n+1}X_nT_x$, where M is a transition metal, X is Carbon and/or Nitrogen, and T_x is a surface termination group [1,2]. Nowadays, MXenes are recognized as a viable and promising technology to eliminate the stability drawbacks in the perspective Halide Perovskite (HaP) photovoltaics [3]. MXenes may help improving the PCE of HaP-based devices through smart and controllable band alignment tuning, while promoting significant life span elongation due to the overall stabilization of HaP structures trough promoting better crystallinity and morphology, passivating grain boundaries, and interacting with undercoordinated lead ions inside the HaP [4-7]. However, while MXenes were introduced into HaPs in various ways, little attention has been paid to the chemistry of these systems. For example, it is not clear what happens to MXenes in halide-containing liquid media before actual perovskite crystallization, although this chemical environment regularly contains corrosive and aggressive species. Since MXenes are highly active and rather gentle materials, the impact of such a surrounding must be carefully investigated.

The ultimate goal of the conducted research was to create durable MXene-HaP "ink" that meets the requirements of ambient stability, predictable and repeatable chemistry, and environmental friendliness. To address this issue, we studied the interaction between $Ti_3C_2T_x$ MXenes and native HaP materials: MAI, PbI_2 and I_2 in organic solvents: DMSO and DMF. While studying various combinations of HaP components, we observed a number of effects, such as: MXene degradation, lead reduction and adsorption, PbI_2/$MAPbI_3$ crystals precipitation or even MXene functional group exchange. These observations were complexly examined using XRD, TEM, EDS, UV-Vis spectroscopy, confocal microscopy, and, with a specific focus, XPS and Raman spectroscopy chemical analysis. Stable MXene-containing inks were used to synthesize reinforced HaP films for structural and optoelectronic characterization. This work addresses the general guideline on the preparation of stable and durable MXene-HaP "inks" for technologically relevant production of MXene-reinforced HaP structures towards tunable and commercially reasonable HaP photovoltaics.

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2D Materials (Tuesday, February 25, 2025 11:10)

Oral Presentation

2D materials

Integration of Single-Layer Graphene on IDA Gold Electrodes and Electrochemical Characterization

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[3]*Azrieli College, Israel*

We report on a novel process for manufacturing and characterizing Graphene electrodes for bioelectrochemical sensing. The study was focused on interdigitated array (IDA) electrodes since they are widely used in electrochemical and biosensing applications. IDAs consist of a series of parallel, alternating electrodes that are closely spaced and interdigitated, giving it a comb-like appearance. IDA electrodes there is a 2D structure with relatively high total surface area, improving current signal in the case of current sensor or capacitance in case of capacitive sensors. IDAs with micron or submicron spacing between the electrodes allow, in some cases, further current amplification using redox cycling.

Graphene is a two-dimensional material made up of a single layer of carbon atoms arranged in a hexagonal lattice. It is a highly versatile material with a range of unique and attractive properties including excellent electrical conductivity, high strength, flexibility, stiffness, and high thermal conductivity. Hence, graphene`s large surface area, high electrical conductivity, chemical stability and well-established surface functionalization schemes, make it an ideal candidate for sensitive and selective detection of a wide range of substances, including small molecules, ions, and biomolecules. Graphene electrodes can be used in various applications, including electrochemical sensing, biosensing, chemical sensing, and environmental monitoring.

The process steps are as follows, First, a single Layer Graphene (SLG) is grown by low-pressure chemical vapor deposition (LPCVD) on a copper substrate. Next, the deposited material is transferred to an IDA chip (Micrux-IDA1) using a wet-transfer method. Next, a lithography process is used to remove the graphene between the electrodes and separate them. The sensor performance was characterized using a variety of analytical techniques, mainly by RAMAN, Cyclic Voltammetry in a standard PBS solution with a Ferri/ferro redox couple and Randles- Sevcik tets. Overall, the use of Graphene electrodes has been demonstrated and further investigation exploring its properties as is, or functionalized, for bio-sensing, is possible.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Invited Lecture

Materials in Archeology

On Ingots and Men: East Mediterranean Copper Trade during the Bronze and Iron Ages

Naama Yahalom-Mack

Several sources of copper were exploited during the Bronze and Iron Ages in the eastern Mediterranean; however, Cyprus was no doubt the richest source. Beginning in the early second millennium BCE, copper from Cyprus circulated in the form of ‘black’, unrefined copper ingots. This is evident from both textual and archaeological evidence. When production increased on the island, copper was cast into a standardized ingot form, generally refined. A similar picture emerges for copper production in the Arabah where 3rd millennium copper is traded in semi-refined form, as bar ingots, whereas in the more systematic endeavour of the late second and early first millennia, copper was traded in a more standardized and refined form. In this talk, the correlation between the refinement of copper and the scale of production and trade, as well as the role of technology in this development, both spatially and chronologically, will be presented and discussed.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Invited Lecture

Materials in Archeology

Archaeometallurgical Approaches to The Analysis of Iron Mining Tools from Nahal ‘Amram, Israel

Adi Eliyahu-Behar

This study investigates four iron mining picks from the ancient copper mines of Nahal ‘Amram in the Arabah Valley, Israel, dated to the Nabataean period (2nd–3rd centuries CE). The exceptional preservation of these rare artifacts enabled detailed archaeometallurgical and provenance analyses, providing valuable insights into Nabataean technological practices and resource utilization.

The analysis employed a suite of advanced methods, including metallography (OM and SEM), indentation hardness testing, chemical analysis of siderophile and lithophile trace elements via LA ICP-MS, and osmium isotopic analysis. The results revealed the use of two distinct alloy types—quench-hardened steel and phosphoric iron—and identified three probable ore sources, highlighting the sophisticated material selection and processing skills of Nabataean blacksmiths.

By integrating multiple analytical techniques, this study demonstrates the potential of archaeometallurgical approaches to address provenance and technological questions. It also enhances our understanding of the interplay between technological innovation and resource networks in the Southern Levant during late antiquity. The findings underscore the importance of such interdisciplinary methods for advancing archaeological research on ancient metallurgical practices.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Invited Lecture

Materials in Archeology

The Nature of the Pumiceous Ash and Tuff used for the Construction of the Sebastos Harbor

Yotam Asscher[1]
University of Haifa, Israel

The most impressive structure built under the king Herod reign was the artificial harbor of the city Caesarea Maritima, named Sebastos in honor of the Emperor (sebastos is Greek for Augustus). The structure was constructed on a shoreline devoid of any natural protective embayment, and given such unfavorable geomorphological conditions, the choice of innovative building materials and techniques was required to protect it from one of the Mediterranean's highest-energy wave environments.

As thoroughly described by the 1st Century CE Roman Jewish historian Josephus Flavius, the construction of Sebastos Harbor "…was to be brought to perfection by materials from other places, and at very great expenses" (JA 15.9.332). These foreign materials were incorporated into large concrete blocks of the underwater foundations, described as "…this he effected by letting down vast stones of above fifty feet in length, not less than eighteen in breadth, and nine in depth..." (JA 10.334-336), and were recently identified as pumiceous ash and tuff sourced from the Phlegraean Fields volcanic district, Italy.

Pumiceous ash and tuff are found to be the key ingredients in constructing underwater foundations, as they contain amorphous aluminosilicate compounds capable of reacting with lime and water to precipitate hydraulic insoluble phases with excellent mechanical properties. The specific chemical nature and mineralogical formation pathways of hydraulic reactions will be discussed here, and a new criteria will be shown for prescreening mortars for these materials based on X-ray powder diffraction (XRD), X-ray fluorescence (XRF) and Fourier transform infrared spectroscopy (FTIR) measurements.

Scholars rely on the writings of Josephus Flavius as the starting point for information about Herod the Great. Recent conservation works and archaeological excavations in Caesarea Maritima allowed material scientists, archaeologists and conservators to find the links between historical texts and Roman concrete in the Sebastos Harbor.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Oral Presentation

Materials in Archeology

The Process of Natural Aging of Pb-Sn Solid Solution in Lead Inclusions in Tin-Leaded Bronzes

Sana Shilstein, Yishay Feldman, Sariel Shalev

Tin-leaded bronzes contain micron-sized lead inclusions (Pb-Sn solid solutions). We have studied archaeological artifacts of ancient and medieval bronzes by the X-ray diffraction method using measurements of the lattice parameter of lead secretions [1]. It has been found that the tin content in the inclusions varies from about 1% at. Sn in ancient bronzes to about 3-5 % at. Sn in modern bronzes. The tin content in lead inclusions in modern bronzes and bronze coins from the mid-19th century turned out to be approximately equal. This means that the initial aging period (approximately 170 years) is not associated with a change in the composition of the solid solution due to the involvement of a small portion of dissolved atoms in the aging process. On the other hand, from ancient times until the early 18th century AD, the tin content in lead inclusions was approximately 1 % at. Sn. This in turn means that the process of complete aging of Pb-Sn solutions in lead inclusions in bronzes occurs over a period of about 350 years.

This also indicates that in the Pb-Sn phase diagram the equilibrium solubility of tin in lead at room temperature should be changed (1% at. Sn instead of 3.5% at. Sn [2]).

In addition, the method used is in principle suitable, for example, for distinguishing antique or Renaissance bronze sculptures from modern fakes.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Oral Presentation

Materials in Archeology

Field Multi-focal Metallography as a Non-destructive Method in Archaeometallurgical Characterization: The Akko Tower Shipwreck as a Test Case

Noam Iddan, Dana Ashkenazi, Deborah Cvikel

Field metallographic replication (FMR) is a well-established method of non-destructive surface examination of industrial metal parts. For example, FRM is widely used in the power generation industry for the in-situ evaluation of the metallurgical state of power pipes. An adaptation and adjustment of this method enabled developing the Field Multi-focal Metallography (FMM) method – direct examination of the surface by using a multifocal microscope. In order to examine the feasibility of the FMM method, an ensemble of ferrous and non-ferrous archaeological findings was examined, all retrieved from the Akko Tower shipwreck, dated to the time following the industrial revolution. The characterization was conducted alongside destructive metallographic testing for comparative purposes.

The results indicated that wrought iron items were made of alloy most likely produced by the ‘puddling’ process and hot-forged to their final shape, whereas their components were joined by forge welding. The grey cast iron items were most probably produced by a low sulphur coke-fuelled blast furnace, casting the molten alloy in a two-part casting die. The composition, microstructure, and the deduced manufacturing processes of these items indicate mid-19th century production, aligning with the ship`s dating. The relative high quality of all ferrous items retrieved from the Akko Tower shipwreck, and their microstructures and compositions, indicated that they were produced by controlled processes according to standards, possibly in the same workshop or according to a single manufacturing protocol. A strong correlation was observed between the destructive and non-destructive metallography methods. The results point to the possible value of non-destructive FMM method in archaeometallurgy in preserving the visual value of the finding, enabling its public display and future study.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Oral Presentation

Materials in Archeology

Crusader Military Activities on the Carmel Coast: the Typology, Imaging, and Metallography of Three Swords

Sara Lantos[1], Yoav Bornstein[1,2], Rabei Khamisy[1,2], Tzilla Eshel[1,2]
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THe presentation examines the Crusader military activities along the Carmel Coast through a detailed analysis of three swords recovered from the marine environment. By employing typological classification, imaging techniques, and metallographic study, we elucidate the swords` construction, dating, and contextual significance within the 12th and 13th centuries AD. The findings reveal insights into the forging techniques employed by medieval artisans and highlight the strategic importance of the Carmel Coast during the Crusades, particularly concerning the presence of military orders. This research contributes to a broader understanding of the maritime and military dynamics in the region during a pivotal historical period.

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Materials in Archeology (Tuesday, February 25, 2025 11:10)

Invited Lecture

Materials in Archeology

Science and Archaeology: Win-Win

Tzilla Eshel[1]
University of Haifa, Israel

The term "crisis of the humanities" encapsulates real challenges—such as reduced enrolment, funding cuts, and debates over practical value of this field of research. Archaeological Science suggests one possible solution: The integration of sciences into humanities, in a way that both parties benefit. However, there are many challenges on the way, and here is just one example:

Lead Isotope Analysis is a geochemical method to date lead. It is based on the radioactive decay of uranium and thorium to lead, creating a unique fingerprint for each lead-containing ore, based on the ratio between the different isotopes of lead. This method is further employed in archaeology to find the source of lead containing finds, mostly metals, and also lead pollution in bones. Although this is a scientific method, there are, surprisingly, several interpretations for the same results. There is one main reasons for this, in my mind: A successful analysis requires the knowledge of both science and archaeology. In my talk, I will discuss the challenges, opportunities and approaches required to make this integration succeed, for lead isotopes, for archaeology, and for humanities in general.

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E. Gutmanas Symposium (Tuesday, February 25, 2025 11:10)

Invited Lecture

Elazar Gutmanas Memorial Symposium

Manipulating the Growth and Form of Biogenic Glass

Igor Zlotnikov

Living organisms form complex mineralized architectures that perform a variety of essential functions. These biological materials are not only responsible for structural support and mechanical strength, but often provide optical, magnetic and sensing capabilities. This diversity in functionality is accomplished using a relatively narrow range of inorganic and organic components arranged into an astonishing variety of highly ordered hierarchical architectures. The control over the shape of the inorganic mineral building units, which in most cases differs significantly from their synthetic and geological counterparts, is executed by the cellular components. Here, growth and form are regulated by generating biochemical and physical boundary conditions that guide the self-assembly of a specific morphology. In the case of crystalline minerals, it is well established that the organic framework secreted by the cellular tissue manipulates the thermodynamics and kinetics of growth to give rise to complex morphologies that contradict the highly symmetrical crystal habit of the pure mineral phase. In essence, incorporated macromolecular content is used to challenge the crystallographic constraints imposed by the physical properties of the mineral. However, the mechanisms by which macromolecular frameworks shape and impose order on inherently disordered amorphous minerals are not well understood. In this work, we describe the formation of skeletal elements of sponges made of amorphous glass. Templated by branched single-crystalline protein filaments, these elements are a paradigm example of symmetry in biological systems. In this talk, I will review all aspects of this extraordinary self-assembly, biomineralization and morphogenesis scheme.

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E. Gutmanas Symposium (Tuesday, February 25, 2025 11:10)

Invited Lecture

Elazar Gutmanas Memorial Symposium

Reactive Synthesis of Ceramic-Metal Composites

Nahum Travitzky[1]
Department of Materials Science, Glass and Ceramics, University of Erlangen-Nuremberg, Germany

Design and development of advanced materials for high performance applications and bringing these materials into use is one of the most challenging tasks of modern engineering. Ceramic-metal composites with enhanced resistance to fracture, creep and oxidation are attractive for automotive, aerospace and defense applications. Ceramic-metal composites (in particularly with interpenetrating networks) are natural candidates for these demanding applications due to their very attractive mechanical properties. These materials can be produced by powder metallurgical or melt casting routes, depending on the efficiency of the process, shape, surface properties and, of course, the required microstructure and properties of the final product.

A comparably innovative reactive approach was used for in situ synthesis of CMCs (e.g., Al_2O_3/TiAl) and MMCs (e.g., $Fe_xCr_yNi_z/Al_2O_3$, $Ni_xCo_yCr_zAl_t/Al_2O_3$). Microstructure and mechanical properties of the fabricated composites have been investigated. In addition, natural ores such as ilmenite ($FeTiO_3$) or picrochromite powder ($FeCr_2O_4$) were also used as a feedstock instead of chemically pure powders to reduce the synthesis cost. A brief overview of our activities in the field of reactive in situ synthesis of metal-ceramic composites will be presented.

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E. Gutmanas Symposium (Tuesday, February 25, 2025 11:10)

Invited Lecture

Elazar Gutmanas Memorial Symposium

Advancing the Knowledge of Dislocation Dynamics: A Simulation Perspective

Dan Mordehai[1]
Faculty of Mechanical Engineering, Technion, Israel

The study of dislocations in crystalline materials, as pioneered by the late Prof. Elazar Gutmanas, has significantly deepened our understanding of material deformationon from its basic building blocks. This presentation delves into contemporary simulation studies, including atomistic modeling, finite element methods, and mesoscale approaches, that extend the knowledge on dislocation dynamics. By simulating dislocation mobility, kink formation, and impurity-dislocation interactions, we aim to refine the understanding of phenomena such as Peierls stress variability, impurity drag effects, and thermally activated processes. The talk will also explore new computational findings on the photoplasticity, echoing Gutmanas` contributions to the field. Through this lens, we celebrate the pioneering contributions of Gutmanas and his peers while highlighting how current simulation paradigms expand upon their legacy.

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E. Gutmanas Symposium (Tuesday, February 25, 2025 11:10)

Invited Lecture

Elazar Gutmanas Memorial Symposium

Cold Sintering Processes: A Historical Perspective on Biomaterials Applications

Aliya Sharipova[1]
Bio- and Medical Technology, Fraunhofer Institute for Ceramic Technologies and Systems IKTS, Germany

Cold sintering (CS) is a non-conventional method for densifying ceramics and metals at significantly lower temperatures than traditional sintering methods (T Tm/2). The concept was first introduced in 1979 by Prof. Elazar Gutmanas from Technion, Israel, who demonstrated that metallic powders could be compacted under high pressure into bulk samples with properties resembling those of dense, sintered materials. This marked a novel approach to processing metal-based materials without high-temperature requirements. In 2016, Prof. Randall at Penn State, USA, extended this concept to ceramics by developing a cold sintering process (CSP) based on a dissolution-precipitation mechanism, enabling ceramic densification at similarly low temperatures.

Cold sintering’s low-temperature conditions provide several advantages, including up to tenfold energy savings and a significant reduction in the carbon footprint. Additionally, its ability to produce near-net-shape components can further reduce manufacturing costs. Most importantly, cold sintering facilitates the development of new material systems, such as composites of ceramics, polymers, or metals, which were previously challenging to fabricate using conventional methods.

Prof. Gutmanas explored cold sintering in various applications, with a notable focus on biomaterials. This talk will present an overview of biomaterials research utilizing cold sintering, beginning with studies initiated in his group in 2010. I will discuss his collaboration with Prof. Sosnik on drug-eluting materials and the subsequent expansion of this process to biometals and bioceramics, including ongoing work at Fraunhofer IKTS in Germany.

Key results to be discussed include the development of iron-based biometals [1], such as metallic scaffolds for bone regeneration [2], and findings on drug loading and release from iron-based biometals [3]. I will also introduce an ongoing project focused on cold sintering of hydroxyapatite-based bioceramics, emphasizing their potential as bone-mimicking replacement materials. The presentation will conclude with recent advances in cold sintering of bioceramics containing metallic lines [4], which show potential for applications in bone-integrated sensors and human-machine interfaces. These structures can improve recording and transmission of electrical signals at human-machine interfaces, addressing key challenges in natural control of prosthetic limbs.

This talk aims to provide a comprehensive overview of cold sintering’s applications in biomaterials, highlighting past achievements, current progress, and future directions.

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E. Gutmanas Symposium (Tuesday, February 25, 2025 11:10)

Invited Lecture

Elazar Gutmanas Memorial Symposium

Reactive Infiltration Synthesis of Additively Manufactured Metal/Ceramic Composites

Alexander Katz-Demyanetz[1]
Israel Institute of Materials Manufacturing Technologies, Technion Research and Development Foundation, Israel

Capillary induced reactive liquid infiltration was utilized for complete densification of porous binder jetting additively manufactured (BJ-AM) ceramic bodies (SiC and WC) resulting in formation of RB-Si/SiC and Cu/W/ZrC metal/ceramic composite materials. Liquid Si and liquid Zr2Cu intermetallic compound have been used as infiltrants for SiC and WC, respectively. Effect of initial capillary geometry (i.e. effective diameter and length), which is caused by initial raw-powders particle sizes and shapes and level of the as-printed open porosity, on Si/residual-Carbon and Zr/WC reaction kinetics and the formed products, was examined by means of density measurements, as well as by SEM/EPMA and XRD. It was found that in the case of RB-Si/SiC synthesis, the amount of residual Carbon remaining in the as-printed pores from the former phenolic-based binder directly affects the amount of secondary SiC, and therefore, the final composite's porosity. In the case of Cu/W/ZrC synthesis, the resulting phase content and porosity of the composite strongly depends on the infiltration parameters (time and temperature), which are responsible for a proper adjustment of Zr2Cu liquid infiltration rate vs WC/Zr reaction rate, and therefore, for a metallic/ceramic phases arrangement in the finally densified Cu/W/ZrC composite material.

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E. Gutmanas Symposium (Tuesday, February 25, 2025 11:10)

Invited Lecture

Elazar Gutmanas Memorial Symposium

Some Reflections on a Promising Trend in Design of Architectured Materials and Engineering Structures

Yuri Estrin[1]
Department of Materials Science and Engineering, Monash University, Australia

This talk is devoted to the emerging area of ‘architectured’ materials. It will touch upon some promising trends in design of such materials but will mainly focus on the concept of topological interlocking (TI). The properties of TI structures are largely governed by the geometry and mutual arrangement of the building blocks from which they are assembled. This approach broadens the materials design space and offers new properties and functionalities. The important features of topological interlocking structures that may be gainfully utilized in design of novel architectured materials include:

- Great tolerance to local failures;
- Enhanced fracture resistance;
- High energy and sound absorption capability;
- Possibility to combine any materials within an integrated assembly;
- Ease of assembly, which makes these structures amenable to robotic manufacturing;
- Ease of disassembly, which permits nearly full recyclability of the blocks.

With this set of properties, one can envisage diverse applications of the topological interlocking systems in structural design and development of architectured materials. An outlook on some of these applications will be given.

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How to Start Writing and Get Your Research Paper Done (Tuesday, February 25, 2025 13:40)

Invited Lecture

How to Start Writing and Get Your Research Paper Done

Olga Degtyareva

This is not a lecture: it’s a hands-on workshop! Bring your laptop and a long-overdue research paper, grant application, or a PhD thesis chapter, and let’s work on it together.

Many researchers struggle with writing, whether it’s a project that keeps getting postponed, a draft that has been forgotten for months, or something urgent with an approaching deadline that feels overwhelming. This workshop is designed specifically for PhD students, postdocs, and early-career researchers who need to break through procrastination and finally make progress.

We’ll tackle the challenges that keep you stuck, help you find your starting point, and guide you through re-animating an old draft or making a fresh start. You’ll leave with clarity, focus, and a realistic, doable plan to keep going after the session, so you can finally get your writing done in a short amount of time.

Join us, get unstuck, and take real action on your writing!

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Materials for Energy (Tuesday, February 25, 2025 14:40)

Invited Lecture

Materials for Energy Storage and Conversion

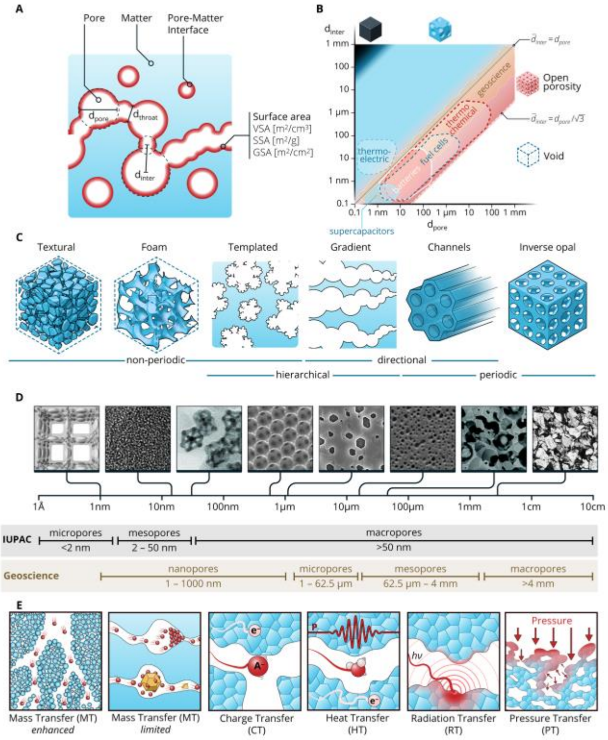
Porosity and Energy: from Fuel Cells to Fracking

David Eisenberg[1]
Schulich Faculty of Chemistry, the Grand Technion Energy Program, and the Resnick Sustainability Center for Catalysis, Technion - Israel Institute of Technology, Israel

Porosity is a key material property in nearly every energy technology in existence: in electrochemical devices (fuel cells, batteries, supercapacitors), in thermal devices (thermoelectrics, solar fuels, geothermal), in fossil fuel extraction (oil, gas, coal) and even in nuclear energy.

Why is porosity so tightly linked to energy conversion and extraction? Fundamentally, a porous material contains two “phases” – matter and void – and the interface between them. Each of these components can participate in the transport of (1) charge, (2) mass, (3) irradiation, (4) heat, and (5) pressure, as well as to participate in their conversion.

In this talk, I will show both fundamental and surprising examples of the role of porosity in energy applications, from electrocatalysts developed in our lab to a broad range of fields. This inter-disciplinary mapping of fundamental links leads to unique unifying insights. Highlighting key materials and characterization methods can help cross-fertilize between diverse fields, and hopefully bring together the diverse and sometimes-disparate porosity communities.



(From: Farber, Eisenberg et al., Science 2025, in press)

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Materials for Energy (Tuesday, February 25, 2025 14:40)

Invited Lecture

Materials for Energy Storage and Conversion

High Entropy Oxides as Materials for Energy Storage and Conversion

Ronen Gottesman[1]
The Institute of Chemistry, Casali Center of Applied Chemistry, and The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

This talk will present an approach to exploring and developing synthetic pathways of high entropy oxides (HEOs) to break present-day limitations and bottlenecks as multi-functional energy-use materials. HEOs have emerged as a new class of remarkably promising materials for energy storage and conversion applications. High configurational entropy stabilizes them as single-phase materials, effectively reducing the Gibbs free energy and overcoming enthalpy-driven segregation. Comprising near-equimolar compositions of 5 or more metal cations, HEOs exhibit remarkable thermodynamic and chemical stability, enhanced properties, and tunable multi-functionalities, presenting material properties between the constituent metal oxides or entirely new ones. Therefore, interest in HEOs is growing exponentially as materials for batteries and photo- and electrochemical fuel synthesis. However, HEOs are still underdeveloped for two significant interrelated challenges: i) material complexity, which often exceeds the robustness of their in-depth characterization and research and development, and ii) synthetic issues of these ceramic compounds, which involve energy-intensive fabrication processes, potentially limiting control of structural and electronic quality and tunable multi-functionalities. In light of these challenges, there is a pressing need for innovative approaches to close synthesis gaps and identify pathways for achieving high-quality multi-functional HEOs to advance their research and development.

In my talk, I will demonstrate our holistic synthesis approach that is based on colloidal and plasma deposition processes combined with rapid photonic heating, using rare earth HEO materials for photoelectrochemical conversion and the model HEO (MgZnCuCoNi)O for electrochemical conversion and energy storage, showing to enhance their properties either as free-standing powder form or functioning (photo)electrodes in energy storage and conversion devices.

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Materials for Energy (Tuesday, February 25, 2025 14:40)

Invited Lecture

Materials for Energy Storage and Conversion

Mixed Conductivity in the TiO2-SrF2 and LaOxFy Systems for Energy Applications

Yatir Sadia[1,2,3], Stephen Skinner[3]
[1]*Material Engineering, Ben Gurion University, Israel*
[2]*Nuclear Research center of the Negev, Israel*
[3]*Material Engineering, Imperial College of London, United Kingdom*

Ionic materials are some of the most interesting materials for a diverse range of applications from superconductivity, semiconductors, ionic conductors, batteries, fuel cells, gas detectors, separation membranes, solar cells and many more. Ionic materials with more than a single ion on their anion site are even more interesting due to the high diversity of properties that can be acquired by slight variations on both the anion and cation site. This is a new approach as most ionic materials in today’s industry and research are used with alloying and doping on the cation site only.

In this talk we will go over some of the properties of hetroanionic materials for energy applications. The ionic-electronic conductivity in the TiO2-SrF2 system will be discussed showing promise as fast fluoride ion conductors. And as interesting thermoelectric material. Additionally, we will discuss the very high ionic conductivity in the LaOxF3-2x system. What is the stability of the materials, at what temperature can they be operated and their peculiar phase changes. Finaly we will discuss some future projects in such systems and new applications such as ionic thermoelectric materials.

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Materials for Energy (Tuesday, February 25, 2025 14:40)

Oral Presentation

Materials for Energy Storage and Conversion

Stabilization of Ti-based MXene Single Flakes Above the Reversible Hydrogen Potential

Brian Rosen[1,3], Sukanta Chakrabartty[1], Haridas Parse[1], Danielle Sviri[1], Mathias Kramer[2], Baptiste Gault[2], Dierk Raabe[2], Noam Eliaz[3], Amir Natan[4], Vipin Kumar[4], Maxim Sokol[3]
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[2]*Max Plank Institue for Renewable Materials, Germany*
[3]*Materials Science and Engineering, Tel Aviv University, Israel*
[4]*Physical Electronics, Tel Aviv University, Israel*

MXenes have gained significant attention, particularly $Ti_3C_2T_z$, as materials with favorable properties for energy storage and conversion applications. The overwhelming majority of electrochemical durability studies are based on durability in the hydrogen evolution window, well below the reversible hydrogen electrode where degradation via electrochemical oxidation is less relevant. Consequently, few strategies have been put forward to protect $Ti_3C_2T_z$ at higher potentials and widen their applicability to electrochemical systems. Here, the electrochemical degradation of pristine $Ti_3C_2T_z$ and tantalum (Ta)- and hafnium (Hf)-sustituted MXenes are reported. X-ray photoelectron spectroscopy and electron microscopy revealed that pristine and Ta-doped MXene went through entirely different degradation mechanisms, and that these mechanisms are driven by electrochemical, rather than chemical effects. Density functional theory is used to explain the role of Ta doping with respect to the binding of oxygen and the formation of metal oxide phases. The influence of the degradation mechanism is observed by accelerated stress tests and anode reversal tests on a polymer electrolyte membrane fuel cell. Therefore, the substitution of titanium (Ti) with other oxyphilic metals in Ti3C2Tz may be an effective route to improve the durability of the otherwise fragile MXene phase.

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Materials for Energy (Tuesday, February 25, 2025 14:40)

Oral Presentation

Materials for Energy Storage and Conversion

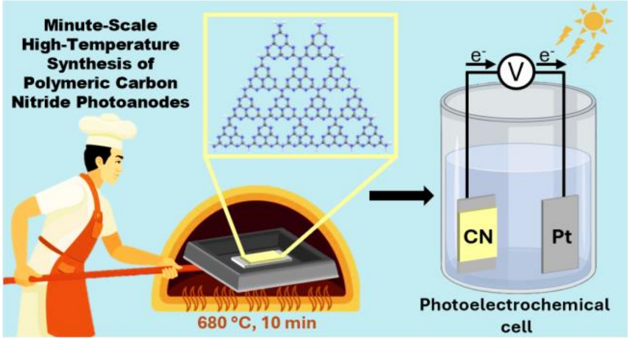
Minute-Scale High-Temperature Synthesis of Polymeric Carbon Nitride Photoanodes

Ayelet Tashakory[1], Sanjit Mondal[1], Venugopala Rao Battula[1], Gabriel Mark[1], Tirza Shmila[1], Michael Volokh[1], Menny Shalom[1]
Department of Chemistry, Ben-Gurion University of the Negev, Israel

Polymeric carbon nitride (CN) materials have emerged as metal-free, low-cost, and environmentally friendly semiconductors in various applications, including photoelectrodes in photoelectrochemical water-splitting. Unlike CN powder, which is used as a dispersed photocatalyst, for applications such as photoelectrochemical cells, light-emitting diodes, and solar cells, the deposition of the CN on a conductive substrate is required. The deposition of CN layers on different substrates can be divided into two main categories: 1) ex-situ deposition of prepared CN powder and 2) in-situ growth of a CN layer directly on the substrate. Generally, the in-situ methods comprise two steps: the first one is the deposition or growth of nitrogen-rich monomers (such as melamine, urea, thiourea, dicyanamide, etc.), forming a film of the monomers on the substrate. The following step is the calcination process, in which these monomers polymerize, forming the final CN electrode.

Most in situ preparation techniques differ in the deposition or growth method of the monomers` film but maintain a similar `standard` calcination process of slowly heating this film to 500–550 °C and keeping the final temperature for several hours, usually under an inert atmosphere. A significant drawback of a long heating process is the possible sublimation and decomposition of the CN monomers and final layer, which may lead to a less uniform film. In addition, from an economical point of view, a long calcination process at a high temperature consumes much energy.

In this talk, I will introduce a facile, scalable, energy-saving, and reproducible synthesis of CN layers on conductive substrates using a fast heating method. In this method, the predesigned CN monomer films are subjected for several minutes (5-20 min) to higher temperatures than the `standard` calcination procedure (650–680 °C). The high-temperature process enables fast condensation of the monomers, and negligible degradation is obtained thanks to the short time at the target temperature. As a result, the formation of a uniform CN layer with excellent contact with the substrate and good activity as a photoanode in PEC is achieved. The optimal CN photoanode reaches photocurrent densities of ~200 µA cm^{-2} at 1.23 vs. RHE in neutral and acidic solutions and 120 µA cm^{-2} in a basic solution.



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Materials for Energy (Tuesday, February 25, 2025 14:40)

Oral Presentation

Materials for Energy Storage and Conversion

Hydrogen Peroxide Formation Enables Efficient Oxygen Evolution in Near-Neutral Zn-Air Batteries

Roman Kapaev[1]
Bar-Ilan University, Israel

Near-neutral Zn-air batteries (ZABs) represent a promising avenue for cost-effective, sustainable energy storage, yet their commercial adoption is hindered by sluggish charge kinetics and limited understanding of underlying mechanisms. This study [1] identifies a novel charge storage pathway in near-neutral ZABs, where the formation and oxidation of dissolved hydrogen peroxide significantly enhance battery performance. During discharge, H_2O_2 forms as a transient species, contributing up to 60% of the total charge capacity in systems utilizing zinc sulfate electrolytes and carbon nanotube (CNT) cathodes. On charge, facile oxidation of H_2O_2 occurs at ~1.5 V vs. Zn^{2+}/Zn, reducing oxygen evolution reaction (OER) overpotentials by 0.2–0.5 V compared to conventional pathways. This mechanism suppresses parasitic carbon corrosion, enhancing cathode durability and energy efficiency. Electrochemical and spectroscopic studies confirm the central role of H_2O_2 in these processes. The stability of H_2O_2 varies with electrode and electrolyte composition, with CNTs providing a more stable environment compared to other carbon materials. This work underscores the critical interplay between electrolyte chemistry and electrode architecture in maximizing H_2O_2-mediated effects, presenting a pathway to higher efficiency and longer-lasting ZABs. By addressing challenges such as H_2O_2 instability, the findings pave the way for practical, sustainable energy solutions.

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Materials for Energy (Tuesday, February 25, 2025 14:40)

Oral Presentation

Computational Materials Science and Machine Learning

Can Vacancy Defects in Graphene Underlayer Improve Hematite`s Catalytic Efficiency in Water Splitting? A First-principles Study

Labanya Bhattacharya[1], Avi Cohen[1], Maytal Caspary Toroker[1,2]
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[2]*The Nancy and Stephen Grand Technion Energy Program, Haifa-3200003, Israel*

Producing hydrogen fuel is playing a key role in achieving the goal of carbon neutrality. Photoelectrochemical (PEC) water splitting is reported to be a nonpolluting technology to produce green hydrogen. Hematite (Fe_2O_3), a metal oxide, has great features as a photoanode material and a catalyst in oxygen evolution reaction (OER). High electron-hole recombination in hematite can be avoided by nanostructuring. Nanostructuring turns hematite sensitive to strain due to stress from the environment such as overlayer, underlayer, or other adsorbates. We find that nano-Fe_2O_3 can be grown on a graphene substrate as the lattice mismatch is negligible. Further, we introduce vacancy defects in graphene to see its effect on hematite`s catalytic efficiency [1]. The study has been performed using density functional theory (DFT)+U methodology. For the hematite having a graphene underlayer, theoretical overpotential is found to be reduced than stand-alone hematite. Carbon vacancies in graphene lead to more charge delocalization which helps to lower the overpotential than pristine graphene. Graphene plays a significant role in reducing the band gap of hematite which is beneficial for light absorption capacity and catalytic efficiency. Graphene underlayer having vacancies have nearly zero band gap which helps charge carriers to be transported to reach the hematite`s surface and that is beneficial for catalysis. The charge dynamics at the graphene-hematite interface has been modeled using a wave propagation simulator. Graphene supported hematite has higher cumulative probability of charge transfer than bare hematite. Graphene supported hematite having carbon vacancies in graphene shows higher cumulative probability of charge transfer than its pristine counterpart [1]. These indicatives for low overpotential, reduced band gap, and improved carrier transport are beneficial to overcome kinetically sluggish OER during water splitting.

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Bio- & Soft Materials I (Tuesday, February 25, 2025 14:40)

Invited Lecture

Bio- and Soft Materials

Inorganic Condensates in Biomaterial Synthesis

Assaf Gal

The formation of inorganic minerals by organisms is a regulated cellular process that occurs in the dense environment of living cells. Traditionally, solution chemistry principles were used to understand such biological mineralization processes. This view is challenged by the overwhelming complexity of mineral morphologies, structures, and growth rates. In our work, we explore the possibility that polymer-mediated phase separation can both serve as a morphogenetic handle and as an enhancer for mineralization. We have shown that macromolecular condensates serve as hotspots for the formation of various mineral types *in vivo*, and established several synthetic systems that recapitulate important aspects of biomineralization. We suggest that the inorganic condensate pathway can be used for developing biocompatible routes for advanced hybrid materials.

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Bio- & Soft Materials I (Tuesday, February 25, 2025 14:40)

Invited Lecture

Bio- and Soft Materials

Amazing Alternative Caseins

Dganit Danino

Casein proteins are both unstructured and amphiphilic; In nature they jointly constitute the milk micelles, but separately they spontaneously self-assemble into classical, soft core-shell micelles of nanometric size. Some years ago we developed beta casein (bCN) micelles as delivery vehicles of bioactives, showing high loading, long stability, and improved bioavailability of very hydrophobic compounds. Now using precision fermentation we produce a friendly and animal-free clean and functional alternative casein that displays similar properties, and with designed modifications even better properties than the natural analogue. The engineered system can be used as a delivery system, as well as, uniquely, a bioreactor for reshaping poorly soluble compounds.

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Bio- & Soft Materials I (Tuesday, February 25, 2025 14:40)

Oral Presentation

Bio- and Soft Materials

Digital Light Processing 3D Printing of Stretchable and Compressible Porous Polymers for Soft Robotics

Ouriel Bliah[1], Seonggun Joe[2], Lucia Beccai[2], Shlomo Magdassi[1]
[1]*Casali Center for Applied Chemistry, Hebrew University of Jerusalem, Israel*
[2]*Soft Biorobotics Perception Lab, Istituto Italiano di Tecnologia, Italy*

This study introduces an approach for fabricating highly stretchable and compressible porous 3D objects for soft robotics applications using vat photopolymerization 3D-printing technology. The printing compositions are based on photopolymerizable water-in-oil (W/O) emulsion, where water droplets function as pore templates and polyurethane diacrylate forms the surrounding stretchable matrix. The emulsion is created by high-shear mixing of the aqueous phase with the continuous phase containing photoinitiators and emulsifiers. Finally, after photopolymerization and subsequent removal of the internal water droplets, an open-cell structure is achieved, exhibiting a remarkable elongation-at-break of 450% and excellent reversible compressibility at 80%. These properties endow the material with both high compliance and strength, which are essential for actuator performance. Furthermore, this method allows the fabrication of high-resolution complex objects with customized porosity, incorporating both macro-pores by design and inherent micro-pores. The potential of these materials is demonstrated through the fabrication of novel actuators for soft robotics, showcasing unique actuation performance, shape adaptability, and high holding force. The high compliance of this material is particularly relevant for actuators as it enables efficient deformation under low energy inputs, enhancing the performance of soft robotic systems.

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Bio- & Soft Materials I (Tuesday, February 25, 2025 14:40)

Oral Presentation

Bio- and Soft Materials

Memory in Bioinspired Capillary Networks and their Perspective Applications

Bat-El Pinchasik[1]
School of Mechanical Engineering, Tel-Aviv University, Israel

Capillary networks are ubiquitous in nature and biology. Understanding these networks is fundamental to comprehending vascular systems in animals, capillary networks in plants, and has extensive applications in medicine and science. However, many questions remain about how these networks regulate and control flow. While we grasp the general principles of capillary networks and their functions, ongoing research explores how these networks dynamically respond to changes, adapt to varying conditions, and whether they retain memory of past states. Establishing a model system of capillary networks allows us to ask new and exciting questions, such as: "Do capillary networks have memory?"

Bioinspired 3D-printed capillary networks enable us to determine whether the wetting state of the liquid in the network depends on the history of actuation—essentially, whether capillary networks can possess memory. This intriguing question opens a new realm of possibilities, such as the potential to encode information within capillary networks, understand how transport responds to external stimuli, explore the interplay between global actuation and local fluid dynamics, investigate the coupling between mechanics and flow, and elucidate how information propagates through capillary networks.

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Bio- & Soft Materials I (Tuesday, February 25, 2025 14:40)

Oral Presentation

Bio- and Soft Materials

Amino-Acid-Based Microstructures as Versatile Organic Photonic Platforms

Handelman Amir

Photonic structures made of organic materials, polymers, live organisms and proteins are getting much interest in recent years due to their potential use in implantable and wearable medical devices, flexible photonics, and photonic circuits for optical communication. In this lecture, I will present some organic materials that could be used for various photonic devices. Specifically, I will show that the amino acid Histidine can guide polarized light. Furthermore, I will show how we deduced Histidine`s linear birefringence from the theory of Generalized Jones Matrix for biaxial crystals. Application of optical switching using Histidine microplates will be also shown.

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Bio- & Soft Materials I (Tuesday, February 25, 2025 14:40)

Oral Presentation

Bio- and Soft Materials

Characterization of Dolomite and Calcite Microcalcifications in Human Breast Tissue

Sahar Gal[1], Mariela J. Pavan[2], Netta Vidavsky[1,2]
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Pathological crystallization in soft tissues often results in biominerals with properties different than their geological or synthetic counterparts. Microcalcifications (MCs) are an example of pathological biominerals that are commonly found in breast tumors, and especially in non-invasive lesions such as ductal carcinoma in situ (DCIS). These MCs are of particular interest for cancer screening and prognosis. Most breast MCs are composed of calcium phosphates (CaP), and their crystal properties are frequently associated with malignancy[1]. However, non-CaP minerals, which are less common and typically linked to benign lesions, have received less attention.

Our study investigated the elemental composition, morphology, and crystal phases of 398 MCs collected from patients diagnosed with DCIS. Using scanning electron microscopy and energy-dispersive X-ray spectroscopy, we characterized the sizes, composition and morphology of the MCs. In addition, Raman spectroscopy provided insights into the crystal phases. Our findings revealed primarily non-CaP MCs, an observation that was likely made possible only by the tissue processing methodology employed, which did not involve harsh conditions. We found that non-CaP MCs were abundant in DCIS lesions, that they exhibited diverse morphologies and sizes, and that they were composed of calcite and dolomite. Dolomite formation in cancer has not been reported previously and may be linked to pH fluctuations in the tumor microenvironment[2]. Our findings suggest a potential association between dolomite MCs and DCIS lesions that progress to invasive cancer, offering insights into the role of MC crystal properties in DCIS prognosis.

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430

Ceramics and Composites (Tuesday, February 25, 2025 14:40)

Invited Lecture

Ceramics and Composite Materials

Self-compensation in Metal Oxides with Application on (Fast) Sintering of MgO

Yoed Tsur[1]
The Wolfson Department of Chemical Engineering, Technion, Israel

Self-compensation is part of the response of a material to doping. Knowing the concentrations of the various point defects in an undoped material in a reference state allows precise calculation of the response at equilibrium. Predicting the native defect concentrations using that "back of an envelope" type of calculation may prove very useful. I will demonstrate that using MgO as a model material in a simple case.[1] However, even that simple case provides some complications to be discussed, e.g., when associates of the native point defects are present in the undoped reference situation.

Next, I will discuss the applications of this approach on regular sintering[1] and flash sintering. Obviously, flash sintering and FAST sintering are extreme examples of far-from-equilibrium cases. Yet, the present approach provides at least a guideline for assessing the availability of agents for the sintering.

Reference

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Ceramics and Composites (Tuesday, February 25, 2025 14:40)

Invited Lecture

Ceramics and Composite Materials

Challenges and Opportunities Utilizing Multilayer MXene as Precursors for Oriented TiC_x in Ceramic Composites

Barak Ratzker[1,2], **Barak Ratzker**[1,2], **Barak Ratzker**[1,2], Or Messer[1], Maxim Sokol[1]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Israel*
[2]*Department of Microstructure Physics and Alloy Design, Max Planck Institute for Sustainable Materials, Germany*

MXenes are 2D carbide and nitride materials with diverse chemistries, mechanical robustness, and high electrical conductivity. This class of 2D materials stands out due to its processability and production scalability. Therefore, there has been growing interest in incorporating them into metal or ceramic matrices to create advanced composite materials. Moreover, MXenes will transform into their respective carbide/nitride MX phases upon heating to high temperatures (>1000°C), offering a pathway to utilize their 2D form to create reinforcement carbides/nitrides with unique morphologies. This work investigated the use of multilayered $Ti_3C_2T_z$ MXene as a precursor for forming bulk TiC_x/Al_2O_3 composites with highly oriented carbide reinforcement by spark plasma sintering. We conducted a side-by-side comparison of the processing, microstructure, and properties against conventional TiC/Al_2O_3 composites. The MXene-derived $TiC_{0.67}/Al_2O_3$ exhibited inferior mechanical properties due to the formation of AlF_3 or $Ti_{2.25}Al_{0.75}O_5$ phases alongside the $TiC_{0.67}$ particles. The MXene fluorine terminations presents another issue of weakening the alumina matrix, leading to significant grain growth and compromised mechanical integrity. Despite these challenges, the proposed approach shows promise, as the desired preferred orientation perpendicular to the applied pressure was achieved. The unique morphology resulted in reducing the percolation threshold, exhibiting high electrical conductivity with roughly one third of the TiC content required in conventional composites. While this approach has clear potential, the findings of this study underscore the need for optimizing the precursor MXene preparation and controlling surface terminations to maximize the benefits of MXene-derived MX phase reinforcements in ceramic composites.

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Ceramics and Composites (Tuesday, February 25, 2025 14:40)

Invited Lecture

Ceramics and Composite Materials

Beyond Thin Films: ALD`s Role in Next-Generation Ceramic Materials

Amnon Rothman[1]
Department of Materials Engineering, Ben Gurion University, Israel

Atomic Layer Deposition (ALD) has emerged as an important deposition method for the precise synthesis of thin-film materials due to its surface-sensitive nature. The ALD process is characterized by its self-limiting surface reactions, promoting a layer-by-layer growth mechanism and allowing for precise control over film thickness conformality and uniformity at the atomic scale.

This presentation explores the role of ALD in advancing ceramics and composite materials, emphasizing its unique advantages in nanostructure fabrication. Beginning with an overview of ALD fundamentals and a comparison to traditional deposition techniques, the discussion highlights its application to thin-film ceramics, focusing on current ceramic materials such as Al_2O_3, TiO_2, and emerging systems like MXenes, silicon carbide (SiC), and silicon nitride (SiN).

Insights into the nucleation and growth mechanisms of ALD-grown noble metals, such as Ru and Pt, provide a foundation for understanding thin-film behavior and optimizing material properties. These findings are extended to address the challenges and opportunities associated with the ALD synthesis of advanced ceramics. Potential applications in microelectronics, energy storage, and protective coatings are discussed, showcasing ALD`s transformative impact on the development of next-generation ceramic materials.

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Ceramics and Composites (Tuesday, February 25, 2025 14:40)

Oral Presentation

Additive Manufacturing

3D Printing of Alumina-based Ceramics through Photopolymerization and Sol-Gel Processes

May Yam Moshkovitz-Douvdevany[1], Shlomo Magdassi[1]
Institute of Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

Additive Manufacturing (AM) has opened new pathways for producing complex, high-precision ceramic structures, especially in applications with critical advanced material properties. This research presents a novel method for fabricating alumina-based ceramics by combining photopolymerization and sol-gel processes. In this method, photopolymerization efficiently forms intricate structures within a particle-free solution of soluble metal salt precursors. The subsequent sol-gel process converts these precursors into alumina, overcoming key challenges in ceramic 3D printing, such as particle settling, light scattering, and high production costs associated with alumina nanoparticles.

This approach yields alumina-based ceramics with finely controlled compositions and microstructures. We achieved materials with high surface areas (up to 1800 m^2/g) and excellent optical transparency (~80%), including amorphous alumina and crystalline γ-alumina, [1] along with doped structures such as ruby gemstones. [2] These properties open up possibilities for high-performance applications in aerospace, biomedical engineering, optics, electronics, and defense sectors.

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Ceramics and Composites (Tuesday, February 25, 2025 14:40)

Oral Presentation

Ceramics and Composite Materials

Development of Ultra-High Temperature Ceramics by Ultra-Fast Sintering

Denis Zolotaryov[1]
Israel Institute of Materials Manufacturing Technologies, TRDF, Technion, Israel

The development of ultra-high temperature ceramics (UHTCs), such as ZrC, ZrB2, TaC, HfC and their composites for applications in hypervelocity vehicles and engine components requiring materials to survive extreme conditions up to 2,000 °C is of the current interest. UHTCs are defined as having melting points over 3,000°C.

The production of such materials is challenging and expensive. However, using novel processes such as ultrafast high-temperature sintering (UHS), it becomes possible to sinter materials in seconds instead of hours, at temperatures of at least 3,000 °C. In this process the sample is sintered inside graphite felt which is heated by applying an electric current. This method can produce UHTCs in a more efficient manner and provides a means to investigate a wide range of materials and compositions quickly.

This presentation concentrates on research utilizing UHS for different ceramics, with a focus on UHTCs. The basic principles of the process were studied on Al2O3 and ZrC. The methodology was based on varying heating rates, temperature of sintering, and dwell-time aimed at finding optimal parameters for densification, as well as studying sintering mechanisms. Microstructural characterization of Al2O3 and ZrC were performed and will be presented.

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Ceramics and Composites (Tuesday, February 25, 2025 14:40)

Oral Presentation

Ceramics and Composite Materials

Impact-Induced Reactivity and Structural Transformations in Ti3SiC2 MAX Phases

Gil Goviazin[1], Dor Aaron Goldstein[2], Barak Ratzker[2], Or Messer[2], Maxim Sokol[2],
Daniel Rittel[1]
[1]*Mechanical Engineering, Technion – Israel Institute of Technology, Israel*
[2]*Department of Materials Science and Engineering, Tel Aviv University, Israel*

This study presents the first evidence of the extraordinary reactive behavior of MAX phase materials, specifically Ti3SiC2, under impact loading. Cylindrical samples of Ti3SiC2 were subjected to Split Hopkinson Pressure Bar (SHPB) tests, with high-speed optical and thermal cameras capturing the process. The investigation into the thermal and spectroscopic properties of these materials has provided crucial insights into the mechanisms driving energy release during the disintegration of MAX phases.

The primary source of energy release was identified as the bulk structural transformation and bond breakage within the material, rather than oxidation. These structural changes include extensive kinking and delamination, along with finer microstructural features such as cracks and planar defects. Although oxidation was observed, it played a secondary role in the energy release process.

The research methodology used in this study has offered valuable insights into the reactivity and dynamic mechanical response of MAX phases. This suggests the need for further investigations to deepen our understanding and develop comprehensive models. The findings pave the way for future quantitative studies on reactive materials and innovative applications, including the potential use of MAX phases as damage-tolerant reactive structural materials (RSMs).

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Quantum Materials (Tuesday, February 25, 2025 14:40)

Invited Lecture

Quantum Materials

Exploring Fast and Ultrafast Dynamics of Matter with Electrons and Photons

Michael Yannai, Matan Haller, Ron Ruimy, Alexey Gorlach, Nicholas rivera Rivera,
Dmitri Basov, **Ido Kaminer**[1]
Technion

Michael yannai1†, matan haller1†, ron ruimy1†, alexey gorlach1, nicholas rivera2, dmitri n. Basov3, ido kaminer1*

Opportunities in nanoscale probing of laser-driven phase transitions

For several decades, optical near-field microscopy facilitated pioneering investigations of photonic excitations at the nanoscale. In recent years, the near-field microscopy of terahertz fields has emerged as an important tool for experiments involving phononic and electronic phenomena, rich spatio-temporal dynamics, and highly nonlinear processes. Building on this foundation, this perspective illuminates the transformative opportunities provided by terahertz near-field microscopy to probe ultrafast phase transitions, helping to tackle previously inaccessible challenges of condensed matter physics. In many systems, laser-driven phase transitions are accompanied by the generation of terahertz pulses with spatio-temporal features governed by the complex physics underlying the phase transition. Thus, characterization of the emitted pulses using terahertz near-field microscopy techniques could support the investigation of ultrafast phase transition dynamics. This approach could, for example, allow the observation of ultrafast topological transitions in quantum materials, showcasing its ability to elucidate the dynamic processes underlying phase changes.

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Quantum Materials (Tuesday, February 25, 2025 14:40)

Invited Lecture

Quantum Materials

Coherent Control of Phonon Anharmonicity

Alon Ron[1]
Tel Aviv University, Israel

Anharmonic lattice vibrations play a key role in many physical phenomena. They govern the heat conductivity of solids, strongly affect the phonon spectra, play a prominent role in soft mode phase transitions, allow ultrafast engineering of material properties, and more. The most direct evidence for anharmonicity is to measure the oscillation frequency changing as a function of the oscillation amplitude. For lattice vibrations, this is not a trivial task, and anharmonicity is probed indirectly through its effects on thermodynamic properties and spectral features or through coherent decay of one mode to another. However, measurement of the anharmonicity of a single Raman mode is still lacking. We show that ultrafast double pump-probe spectroscopy could be used to directly observe frequency shifts of Raman phonons as a function of the oscillation amplitude and disentangle contributions from quasi-harmonic sources such as temperature and changes to the carrier density in the thermoelectric material SnTe. Our results have dramatic implications for the material engineering of future thermoelectrics. Moreover, our methodology could be used to isolate the basic mechanisms driving optically induced phase transitions and other nonlinear phenomena.

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Quantum Materials (Tuesday, February 25, 2025 14:40)

Invited Lecture

Quantum Materials

Features of Uniform and Non-Uniform Strain in Transition-Metal Dichalcogenides Mono-layers

Moshe Harats[1]
Department of Materials Engineering, Ben Gurion University of the Negev, Israel

One of the most appealing features of 2-dimensional materials is their elastic properties which makes them excellent candidates for future flexible electronic and photonic devices. It is therefore of high importance to reveal their physical and optical properties under elastic deformations. In the first part of my talk I will focus on the role of spatially non-uniform strain. In graphene, non-uniform strain can form pseudo-magnetic fields that show the existence of Landau levels without an external magnetic field [1]. For transition-metal dichalcogenides, the effect of “funneling” – the transport of neutral excitons to the point of maximum strain – has been proposed [2]. In this work we show 2 distinct experimental setups that show that although funneling was believed to be the more dominant process arising from non-uniform strain in transition-metal dichalcogenides, a different effect occurs where excitons transform to negatively charged trions. This is shown both for samples strained by an AFM tip [3] (Fig. 1a), and for samples strained using air pressurized membranes [4] (Fig. 1b). To understand the discrepancies between different experiments we develop a theory based on the drift-diffusion of the excitons and we predict that by using heterostructures the funneling efficiency can be increased significantly [5].

I will present new results of the role of uniaxial strain on the emission properties of excitons and trions at room temperature and in particular, their angular emission properties. Using a k-space imaging setup we can resolve the angular and spectral response of the different optical excitations under uniaxial strain.

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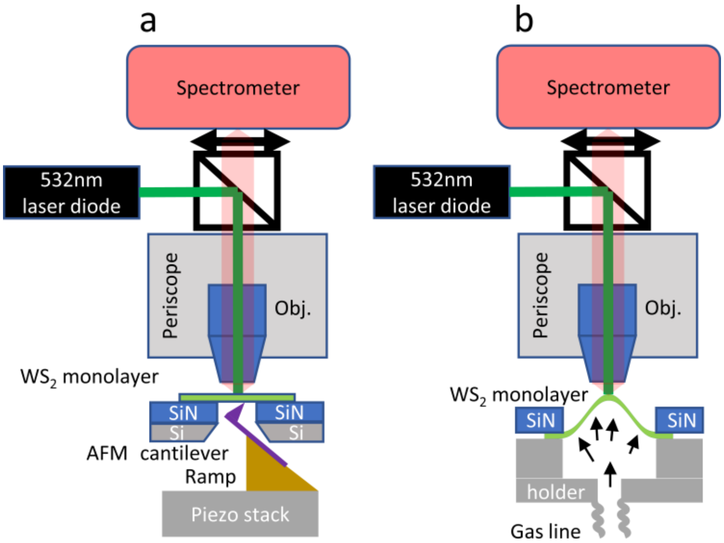

Fig. 1 (a) The experimental setup where the sample is strained using the nanoindentation technique, by using the AFM tip. (b) The experimental setup where the sample is strained with air pressure – the bulge test.

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Quantum Materials (Tuesday, February 25, 2025 14:40)

Oral Presentation

Quantum Materials

Collective Excitations in Perovskite Quantum Dot Superlattices and Heterostructures

Yehonadav Bekenstein[1], **Shai Levy**[1]
Materials Science and Engineering, Technion – Israel Institute of Technology, Israel

Collective superfluorescent emission was reported for halide perovskite nanocrystal superlattices. It was confirmed to be coherent, stronger, and faster than spontaneous emission, surpassing standard isolated nanocrystals. The emission is similar to the famous Dicke superradiance first reported in the 1950s. However, a deeper inspection of the various reports raises questions regarding the limits of such an effect. In particular, natural linewidth-broadening reflects intrinsic energetic state variations between nanocrystals and excitonic interactions, which will prevent such collective emissions. I will describe two different colloidal schemes that enable the experimental testing of these ideas namely colloidal nanocrystal superlattices and perovskite heterostructures.

In both examples, interactions between excitons dominate the resulting collective emission properties. Superlattices made of weakly confined nanocrystals showed a red-shifted collective emission burst with a faster emission rate, showcasing key characteristics of superfluorescence (bunched light). In contrast, the exact composition of superlattices made of much smaller, strongly confined nanocrystals showed a blue-shifted emission burst. Further emphasis on the role of confinement of the neighboring excitons was achieved via testing same-size nanocrystals but engineered quantum confinement by a modified dielectric environment (halide composition). We assign these contrasting modes of collective emission to dipole-dipole interactions between neighboring excitons in the superlattice. Careful engineering of the quantum confinement results in either head-head exciton orientation (H-aggregates) or head-tail interaction (J-aggregates). Further indication that quantum confinement changes the preferred alignment/ interaction of transition dipoles comes from the angular-dependent emission patterns.

In a second example, we explore excitons in colloidal nanoparticles with periodic heterostructures within the material. We have developed a colloidal synthesis for nanocrystals that periodically incorporates two distinctive structures: a perovskite corner-sharing octahedra of PbBr4 and an edge-sharing (PbBr2)2AMTP2 decahedra, creating the edge-perovskite heterostructure. Our new colloidal synthesis demonstrates size control over the resulting nanocrystal and indicates quantum confinement effects compared to the bulk material. A clear double peak in the emission spectrum indicates non-trivial excitonic behavior and potentially correlated emission.

By comparing the two examples, I will convey the importance of excitonic interaction in achieving correlated emission from perovskite nanocrystals.

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Quantum Materials (Tuesday, February 25, 2025 14:40)

Oral Presentation

Quantum Materials

-Intertwined Topological Phases in $TaAs_2$ Nanowires with Giant Magnetoresistance and Quantum Coherent Surface Transport

Anand Roy, Anna Eyal, Roni Majlin Skiff, Barun Barick, Samuel D. Escribano, Olga Brontvein, Katya Rechav, Ora Bitton, Roni Ilan, Ernesto Joselevich

Nanowires (NWs) of quantum materials are emerging as an exciting platform to probe, effectively tune, and engineer new quantum phenomena that are hard to access in bulk materials. Specifically, if made from topological materials, their quasi-one-dimensional (1D) nature and large surface-to-bulk ratio unlock new expressions of topology and highlight the role of topological surface states (TSS). The surface is the most interesting part of these materials, where topologically non-trivial electronic states (TSS) harboring quasiparticles can exhibit extremely high mobilities, giant magnetoresistance, magnetochiral currents, high-speed dissipationless electronics, and Majorana particles for the defect-tolerant quantum computation. Nevertheless, probing and extracting transport features of quasiparticles associated with TSS is strenuous and requires meticulous efforts to enhance the signal from these states and suppress the overwhelming bulk electronic states. To achieve this experimental realization of low dimensional (1D/2D) nanostructures of topological materials with a high surface-to-bulk transport ratio is desired. We report a novel synthetic approach to grow quasi-1D nanowires of rich topological material $TaAs_2$ encapsulated in a functional all-around SiO_2 dielectric shell and study their extraordinary magnetotransport properties. The SiO_2 shell protects the surface from degradation and can be locally etched to create ohmic contacts at specific locations, while the rest of the nanowire surface remains pristine and protected, allowing us to probe topologically non-trivial states and magnetotransport features, including metal-to-insulator transition and strong signatures of topologically non-trivial transport at remarkably high temperatures, direction-dependent giant positive and negative magnetoresistance arising from intertwined mixed topological phases, and a double pattern of Aharonov-Bohm oscillations, demonstrating coherent surface transport consistent with the two Dirac cones of a WTI surface. The coexistence and susceptibility of these topological phases to external stimuli are remarkable and can have potential applications in spintronics and nanoscale quantum technology. Furthermore, we will demonstrate a unique methodology to grow large-area epitaxially guided, highly orientated NWs of quantum materials, showing potential for integrating them in large-scale quantum nanotechnology.

Reference

Intertwined topological phases in $TaAs_2$ nanowires with giant magnetoresistance and quantum coherent surface transport. (https://arxiv.org/abs/2411.15974)

Anand Roy*, Anna Eyal, Roni Majlin Skiff, Barun Barick Samuel D. Escribano, Olga Brontvein, Katya Rechav, Ora Bitton, Roni Ilan and Ernesto Joselevich*

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Quantum Materials (Tuesday, February 25, 2025 14:40)

Oral Presentation

Quantum Materials

Quantum Relativistic Materials

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Center for Astrophysics, Geophysics, and Space Sciences (AGASS), Ariel University, Ariel University
FEL User Facility, Ariel University, Ariel University

In a paper discussing Newton`s third law in the framework of special relativity for charged bodies [1], it was suggested that one can construct a practical relativistic motor provided high enough charge and current densities are available. As on the macroscopic scale charge density is limited by the phenomena of dielectric breakdown, it was suggested to take advantage of the high charge densities which are available on the microscopic scale [2,3,4]. A preliminary analysis of this option denoted "quantum relativistic material" will be described in this presentation. In such materials the electron must travel in a close proximity to the nucleus and yet the material must be conductive. A relativistic motor possesses the following attributes:

- Allows 3-axis motion (including vertical)
- No moving parts
- Zero fuel consumption
- Zero carbon emission
- Needs only electromagnetic energy (which may be provided by solar panels).
- Ideal solution for space travel in which currently much of the space vehicle mass is devoted to fuel
- Highly efficient, in principle kinetic energy can be converted back to electromagnetic energy.

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Mechanical Properties & Failure (Tuesday, February 25, 2025 14:40)

Invited Lecture

Mechanical Properties and Failure

The Fundamental Physics of the Onset of Frictional Motion: How Does Friction Start?

Jay Fineberg[1], Shahar Gvirtzman[1]
The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

Recent experiments have demonstrated that rapid rupture fronts, akin to earthquakes, mediate the transition to frictional motion. Moreover, once these dynamic rupture fronts (“laboratory earthquakes”) are created, their singular form, dynamics and arrest are well-described by fracture mechanics. Ruptures, however, need to be created within initially rough frictional interfaces, before they are able to propagate. This is the reason that “static friction coefficients” are not well-defined; frictional ruptures can nucleate for a wide range of applied forces. An important open question is, therefore, how the nucleation of rupture fronts actually takes place. We experimentally demonstrate that rupture front nucleation is prefaced by extremely slow, aseismic, nucleation fronts. These nucleation fronts, which are often self-similar, are not described by our current understanding of fracture mechanics. The nucleation fronts emerge from initially rough frictional interfaces at well-defined stress thresholds, evolve at characteristic velocity and time scales governed by stress levels, and propagate within a frictional interface to form the initial rupture from which fracture mechanics take over. We will briefly describe a new theoretical description of the nucleation process obtained by means of a nontrivial extension of fracture mechanics. This theory quantitatively describes all of the experimentally observed features of the extremely slow nucleation process and merges seamlessly with the accepted fracture mechanics description of rapid dynamic ruptures. These results are of fundamental importance to questions ranging from earthquake nucleation and prediction to processes governing material failure.

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Mechanical Properties & Failure (Tuesday, February 25, 2025 14:40)

Invited Lecture

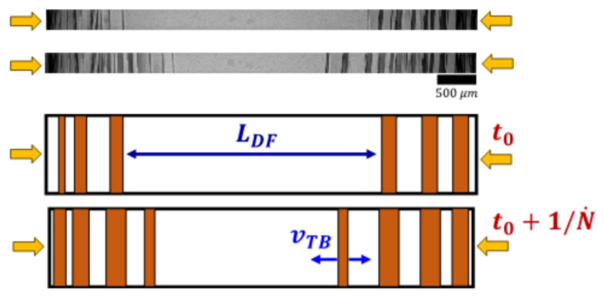
Mechanical Properties and Failure

Dynamics of Deformation Twinning in Magnesium

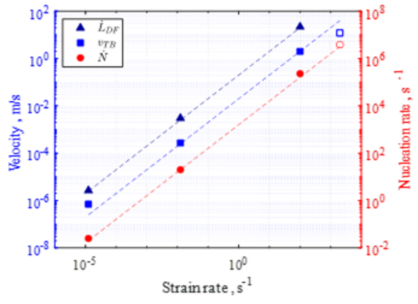
Eilon Faran[1], Doron Shilo[1]
Faculty of Mechanical Engineering, Technion, Israel

Twinning is a primary deformation mechanism in engineering hexagonal close packed (hcp) alloys such as magnesium (Mg), titanium (Ti), cobalt (Co), and zirconium (Zr). Therefore, understanding the underlying twinning mechanisms is fundamentally important. In this study, we investigate the dynamics of extension twins in single-crystal magnesium employing unique experimental methods to tracking individual interfaces across various length and time scales. Specifically, we performed uniaxial compression experiments coupled with direct optical imaging. The mechanical experiments spanned a strain rate range of seven orders of magnitude, between , covering all rates of engineering applications of magnesium and its alloys.

Across the entire strain rate range, the twinning transformation follows a self-similar pattern of twin nucleation and thickening. Deformation fronts initiate at the edges of the sample and propagate toward the center, creating parallel twins with characteristic thicknesses and distances from each other. The velocity of these deformation fronts scales linearly with the applied external strain rate and a nearly uniform resolved shear stress is measured over the entire strain rate range. This unique process is attributed to the constant ratio between the nucleation rate and sideways velocity of individual twin boundaries, both of which are proportional to the applied strain rate. Our results indicate that, across the large strain rate range investigated in this study, the evolution mechanism of extension twinning is practically rate independent [1]. Furthermore, by coupling unique acceleration measurements to the mechanical experiments, we uncover novel insights into the temporal characteristics of the nucleation events, showing that their duration is at the microsecond time scale [2].



Extension twinning evolves via a self-similar mechanism across a wide range of strain rates.



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Mechanical Properties & Failure (Tuesday, February 25, 2025 14:40)

Invited Lecture

Mechanical Properties and Failure

Structural Motifs in Soft Fibrous Tissues: Unraveling Structure-Mechanics Relationships to Inspire Biomimetic Material Design

Mirit Sharabi[1]
Mechanical Engineering, Ariel University, Israel

Over millions of years, nature has refined the design of soft fibrous tissues (SFTs) to achieve exceptional mechanical performance that engineered materials have yet to replicate. These remarkable properties stem from simple, repeating building blocks arranged into intricate structural motifs, which enable diverse mechanical functions. While these motifs are universal across SFTs, their unique composition defines each tissue’s specific physiological role.

Despite the critical need to replicate the structural integrity, mechanical properties, and long-term functionality of natural tissues, the fundamental structure-mechanics relationships governing SFTs remain incompletely understood. This knowledge gap limits advancements in designing tissue constructs and implantable materials with hierarchical functionality akin to native tissues.

In this presentation, I will highlight recent progress in understanding how structural motifs in SFTs contribute to their optimal mechanical behavior and demonstrate how these insights inform the design of fiber-reinforced soft composites in my lab. Applications include bioengineering materials for meniscal tissue, intervertebral discs, and blood vessels.

By unraveling the connections between SFT motifs and their mechanical properties, we aim to establish nature-inspired design principles that advance the creation of complex, bioengineered soft-tissue analogs with transformative potential for biomedical applications.

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Mechanical Properties & Failure (Tuesday, February 25, 2025 14:40)

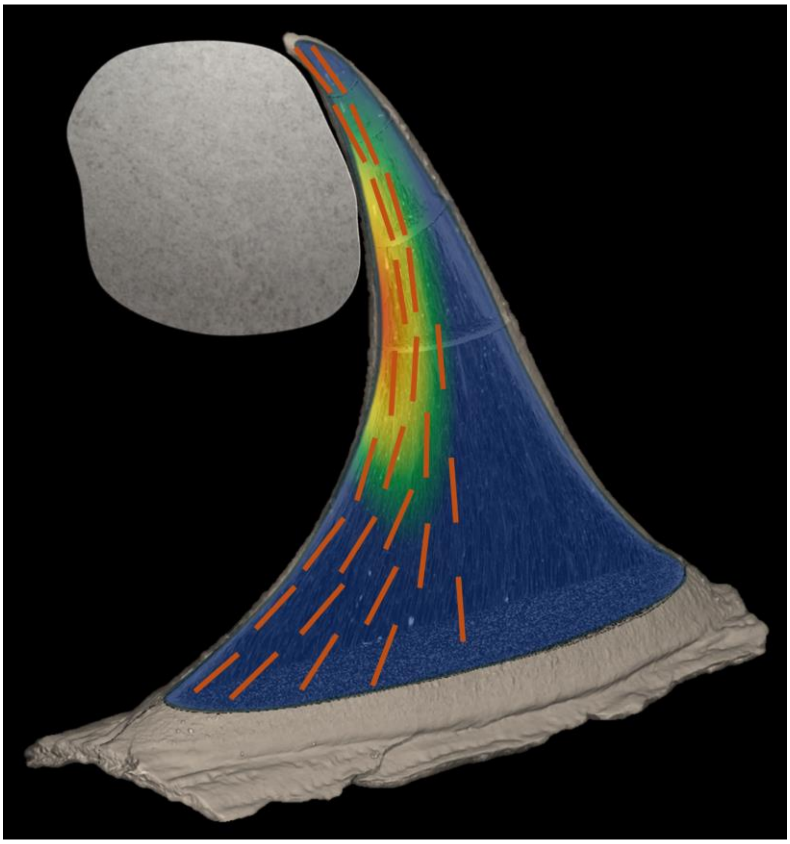
Oral Presentation

Bio- and Soft Materials

How Do Roses Build Failure-resistant Prickles?

Benny Bar-On, Liat Levavi

Rose prickles are small-scale, plant-based anchoring tools of multifunctional biomechanical roles, combining physical defense against herbivores and growth support on surrounding objects. By employing multiscale structural observations, nanomechanical characterizations, and finite element simulations, we unveil that the dog rose (R. Canina) prickle incorporates complementary structural-mechanical modifications at different length scales, resulting in macroscopic stress-locking effects that provide the prickle with extreme damage resistant capabilities and secure its functional form against catastrophic failures. These novel functional design strategies, unique to plant-based biomechanical tools, may promote micro-engineered material designs for futuristic anchoring platforms.



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Mechanical Properties & Failure (Tuesday, February 25, 2025 14:40)

Oral Presentation

Mechanical Properties and Failure

A Critical Analysis on the Predictive Capabilities of Different Criteria for Ductile Failure Initiation in Metallic Materials

Elad Priel[1,2], Nitzan Rom[3], Jacob Bortman[4]
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[2]*Materials Engineering, NRCN, Israel*
[3]*Israel Atomic Energy Commission, Israel*
[4]*Mechanical Engineering, Ben Gurion University, Israel*

Predicting ductile damage in metallic materials is a challenging topic. When the component has an initial crack, theories and tools from fracture mechanics are employed. However, when analyzing failure of a ductile material component, which does not contain a macroscopic initial crack, several approaches are reported in the literature.

In the current study, four different ductile failure criteria were implemented in the finite element framework and used to study the ductile failure process of Al2024 and Al7075 specimens. The failure criteria included stress based, energy based and strain based formulations. Several different sets of experiments were used to determine the model parameters. Then these same parameters were used to predict failure initiation for a different set of validation experiments with different geometries and under a complex stress and strain state. A critical analysis of the performance of the different ductile failure criteria was then conducted.

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Mechanical Properties & Failure (Tuesday, February 25, 2025 14:40)

Oral Presentation

Mechanical Properties and Failure

Strength of Precipitates in Ni-Al and Ni-Al-Fe Alloys

Igor Efremenkov, Michael Aizenshtein[1], Eugene Zaretsky[2], Shmuel Hayun[3]
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[2]*Department of Mechanical Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel*
[3]*Department of Materials Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel*

Abstract

The present research combines Transmission Electron Microscopy and planar impact testing to investigate the geometry, concentration, and individual strengths of Ni3Al precipitates in Ni-Al and Ni-Al-Fe alloys. The study focuses on homogenized and aged samples of binary (88.5% Ni, 11.5% Al) and ternary (79.3% Ni, 10.2% Al, 10.5% Fe) systems. A detailed analysis of experimental results reveals significant differences between the structures of the Ni3Al precipitates in these alloys. In the binary Ni-Al alloy, precipitates are predominantly small and dense spheres with an average diameter of 4 nm. Conversely, the ternary Ni-Al-Fe alloy exhibits larger and loose spherical precipitates, averaging 50 nm in diameter. A key finding of this study is the superior strength of smaller precipitates, which are approximately 40% stronger than their larger counterparts. The latter are identified as regions of Ni-based solid solution densely packed with minuscule, 2 nm-diameter, islands of the ordered Ni3Al phase. This work provides valuable insights into the mechanisms of precipitation hardening in Ni-Al and Ni-Fe-Al alloys. By understanding the effects of aging conditions, the characteristics of precipitates, and Peierls stress, this study lays a foundation for optimizing the design and processing of these alloys for various engineering applications where enhanced mechanical properties are crucial.

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Unveiling the Art of Self-Assembly in the Creation of Diverse Biomaterials (Wednesday, February 26, 2025 09:00)

Invited Lecture

2D materials

Unveiling the Art of Self-Assembly in the Creation of Diverse Biomaterials

Ulyana Shimanovich[1]
Weizmann Institute of Science, Israel

The Abstract is: Natural proteins exhibit structural and functional properties honed by millions of years of evolution, serving as biological analogs to synthetic polymers. Silk, in particular, is a protein-based biopolymer renowned for its exceptional mechanical properties, including high strength-to-weight ratio, self-healing ability, biocompatibility, and biodegradability. Despite its significance, the mechanistic pathways governing silk fiber formation and the evolution of its physical properties remain poorly understood, limiting efforts to replicate its performance in synthetic polymer systems. In our research, we utilized an ensemble of advanced analytical techniques to investigate silk feedstock processing in vivo at nano- to micron-scales within the silk gland of Bombyx mori silkworm. The results from our investigation offer a deeper understanding of silk's hierarchical organization and hold potential for advancing the development of bioinspired synthetic polymers with enhanced mechanical performance.

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Materials Science Challenges in Developing High Energy, Safe and Durable Rechargeable Batteries (Wednesday, February 26, 2025 09:45)

Invited Lecture

Materials for Energy Storage and Conversion

Materials Science Challenges in Developing High Energy, Safe and Durable Rechargeable Batteries

Doron Aurbach[1]
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Materials, and INIES – Israel National Institute of Energy Storage, Bar Ilan
university, Israel

The development of high energy density, long running rechargeable Li ion batteries that power successfully all mobile electronic devices, can be considered as the greatest success of modern electrochemistry.

This lecture provides examples of developing high energy density rechargeable batteries based on systematic studies of new materials.

The successful development of commercial reliable, durable and safe rechargeable lithium batteries resulted from extensive basic scientific work in which complex electrodes, electrolyte solutions and reactive interfaces of these batteries are explored by sophisticated electroanalytical tools in conjunction with advanced spectroscopic and microscopic techniques.

The success of Li ion battery technology to conquer power sources markets, especially for mobile electronic devices, promotes electromobility, which is a major challenge today in the field of electrochemical power sources. This presentation has two main themes: To provide vital examples how fundamental work in electroanalytical chemistry promotes development of reliable secondary batteries, emphasizing the use of in-situ analytical tools; To examine what is the true horizons for advanced high energy density batteries that can promote further the electromobility revolution. Regarding the first theme, we pioneered the application of *in-situ* FTIR and Raman spectroscopies, AFM, STM, QCM, for the study of highly reactive Li electrodes in the electrolyte systems relevant to secondary Li batteries. With these methodologies we deciphered complex side reactions and passivation mechanisms of all kinds of electrodes relevant to the electrochemical energy storage & conversion field. We demonstrated comprehensive studies of a wide variety of Li ions intercalation cathodes by a complementary use of fine electroanalytical tools, in conjunction with spectroscopic, microscopic and diffractometric measurements, through which we could understand ions insertion mechanisms into host electrodes. Regarding the second them, the limiting factor in Li-ion batteries in terms of energy density, cost, potential, durability and cycling efficiency are the cathode materials used. We examined most energetic cathode materials and novel approaches developed for their stabilization. We describe in this lecture promising electrode materials and methodologies for their stabilization by doping, coating, and affecting electrodes surface chemistry using active additives. Most important cathode materials for high energy density batteries are elemental sulphur and lithiated transition metal oxides comprising the 5 elements Li,Ni,Co,Mn,O at different stoichiometries that determine voltage and specific capacity. We explain how the stoichiometry dictates basic cathodes properties. We discuss the renaissance of Li metal-based rechargeable batteries. We have learned how the stabilize Li metal anodes in rechargeable batteries using reactive electrolyte solutions that induce excellent passivation through controlled surface reactions. We report on fluorinated co-solvents that open the door for a very rich surface chemistry which forms passivating surface films that behave as ideal solid electrolyte interphase (SEI) on both anodes and cathodes in advanced secondary Li batteries. This field provides fascinating examples how systematic basic scientific work leads to development of most practical devices for energy storage & conversion.

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Computational Materials Science I (Wednesday, February 26, 2025 11:00)

Invited Lecture

Mechanical Properties and Failure

Thermodynamic Theory of Dislocation-Mediated Plasticity

Alexander Umantsev[1]
Department of Chemistry, Physics, and Materials Science, Fayetteville State University, United States

Motion of dislocations is a common mechanism of plasticity in many materials. Acoustic emissions (AE) and stress bursts turned out to be integral parts of this mechanism. Adequate description of these processes is an important goal of Materials Theory, which aims to describe mechanical properties of materials and their reliability in service. In this presentation I will introduce a novel approach to dislocation plasticity [1,2] capable of describing AE events and stress bursts and discuss computational experiments intended to model the processes of compressive creep and shock compression in samples of various makeup and sizes. It turns out that the AE events self-organize into the dislocation avalanches, which propagate at a speed determined by the conditions of loading. In the compressive creep experiments the avalanches arrange into slow moving slip bands while in the shock compression experiments the avalanches move faster than sound.

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Computational Materials Science I (Wednesday, February 26, 2025 11:00)

Invited Lecture

Computational Materials Science and Machine Learning

Predicting Two-Dimensional Semiconductors Using Conductivity Effective Mass

Lee Burton

We investigate the relationship between the conductivity effective mass and exfoliation energy of materials to assess whether automatic sampling of the electron band structure can predict the presence of and ease of separating chemically bonded layers. We assess 22,976 materials from the Materials Project database, screen for only those that are thermodynamically stable and identify the 1,000 materials with the highest standard deviation for p-type and the 1,000 materials with the highest standard deviation for n-type internal conductivity effective mass tensors. We calculate the exfoliation energy of these 2,000 materials and report on the correlation between effective mass and exfoliation energy. A relationship is found which is used to identify a previously unconsidered two-dimensional material and could streamline the modelling of other two-dimensional materials in the future.

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Computational Materials Science I (Wednesday, February 26, 2025 11:00)

Invited Lecture

Computational Materials Science and Machine Learning

Towards Fully Automated and Universal Metallographic Image Analysis Using AI Methods

Ofer Beeri[1], Inbal Cohen[2], Matan Rusanovsky[1], Julien Robitaille[3], Francis Q. Lauzon[3], Shai Avidan[2], Gal Oren[4,5]
[1]*NRCN, Israel*
[2]*Tel Aviv University, Israel*
[3]*Clemex Technologies, Canada*
[4]*Stanford University, USA*
[5]*Technion, Israel*

Metallography is a fundamental and widely utilized method for characterizing the microstructure of materials. Typically, metallographic images are analyzed manually or semi-automatically by an expert, often with the assistance of computer software. However, to the best of our knowledge, no fully automated tool for metallographic image analysis currently exists. This gap can likely be attributed to the imperfect nature of features on the metallographic surface, such as unclear boundaries between precipitates and the matrix, incomplete revelation of grain boundaries, and other challenges. Additionally, the considerable variability in microstructures across different materials, as well as within samples of the same material or even across different areas of the same sample, further complicates the analysis. These factors make traditional image analysis methods inadequate. As with other fields where conventional methods are insufficient, the application of emerging artificial intelligence (AI) and machine learning (ML) techniques offers a promising alternative.

In this study, AI-driven computer vision methods were developed to create a fully automated tool for the quantitative analysis of metallographic images, including the detection of inclusions and grain boundaries. The work also encompasses the development of several quantitative analysis techniques, as well as a novel algorithm for the automatic detection of inclusion anomalies. The challenges encountered during the research and the various approaches employed to address these challenges are presented and discussed.

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Computational Materials Science I (Wednesday, February 26, 2025 11:00)

Computational Materials Science and Machine Learning

Accurate Solid-State Electronic and Optical Excitations from Non-Empirical (Time-Dependent) Density Functional Theory

Guy Ohad[1], Stephen E. Gant[2,3], Dahvyd Wing[1], Michal Hartstein[1], Jonah B. Haber[2,3],
María Camarasa-Gómez[1], Ayala V. Cohen[1], Francisca Sagredo[2,3], Marina R. Filip[4],
Tim Gould[5], Jeffrey B. Neaton[2,3,6], Leeor Kronik[1]
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[6]*Kavli Energy NanoSciences Institute at Berkeley, University of California, Berkeley, CA, United States*

Accurate prediction of the electronic structure of molecules and solids, entirely within density functional theory, has been a long-standing challenge. Optimal tuning of range-separated hybrid functionals has emerged as a highly accurate method for predicting fundamental gaps of molecules by enforcing the ionization potential (IP) theorem. Recently, we developed a simple and inexpensive method for solid-state band gap predictions based on an *ansatz* that generalizes the IP theorem to the removal of charge from a localized Wannier function. Here, we present applications of the method to three-dimensional solids, notably simple semiconductors and insulators, halide perovskites, and metal oxides, demonstrating quantitative accuracy in band gaps and optical absorption spectra with respect to experiment and a comparable level of accuracy to many-body perturbation theory calculations. We further demonstrate the merit of using the optimally tuned eigensystem as a starting point in combined *GW* plus Bethe-Salpeter calculations. Additionally, we demonstrate the usefulness of the approach for low-dimensional systems, including one-dimensional molecular chains and two-dimensional van der Waals materials.

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Computational Materials Science I (Wednesday, February 26, 2025 11:00)

Oral Presentation

Computational Materials Science and Machine Learning

Exploring the Optical Properties of Defects in Nanomaterials through Electronic Structure Calculations

Tamar Goldzak[1]
Engineering, Bar Ilan University, Israel

Defects in nanomaterials are crucial for understanding their optoelectronic properties, including quantum yield, absorption, and emission spectra. These properties significantly impact the performance of optoelectronic devices like solar cells and quantum detectors. Additionally, they play a pivotal role in advancing quantum information technologies, such as the development of novel qubits. Providing an accurate quantum mechanical description of excited-state properties has long been a challenge, particularly for complex molecular systems such as colloidal nanocrystals (NCs) and defects in 2D materials, which consist of hundreds to thousands of atoms. First-principle electronic structure methods are essential for achieving a microscopic quantum mechanical understanding of excited-state phenomena and structural properties. These calculations inherently account for many-body correlation effects, providing insights into energy and charge transfer mechanisms at the atomic level. They also serve as valuable tools for exploring novel materials and guiding new synthesis pathways. In this presentation, I will explore recent advancements in the development and application of electronic structure methods for complex nanomaterial systems that conventional approaches cannot effectively address. The focus will center on employing Density Functional Theory (DFT)-based methods to calculate excited states and absorption spectra, with a particular emphasis on colloidal nanocrystals (NCs) and defects in 2D materials. The first part of the presentation will examine how nanocrystals (NCs), their surface structures, and defects influence the excited-state manifold and impact spectroscopic properties. In the second part, we will showcase a collaborative effort combining theoretical modeling and experimental studies to unravel the atomic structure and chemical composition of chromium (Cr) color centers in hexagonal boron nitride (hBN). By combining simulations with experimental data, we aim to establish a direct correlation between the atomic structure of these defects and their optical characteristics.

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Computational Materials Science I (Wednesday, February 26, 2025 11:00)

Oral Presentation

Computational Materials Science and Machine Learning

Structure and Properties of Graphullerene: a Semiconducting Two-Dimensional C60 Crystal

Uri Argaman, Guy Makov

Graphullerene is a recently discovered, two-dimensional allotrope of carbon formed from C_{60} molecules. It has been synthesized in the form ($C_{60}Mg_4$)n and subsequently transformed into $(C_{60})_n$ by removal of the Mg atoms. Ab initio calculations are employed to examine the structure and properties of this material. Structurally, graphullerene is composed of strained C_{60} molecules. Each of these molecules is connected to six neighbors in a hexagonal network with a total of eight chemical bonds. We find this structure to be meta-stable, owing to the strain produced by the covalent bonding of the molecules. However, the inclusion of Mg atoms transforms the cohesion energy from negative to positive values by forming additional C-Mg bonds, creating an energetically stable material. In the absence of Mg, this allotrope is a pure carbon semiconductor with an indirect band gap. Phonon spectrum calculations confirm the dynamical stability of the material and yield its in- and out-of-plane sound velocities. In addition, symmetry breaking of the C_{60} molecules results in a distribution of bond lengths and creates vibrational modes that serve as a signature of graphullerene.

Reference: npj Computational Materials (2023) 211

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Surfaces & Interfaces (Wednesday, February 26, 2025 11:00)

Invited Lecture

Surfaces and Interfaces

Quantitative Surface Optical Imaging and Spectroscopy

Adi Salomon

Numerous processes unfold at or in close proximity to surfaces or at interfaces, including biofilm growth, crystallization, transport, signaling across cellular membranes, and various chemical processes. Yet, after three decades of progress in nanoscience and nanotechnology, obtaining detailed information about processes occurring at interfaces has been challenging. Microscopy is not an exception in this, as selectively studying dynamic near-surface processes invokes optical near fields. Yet, quantitative measurements along the microscope’s optical axis with nanoscale resolution remain challenging.

With the exception of DNA origami that offer a single-point measurement, there are no nm-axial structures for metrology and calibration across the field-of-view of the objective.

Is it feasible to devise a user-friendly nanoscale axial ruler for optical microscopy users?

In this presentation, I will unveil our recent advancements in ’smart` surfaces, enabling the decoding of information within the near field regime, including axial distance of emitters, polarization, and molecular specificity. Various far field optical techniques, such as total-internal reflection fluorescence microscopy (TIRF), super-critical angle fluorescence (SAF) analysis by back focal plane (BFP) imaging, second harmonic generation (SHG), and surface-enhanced Raman scattering (SERS) will be presented

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Surfaces & Interfaces (Wednesday, February 26, 2025 11:00)

Invited Lecture

Surfaces and Interfaces

High Purity Nanoporous Metallic Films: Direct Synthesis and Catalytic Applications

Hannah-Noa Barad[1]
Department of Chemistry, Institute of Nanotechnology & Advanced Materials, and
Israel National Institute of Energy Storage (INIES), Bar-Ilan University, Israel

Morphology of materials is highly important because it affects many properties such as, active sites, surface energy, and surface area, which can lead to tunable characteristics, for example in electrocatalysis. Nanoporous metallic networks (NPMs), a morphology of interest in catalysis, contain many uncoordinated surface atoms and highly curved ligaments with high energies that can have a large effect on catalytic performance. Self-supported nanoporous metal structures have been previously prepared by dealloying of a master alloy,[1] which is a wet chemical method. In this method, Ag is etched from an Au-Ag alloy. This always results in NPMs containing residual amounts of the etched metal (Ag), preventing the synthesis of high-purity structures. Thus, the catalytic properties of pure NPMs cannot be studied due to metal \`impurities\` remaining in the structure. Although these \`impurities\` may contribute to catalytic activity and stability by changing the surface properties, it is difficult to control them and the systematic investigation of the \`impurity\` effect is almost impossible.

Here, we present NPMs fabricated by using a physical vapor deposition method, known as glancing angle deposition (GLAD) to form nanoporous ultra-thin metal mesh structures, in a unique direct synthesis method,[2] unlike most wet chemical synthesis methods used to prepare NPMs, which result in chemical waste. The nanostructured metal mesh films are suitable for catalysis as they are extremely pure and highly porous, and contain very curved ligaments, different crystal motifs, and many grain boundaries on their surfaces. We present nanoporous gold films (NPGF) and nanoporous Ni films (NPNF) as examples. We show that the NPGF electrochemical structural stability is remarkably higher than that of dealloyed nanoporous gold, which is a result of the high amount of grain boundaries in the NPGFs. Moreover, the electrocatalytic performance of methanol oxidation is investigated and the results show high catalytic activity for pure NPGF.[3] For the NPNFs we measure activity as urea oxidation catalysts in the presence of borate anions. The NPNFs show much higher activity and stability towards urea oxidation, which we relate to the porous surface of the catalyst.[4] The GLAD method we developed can be applied to various metals as well as oxides and enables precise mixing or doping of the different materials composing the NPMs. The high porosity, active sites, and elemental mixing abilities will lead to new materials with interesting surface properties and activities as electrocatalysts.

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Surfaces & Interfaces (Wednesday, February 26, 2025 11:00)

Invited Lecture

Surfaces and Interfaces

Surface Engineering on Gold: From Atomic Steps to Nanoporous Structures and Directed Nanowire Growth

Lotan Portal, Rotem Zilberberg, Iryna Polishchuk, Maria Koifman Khristosov,
Alexander Katsman, **Boaz Pokroy**[1]
Materials Science and Engineering, Technion Israel Institute of Technology, Israel

This presentation will highlight research in surface engineering on gold, ranging from atomic-level modifications to the development of nanoporous structures and directed nanowire growth. I will begin by discussing the enhancement of atomic steps through template stripping, which improves monolayer ordering and defect management. Further, I will demonstrate how the formation of nanoporous gold can be controlled through gold-germanium eutectic transformations, emphasizing the role of interfacial phenomena in morphological control. Additionally, I will explore the directed growth of gold nanowires, templated by dislocation lines in cases where the gold alloy has undergone significant plastic deformation prior to dealloying. This research offers crucial insights into the mechanisms of surface engineering on gold, highlighting its potential applications in catalysis, sensing, optics, and beyond.

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Surfaces & Interfaces (Wednesday, February 26, 2025 11:00)

Oral Presentation

Bio- and Soft Materials

Electrofreezing of Super-Cooled Water as Induced by an Al Electrode

Shiri Dishon Ben Ami[1], Leah Fuhrman Javitt[1], Shakir Ali Siddiqui[2], Hagai Cohen[3],
Kshatresh Dutta Dubey[2], Meir Lahav[1], Igor Lubomirsky[1]
[1]*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*
[2]*Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence, India*
[3]*Chemical Research Support, Weizmann Institute of Science, Israel*

Understanding ice nucleation is of central importance in a variety of areas, such as the earth's climate system and food preservation. At temperatures close to 0°C and under atmospheric pressure, water freezes into ice with a hexagonal lattice structure. Clean water can be super-cooled homogeneously to low temperatures as -42°C, without freezing. The electrofreezing process has been investigated since 1861, however, numerous different mechanisms are still under debate.

Here we report that water freezes without super cooling (-0.5C) on aluminum electrodes when 50V is applied.[1] To explain it, we suggest a chemical mechanism of electrofreezing. We demonstrate that hydrated Al^{3+} or hydrated $Al(OH)_3$ act as ice makers on or near the electrode surface. The presence of ice making ions changes the weak water-water interactions at neutral pH to stronger interactions of coordinated acidic water molecules with surrounding Bronsted-Lowry basic one. Specifically, hydrated $Al(OH)_3$ induces icing faster than hydrated Al^{+3}. We use an experimental system together with MD simulations to show that the presence of the ice-making ions in the water, together with the electric field, are both crucial for inducing icing without supercooling.

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Surfaces & Interfaces (Wednesday, February 26, 2025 11:00)

Oral Presentation

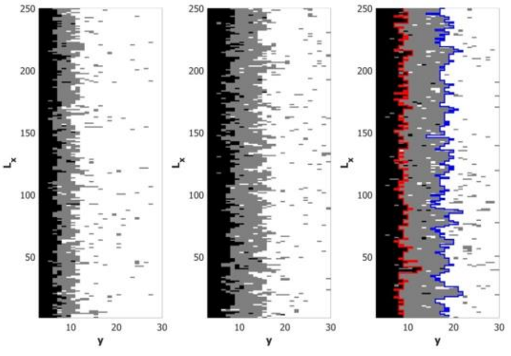
Surfaces and Interfaces

Precursor and Bulk Dynamics of Thin Film Spreading

Haim Taitelbaum[1], Meital Harel[1]
Department of Physics, Bar Ilan University, Israel

One of the manifestations of thin film spreading is the phenomenon of a precursor spreading in front of an advancing droplet. The microscopic characteristics of the precursor dynamics are still not fully understood. We study thin film spreading using a driven lattice-gas model of two layers, representing the bulk and the precursor film, first suggested by Abraham et al [1]. By changing the relations between the Hamaker constant (van der Waals interaction), the nearest neighbor interaction (surface tension) and the temperature, we study the effects of these parameters on the scaling exponents describing the spreading of both layers.

We find that the scaling exponents of both layers are neither universal [2] nor monotonic [3], and show that they strongly depend on these parameters, reflecting the competition between the various mechanisms that drive the system. We discuss our results in the context of the well-known Tanner and Lopez laws for bulk dynamics of spreading droplets. We also discuss results recently reported for this problem in band [4] and circular [5] geometries.



Top view snapshots of the interface evolution (from left to right) in the lattice gas model. Precursor (blue) and bulk (red).

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Surfaces & Interfaces (Wednesday, February 26, 2025 11:00)

Oral Presentation

Surfaces and Interfaces

Tailoring the Chemistry and Morphology of Vertically Aligned Carbon Nanotubes Forests, Implications for Smart Electrodes

Lev Rovinsky[1], Noa Lachman[1]
Materials Science and Engineering, Tel Aviv University, Israel

Vertically aligned carbon nanotubes (VACNT) combine three advantageous traits: immense specific surface area, excellent thermal and electric conductivities, and controllable directionality. Thus, VACNT attract attention for anisotropic nanocomposites useful in applications such as supercapacitors, transistors, water purification, thermal management, and dry adhesives. The varying waviness, and high anisotropy VACNT hinders adhesion and therefore processability, thus requires adjustment. Because VACNT structures are susceptible to capillary forces, most wet surface treatments become impractical, leaving only gas-based methods as viable options. The field of gas-based VACNT surface treatment is underdeveloped, with limited control over processes outcome. The introduced methodology enhances the process controllability, enabling gently adjusting the oxygen content on VACNT nanotube surfaces, as well as their nanomorphology and entanglement. The samples are gradually heated to between 430 and 500 °C to weaken the C-C bonds without really breaking them, enabling their adjustment, by introduction of either air or Ar through the reactor. Argon causes removal of excess oxygen contamination and nanotubes straightening, while air enables introduction of additional oxygen functional groups. This method augments the nanocomposite homogeneity, enhancing accessibility towards more active sites for current application performance, amplifying biomedical sensing signal, catalytic activity and heat dissipation. Additionally, by introduction of other gases, unfulfilled predictions could be enabled, and the current state-of-the-art can be expanded.

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Additive Manufacturing I (Wednesday, February 26, 2025 11:00)

Invited Lecture

Additive Manufacturing

4D Bioprinting of Engineered Tissues

Shulamit Levenberg[1]
Biomedical Engineering, Technion - Israel Institute of Technology, Israel

4D bioprinting introduces a transformative dimension to tissue engineering by integrating time as a critical factor in bioprinted constructs. It leverages dynamic materials and stimuli-responsive strategies to create constructs capable of morphing, growing, or adapting post-fabrication. This paradigm shift opens new horizons for engineering functional tissues that respond to environmental changes, enabling enhanced integration, repair, and functionality in vivo.

Fabricating living tissues is inherently a dynamic process. Cells actively interact with biomaterials during both the fabrication and maturation phases, significantly influencing the shape, size, mechanical properties, and extracellular matrix (ECM) composition of the resulting tissue. While acellular 3D printing offers high fidelity, introducing cells often results in constructs that undergo substantial transformations during post-printing cultivation. These transformations can lead to tissues with morphologies and properties that differ greatly from the original design. In our studies we explored how 4D bioprinting can embrace and harness these dynamic processes. With development of biomaterials and bioprinting strategies designed to anticipate and accommodate temporal changes, we can optimize final tissue outcomes. By leveraging the inherent dynamism of living systems, 4D bioprinting offers the potential to create more functional and biologically relevant constructs.

565

Additive Manufacturing I (Wednesday, February 26, 2025 11:00)

Invited Lecture

Additive Manufacturing

Overview of Mechanical, Metallurgical, and Physical Properties of PBF Ti-6Al-4V

Amnon Shirizly[1]
Rafael, Israel

Ti-6Al-4V is extensively used in the aerospace industry due to its exceptional mechanical and physical properties, as well as its high specific strength. The adoption of powder bed fusion (PBF) technology allows engineers to design and manufacture complex geometries that are otherwise unachievable with traditional methods. This includes parts with lattice structures and/or cooling channels that would be impossible to produce or would require assembly from multiple components.

This presentation will provide an overview of the mechanical properties of PBF Ti-6Al-4V, with a particular focus on tensile strength, fracture toughness, and fatigue performance after stress relief, with or without hot isostatic pressing (HIP). Additionally, we will explore metallurgical and physical properties, highlighting the potential for innovation with new hybrid structures.

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Additive Manufacturing I (Wednesday, February 26, 2025 11:00)

Invited Lecture

Bio- and Soft Materials

Soft 3D-printable Multifunctional Ionic Materials for Physical AI

Aslan Miriyev[1]
Department of Mechanical Engineering, Ben-Gurion University, Beer Sheva, Israel

Physical AI (PAI) involves creating nature-like physical systems with the capabilities of intelligent organisms. Multifunctionality is a defining feature of many natural organisms, and similarly, it is an essential characteristic of PAI. Ionic electroactive gels (IEGs) show numerous benefits as candidates for use in the field of PAI, thanks to their multifunctionality and ability to transform electrical energy into mechanical energy (and vice versa) under low voltages and currents. They can serve as actuators, sensors, and supercapacitors and hold high potential for 3D-printing-mediated fabrication. In my talk, I will discuss how the multifunctionality of IEGs contributes to the development of various parts of the intelligent body puzzle. Specifically, my talk will include an exploration of mixed ion-electron conductivity ionogel/single-walled carbon nanotube (ISMC) composites for multisensors, ionogel and ionic eutectogel soft wires (i-Wi), and a novel sustainable ionic eutectogel-based sensing mechanism with dual capacitive and resistive responses (Perf-iGel) for diagnostics and rehabilitation. The discussed materials are fully 3D-printable using UV-assisted (ISMCs, i-Wi) and direct ink writing (Perf-iGel) 3D-printing techniques, allowing for tailored design for specific functional needs. These materials are being combined in electromechanical systems designed to exhibit actuation, sensing, and power functions. Built using soft matter with similar chemistry, such systems pave the way for self-control mediated by learning-based methods.

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Additive Manufacturing I (Wednesday, February 26, 2025 11:00)

Oral Presentation

Additive Manufacturing

Exploring New Pathways for Directed Assembly

Hagay Shpaisman[1]
Chemistry Department & Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel

While numerous chemical procedures have been developed to produce microstructures, achieving on-demand patterns remains challenging. Current micro-fabrication methods typically involve multiple steps and necessitate an initial template for self-organization. However, directed assembly, achieved by applying external fields to materials, can induce a state of local equilibrium with complex spatial organization.

We present a novel concept based on the idea that mechanical forces arising from standing acoustic waves or flow directed by local laser heating can be utilized to direct not only preformed nanoparticles but also products of ongoing chemical reactions. These forces determine the spatial distribution of the formed materials, their mesoscopic structure, amorphousness/crystallinity ratio, the kinetics of the reaction, and could facilitate various composite formations. A key feature of this approach is its modularity, as it could be implemented across various material systems.

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Additive Manufacturing I (Wednesday, February 26, 2025 11:00)

Oral Presentation

Additive Manufacturing

Controlled Stretchable Lotus Leaf effect by Digital Light Processing

Noa Trink[1], Shlomo Magdassi
Institute of Chemistry, Casali Center, The Hebrew University of Jerusalem, Israel

The field of additive manufacturing, also known as 3D printing, has experienced a significant expansion in recent years. A particularly intriguing aspect of this field involves its application in developing soft materials. The phenomenon of superhydrophobicity is inspired by the lotus leaf effect and is characterized by extreme water repellency and self-cleaning. Combining superhydrophobicity with 3D printing of stretchable materials makes it possible to achieve high-performance flexible and stretchable structures with tunable superhydrophobicity and self-cleaning properties.

In this research [1], stretchable 3D structures with superhydrophobic properties were fabricated utilizing digital light processing printing. The printing compositions comprise silicone urethane acrylate and dispersed hydrophobic silica particles. The structures consist of arrays of printed pillars, with both pillar dimensions and spacing that adjust in response to stretching. Therefore, the resulting superhydrophobicity is programmable and can be controlled according to the degree of applied stretch. Top of Form The tuned wetting properties can find diverse applications in soft robotics, medicine, agriculture, and other areas where substrates may be exposed to pathogens, dirt, and corrosive elements.

(1) Trink, N.; Magdassi, S. Tunable Lotus Leaf Effect by Three-Dimensionally Printed Stretchable Objects. ACS Appl Mater Interfaces 2024. https://doi.org/10.1021/acsami.4c14238.

310

Additive Manufacturing I (Wednesday, February 26, 2025 11:00)

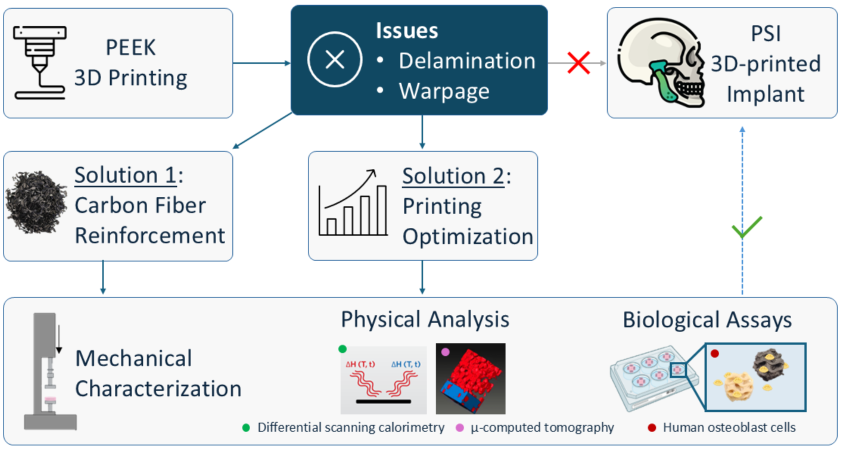
Oral Presentation

Additive Manufacturing

3D-Printed Patient-specific Bone Reconstruction Implants Based on Poly Ether Ether Ketone (PEEK)

Itamar Tulpan[1], Sahar Halevy[1], Sivan Hazan[1], Galit Katarivas Levy[1]
Department of biomedical engineering, Ben Gurion University, Israel

Recent advancements in additive manufacturing have revolutionized bone reconstruction methods, enabling the design of customized implants tailored to specific clinical needs. While metals such as titanium and its alloys are the most widely used materials for bone reconstruction, they come with significant limitations, including stress shielding, high specific weight, and challenges in radiographic imaging. Poly-ether-ether-ketone (PEEK), a high-performance thermoplastic polymer, has emerged as a promising biomaterial for bone reconstruction applications due to its excellent biological, mechanical, and chemical properties. However, PEEK also has drawbacks, such as inadequate mechanical strength for load-bearing applications and the high cost and complexity of manufacturing. To address these challenges, efforts have focused on optimizing 3D printing parameters and enhancing PEEK by integrating reinforcing materials, such as carbon fibers (CF), to create PEEK composites. This study presents an optimization process aimed at improving the printability and mechanical properties of 3D-printed PEEK and PEEK-CF, evaluating their potential as load-bearing bone reconstruction implants. The printed samples were assessed through compression and tension tests, fractographic analysis, µ-computed tomography, and differential scanning calorimetry. Additionally, biocompatibility and cytotoxicity were examined in vitro. The results demonstrated enhanced properties for both PEEK and PEEK-CF, with PEEK-CF exhibiting superior printability, including fewer printing defects, reduced warping, and improved dimensional accuracy. Both materials also showed favorable biocompatibility. These findings suggest that 3D-printed PEEK and PEEK-CF implants hold significant promise for load-bearing bone reconstruction applications, potentially overcoming the limitations of traditional metallic implants.



578

Functional Materials (Wednesday, February 26, 2025 11:00)

Invited Lecture

Functional Materials

Pyrolytic Radical Polymerization of Molecular Covalent Crystals

Elena Meirzadeh[1]
Molecular chemistry and materials science, Weizmann Institute of Science, Israel

To unlock future technologies like quantum computing, nano-transistors, and energy storage, chemists must overcome the limitations of current material synthesis methods. In this context, single crystals are essential for accurately exploring a material's intrinsic properties without distortions caused by grain boundaries or defects. While solid-state synthesis has proven effective for crystallizing inorganic covalent networks, solution polymerization often results in or polycrystalline powders due to the insolubility of covalent extended networks. Furthermore, the range of structures achievable through solid-state synthesis is restricted, as atomic composition limits the number and geometry of covalent bonds.

To address these limitations, we explore the use of molecular building blocks, such as polycyclic aromatic hydrocarbons, as precursors for the solid-state synthesis of covalent crystals with tunable structures and properties. Our approach leverages reduction-driven and thermally induced polymerization to promote the formation of intermolecular covalent bonds, enabling the design of crystalline materials with enhanced structural precision and functionality. This synthetic approach opens new pathways for the synthesis of molecular covalent crystals, bridging the gap between organic and inorganic material design for next-generation technologies.

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Functional Materials (Wednesday, February 26, 2025 11:00)

Invited Lecture

Functional Materials

On the Role of Twinning in Phase Transitions of Ferroelectric Perovskites

Semën Gorfman[1]
Materials Science and Engineering, Tel Aviv University, Israel

Many ferroelectric materials undergo transitions between phases of different crystallographic symmetry [1], driven by the structural flexibility of a perovskite framework and its various distortion modes. These transitions are central to such exceptional physical properties of perovskite-based materials as giant electromechanical coupling and enhanced dielectric susceptibility. Despite decades of research, some key questions remain unresolved, particularly regarding the role of domain microstructures in phase transition pathways. This is true even for well-studied transitions, such as cubic-to-tetragonal transformation in $BaTiO_3$ at 125 C. It is assumed that domain formation within the tetragonal phase enables mismatch-free coexistence of cubic and tetragonal regions, as introduced by the Weschler-Lieberman-Read (WLR) crystallographic theory [2]. Yet, experimental characterization of such domain assemblages remains rare and challenging because most commonly used microscopy techniques have limited power to investigate domains microstructures.

In this study, we advance single-crystal X-ray diffraction techniques to investigate domain microstructures during cubic-tetragonal phase transitions. First, we developed the formalism which help investigating coherent twin relationship in single-phase ferroelectrics of tetragonal, rhombohedral and monoclinic symmetry [3,4] using X-ray diffraction. Next, we modified the WLR model to derive formulas describing the orientation relationships between the basis vectors of real and reciprocal lattices of the cubic phase and tetragonal domains. These derivations allowed us to predict the separation of Bragg peaks for 24 possible variants of coexistence. We applied this technique for the investigation of cubic-tetragonal phase transition in PMN-35PT crystal at the phase coexistence temperatures [5].

Our results enhance the capability of X-ray diffraction as a bulk-penetrating and non-destructive tool for investigating domain microstructures in phase transitions. They provide new insights into orientation relationships that are critical for understanding physical properties in ferroelectrics and other functional materials.

[1] Howard, C. J. & Stokes, H. T. Structures and phase transitions in perovskites – a group-theoretical approach. Acta Crystallogr. A 61, 93–111 (2004).

[2] Lieberman, D. S., Wechsler, M. & Read, T. Cubic to orthorhombic diffusionless phase change—experimental and theoretical studies of AuCd. Journal of Applied Physics 26, 473–484 (1955).

[3] Gorfman, S., Spirito, D., Zhang, G., Detlefs, C. & Zhang, N. Identification of a coherent twin relationship from high-resolution reciprocal-space maps. Acta Crystallogr. A Found. Adv. 78, 158–171 (2022).

[4] Biran, I. & Gorfman, S. Permissible domain walls in monoclinic MAB ferroelectric phases. Acta Crystallogr A Found Adv 80, 112–128 (2024).

[5] Biran, I., Bosak, A., Ye, Z.-G., Levin, I. & Gorfman, S. Lattice match between coexisting cubic and tetragonal phases in PMN-PT at the phase transition. Appl. Phys. Lett. 124, (2024).

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Functional Materials (Wednesday, February 26, 2025 11:00)

Invited Lecture

Functional Materials

Non-Ergodic-Induced Negative Differential Piezoresponse in Relaxor Ferroelectrics

Cecile Saguy, Benjamin Kowalski, Alp Sehirlioglu, **Yachin Ivry**[1,4,5]
[1]*Solid-State Institute, Technion−Israel Institute of Technology, Israel*
[4]*Department of Materials Science and ENgineering, Technion−Israel Institute of Technology, Israel*
[5]*The Nancy and Stephen Grand Technion Energy Program (GTEP), Technion−Israel Institute of Technology, Israel*

Relaxor ferroelectric materials are the core for a broad range of advanced electro-mechanical energy-conversion technologies, including biomedical imaging, accurately controlled motors and electric-charge generators. The strong electro-mechanical coupling that these materials exhibit stems from a unique competition between long-range and short-range ordering of ions that form their crystallographic structure, and that the ordering can be tuned electrically. While relaxor-based applications are found in everyday technologies, the basic ordering mechanism in relaxor ferroelectrics has yet remained elusive. In particular, limited nanoscale observation tools hinder the determination of the transition from short-range to long-range ordering, which is classified as a unique transition from an ergodic to a non-ergodic state.

Here, we used piezoresponse-force microscopy to observe directly the ergodic-to-non-ergodic transition in the seminal relaxor ferroelectric PMN-PT. These results were backed up by macroscopic dielectric measurements. The controlled ergodicity was then used to demonstrate unprecedented differential-negative-piezoresponse behavior, which spans a broad temperature range. Bearing in mind the direct relationship between piezoresponse and capacitance, relaxor ferroelectrics are thus found promising not only for power-generation applications, but also as an excellent platform for the emerging technology of low-power negative-capacitance transistors.

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Functional Materials (Wednesday, February 26, 2025 11:00)

Oral Presentation

Functional Materials

Melt Alloying of Two-Dimensional Hybrid Perovskites: Composition-Dependence of Thermal and Optical Properties

Arad Lang[1], Celia Chen[1], Chumei Ye[1], Lauren N. McHugh[2], Xian Wei Chua[3], Samuel D. Stranks[3], Sian E. Dutton[4], Thomas D. Bennett[1]
[1]*Materials Science and Metallurgy, University of Cambridge, United Kingdom*
[2]*Department of Chemistry, University of Liverpool, United Kingdom*
[3]*Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom*
[4]*Cavendish Laboratory, University of Cambridge, United Kingdom*

Melt processing is a common practice for handling materials. In classic metallurgy, for example, it is widely used for alloying: the pure metals are heated above their melting point, followed by mixing and subsequently cooling. This process often yields alloys with distinct thermal, electrical, and optical properties compared to their constituent metals, primarily dictated by the chemical composition, i.e., each metal`s identity and relative amount.

Recently, it was shown that two-dimensional hybrid organic-inorganic perovskites (2D-HOIPs), with the chemical formula of (RNH3)2MX4 (where R is an organic moiety, M is a divalent metal cation, and X is a halide) can undergo melting upon heating. These materials demonstrate a tremendous potential to be implemented in next-generation optoelectronic applications. Leveraging this meltability offers a promising solvent-free fabrication approach with potential enhancements in performance metrics.

In this research, we demonstrate the applicability of melt-alloying to a binary 2D-HOIPs system, specifically analysing $(1\text{-MHA})_2PbI_4$ (where 1-MHA = 1-methylhexylamine) and $(S\text{-NEA})_2PbBr_4$ (where S-NEA = (S)-(−)-1-(1-naphthyl)ethylamine), which are examples of liquid-forming and glass-forming 2D-HOIPs, respectively. The blends, formed by melt-alloying, were shown to be chemically and structurally homogeneous. Thermal analysis has revealed significant changes in both melting and glass transition temperatures, compared to the pure 2D-HOIPs. Furthermore, optical absorbance and circular dichroism measurements have shown melt- and recrystallisation-induced variations in both the band gap of these blends and their response to polarised light.

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Functional Materials (Wednesday, February 26, 2025 11:00)

Oral Presentation

Functional Materials

Preparation and Core-electron Spectroscopy of Y- or Sc- Doped AlN Films

David Ehre[1], Asaf Cohen[1], Sergey Khodorov[1], Igor Lubomirsky[1], Ellen Wachtel[1],
Hagai Cohen[2], Junying Li[3], Anatoly Frenkel[3]
[1]*Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*
[2]*Chemical Research*

Support, Weizmann Institute of Science, Israel
[3]*Materials Science and*

Chemical Engineering, Stony Brook University, New York, United States

Thin films of doped aluminum nitride, $(Al_{1-x}Do_x)N$, have evoked significant interest during the last decade as a lead-free, biocompatible, environmentally friendly piezoelectric/ferroelectric material. Chemical stability, large thermal conductivity, large elastic modulus and compatibility with Si-based microfabrication methods make $(Al_{1-x}Do_x)N$ thin films a most promising candidate as active materials for piezoelectric MEMS and ferroelectric devices. However, depositing fully oriented (001) films without DoN (Do=Sc, Y) segregation remains challenging, despite almost two decades of intensive development. This is because both ScN and YN are completely immiscible with AlN in bulk form. This is the driving force for their segregation and loss of orientation during deposition. Here, we describe the preparation of 2 µm thick wurtzite textured,$Al_{1-x}Do_xN$ (Do= Sc, x=0.25, 0.30 or Y, x=0.25) sputtered thin films as well as the investigation of the local environments of Sc and Y using X-ray absorption (XAS) and photoelectron (XPS) spectroscopies. We present evidence from the X-ray absorption fine structure (XAFS) spectra that, when x=0.25, both Sc^{+3} and Y^{+3} ions are able to substitute for Al^{+3}, thereby acquiring four tetrahedrally coordinated nitrogen ligands, i.e., coordination number (CN) of 4. On this basis, the crystal radius of the dopant species in the wurtzite lattice, not available heretofore, could be calculated. By modelling the scandium local environment, extended XAFS (EXAFS) analysis suggests that, when x increases from 0.25 to 0.30, CN for a fraction of the Sc ions increases from 4 to 6, signaling octahedral coordination. This change occurs at a dopant concentration significantly lower than the reported maximum concentration of Sc (42 at% Sc) in wurtzite (Al, Sc)N. XPS provides support for our observation that the local environment of Sc in (Al, Sc)N may include more than one type of coordination.

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Functional Materials (Wednesday, February 26, 2025 11:00)

Oral Presentation

Functional Materials

Synthesis and Nonlinear Optical Characterization of Para Red Azo Dye Crystals

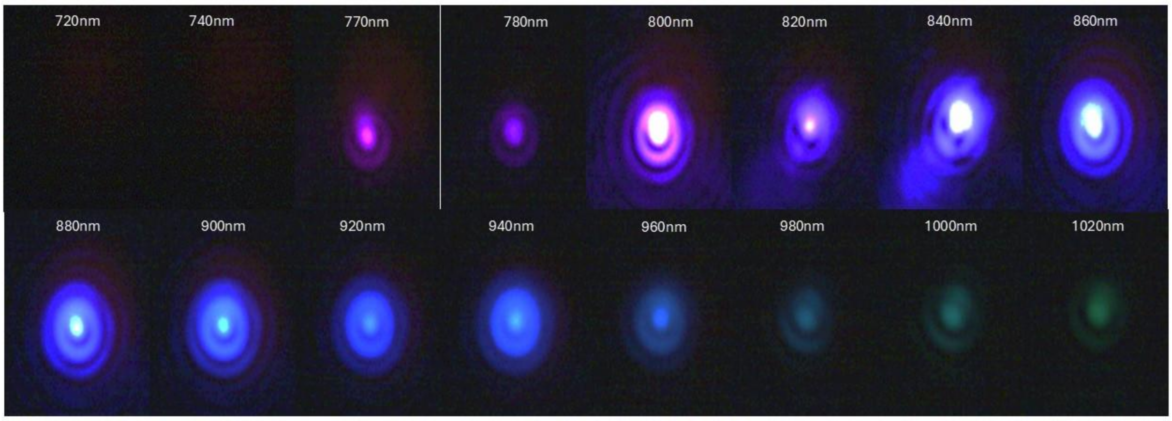
Alon Krause[1], Tchiya Zar[1]
Chemistry, Bar Ilan University, Israel

This work investigates the synthesis and characterization of nonlinear optical organic crystals based on the azo dye Para Red, which possesses a molecular and crystal structure that promote nonlinear activity due to a large conjugated system, donor-acceptor groups, and a non-centrosymmetric crystal group. Those highly stable crystals give rise to both SHG and 2 photon excitation fluorescence.

A novel de-sublimation technique that we developed for the growth of Para Red crystals results in different polymorphs belonging to the symmetry groups Pn and P212121 , forming needle and thin plate shapes, which function respectively as J and H aggregates. The plate crystals have a millimeter scale with thicknesses between half a micron to two microns. These crystal plates were found to have distinct nonlinear properties, with conversion efficiency of 1.4x10-8 and stability of hours under fs laser illumination. These nonlinear optical responses are higher than those present in crystals made in conventional evaporation or cooling crystallization.

The crystal structures were determined by using single crystal X-ray diffraction, and the physical dimensions were measured by Optical and Electron Microscopies. The optical activity was examined linearly and nonlinearly using a custom-made scanning SHG setup, and imaging. It is shown that the resulting Para red crystals provide uniform SHG activity, over a wide range of wavelengths, up to ~5 times more efficient than industry standard materials such as BBO.

These properties make these crystals promising candidates for practical applications in photonic devices and in photonics in general, including frequency doubling, Terahertz generation, calibration of advanced nonlinear optical microscopes and detection of plasmonic nanocavities.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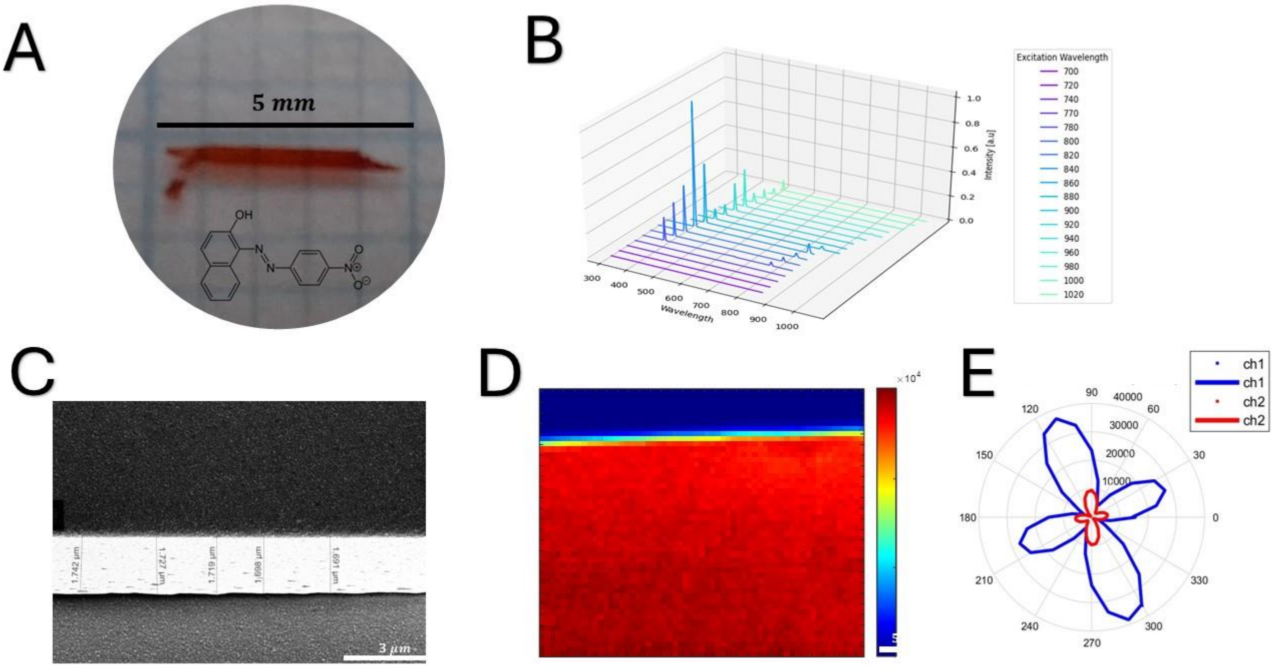
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Physical Metallurgy (Wednesday, February 26, 2025 11:00)

Invited Lecture

Physical Metallurgy

Heusler Alloys for Spintronics and Magnetocaloric Applications: Understanding through the Lens of Diffraction Techniques

Pnina Ari-Gur[1], Amila Madiligama[2], Sven Vogel[3], Viktor Koledov[4]
[1]*Mechanical & Aerospace Engineering, Western Michigan University, USA*
[2]*Physics, Penn State DuBois, USA*
[3]*Los Alamos National Laboratory, USA*
[4]*Russian Academy of Science, Moscow, Russia*

Heusler alloys may demonstrate unique combinations of properties, such as, ferromagnetism (sometimes even when the alloy is made of non-magnetic elements), antiferromagnetism, and superconductivity. Their properties critically depend on their crystalline structures, chemical order, structural phase transformations, and crystallographic texture. Because of the interplay between magnetic and crystallographic structures, a combination of diffraction techniques is essential for the understanding of their properties and behavior.

A major contribution to the giant magnetocaloric effect is the entropy change during the structural phase transformation from austenite (typically cubic $L2_1$, Fig.1) to a lower symmetry martensite. Its magnitude depends on the structure and the modulation of the martensite. Heusler alloys studied for the magnetocaloric effect are of non-stoichiometric composition. The site occupancy determines the chemical order and hence, the exchange interaction between atoms and, as a result, the magnetic nature of the phase. The chemical order is studied by a combination of x-ray and neutron diffraction because the sensitivity of each technique to different atoms is different.

Neutron diffraction (as opposed to x-rays) is needed to identify antiferromagnetic phases. Antiferromagnetic materials are considered “the future of spintronic applications thanks to the numerous interesting features they combine” [1]. This property is important for the magnetocaloric effect as well, because of the contribution of the magnetic phase transformation to the overall entropy change. Neutrons, having their own magnetic moment, will distinguish between identical chemical atoms with different magnetic moments and hence the magnetic state.

Crystallographic texture often results from the processing route used. In magnetic materials it affects the direction of the magnetization easy axis in the sample. Fig. 2 shows the texture in a heat exchanger, made of Ni50Mn18.75Cu6.25Ga25 by additive manufacturing [2].

Support by several NSF grants and the Department of Energy, Office of Science (Advanced Photon Source) under Contract DE-AC02-06CH1137 are acknowledged.

[1] Baltz, V., Manchon, A., Tsoi, M., Moriyama, T., Ono, T. and Tserkovnyak, Y., 2018, Antiferromagnetic Spintronics. Reviews of Modern Physics, 90(1), p.015005.

[2] Heat exchanger manufactured by Rafał Wróblewski, Prodziekan ds. Studenckich, Wydział Inżynierii Materiałowej, Politechnika Warszawska, Poland.

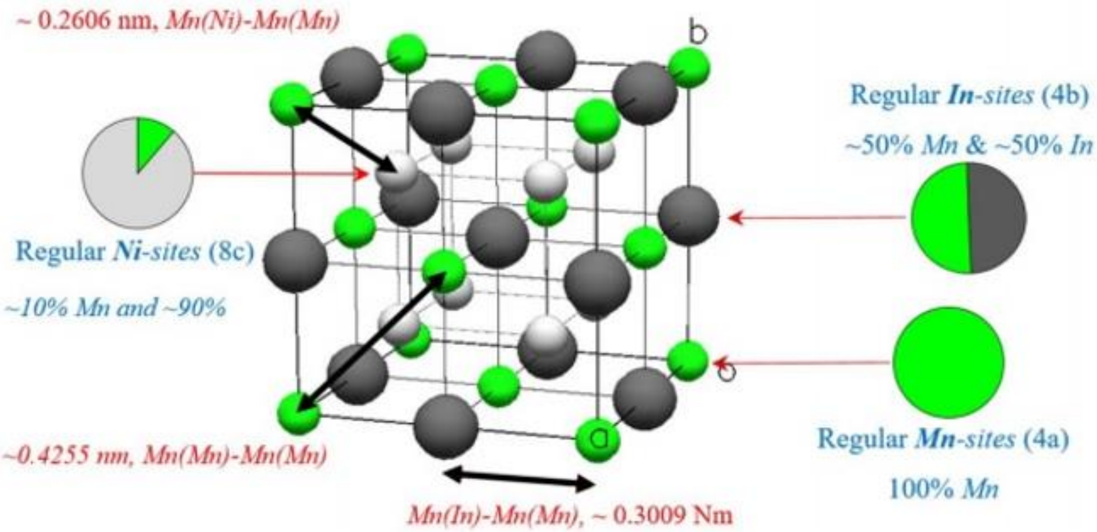

Fig. 1. Austenitic L21 (a=0.6018 nm) of Ni45Mn43In12 (314 K, 4 T). Site occupancies of the Mn (green), In (black), and Ni (silver) and the interatomic distances between different crystallographic sites are shown.

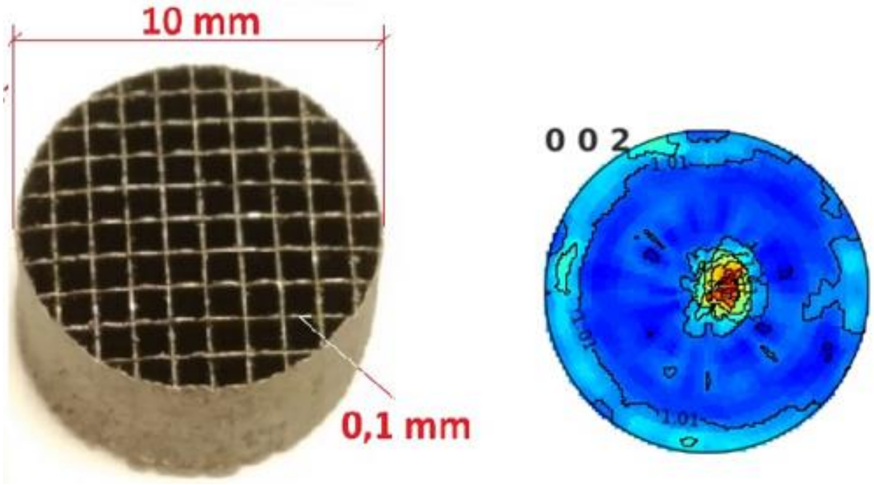

Fig. 2. Heat exchanger made by additive manufacturing (Ni50Mn18.75Cu6.25Ga25), demonstrates [001] preferred orientation along the build direction. This is the magnetization easy axis in this I 4/m m m martensite.

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Physical Metallurgy (Wednesday, February 26, 2025 11:00)

Invited Lecture

Surfaces and Interfaces

Local Electrical Properties of Grain Boundary Complexions in Alloys

Hanna Bishara

Grain boundaries (GBs) significantly affect the electrical properties of metallic and semi-conductor materials. The GB structural, thermodynamic and chemical characteristics heavily depend on the relative orientation of its adjacent grains, composition, and processing. Therefore, the GBs electrical properties are expected to span over a spectrum of values. Yet, the relationship between the boundary’s characteristics and their electron transport properties is not well-understood. Revealing the contribution of different GB complexions to electrical resistivity would pave the path for novel defect engineering to optimize the performance of conductors and functional alloys. This talk presents studies on the impact of complexion`s character on its resistivity, focusing on local electrical characterization of individual GB segments.

The talk initially introduces an experimental procedure to measure the local electrical resistivities of GB segments with high sensitivity and spatial resolution in-situ scanning electron microscopy (SEM). These segments are characterized by electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), and atom probe tomography (APT), in addition to molecular dynamics (MD) simulations. The measured electrical properties are coupled with the boundaries’ structural characteristics and thermodynamic excess properties. Multiple materials system will be addressed, namely, pure Cu, Cu alloys, Al alloys, and Heusler thermoelectric alloys. In addition to the GB resistive nature, the lecture reports unexpected trends of conductive GB complexions in the Heusler alloys. Such complexions are more conductive than the grain interior, due to segregation phenomena.

The novel results contribute to a better understanding of the defects’ resistivity and opens new horizons in knowledge-based defect engineering of smart materials. The present research is promising to be applied on phase boundaries and internal interfaces in general.

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Physical Metallurgy (Wednesday, February 26, 2025 11:00)

Invited Lecture

Physical Metallurgy

Structural Materials for Nuclear Fusion Energy: Knowledge Gaps and Opportunities in Metallic Materials Innovation

Aleksandra Baron-Wiechec[1], Haishan Zhou[2], Yuping Xu[2]
[1]*Materials Science and Engineering, Guangdong Technion – Israel Institute of Technology, China*
[2]*Fusion Reactor Materials and Components Division, Institute of Plasma Physics,*

Chinese Academy of Sciences, China

One of the future solution for energy source problems is a nuclear fusion, potentially unlimited, safe, no carbon emitting process. Nuclear fusion is the same process that powers stars and our Sun.
The most advanced design for the demonstration fusion power plant utilizes the tokamak concept, in which a burning plasma is confined by magnetic field in a torus-shaped vacuum vessel. The fuel - a mixture of Deuterium (D) and Tritium (T) - heated to temperatures in excess of 150 million °C, forms hot plasma. There are numbers of critical issues, primarily related to materials science and engineering, which requires significant innovation, before bringing the fusion power to the electricity grid.

Some of the operational requirements of the structural materials in fusion power plants are beyond today's experience. This includes high heat load, steep temperature and stress gradients, high energy neutron irradiation damage, formation of dust due to plasma – reactor's walls interaction, hydrogen isotopes permeation as well as corrosion of structural materials. Joint European Torous (JET) in the UK, as well as Comprehensive Research Facility for Fusion Technology (CRAFT) being currently constructed in China are two major examples of the facilities dedicated to address various fusion materials related challenges. CRAFT specifically will be testing the large-scale components before final decision on the technology and materials choice for the future power plants, bridging the materials engineering and technological gaps, and establish standard methodologies for manufacturing key materials and component.

This presentation is aimed to provide a snapshot of the unique topics relevant to metallic materials in nuclear fusion reactor environment. Examples of H isotopes retention studies (also referred to as "fuel retention") carried at the world's largest nuclear fusion experimental reactor JET, results of a hydrogen permeation study in the nuclear fusion relevant steels, and assessment of magnetic-field assisted corrosion of metallic structures of the fusion reactor cooling system will be discussed.

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Physical Metallurgy (Wednesday, February 26, 2025 11:00)

Oral Presentation

Physical Metallurgy

Recovery and Recrystallization of Deformed Metal Nanoparticles

Jonathan Zimmerman[1], Eugen Rabkin[1]
Technion - Israel Institute of Technology, Israel

Metallic nanoparticles are utilized in a growing number of applications such as catalysis, drug delivery, sensing and optoelectronics due to their unique and tunable properties. Recrystallization has great potential to further enhance the tunability of nanoparticles, but despite historically being a primary method for manipulating the properties of bulk metals, it was never applied to individual metal nanoparticles. We studied thousands of initially pristine, single crystal platinum nanoparticles during a recrystallizing anneal after compressive deformation. We found that the compressive deformation causes a dramatic change in particles orientation, misaligning them by up to 28 degrees with respect to their stable orientation. During the recrystallizing anneal a large fraction of the nanoparticles retained their new misaligned orientation and changed their shape to match this new orientation. We observed the nucleation of new grains at the onset of recrystallization, however, in the smallest particles these grains stopped growing and annihilated into the deformed matrix. We found that the critical particle diameter for recrystallization is about 500 nm: In smaller particles the recovery of the deformed microstructure is so fast that a recrystallized nucleus loses the driving force for growth and collapses under the action of capillary driving pressure. Finally, a model was developed to describe this phenomenon. It was shown that the critical diameter for recrystallization depends on grain boundary energy, mobility, and recovery kinetics of deformed microstructure.

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Physical Metallurgy (Wednesday, February 26, 2025 11:00)

Oral Presentation

Physical Metallurgy

Dynamics of Martensitic Transformations

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Our hypothesis is that the nucleation of martensite is not led by a single or a few atoms but it is a "joint venture" of many atoms. Coordinated atomic motion is not an extraordinary behavior: oscillatory waves are natural motion modes that fulfill the equations of motion when the energy landscape is ascending. In certain unstable lattices there are certain waves that are able to bring up structural transitions. They have negative ω^2 roots of the dynamic equations, which predict diverging atomic displacements due to a descending energy landscape. Indeed, observation of the atomic motion in the core of the martensitic nuclei in molecular dynamics (MD) simulations show a coordinated motion of a group of atoms that cause relative shear displacements and twin formation, which has an envelope of a transverse wave.

We have solved the dynamic equations of an unstable austenitic lattice and found that a transverse acoustic branch is unstable (has negative ω^2) at 0oK. Then we applied the spectral analysis method to extract the dispersion relation from MD simulation of the same lattice. We found that the same transverse acoustic branch of oscillatory modes exists at elevated temperatures with real frequencies. Now we invoke the understanding that phonon lifetime or mean free path decreases with increasing temperature due to interactions between phonons. We thus assume that the transverse acoustic modes are stable when they have short lifetime or free path, but are unstable when their free path are long. Calculation of the potential energy of lattices that contain static modulations of different paths confirms that the energy is ascending with increasing amplitude of the modulations with short free path (indicating stable oscillatory motion) but it is descending when the free path increases, indicating instability of the lattice with respect to the transvers acoustic modes.

The hypothesis is in-line with an important experimental observation: the appearance of martensite is gradual; its fraction usually increases gradually with lowering the temperature around Ms. It conforms with the statistical nature of the free path of phonons, so that more phonons with long enough free path gradually appear as the temperature decreases.

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Physical Metallurgy (Wednesday, February 26, 2025 11:00)

Oral Presentation

Physical Metallurgy

Stress Relaxation and Anisotropy in Zircaloy-4 Cladding: Insights from Uniaxial and Biaxial Testing under Pellet-Cladding Interaction Conditions

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What governs the enhanced stress relaxation and deformation behavior of Zircaloy-4 cladding under reactor-relevant stress states? This study delves into this critical question through a comprehensive investigation of cold-worked, stress-relieved (CWSR) Zircaloy-4 (Zry-4), employing state-of-the-art experimental techniques and advanced computational modeling. By integrating mechanical testing under varying loading modes, detailed microstructural characterization, and viscoplastic self-consistent (VPSC) simulations, we identify the key deformation mechanisms and their implications for nuclear fuel performance.

Our findings[1-3] show that internal pressurization, representative of pellet-cladding interaction (PCI) loading, induces higher resolved shear stresses on basal slip systems than uniaxial tension. This stress state promotes a complex interplay between basal and prismatic slip systems, leading to enhanced stress relaxation and reduced mechanical anisotropy at elevated temperatures. In contrast, uniaxial tension maintains prismatic-dominant deformation, resulting in temperature-independent anisotropy.

These insights into the relationship between stress state, temperature, and anisotropic deformation provide a foundation for optimizing cladding design and improving reactor safety.

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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Invited Lecture

Bio- and Soft Materials

Bioinspired Materials for Biomedical Applications

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The emerging demand for tissue engineering scaffolds capable of inducing bone regeneration using minimally invasive techniques prompts the need for the development of new biomaterials. One promising route is molecular self-assembly, a key direction in current nanotechnology and material science. In this approach, the physical properties of the formed supramolecular assemblies are directed by the inherent characteristics of the specific building blocks. Molecular co-assembly at varied stoichiometry substantially increases the structural and functional diversity of the formed assemblies, thus allowing tuning of their architecture and physical properties.

Here, in line with polymer chemistry paradigms, we applied a co-assembly approach using hydrogel-forming peptides, resulting in a synergistic modulation of their mechanical properties to form extraordinarily rigid hydrogels that supported osteogenic differentiation based on cells-mechano-sensing. Furthermore, we designed a multi-component scaffold composed of polysaccharides, short self-assembling peptides, and bone minerals. We demonstrate the formation of a rigid yet injectable and printable hydrogel without the addition of cross-linking agents. The formed composite hydrogel displays a nanofibrous structure, which mimics the extracellular matrix and exhibits thixotropic behavior and a high storage modulus. This composite scaffold can induce osteogenic differentiation and facilitate calcium mineralization.

This work provides a conceptual framework for utilizing co-assembly strategies to push the limits of nanostructure physical properties obtained through self-assembly to design new biomaterials for tissue engineering and personalized medicine applications.

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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Oral Presentation

Bio- and Soft Materials

Effect of Binary Mechanical Environment on T-cell Function.

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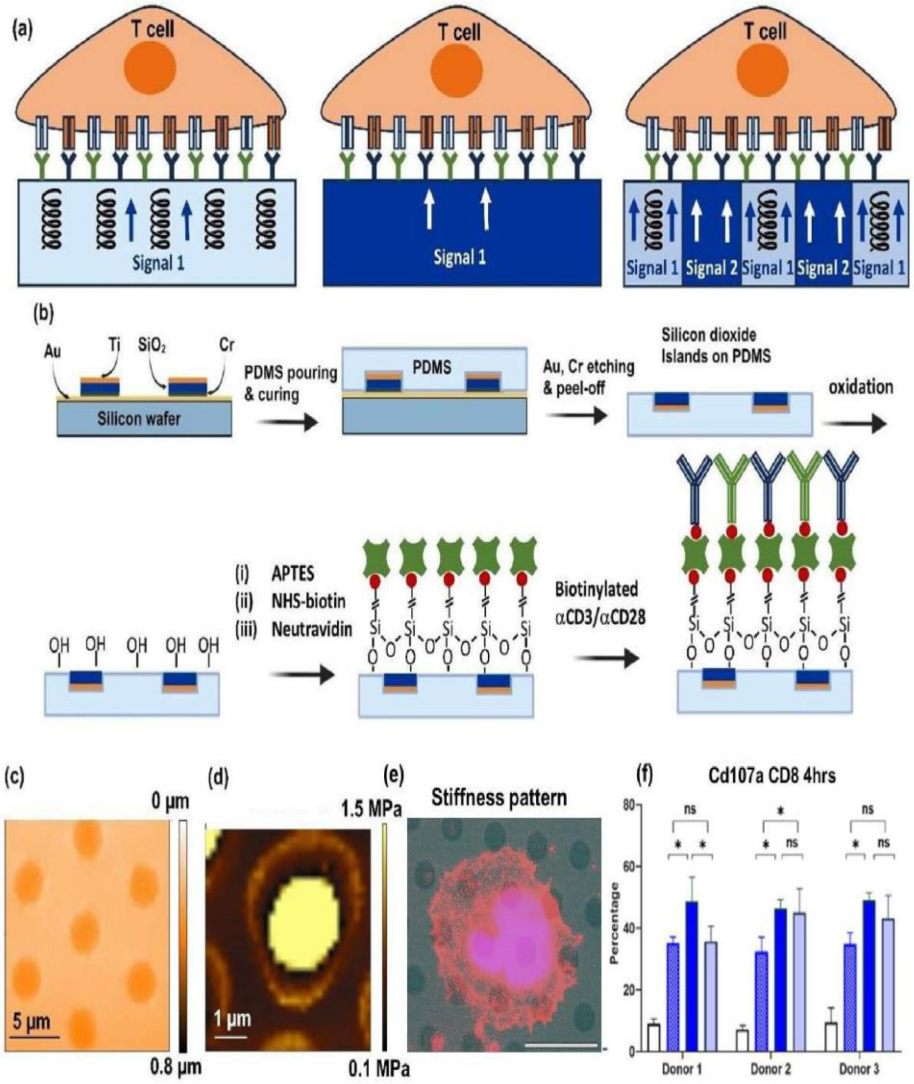
Health Sciences, Ben-Gurion University of the Negev, Israel

Recent studies indicate that T cells are mechanosensitive, and their activation depends on the mechanical properties of their environment, including target cells, professional antigen-presenting cells, and surrounding tissues. This mechanosensing was demonstrated ex vivo by showing that T cells activated on surfaces of varying stiffness adjust their responses accordingly. However, in all these studies, T cells were stimulated ex vivo by homogeneous mechanical environments, whereas their natural environment can be heterogeneous, providing multiple mechanical stimuli simultaneously. For example, antigen-presenting cells such as dendritic cells, macrophages, and B cells, as well as endothelial cells within blood vessels, expose T cells to different mechanical cues, often at the same time. In bones, T cells encounter both the cortical bone, with elasticity in the range of tens of GPa, and the bone marrow, with elasticity in the range of a few kPa. Similarly, tumor tissue comprises multiple components with varying elasticities: tumor cells (~1–10 kPa), fibroblasts (~5–10 kPa), immune cells (~100 Pa), and extracellular matrix, whose primary components include fibronectin (~1–15 MPa) and collagen (~5–10 GPa). This raises a long-standing question: when T cells receive two or more mechanical stimuli simultaneously, do they average their responses to these stimuli, or does one stimulus dominate? Addressing this question has so far been limited due to the lack of ex vivo model environments capable of delivering simultaneous mechanical stimuli.

Here, we engineered a novel model system for T cell stimulation that mimics the mechanical complexity of the T cell environment and studied its effects on T cell activation. The system consisted of a micropattern of alternating soft and stiff microdomains. The micropattern was fabricated by photolithographic patterning of silica lines, which were then mechanically embedded within soft polydimethylsiloxane (PDMS). The pattern was uniformly functionalized with activating and costimulatory ligands essential for biochemical signaling. T cells were plated on these patterns as well as on homogeneous soft and stiff surfaces for comparison. We found that T cells did not average the mechanical signals. Instead, they responded similarly to those on a homogeneously soft surface, exhibiting lower activation compared to those on a stiff surface. Interestingly, long-term exposure to these patterns enhanced the proliferation of central memory and effector T cell phenotypes, similar to the response observed in stiff environments. These findings reveal the non-linear nature of T cell mechanosensing and suggest that mechanical heterogeneity plays a critical role in modulating T cell responses. This provides new insights into T cell activation and has potential implications for immunotherapies.

*J.J Pandit et.al, Under revision in Acta Biomaterialia.



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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Oral Presentation

Bio- and Soft Materials

Shaping Molecular Crystals: The Role of Polymers and Small Molecules

Dolev Brenman-Begin[1], Zohar Eyal[1], Rachael-Lynn Deis[1], Anna-Eden Kossoy[2],
Iddo Pinkas[2], Tatyana Bendikov[2], Lyudmila Veikhman[2], Dvir Gur[1]
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Controlling the three-dimensional morphology of crystals is crucial for optimizing their optical, mechanical, and electronic properties, yet achieving precise control is often challenging. In contrast, organisms meticulously control every aspect of crystal morphology and size, though the mechanisms behind this are not completely understood. In nature, organisms form a diverse array of organic and inorganic crystals, each serving distinct functional roles. These crystals grow within specialized organelles, with guanine being one of the most common organic materials utilized. Anhydrous guanine crystals are particularly interesting due to their plate-like morphology and high anisotropic refractive index, which results from the stacking of hydrogen-bonded molecular layers along the (100) plane. Our previous work revealed that biogenic guanine crystals in zebrafish form via heterogenous nucleation as thin leaflets on amyloid fibers, which serve as templates, incorporating substantial amounts of organic dopants like hypoxanthine.[1, 2] However, the precise interactions and chemistries of amyloid fibers and dopants in the crystallization process remain poorly understood. In this study, we investigate the effects of polymers, acting as amyloid fiber analogs, and organic dopants on the in-vitro formation of guanine crystals. Using spectroscopic and microscopic techniques, we demonstrate that the polymer backbone and its functional groups play a crucial role in determining crystal morphology. Hydrophobic functional groups containing carbonyl moieties slow growth along the π-π stacking direction, leading to a plate-like morphology similar to natural biogenic crystals. Conversely, hydrophilic functional groups interact with guanine`s hydrogen bonds, resulting in bulky, thin crystals (Figure 1, A-B). Additionally, increased levels of hypoxanthine result in broader crystals with prominent (012) facets and reduced (010) facets (Figure 1C). Given that the growth of a crystallographic facet is inversely related to its expression, our findings indicate that hypoxanthine selectively inhibits growth along the (012) plane.

By elucidating the roles of polymers and dopants in crystal formation, our work offers insights that could guide new approaches to controlling crystal growth and morphology, toward the rational design of crystals with tailored properties.

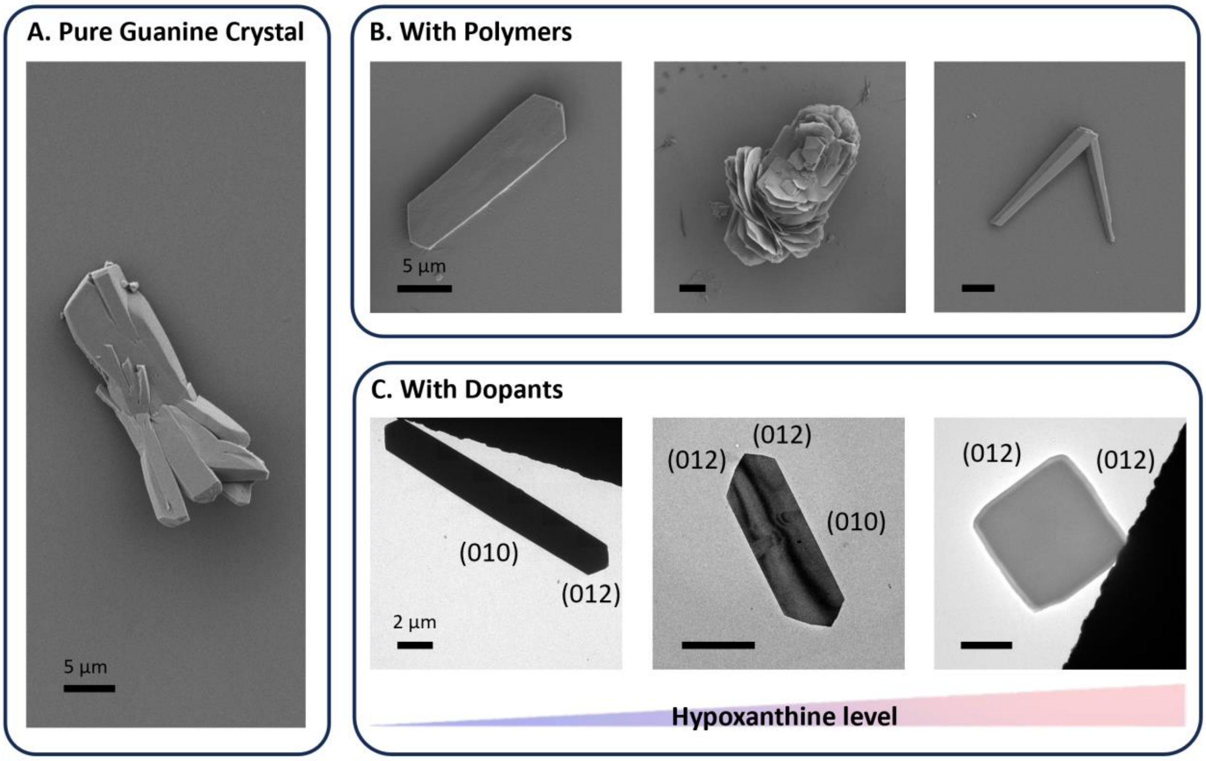

Figure 1. The effect of polymers and organic dopants on crystal morphology. A. A Scanning electron microscope image of pure guanine crystals, B. Scanning electron microscope images of guanine crystals formed with different polymers (from left to right: PVP-co-VA, Polyvinyl acetate & Polyacrylamide), and C. Transmission electron microscope images of guanine crystals formed with increasing levels of hypoxanthine (left to right) and PVP-co-VA.

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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Oral Presentation

Bio- and Soft Materials

Enhanced Mechanophore Activation in Hydrogel Networks Driven by Pre-Tension

Meytal Forer[1,2], Alessio Maselli[2,3], Yifan Liao[2], Josh Grolman[2]
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Mechanophores, molecules that change color and structure when force is applied, have the potential to revolutionize biomedical research due to many diseases that have mechanical driving factors, like the metastasis of cancer. However, there is a gap between the activation sensitivity of the mechanophore attached in the polymer chain, compared to the actual force needed to activate the mechanophore when combined in the network. The force propagation pathway in a network to the mechanophore remains widely unknown, resulting in a lack of sensitivity unsuitable for biological systems. Here we show activation of SP in alginate hydrogel networks, directly related to the cross-linking bond strength of the network by testing ionic cross-linked and covalent cross-linked gels. We also found that the reversibility of the ring-closing reverse reaction that resets the mechanophore is related to crosslink strength and network architecture. Our results set the stage for mechanophore incorporation in biomaterials and enable them to be used in furthering the field of mechanobiology.

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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Oral Presentation

Advanced Characterization Methods

Study of the Active Site in Azurin Blue Copper(II) Protein with Cryogenic X-ray Photoelectron Spectroscopy

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[2]*Department of Molecular Chemistry & Materials Science, Weizmann Institute of Science, Israel*

Solid-state electron transport (ETp) through the blue copper protein Azurin (*Az*) is well studied[1-3] due to its potential capability for diverse functional electronic devices. X-ray and Ultraviolet Photoelectron Spectroscopies (XPS, UPS) with their high surface sensitivity have been used extensively to study the electronic and chemical structure of *Az*, especially as a thin films or monolayers on solid surfaces.[1-3]

XPS measurements of the active site of *Az* protein and, especially, the Cu(II) ion is not a straightforward task, due to its very low concentration (one Cu atom per $C_{607}N_{164}O_{194}S_9Cu$ protein molecule) and sensitivity to X-ray exposure. Az solution has strong blue color caused by paramagnetic complex of Cu(II) with sorrounding ligands comprising the active site of the protein. We found that after prolonged XPS measurements the blue color is changed to dark brown and the Cu ion, most probably, is reduced to the (+1) or neutral (0) state, as the Cu 2p spectrum takes on the shape, characteristic for diamagnetic Cu(I)-Cu(0).

To preserve the protein from deterioration as a result of its exposure to the X-ray beam, we performed XPS measurements under cryogenic conditions. In this procedure, the liquid sample is frozen during the loading, using the fast freezing method,[4-5] and remains frozen up to it removal from the XPS instrument. We also deposited thin protein layers on gold TEM grids coated with about 20 nm layer of amorphous carbon. Formation of the thin protein layer on the conducting grid prevents accumulation of positive charge, as usually observed during cryo-XPS measurements, allowing performance of these measurements without application of a low energy electron flood gun. The role of the substrates and other possible reasons for Cu reduction will be discussed.

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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Oral Presentation

Bio- and Soft Materials

The Mechanics of PEGDA Hydrogels: from Microstructure to Macroscopic Behavior

Michal Levin[1], Yongkui Tang[2,3], Claus Eisenbach[3,4], Megan Valentine[2,3], Noy Cohen[1]
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[4] *Institut for Polymerchemie, University of Stuttgart, Stuttgart, Germany*

Poly(ethylene glycol) diacrylate (PEGDA) hydrogels are a widely used material in biomedical applications, such as tissue engineering and drug delivery. This is thanks to PEGDA`s biocompatibility and mechanical stability under various loadings. From a chemical and microstructural viewpoints, this material forms a complex three-dimensional network called **bottlebrush**, consisting of stiff rod-like polyacrylate (PA) cores that connect soft random coils of poly(ethylene glycol) (PEG) chains. To the best of our knowledge, such complex networks, that are fundamentally different from classic polymeric gels, have not been studied through theoretical modeling yet.

The aim of this talk is to present a microscopically motivated and energy-based model to describe the mechanical behavior of PEGDA. By considering the contribution of all components – the PA rods and the PEG chains, as well as the PA-PA mechanical interaction, we explain the macroscopic mechanical response of the network under loading.

The results of our work reveal that when subjected to external load, the soft PEG chains elongate and shorten and apply forces on the stiff PA rods, causing them to bend and thus absorb the external energy. Considering various systems with changing ratios of PEG chain to PA rod lengths, we discovered that PA-PA interactions are an important factor, specifically in the case of long PA rods. Next, our model was fitted to experimental results of nine hydrogel samples with varying molecular weights that were compressed uniaxially. We found out the influence of PEGDA molecular weight on the macroscopic mechanical response and explained it through microstructural behavior.

The findings from this work can be implemented to program the properties and response of PEGDA hydrogels through experimental modifications, by varying the molecular weight and concentration of the fabricated PEGDA. Control over the mechanical response of this material is crucial for its applications in the biomedical field.

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Bio- and Soft Materials II (Wednesday, February 26, 2025 11:00)

Oral Presentation

Bio- and Soft Materials

Short Peptides as Tools for Novel Bioink Formulation in Tissue Engineering

Francesca Netti[1,2,3], Moran Aviv[1,2,3,4], Yoav Dan[1,2,3], Safra Rudnick-Glick[1,2,3],
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The development of advanced bioinks for 3D bioprinting relies on the ability to seamlessly combine biocompatibility, mechanical robustness, and printability. Short peptide-based hydrogels, such as fluorenylmethoxycarbonyl diphenylalanine (Fmoc-FF), have emerged as versatile tools for bioink design due to their self-assembly properties and capacity to interact with various polymers. In this study, we investigate the use of Fmoc-FF peptides as a platform for fabricating novel bioink formulations by incorporating polymers like gelatin. Gelatin is a widely utilized biomaterial for its biocompatibility and extracellular matrix (ECM) mimicking properties. However, its reliance on UV crosslinking poses challenges, as the process can harm cells and reduce overall cell viability. To eliminate the need for post-printing crosslinking, we employed a novel approach by modifying Fmoc-FF peptides with ethylene glycol (EG) motifs. This modification enhanced the peptides hydrophilicity, elasticity, and ability to stabilize polymer networks. The modified Fmoc-FF peptides were successfully used to integrate gelatin into a cohesive bioink matrix. This new formulation provided structural stability and tunable mechanical properties, enabling the creation of 3D-printed scaffolds while maintaining high cell viability. By eliminating cytotoxic crosslinking processes, this approach offers a significant advantage in the fabrication of bioinks. This study underscores the transformative potential of short peptides as functional tools in the design of innovative bioink formulations. These advances pave the way for the development of versatile, biocompatible scaffolds for tissue engineering and regenerative medicine applications.

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Computational Materials Science II (Wednesday, February 26, 2025 14:30)

Invited Lecture

Computational Materials Science and Machine Learning

Computational Thermodynamics: Principles and New Applications to Electrodeposition of Reactive Metals from Molten Salts

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Thermodynamic calculations are an invaluable tool for predictions for the understanding and design of materials and processes. In the last decades, the way thermodynamic theory is applied to problems in chemistry and materials science has evolved significantly. Rather than the examination of particular reactions, the thermodynamic calculation is performed by Gibbs energy minimization. In the CALPHAD (CALculation of PHAse Diagrams) method, thermodynamic models are constructed for the Gibbs energy of all the phases in a system over the widest possible range of temperatures, pressures and compositions. Such models include adjustable parameters that are determined by fitting to experimental results or results of ab-initio calculations. The calibration proceeds from unary to binary to ternary systems whereas predictions for higher order systems are obtained by extrapolations. CALPHAD model predictions include equilibrium phase composition, phase composition following rapid solidification as well as driving forces for kinetic simulations (e.g. using phase-field methods).

Today CALPHAD calculations are applied to a wide variety of materials systems such as multicomponent alloys [1,2], oxides and salts. Current CALPHAD software can handle several type of equilibrium conditions: Temperature, Pressure, constraints on system composition as well as constraints on chemical potentials or activities. It does not allow electrical potential with respect to some electrode to be set as an equilibrium condition. For certain situations this problem can be circumvented by considering other, equivalent constraints. Recently, this approach was applied to the electrodeposition of reactive metals such as Titanium and rare earths form molten chloride salts [3]. Thermodynamic calculations predict which phase is deposited at a certain electrical potential from a salt of a given composition, in the limit of zero current. With CALPHAD software, models and databases, predictions of can take into account non-stoichiometric phases, as well as complex behavior of molten salt solutions. Consistency is achieved between predictions of electrodeposition and other phase equilibria.

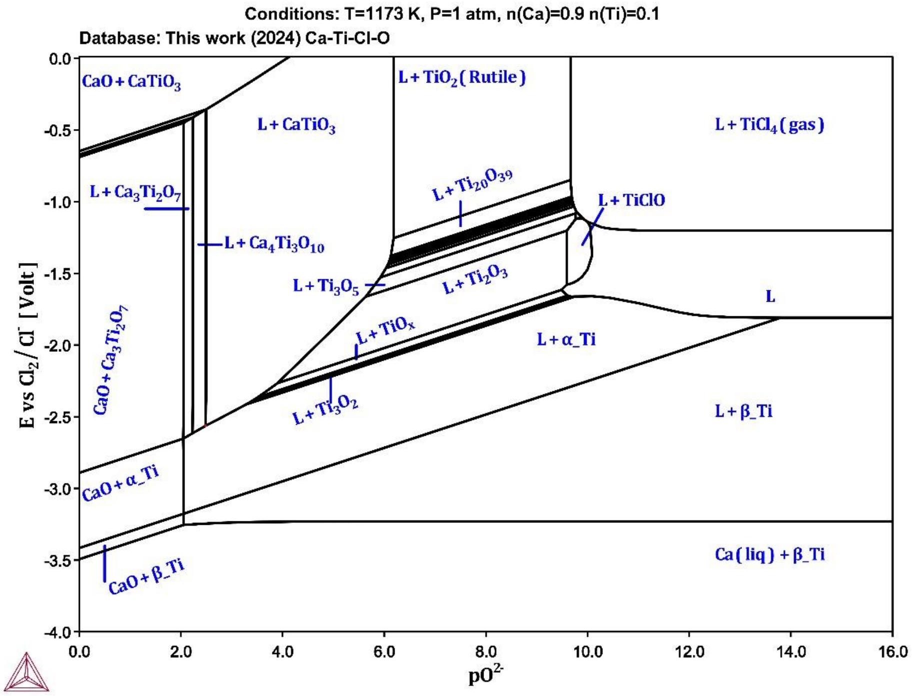

Figure 1: A Littlewood phase stability diagram for electrodeposition of Titanium from molten $CaCl_2$ salt. The x-axis is where is the activity of the oxide ion in analogy to pH. The y-axis is the potential vs a Cl_2/Cl^- electrode in equilibrium with Cl_2 gas at atmospheric pressure. The fields on the diagram are the stable phases. Calculation of the diagram with CALPHAD software and database permits the creation of more detailed diagrams than was possible by traditional methods.

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Computational Materials Science II (Wednesday, February 26, 2025 14:30)

Invited Lecture

Computational Materials Science and Machine Learning

Light-Matter Interaction Dynamics with Ab Initio Data-Driven Computations

Sivan Refaely-Abramson

Excited-state processes are essential for emerging applications in materials, from energy conversion to quantum information science. The associated generation and relaxation mechanisms are often coupled to quantum selection rules, stemming from the underlying material structure. In this talk, I will discuss the relation between excited-state evolution and structural design in low dimensional semiconductors. I will present our bandstructure theoretical and computational approaches to calculate phonon-assisted exciton interaction dynamics as a function of the underlying structure and discuss the importance of many-body effects in the excited state relaxation and dephasing mechanisms. I will further discuss our ab initio – based data-driven approaches to explore excited-state relaxation upon phonon scattering, offering new design principles to achieve light-induced quantum coherence in semiconducting materials.

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Computational Materials Science II (Wednesday, February 26, 2025 14:30)

Invited Lecture

Computational Materials Science and Machine Learning

Charge Transport through Catalytic Materials

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Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Israel

Functional materials are important for applications in the fields of catalysis and renewable energy. Specific functionalities include charge transport through electronic material components as well as catalytic reactivity on material surfaces. In the talk, I will advocate that there is a relation between charge transport efficiency and reactivity, and therefore developing novel algorithms that calculate both are important for better understanding of intrinsic material limitations. We cover our latest results in developing and using charge transport calculation methods and demonstrate them on catalytic materials. Our home code is developed on a user-friendly GUI and enables to use widely available Density Functional Theory results as input. The methodology is demonstrated on several semiconducting materials.

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Computational Materials Science II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Computational Materials Science and Machine Learning

Surface Tension Calculations in Liquid Metals Using First Principles and Machine Learning

Netanela Cohen[1], Oswaldo Diéguez

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Surface tension, a fundamental property of liquids, plays a crucial role in various phenomena, from a steel wire ‘floating’ on water to materials processing. Despite centuries of investigation, challenges persist in predicting surface tension due to limitations in empirical force-fields in computational methods like molecular dynamics (MD). Furthermore, these force-fields often struggle to accurately predict properties under different conditions than those in which they were fitted, emphasizing the need for tailored approaches or even force-field-free methods.

Our research aims to overcome this challenge by developing efficient computational methods for calculating the surface tension of liquids, focusing on elemental liquid metals. For this purpose, we use *ab initio* molecular dynamics (AIMD) and machine learning force fields (MLFF), both of which combine molecular dynamics and Kohn-Sham density functional theory. By eliminating the dependence on empirical force fields, these two approaches are likely to enhance accuracy and transferability across diverse liquid systems, potentially enabling the study of their properties under varied conditions.

Emphasizing computational efficiency, we present the results of our surface tension calculations using an approximation based on the work of cohesion. We assess the performance of this approximation in liquid metal systems, and validate our computational approaches by comparing the MLFF results with AIMD simulations and available experimental data.

By refining the methods discussed, we aim to establish a robust and transferable framework for the calculation of surface tension, contributing to a deeper understanding of liquid behavior and advancing predictive in materials science.

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Computational Materials Science II (Wednesday, February 26, 2025 14:30)

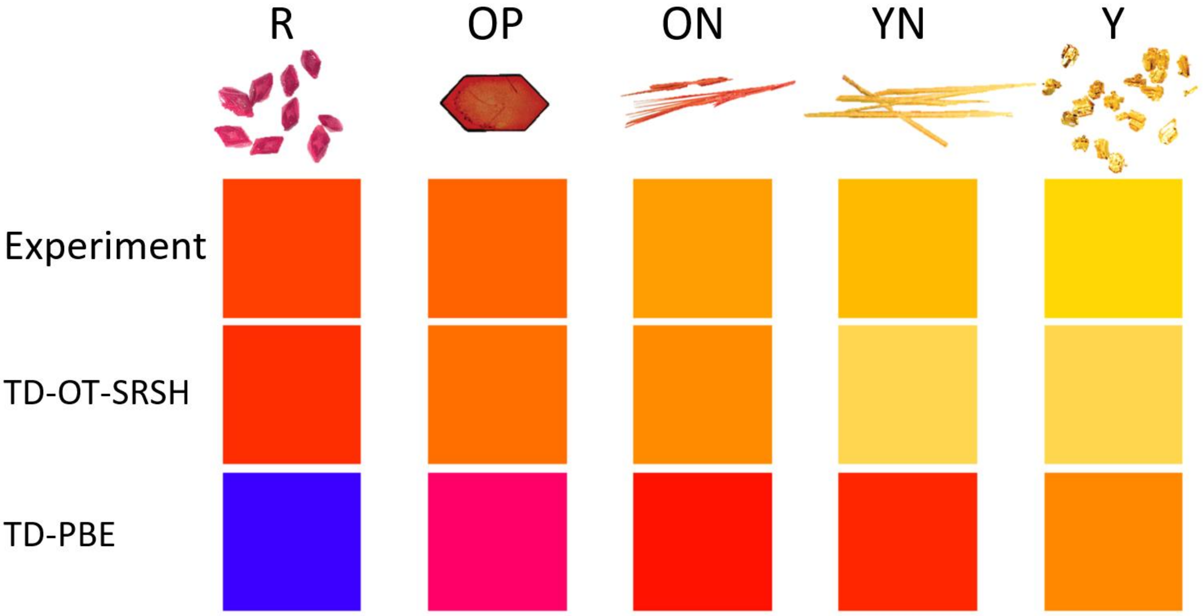
Oral Presentation

Computational Materials Science and Machine Learning

Predicting and Understanding Color Polymorphism in ROY from First Principles

MICHAL HARTSTEIN[1], Guy Ohad[1], Leeor Kronik[1]
Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

Color polymorphism is an intriguing phenomenon, in which different polymorphs of the same molecular solid exhibit different perceived colors. While spectacular, this color polymorphism corresponds to relatively modest spectral changes. It is therefore a long-standing challenge for time-dependent density functional theory. Here, we show that the experimentally observed colors of 5-methyl-2-((2-nitrophenyl)amino)thiophene-3-carbonitrile, known as ROY for its red, orange, or yellow polymorphs, can be predicted accurately using non-empirical optimally-tuned screened range-separated hybrid (OT-SRSH) functionals. Moreover, we use the polarizable continuum model (PCM) to assess the effect of different contributing factors, e.g. molecular conformations, dielectric effects, and intermolecular interactions, on the varying polymorph colors.



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Computational Materials Science II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Computational Materials Science and Machine Learning

Nonlinear Self-calibrated Spectrometer with Single GeSe-InSe Heterojunction Device

Rana Darweesh[1,2], Rajesh Kumar Yadav[1,2], Elior Adler[1,2], Michal Poplinger[1,2], Adi Levi[1,2], Jea-Jung Lee[3], Amir Leshem[1], Ashwin Ramasubramaniam[4,5], Fengnian Xia[3], Doron Naveh[1,2]
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Computational spectrometry is an emerging field that uses photodetection in conjunction with numerical algorithms for spectroscopic measurements. Compact single photodetectors made from layered materials are particularly attractive since they eliminate the need for bulky mechanical and optical components used in traditional spectrometers and can easily be engineered as heterostructures to optimize device performance. However, such photodetectors are typically nonlinear devices, which adds complexity to extracting optical spectra from their response. Here, we train an artificial neural network to recover the full nonlinear spectral photoresponse of a single GeSe-InSe p-n heterojunction device. The device has a spectral range of 400 to 1100 nm, a small footprint of ~25 × 25 square micrometers, and a mean reconstruction error of $2 \times 10{-}4$ for the power spectrum at 0.35 nanometers. Using our device, we demonstrate a solution to metamerism, an apparent matching of colors with different power spectral distributions, which is a fundamental problem in optical imaging.

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Materials for Extreme Conditions (Wednesday, February 26, 2025 14:30)

Invited Lecture

Materials under Extreme Conditions

The Influence of Solutes and Fields on Anisotropic Grain Growth of Alumina

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Grain growth occurs alongside densification during the sintering of polycrystalline ceramics. The size and shape of grains can significantly influence a material`s properties, while grain boundary motion can lead to the occlusion of second-phase particles and pores, altering residual stress fields and strengthening mechanisms. Understanding the factors driving morphological changes is therefore critical. Although dopants are often used to limit grain growth via solute-drag, recent studies have shown that certain dopants can accelerate grain growth. In alumina, dopants can also alter the relative anisotropic grain boundary mobility, causing notable changes in morphology and properties.

This presentation examines anisotropic grain boundary mobility by measuring the interface motion of oriented single crystals of sapphire into undoped and Ca-doped polycrystalline alumina. The findings show that while Ca increases the mean mobility, it dramatically enhances the mobility of boundaries parallel to the rhombohedral plane, resulting in elongated grains. These results are compared with the effects of electric fields on grain growth in dense alumina, highlighting the role of oxygen vacancies in this process. Finally, the role of disconnections as the mechanism for grain boundary motion will be discussed.

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Materials for Extreme Conditions (Wednesday, February 26, 2025 14:30)

Invited Lecture

Materials under Extreme Conditions

Directed Energy Deposition (DED) of Refractory Ultrahigh Temperature Ceramics (UHTCs) for Extreme Environments

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Directed Energy Deposition (DED) is a branch of additive manufacturing (AM) in which a focused energy source (laser, electron beam, or arc) melts the feedstock (either powder or wire) at a specific point and creates a melt pool, often shielded with an inert atmosphere.1,2 In this presentation I will review the R&D in my group towards processing by DED of refractory coatings such as carbides and borides on different substrate materials (e.g. pure tungsten and Inconel). In the case of SiC, for example, the high-energy deposition leads to the formation of a relatively dense graded coating. Additionally, partial mixing of SiC with the underlying refractory metal is observed, resulting in a robust composite material. DED processing is reported to offer a viable method for fabricating chemically and functionally graded coatings for advanced high-temperature applications.

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Acknowledgement

We are grateful for the financial support from the Israel Ministry of Defense (grant no. 4440783376).

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Materials for Extreme Conditions (Wednesday, February 26, 2025 14:30)

Invited Lecture

Materials for Security and Defense

Ceramic Matrix Composites – Challenges and Development Approach for Military Applications

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Ceramic Matrix Composites (CMCs) are revolutionizing the aerospace and military industries by offering exceptional properties like high temperature resistance, low specific mass and superior strength at high temperatures. These materials enable the development of advanced structures, capable of withstanding extreme operating conditions.

However, challenges remain in the widespread adoption of CMCs. This includes complex manufacturing processes, high costs and concerns regarding reliability and damage tolerance. To address these issues, an advanced development approach that combines fabrication techniques, material properties, material modeling and advanced testing was adopted.

This work will demonstrate this development approach and some of the challenges on the way to proving CMCs as a material solution for high temperature structures with standing temperature exceeding 1300°C such as, leading edges, engine components and more.

By overcoming these challenges, CMCs have the potential to significantly enhance the performance and efficiency of aerospace and military systems, leading to groundbreaking advancements in propulsion, structural components and thermal protection systems.

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Materials for Extreme Conditions (Wednesday, February 26, 2025 14:30)

Oral Presentation

Materials under Extreme Conditions

AlFeCoCrNi$_x$ (with x=1.2, 2.1, 2.6) High Entropy Alloys: Microstructure, Properties and Heavy Ion Irradiation Resilience

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The development of fusion and fission reactors requires advanced structural materials that can maintain performance under extreme conditions, such as high temperatures and irradiation doses. High Entropy Alloys (HEAs) [1], which are multicomponent concentrated solid solution alloys, have emerged as promising candidates for radiation-resistant materials due to the retarded energy dissipation, and suppressed damage accumulation [2]. In addition, HEAs exhibit superior mechanical properties, including high strength, ductility, and improved fracture toughness. However, these materials are susceptible to order-disorder phase transformations, which can significantly alter their mechanical properties.

Our previous research [3] evaluated the irradiation resilience of AlCoCrFeNi dual-phase (ordered and disordered Body Centered Cubic (BCC/B2)) HEAs, indicating their stability. Additionally, studies on Face Centered Cubic (FCC)-based HEAs have demonstrated exceptional stability under irradiation [4]. To further enhance the radiation resistance and mechanical properties of HEAs and propose them as candidates for structural materials in the nuclear industry, the current research explores the eutectic alloy concept (alternating FCC/BCC (or their ordered variants L12/B2) lamellas) as a strategy.

In the AlCoCrFeNi$_x$ system, the microstructure varies significantly with the Ni content, transitioning from dendritic morphology ($1.0 \leq x \leq 1.5$) to eutectic structure ($x = 2.1$) consisting of alternating soft L12 and hard B2 phases, and finally to oriented cellular structure ($x \geq 2.4$) [5]. Considering that microstructure and grain boundary density play a major role in radiation resilience, this system was chosen for the current study as an interesting candidate with varying microstructure, high grain boundary density, and potential order/disorder phase transformation.

In this research, AlCoCrFeNi$_x$ HEAs with varying Ni content ($x = 1.2$, 2.1, and 2.6) were studied using X-ray diffraction, scanning and transmission electron microscopies, and microhardness methods. Following prolonged heat treatment at 900°C, these alloys exhibited exceptional microstructural stability. Furthermore, characterization of these alloys subjected to irradiation with Ne ions at varying doses (0.5, 1, and 1.5 DPA) revealed minor microstructural changes. In all three samples, the B2 phase remained stable and did not undergo a phase transition to the disordered phase even after exposure to the highest dose of irradiation used in this study. As for the FCC/L12 phases, in the eutectic and hypereutectic microstructures, the phase changed from L12 to FCC, indicating a decrease in the order parameter as a function of irradiation and Ni content.

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Materials for Extreme Conditions (Wednesday, February 26, 2025 14:30)

Oral Presentation

Materials for Security and Defense

Implementation of Time-domain Frequency-dependent Acoustic Drag to Model the Shock Attenuation Characteristics of Methyl Cellulose Hydrogel

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Methyl cellulose is a unique material that display a liquid-solid phase transition when heated. Previous researches found that the solidification energy can be supplied as a mechanical impact, and not only as heat (Parvari, Rotbaum, Eichen, & Rittel, 2018). The endothermic solidification of the gel under impact, absorbs some of the impact energy (Rotbaum, Parvari, Eichen, & Rittel, 2019). In a previous work, the frequency-dependent attenuation of methyl cellulose was modeled for different compositions and thicknesses (Guetta, Varfman, & Rittel, 2020).

The frequency-dependent attenuation of the gel was implemented into a finite-element routine. The gel is modeled as an ‘acoustic medium’ with a drag coefficient that controls the attenuation. Commercial FE softwares, do not support a frequency-dependent drag coefficient in time-domain simulations. Frequency-dependent attenuation is usually set by calibrating a “Prony series” of springs and dashpots, according to a measured frequency response function.

In this work, we suggest a new methodology for implementing a frequency-dependent acoustic drag in time-domain FE simulations. The incident pulse, which can be obtained experimentally or from another FE simulation, is decomposed into its frequency content. A series of single-frequency simulations is then performed, each simulation with the appropriate amplitude and drag coefficient. A closed formula is developed for the acoustic drag according to the frequency response function. The single-frequency simulations are performed with the same mesh and time increments. Finally, the nodal pressure of all single-frequency simulations is summed and the recomposed transmitted pulse is obtained.

The suggested method is validated and compared to experimental incident and transmitted signals. The impact mitigation ability of methyl cellulose for two complex 3D cases, namely an armor plate and a combat helmet, is illustrated. Although this methodology is elaborated on methyl cellulose hydrogel, it applies to any shock absorbing material for which the frequency-dependent drag can be determined.

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Materials for Extreme Conditions (Wednesday, February 26, 2025 14:30)

Oral Presentation

Ceramics and Composite Materials

Microstructure and Properties of Ultra High Temperature Ceramic Matrix Composite Produced by Infiltration of Eutectic Zr-Si into Carbon-Carbon Preform

Neta Kurz[1], Eugen Rabkin[2], Itamar Gutman[1]
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Ceramic Matrix Composites (CMC) are advanced materials designed for high-temperature environments, combining high strength and fracture toughness. One of the leading CMC materials for high-temperature aerospace structures is the C/C-SiC based on high strength carbon fibers, protected by a high temperature resistant silicon carbide (SiC) matrix. These composites can be produced using Reactive Melt Infiltration (RMI) with silicon. However, SiC matrix cannot withstand working temperatures above 1600ºC for extended periods.

The development of CMCs capable of withstanding extreme temperatures necessitates the modification of the matrix material towards Ultra-High Temperature Ceramics (UHTCs). This requires novel approaches using different alloys to infiltrate the porous C/C body, producing a high content UHTC matrix such as zirconium carbide (ZrC).

In this work we produced the UHTCMC samples by the infiltration of a eutectic binary alloy Zr-8.8at%Si. This eutectic alloy allows reduced processing temperatures, thereby decreasing the fiber-melt reactivity that could lead to a severe degradation of the carbon fibers during the reactive infiltration process. Furthermore, we studied the effect of infiltration parameters on the reaction mechanism and the development of the final microstructure. The compression tests were performed to investigate the effect of processing parameters on the mechanical properties of the resulting UHTCMC samples. The results of this research demonstrate a feasibility of lowering the infiltration temperature to produce a more cost effective UHTCMC.

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Materials Physics (Wednesday, February 26, 2025 14:30)

Invited Lecture

Semiconductors and Electronic Materials

Charge Transport in Calcium-Manganate Oxides for Thermoelectric Applications

Yaron Amouyal

Thermoelectric (TE) technology can convert waste heat into useful electrical power, thereby providing appropriate solutions for sustainable and clean energy demands. The most significant challenges today are developing inexpensive materials with improved TE conversion efficiency that sustain adequately high temperatures. Metal-oxide TE compounds are promising candidates for such applications, and it is essential to obtain fundamental understanding of their electrical and thermal conduction mechanisms. In this talk we will introduce strategies to develop TE oxides with improved properties, which are based on experimental procedures, including materials synthesis, TE transport property measurements, and high-resolution electron microscopy, and are supplemented by density functional theory (DFT) calculations.

We investigate heat and charge transport kinetics of bulk polycrystalline Y- and La-doped $CaO(CaMnO_3)_m$ Ruddlesden-Popper layered compounds, comprising m-perovskite sub-cells separated by CaO-planes, which are tuned by altering the crystal periodicities, aiming at enhancing charge transport and suppressing heat transport. Selective doping of Ca_2MnO_4 (m=1) and $Ca_3Mn_2O_7$ (m=2) at preferred lattice sites enables us manipulating the energy barriers for charge carrier transport, thereby enhancing their TE power factor. We find that Y-doped compounds of the $Ca_{1-x}R_xMnO_3$ series (m=∞) with $R = Y$ and La ($0 \leq x \leq 0.13$) are usually more conductive than their La-doped counterparts. Analysis in terms of the small polaron hopping model reveals that Y-doping reduces conduction activation energies, resulting in higher charge carrier mobility. This is associated to softening of interatomic bonds, which is more pronounced for Y-doping compared to La-doping, pointing on fundamental correlations between charge carrier dynamics and elastic properties. Remarkably high TE power factor values were recorded for the $Ca_{0.97}La_{0.03}MnO_3$ compound, i.e., 300 $\mu Wm^{-1} K^{-2}$ at 1050 K. These values are preserved for a wide temperature range, rendering this compound a good candidate for heat-to-electrical power generation at elevated temperatures.

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Materials Physics (Wednesday, February 26, 2025 14:30)

Invited Lecture

Semiconductors and Electronic Materials

Chalcogenides for Extreme Light-Matter Interactions

Tomer Lewi[1]
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In nanophotonics, small mode volumes, narrow resonance linewidths and large field enhancements, fundamentally scale with refractive index values and are key for many implementations involving light-matter interactions. Chalcogenides are excellent candidates for implementing nanophotonic and metasurface devices as they possess ultra-high permittivities and support large modulation of optical constants through various physical mechanisms. In this talk, I will present our latest results on extreme light-matter interactions in nanophotonics using ultra-high index chalcogenides. I start by discussing the optical properties of Bi2Te3 and Bi2Se3 Topological Insulators (TIs) nanostructures. Using polarized far-field and near field nanospectroscopy, we demonstrate that Bi2Se3 nanobeams exhibit mid-infrared resonant modes with 2π phase shifts across the resonance. Employing scattering-type Scanning Near-field Optical Microscopy (s-SNOM), we reveal local variations in the optical constants of these nanostructured TIs and outline the role of the imaginary component of the refractive index in the observed phase shifts. We further demonstrate that Bi2Te3 metasurfaces exhibit deep-subwavelength resonant modes utilizing their record high giant index value peaking at n~11. Finally, we present ultrafast spatiotemporal nanospectroscopy investigations on PbTe resonators and discuss how the anomalous thermo-optic effect in lead chalcogenide can be harnessed for implementing temperature invariant metasurfaces.

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Materials Physics (Wednesday, February 26, 2025 14:30)

Invited Lecture

2D materials

Designing Nickelates for High-temperature Superconductivity

Muntaser Naamneh, Yoav Mairovich

Since the discovery of superconductivity in cuprates, there has been a concerted effort to find materials with similar electronic or atomic structures for comparison. Such systems offer the opportunity to explore both the similarities and differences, shedding light on the key factors driving superconductivity. In this talk, I will present our work on synthesizing superconducting infinite-layer nickelates via a topotactic reaction and exploring their magnetic properties using transport measurements. We find that these nickelates exhibit behavior reminiscent of electron-doped cuprates, including the presence of static or quasi-static magnetic order. These findings not only highlight key similarities with cuprates but also provide new avenues for understanding the complex interplay between superconductivity and magnetism in these intriguing materials.

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Materials Physics (Wednesday, February 26, 2025 14:30)

Invited Lecture

Surfaces and Interfaces

Probing Phase Transitions and Stability within Molecular Ices by the Discharge of Weakly Bound Electrons and Ions

Roey Sagi[1,2], Micha Asscher[2]
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[2]*Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel*

Molecular ices and their internal structures are important and relevant to studies of thin films known as analogs to icy particles (grains) in the interstellar medium (ISM). Interaction of molecular films with low energy electrons and ions is a fundamental process that occurs throughout the universe. It results from the interaction of condensed matter with high-energy radiation, e.g., cosmic rays, γ-rays, X-rays, UV light, ion beams and free electrons, with implications on diverse fields, including environmental and life sciences, medicine, as well as astrochemistry. Discharge of weakly bound, positive and negative charges upon annealing of atomic and molecular ices (acting as nanocapacitors) is demonstrated as a uniquely sensitive detection method of low temperature structural changes occuring within condensed molecular films once annealed. This is monitored by employing temperature-programmed contact potential difference (TP-ΔCPD) measurements utilizing an in-vacuum noninvasive Kelvin probe. Various polar organic molecules, water among them, spontaneously form polar ices upon their condensation under ultrahigh vacuum (UHV) and cryogenic conditions. The polarization reflects the internal morphology of the film, primarily the degree of net molecular orientation. As in amorphous solid water (ASW) and other hydrogen bond forming molecular films, polarization also reflects the degree of film porosity, since a net dipole alignment tends to evolve at pore walls. The polarization increases with increasing film thickness and generally decreases at increasing growth temperatures. Structural changes in molecular ices are accompanied by macroscopic movement of molecules, thus, in cases of polar molecules changes in film polarization follow molecular rearrangement. Bombarding the ices with low-energy charges (either positive or negative) results in their population at shallow traps nearby the interface of the film with the vacuum. The charged films obey classical plate capacitor physics and may develop extremely high internal electric fields, 10^8-10^9 V m^{-1}. Such fields manipulate for example the orientation of guest molecules embedded within the host ice and may further catalyze their reactivity. Molecular movement upon annealing leads to film discharge at temperatures correlated to the growth conditions [1], in a similar manner to a phenomenon we term '*inverse volcano*' [2]. There, guest molecules migrate towards the interface with the substrate that supports the host films during their crystallization, in contrast to the direct 'volcano effect', in which coadsorbed guest molecules explosively desorb from the host films to the vacuum. The main advantage the Kelvin probe has over mass spectrometry is the capability to sense dynamic processes at temperatures significantly lower than the onset for desorption. Film charging thus enables the detection of structural changes occurring in nonpolar films, significantly enhances the depolarization signal recorded in polar ones, and provides information on the restructuring kinetics. Overall, the thermal behavior of these films provides an insight into processes that may occur at the ISM.

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Materials Physics (Wednesday, February 26, 2025 14:30)

Invited Lecture

Nanomaterials

Metasurfaces: From Science to Applications

Uriel Levy[1]
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We present our recent work related to metasurfaces. This includes new materials platforms such as silicon rich nitride demonstrating an important interplay between real and imaginary parts of the refractive index, and lithium niobate for obtaining tunability. We also demonstrate tunability based on the integration of metasurfaces with MEMS technology. Advanced imaging in 2D and 3D with metalenses is also demonstrated. Finally, we demonstrate the enhancement of light-matter interactions using hyperbolic metamaterials cavities.

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Materials Characterization (Wednesday, February 26, 2025 14:30)

Invited Lecture

Advanced Characterization Methods

Discovering Order in Meta-Stable Materials with SNEM

Yevgeny Rakita[1]
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Understanding the factors that control the evolution of meta-stable materials is of utmost importance if one wishes to control and harness their properties at various length-scales. Glasses, for example, play an important role at the forefront of technology, e.g., in IR optoelectronics, neuromorphic computation, space materials, medicine, energy conversion, and energy storage, and while they play such important role in our lives, they are often understood much less than the ordered crystals with similar composition. In fact, most of the material systems we are dealing with in our daily lives are not perfectly ordered, and the spectrum of structural order we are required to understand is much broader than what textbooks address.

A central gap that lacks understanding is the order of disordered (or quasi-ordered) materials at the *nano-scale.* Going back to glasses – glasses are multi-state kinetically-stabilized systems, and what mostly defines them is their chemical and structural *local* short-range and medium-range order, which is never homogenous once one looks close enough. Physical models often address glasses as homogenous arrangements of atoms with some statistical distribution of distances between atoms and between the chemical identity of atoms. However, at the nano-scale, one will often find that this homogeneous picture is incorrect. The origin of the gap is the lack of a tool that will be able to disentangle changes in order motifs at such high magnifications, namely – a few nanometers.

In this talk, I will present the Scanning Nano-structure Electron Microscopy (SNEM) [1] – a methodology that uses a transmission electron microscope (TEM) to gather multiple layers of information about the local chemistry, order, and electron density at the same time, providing us with a very rich set of information about local order and chemistry: the chemical contrast will come from EDS / EELS measurements, the structural contrast will come from 4D-STEM measurements, and the electron density contrast from HAADF. SNEM combines physically-meaningful relational datasets, where together with routine synchrotron-based pair-distribution-function (PDF) analysis and Machine-Learning algorithms, we follow the correlation between chemical and structural information at the nano-scale in disordered material systems. I will start with an example of Zr65Cu17.5Ni10Al7.5 bulk metallic glass (BMG), where we show that nucleation events may be predetermined by local ordering that is chemically ordered but not necessarily structurally ordered. We also show that chemical variabilities at the nano-scale may effectively control nucleation at the nano-scale, which is a critical feature to control in memory and computation devices, for example, when using phase-change memory materials (PCM). Besides BMG, we will demonstrate the usefulness of SNEM in several other use cases, including multi-component metallic and semiconducting alloys and bio-crystals.

Further reading:

1. Y. Rakita, "Mapping structural heterogeneity at the nanoscale with scanning nano-structure electron microscopy (SNEM)." Acta Materialia. 242 (2023) 118426.

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Materials Characterization (Wednesday, February 26, 2025 14:30)

Invited Lecture

Advanced Characterization Methods

Elucidating the Structure and Composition of Buried Interfaces with New Solid State NMR Methods

Michal Leskes[1]
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

Buried interfaces play a central role in the function of energy storage and conversion materials. Some examples include the catalytically active interfaces formed between different oxides or charge transfer processes across heterogenous interfaces formed in solar, fuel and battery cells. As such there is great interest in probing the chemical composition and structure of such interfaces. However, the limited quantity, inaccessibility, heterogeneity and disorder of buried interfaces limit our ability to characterize them by conventional diffraction and microscopy tools.

Solid state NMR spectroscopy is one of the best tools to determine the chemical composition of solids, yet the inherent low sensitivity of NMR prevents the detection of interfaces. In recent years, the development of Dynamic Nuclear Polarization (DNP), a process in which the high electron spin polarization is transferred to surrounding nuclear spins thereby increasing NMR sensitivity by orders of magnitude, has completely transformed the breadth of applications and systems that can be studied with solid state NMR. In this talk I will survey recent developments in the field, focusing on the development and application of DNP from endogenous polarization sources such as paramagnetic metal ions. I will describe the basic principles of the approach and demonstrate how it can be applied to selectively probe buried interfaces with high sensitivity. I will show how we can gain unique chemical and structural information on nanometer thick interfacial layers and the application of the approach to obtain unprecedented atomic-scale insight into heterogenous native and artificially formed surface layers in battery materials.

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Materials Characterization (Wednesday, February 26, 2025 14:30)

Invited Lecture

Advanced Characterization Methods

Point Spread Function Engineering in Optical Microscopy - Why and How to Ruin a Perfectly Good Microscope

Yoav Shechtman[1]
Technion, Israel Institute of Technology, Israel

The point spread function (PSF) of an imaging system is the system`s response to a point source. To encode additional information in microscopy images, we employ PSF engineering – namely, a physical modification of the standard PSF of the microscope by additional optical elements that perform wavefront shaping. I will describe how this method, combined with advances in machine learning, enables unprecedented capabilities in localization microscopy. I will also discuss recent results on additive-manufacturing of highly precise optics using printers that seemingly do not possess the necessary resolution.

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Materials Characterization (Wednesday, February 26, 2025 14:30)

Oral Presentation

2D materials

X-Ray Diffraction Analysis of Layered Compounds: from Regular Structures to Nanoparticles with Curved Turbostratic Layers

Yishay Feldman[1]
Department of Chemical Research Support, Weizmann Institute of Science, Israel

Layered materials have strong covalent bonds within the layer and weak van der Waals forces between the layers. These structural features allow the layers to be stacked turbostratocally [1], like a pile of randomly stacked cards, where the individual cards are parallel to each other at the same interlayer distance but are random in translation and rotation around the normal to the cards. X-ray patterns of such structures are characterized by the fact that some of the peaks are highly asymmetric. For example, clay often consists of minerals that have partially turbostratic layers. Although their X-ray patterns are usually difficult to analyze; these asymmetrical peaks provide additional structural information because, as will be recalled, they always correspond to specific lattice planes.

Another distinctive feature of layered compounds is the ability of the layers to bend. The best example is the formation of carbon nanotubes and fullerenes, but even a layer of a few atoms can also bend and fold. In 1930, Pauling, analyzing the structure of kaolinite, which has slightly asymmetric layers consisting of aluminum oxide octahedra on one side and silica tetrahedra on the other, suggested that structures with mismatched two halves of the layer could naturally bend [2]. His idea has been well confirmed for materials such as asbestos [3]. However, in the nineties, Tenne`s group at the Weizmann institute showed that under certain conditions, even symmetrical triatomic layers of MS2 (M=W, Mo) can fold into nanotubes or fullerene-like nanoparticles [4, 5]. Moreover, although such curved layers are clearly under stress, these multilayer nanoparticles have proven to be stable and, furthermore, show promising properties [6].

X-ray diffraction patterns of multilayer nanoparticles with layers folded into a cylindrical or nearly spherical structure are highly inhomogeneous: the peaks have inconsistent broadenings, and some peaks are highly asymmetrical. This means that, in addition to the anisotropy of coherent scattering length and microstrains in such nanoparticles, their layers are also turbostratic to varying degrees. Various results of the analysis of these structures will be presented [5, 7], as well as examples of using the features of complex X-ray patterns as an additional tool for solving specific problems [8].

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Materials Characterization (Wednesday, February 26, 2025 14:30)

Oral Presentation

Advanced Characterization Methods

Interplanar Spacing Metrology at 30 fm Uncertainty Using Scanning Transmission Electron Microscopy

Amram Azulay[1], Itai Silber[2], Yoram Dagan[2], Amit Kohn[1]
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Atomic-scale metrology in scanning transmission electron microscopy (STEM) is based on measuring distances between atomic columns in crystals and is therefore necessary for structural characterization. Furthermore, it enables to locally resolve strain in crystals [1] and calibrate the pixel size in STEM. We present a method dedicated to the evaluation of interplanar spacing (d-spacing) based on an algorithm including curve fitting of processed high-angle annular dark-field STEM (HAADF STEM) signals. By exploring simulated data of perovskite cubic $SrTiO_3$, we confirm that our proposed method is unbiased. Then, we examine experimental data to learn how electron dose, sampling resolution, and statistical sampling affect the mean and precision values of measured d-spacings. For single d-spacing measurements using a probe corrected STEM, we find that uncertainty ranges between 1 and 3 pm. By measuring numerous d-spacings in an automated and statistical approach, uncertainties of mean values as low as 30 fm, corresponding to some parts in 10^4, were achieved. Therefore, we offer to calibrate TEMs using this method as it can measure lattice parameters at uncertainties comparable to reports using x-ray diffraction measurements.

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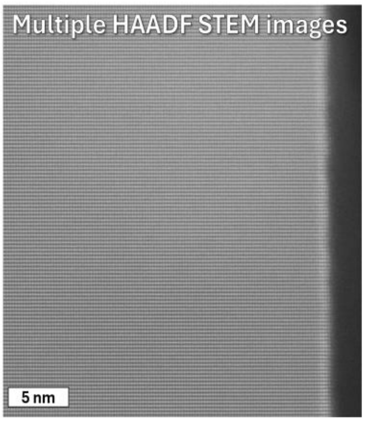

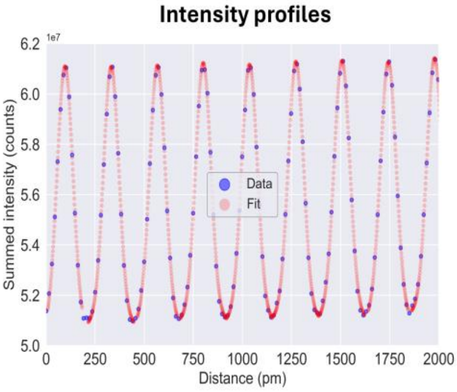

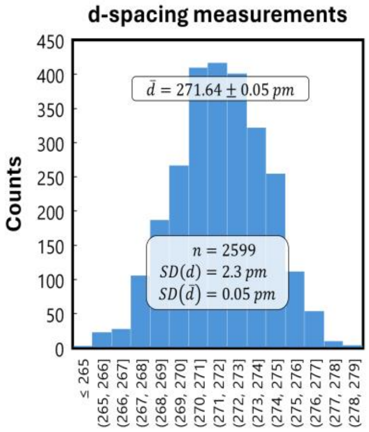

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Materials Characterization (Wednesday, February 26, 2025 14:30)

Oral Presentation

Advanced Characterization Methods

Advanced and Future Logic Device Architecture: Challenges and Solutions in Materials Metrology

Yovav Kalifon[1]
CTO group, Nova Ltd., Israel

INTRODUCTION

Since the semiconductor industry`s inception, traditional scaling has reduced the cost per transistor by shrinking gate oxide thickness and optimizing doping profiles. Modern scaling strategies [Fig. 1] include innovative materials and device architectures like strained channels, high-k metal gates (HKMG), and fin field-effect transistors (FinFETs). The International Roadmap for Devices and Systems (IRDS) indicates that scaling below 5-nm nodes will face significant challenges, highlighting the importance of materials research[1,2]. Integrating novel materials, reducing feature sizes, and shifting to 3D structures pose substantial challenges to materials characterization and contamination analysis, crucial for process development and quality assurance.

As the industry advances towards future logic devices like Gate All Around (GAA), material-related challenges will intensify[3,4]. Material selection must match electrical properties, ensure adequate isolation, and simplify processing. The demand for characterization accuracy increases with technology node advancement, necessitating the evolution of lab techniques into high-volume manufacturing (HVM) methodologies[5]. Advanced material metrology tools, currently used in labs, are essential for identifying process deviations and must transition to inline applications to enhance process control.

GATE-ALL-AROUND MATERIAL CHALLENGES

GAA architecture offers enhanced performance and cost per transistor, but it poses significant manufacturing and monitoring challenges [Fig. 2]. Uniform thickness, material composition, and Silicon:Silicon-Germanium (Si:SiGe) superlattice quality are vital for electrical performance and must be controlled throughout manufacturing. The transition to monolithic Complementary Field-Effect Transistors (CFET) further intensifies these challenges[6].

FROM LAB TO FAB INLINE SOLUTIONS

To control advanced node manufacturing, chip manufacturers rely on various metrology tools, many of which are lab-based. These include imaging methodologies like Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and the array of techniques within the Scanning Probe Microscopy (SPM) family, including Atomic Force Microscopy (AFM), and spectroscopic techniques encompassing Infrared (IR), Raman Spectroscopy, X-ray Photoelectron Spectroscopy (XPS), Rutherford Back Scattering (RBS), Secondary Ion Mass Spectrometry (SIMS), Electron Energy Loss Spectroscopy (EELS), Atom Probe Tomography (APT), and more.

Transitioning lab techniques into the fab introduces industrial requirements such as: automation, connectivity, control layers, tool matching, high uptime, and more. Furthermore, technology performance enhancement and adding data-analysis algorithms are crucial considerations in evaluating candidate metrologies for HVM, where it becomes essential to accurately capture and convert detailed raw data into actionable insights, allowing informed decision-making.

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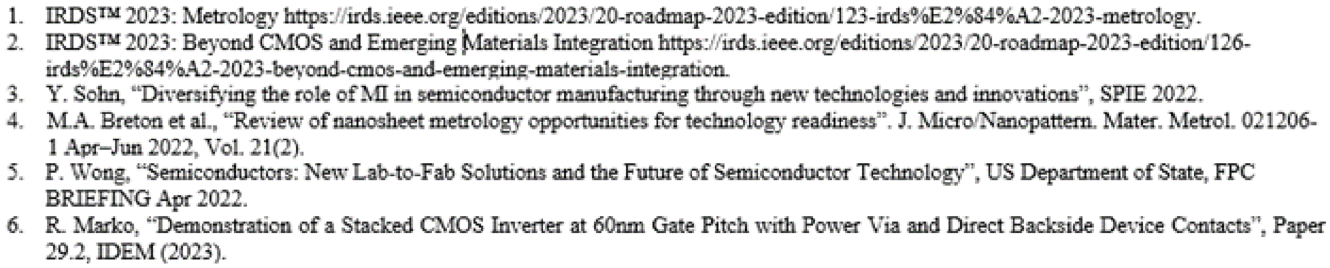

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KEYWORDS
Inline metrology, Materials metrology, Gate-All-Around, Nanosheets, Lab-to-Fab

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Corrosion & Electrochemistry (Wednesday, February 26, 2025 14:30)

Invited Lecture

Corrosion and Protection of Materials

Synthesis of Functional Coatings Using the Molten Salt Plasma Electrolytic Oxidation

Konstantin Borodianskiy[1], Yuliy Yuferov[1]
Chemical Engineering, Ariel University, Israel

Functional coatings are essential in materials science and engineering, significantly improving the performance and properties of various substrates for diverse applications. Plasma electrolytic oxidation (PEO) emerges as a leading technique among surface treatment methods. This environmentally friendly electrochemical process produces highly adhesive surfaces on non-ferrous metals such as aluminum, titanium, magnesium, and zirconium. These coatings typically offer superior wear and corrosion resistance and, in some cases, enhanced bioactivity. While PEO is traditionally conducted in aqueous electrolytes, its application in molten salts has demonstrated greater effectiveness, enabling the treatment of larger surface areas with improved purity.

In this study, functional coatings were developed on aluminum, titanium, and zirconium alloys using PEO treatment in molten salt electrolyte. A comprehensive analysis followed, including microstructural examination via electron microscopy and phase composition determination through X-ray diffraction. Additionally, the coatings` corrosion resistance, adhesion performance, and bio-response were evaluated using potentiodynamic polarization, tensile strength testing, and in vitro experiments. The results confirmed the successful synthesis of highly adherent ceramic functional coatings with significantly enhanced surface properties, paving the way for future research for broader industrial applications and exploring their potential in emerging fields such as biomedical implants.

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Corrosion & Electrochemistry (Wednesday, February 26, 2025 14:30)

Invited Lecture

Corrosion and Protection of Materials

Enhancing the Efficiency and Stability of Reversible Zinc and Iron Electrodeposition in Mildly Acidic Electrolyte Solutions

Daniel Sharon[1]
Institute of Chemistry, The Hebrew University of Jerusalem, Israel

The global shift toward renewable energy has highlighted the critical need for large-scale, safe, and environmentally sustainable energy storage systems. Rechargeable aqueous batteries, utilizing abundant and cost-effective metals like zinc and iron, offer a promising solution. However, their practical implementation is hindered by challenges such as uncontrolled metal deposition, corrosion, and interfacial instability.

This presentation explores the electrochemical and corrosion phenomena affecting zinc and iron anodes in mildly acidic aqueous environments. Through advanced in-situ and ex-situ techniques, we uncover the fundamental mechanisms driving anode degradation and demonstrate how tailored electrolyte compositions and surface engineering can significantly enhance the efficiency and stability of these critical battery components.

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Corrosion & Electrochemistry (Wednesday, February 26, 2025 14:30)

Invited Lecture

Corrosion and Protection of Materials

Corrosion Performance of Biomaterials in Physiological Environments

Galit Katarivas Levy[1]
Biomedical Engineering, Ben-Gurion University of the Negev, Israel

Biomaterials used in medical implants must exhibit superior corrosion resistance to ensure safety, longevity, and biocompatibility in physiological environments. While metallic biomaterials such as stainless steel, titanium alloys, and emerging biodegradable metals (e.g., magnesium and zinc alloys) have been widely studied, emerging composite implants combining metals and polymers present new opportunities to tailor corrosion behavior to specific clinical needs. Yet, these hybrid systems also introduce complexity, as interactions among constituents can significantly influence their surface reactivity and degradation mechanisms. In this talk, I will present our novel topology design strategy for metal-metal and metal-polymer composites by infiltrating an Al/PEI melting into additive manufacturing (AM) fabricated Ti lattice structures (Cubic and BCCZ). A primary focus is placed on the formation and role of the interface zone between the lattice structure and the matrix, which critically influences the composite's final properties. Our findings reveal that both AM-Ti lattices infiltrated with Al or PEI matrix form a continuous bond via the development of a robust interface zone, resulting in solid composite systems. Transitioning the lattice structure design from Cubic to BCCZ increases the surface area fraction, significantly reducing casting defects and porosity in the Al matrix. Both Ti-Al composite systems demonstrate superior mechanical performance, surpassing the rule-of-mixtures predictions and the individual materials, likely due to the continuous and well-bonded interface zone. Furthermore, corrosion resistance studies indicate that the composition and morphology of the interface zone significantly affect the composites` corrosion behavior, providing insights into optimizing the interface for enhanced durability in corrosive environments. This study underscores the critical role of lattice architecture in tailoring corrosion behavior, mechanical properties, and interface zone characteristics of Ti-Al and Ti-PEI composite systems. Our results lay the foundation for further exploration of composites with exceptional corrosion, mechanical and physical properties, opening new avenues for advanced material design.

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Corrosion & Electrochemistry (Wednesday, February 26, 2025 14:30)

Materials for Energy Storage and Conversion

One-step Synthesis of Single Atom Catalysts (SACs) on Nanocarbons Using Thermal Delamination: A New Paradigm For High Performance, Binder-Free, Electrodes for Water Splitting

Daniel Nessim

Single atom catalysts (SACs) can enable a sustainable energy scenario, as they are cheaper (atom economy), more selective, durable, and efficient than the precious metals (PGM) currently used in electrochemical energy conversion technologies. To bring SACs to the market, the major challenges are the achievement of a high site density of SACs and the lack of an economical and scalable synthesis.

We produced SACs@nanocarbon using an innovative one-step chemical vapor deposition (CVD) synthesis based on temperature-controlled delamination of multilayer mixed metal films from a substrate with concurrent reactions with precursor gases and dopants to obtain a self-standing (no binder), high surface area doped carbon electrode bearing nickel SACs (not-PGM). These electrodes with nickel SACs performed well for water splitting, both in performance (low OER overpotential of 290mV @ 10mAcm-2; low HER overpotential of 230mv @ 10mAcm-2) and durability (over 20,000 cycles).

In this presentation, we will discuss the main phenomena are at play, including nucleation, growth, and doping of the nanocarbons; dewetting of thin metal films on the nanocarbons to form the SACs; thermal detachment of selected weak-adhesion thin films; and multiple gas-solid phase reactions in the CVD reactor. Given the inherent scalability of CVD, this technique could be used industrially with large reactors to produce large area electrodes and become a new benchmark for water splitting and other electrocatalytic reactions.

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Corrosion & Electrochemistry (Wednesday, February 26, 2025 14:30)

Oral Presentation

Corrosion and Protection of Materials

Sulfur Corrosion in Copper within Insulating Liquids

Grisaru Marius[1]
Consulting Marius Grisaru, Israel

Sulfur corrosion in insulating liquids, particularly in oil-immersed power transformers, poses a significant threat to the reliability and longevity of electrical equipment. This study investigates the mechanisms of sulfur corrosion on copper conductors within insulating liquids, focusing on the formation of copper sulfide deposits. The research highlights the role of corrosive sulfur compounds, such as dibenzyl disulfide (DBDS), in accelerating the corrosion process (Griffin & Lewand, 2011). The study elucidates the local enrichment of acids and copper ions at copper-insulating paper contacts through accelerated thermal aging experiments and advanced analytical techniques, including SEM/EDX, ICP-AES, and precipitation methods. The findings reveal that copper sulfide formation significantly deteriorates the dielectric properties of oil-paper insulation, reducing its electrical breakdown strength (Li et al., 2011).

Sulfur compounds in transformer oils can react with copper conductors to form copper sulfide, leading to the deterioration of electrical insulation and eventually causing transformer failure. This corrosion process is influenced by various factors, including temperature, moisture, and the presence of corrosive sulfur compounds. The study conducted accelerated thermal aging tests on copper-insulating paper samples immersed in mineral oil containing DBDS. The samples were aged at different temperatures to simulate the operating conditions of power transformers. The results showed a significant increase in copper sulfide deposition on the copper surfaces with increasing temperature and aging time (ASTM International, 2015).

Advanced analytical techniques were employed to characterize the corrosion products and understand the mechanisms involved. Scanning Electron Microscopy (SEM) coupled with Energy Dispersive X-ray Spectroscopy (EDX) revealed the morphology and elemental composition of the corrosion products. Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES) was used to quantify the amount of sulfur in the oil and on the copper surfaces. Precipitation methods were employed to isolate and identify the sulfur compounds responsible for the corrosion.

The study also explored potential mitigation strategies to prevent sulfur corrosion in insulating liquids. The use of metal passivators, such as benzotriazole (BTA) and Irgamet® 39, was investigated. These additives significantly reduced the formation of copper sulfide on the copper surfaces. The effectiveness of the passivators was evaluated through long-term aging tests and analytical techniques (Krauter et al., 2015). The findings suggest that incorporating metal passivators into transformer oils can enhance the durability and reliability of oil-immersed power transformers.

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Corrosion & Electrochemistry (Wednesday, February 26, 2025 14:30)

Oral Presentation

Materials for Energy Storage and Conversion

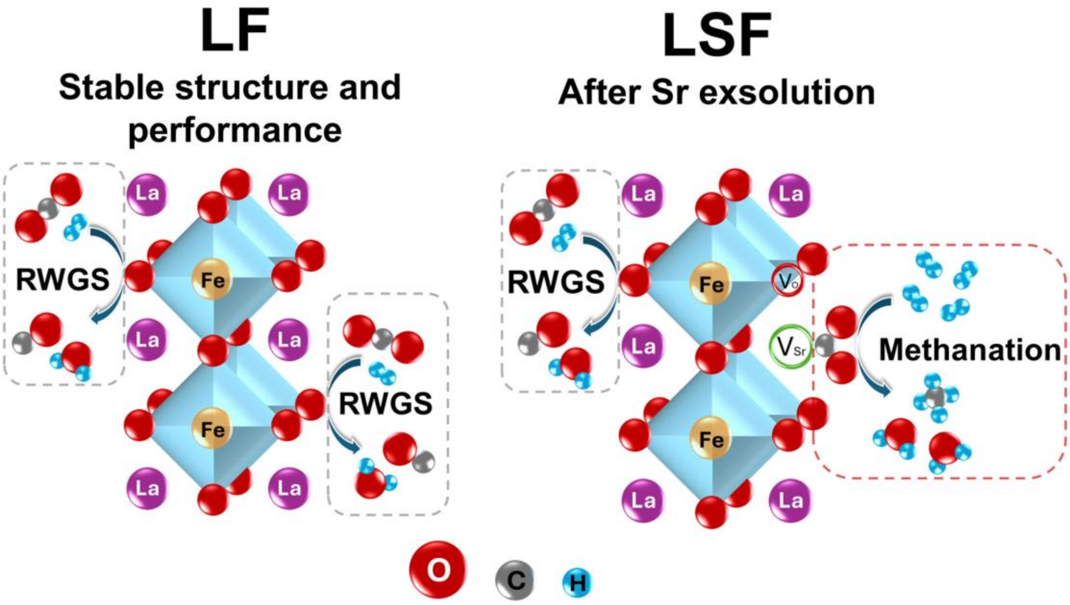
Performance of $LaFeO_3$ and $La_{0.8}Sr_{0.2}FeO_3$ perovskites in Reverse Water-Gas Shift

Gal Sror[1], Leonid Vradman[2], Miron Landau[1], Moti Herskowitz[1]
[1]*Chemical Engineering, Blechner Center for Industrial Catalysis and Process Development, Ben-Gurion University of the Negev, Be'er-Sheva, Israel*
[2]*Department of Chemistry, Nuclear Research Centre-Negev, Be'er-Sheva, Israel*

The steady increase in CO_2 atmospheric concentration is one of the main drivers of global warming. Utilizing CO_2 waste as feedstock for renewable energy sources and value-added products is a crucial step to advance decarbonization. A promising option to convert CO_2 is through the reverse water-gas shift reaction (RWGS) - $CO_{2(g)}+H_{2(g)}\rightleftharpoons CO_{(g)}+H_2O_{(g)}$. The product of this process constitutes a raw material (Syngas – H_2/CO mixture) for eFuels production through Fisher-Tropsch synthesis (FTS).

The RWGS is an endothermic oxygen-transfer reaction, performed at elevated temperatures (500°C-800°C). Perovskite-oxides can function as RWGS catalysts due to their thermal stability, oxygen storage capacity and redox ability. In general, H_2 reacts with oxygen from the perovskite lattice, creating oxygen vacancy that facilitates CO_2 conversion to CO [1]. However, perovskites can suffer structural and compositional changes during reaction [2]. These changes can affect the oxygen transfer process (i.e. catalytic activity) and enable new reaction paths. In the case of RWGS, methanation is a competing reaction, thermodynamically favored at low temperatures (500°C) - $CO_{2(g)}+4H_{2(g)}\rightleftharpoons CH_{4(g)}+2H_2O_{(g)}$. This reaction consumes valuable H_2 that harms the process yield and hampers low-temp RWGS operation which is desired to improve energy efficiency. Hence, the structural stability of the perovskite at reaction conditions is a key property to maintain catalytic activity and avoid the possibility of methanation.

Here, we synthesized and tested $La_{0.8}Sr_{0.2}FeO_3$ (LSF) and $LaFeO_3$ (LF) perovskites as steady-state RWGS catalysts (100h). The effects of operating conditions, phase transformations, and nature of active sites on the catalytic performance are studied. LSF underwent Sr exsolution [3] leading to evolution of cationic vacancies that strongly adsorb CO_2. At sufficient H_2 concentration ($H_2/CO_2 4$), the adsorbed CO_2 is converted to CH_4, thus reducing the CO selectivity and consuming additional H_2. LF yielded stable CO_2 conversion with no detected CH_4 at all tested conditions (500°C-800°C, $H_2/CO_2=0.3\text{-}8$). Syngas with relevant ratios for eFuels synthesis (0.72/CO2) was obtained with LF at 700°C and $0.32/CO_2 1$.



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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Additive Manufacturing

Additive Manufacturing of Hypereutectic Al-Si Alloys

Dr. Tatiana Vompe[1]
The Israel Institute of Materials Manufacturing Technologies, Technion Research and Development Foundation, Israel

Hypereutectic Al-Si alloys are of great interest for applications in the automotive, aerospace, and electronics industries because of their low weight and thermal expansion, superior mechanical and tribological properties compared to low-Si Al-Si alloys. Additive manufacturing techniques for these alloys offer not only the opportunity in geometrical design but also in composition formation. Microstructural evolution during solidification is a critical factor in determining the final physical and mechanical properties of Al-Si alloys.

The aim of the work was to receive highly dense and cracks-free samples, and to study the microstructure, physical and mechanical properties of hypereutectic Al-Si alloys produced by Selective Laser Melting from pre-alloyed powders.

The specimens were manufactured using EOS M290 LPBF system equipped with 400 W Nd-YAG laser in Ar atmosphere. The influence of the printing process parameters (laser power 350 – 370 W, scanning speed 800 – 2100 mm/s, hatch spacing 0.09 – 0.13 mm) on properties of AlSi40 alloys were investigated using the design of the experiment approach and optimal parameters were found.

Samples from hypereutectic Al-Si alloy with high dense 99 %, tensile strength 423 MPa, yield strength 280, Young’s modulus 93 GPa were successfully produced by SLM. This study contributes to optimizing additive manufacturing processes for advanced aluminum-based materials.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Additive Manufacturing

Inconel 939 Superalloy - The Effect of Portevin-Le Chatelier on Additively Manufactured and Casted Alloy

Moshe Nahmany[1,2], Danny Moreno[1], Yohanan Nahmana[1], Matan Zakai[1], Ariel Yehuda Cohen[1], Moshe Shapira[1], Ronny Shneck[3]
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Inconel 939 is a γ’ precipitate-hardened Ni-based superalloy, widely used in recent decades for fabricating high-temperature-resistant cast components, such as fuel nozzles, turbine castings, and gas turbine vanes and blades. The relatively new additive manufacturing (AM) technology for Ni-based superalloys presents challenges but also improves the ability to produce complex parts while enhancing R&D outcomes and reducing both costs and Time to Market (TTM).

PLC bands and Lüders bands can be explained by the difference between Static Strain Aging (SSA) and Dynamic Strain Aging (DSA). The DSA effect is characterized by repeated load drops in the stress-strain curve.

In the current work, a distinctive trend of cyclic flow is detected during the Portevin-Le Chatelier (PLC) effect in additively manufactured (AMed) and cast IN939 under constant strain rate tensile tests. The PLC segment of the tensile test reveals specific features and behaviors in the typical cycle, stress-strain local strain, and total rise and drop stresses. Characterization of γ′ precipitates, using HR-SEM, demonstrated different morphologies, which were proposed to be correlated with the PLC-region behavior.

This investigation describes and analyzes the “rise and fall” cyclic behavior of the stress-strain curve, attributed to the PLC phenomenon. This phenomenon significantly impacts the interpretation of mechanical behavior and, consequently, the application of materials, particularly in high-stress or high-strain scenarios, as required for the service life of Ni-based superalloys.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Additive Manufacturing

Fabrication of Full Dense SiC-Si Composites using Directed Energy Deposition

Vladimir Popov[1], Shir Andreev Batat[1], Noam Eliaz[1]
Materials Science and Engineering, Tel Aviv University, Israel

Conventional additive manufacturing techniques for producing SiC-Si composites generally involve the binder jetting of SiC, followed by liquid silicon infiltration. This multi-step process is both time and energy-intensive, often leading to prolonged lead times and increased manufacturing costs. This research proposes a more efficient approach: direct additive manufacturing of SiC-Si composites using Directed Energy Deposition (DED) with blended SiC and pure Si powders. For the DED trials, various substrates were used: made of pure titanium, stainless steel, tungsten, and aluminum. The proposed method significantly streamlines the production process, reducing lead time and enhancing material density. The goals of this research work were to investigate the interface between DED`ed composite and metal substrate; density measurements of the printed composites; and study of how the chemical composition of the samples is affected by the selected metal substrate. The DEDed composite samples were subjected using optical and scanning electron microscopy (SEM) to evaluate the microstructure. Phase composition was determined through X-ray diffraction (XRD), and mechanical properties were assessed using hardness tests. Adhesion tests were applied for the interface measurements. Experimental findings confirm that the DED process yields in-situ manufacturing of high-dense SiC-Si composites, promising substantial improvements in manufacturing efficiency and material performance.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Ceramics and Composite Materials

“Writing” Crystal Phases in Amorphous Calcium Carbonate via Bio-Inspired Laser-Induced Patterned Transformations

Hadar Shaked, Iryna Polishchuk, Niv Ben-Arie, Daniela Dobrynin, Javier Gainza,
Alexander Katsman, Boaz Pokroy

The precise control in biomineralization over various phases has inspired us to study a novel laser-induced crystallization route. To this end, we employed laser-induced crystallization in a magnesium-stabilized amorphous calcium carbonate (ACC) environment to generate four distinct phases: calcite, stable dehydrated ACC, monohydrocalcite, and hydromagnesite in a patterned manner. We characterized the energy range, determined by laser power and speed, required for each phase formation and demonstrated the reproducibility of this process. Our approach enables precise patterning in the ACC environment, where laser-affected areas undergo phase changes while the rest remains unaltered. Furthermore, we investigated the controlled production of monohydrocalcite and hydromagnesite under varying thermal conditions, examining the influence of substrate composition, ACC stability, and repeated exposure on phase formation. We propose an explanation for the observed phases and demonstrate impressive control over polymorph location, enabling calcite patterning within an ACC matrix. This research explores laser patterning within a bio-inspired framework and advances our understanding of out-of-equilibrium phase formation processes inspired by biomineralization.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Additive Manufacturing

3D-printing of Functional, Mineral-Infused Substrates for Coral Settlement Enhancement

Almog Sulam, Iryna Polishchuk, Boaz Pokroy

Corals are marine organisms that form their exoskeletons through the process of biomineralization. Their exoskeletons are mainly composed of calcium carbonate in its aragonitic phase and trace amounts of elements, such as Mg and Sr. Before biomineralizing, corals undergo a settlement stage, where they attach to a substrate for further growth. This process is influenced by biological cues, mineral composition, and surface roughness. Corals are vital to ocean health, as they provide habitat and food security to many other marine species. However, anthropogenic greenhouse gas emissions are causing corals to face significant stress, threatening their survival. As previous studies have shown that their settlement can be manipulated, this research focuses on developing highly customizable settlement substrates through 3D-printing. Such 3D-printed substrates contain varying mineral concentrations and include variations in surface roughness, features, and geometries. This research employs several 3D-printing methods, such as selective laser sintering (SLS) and fused deposition modeling (FDM). Using SLS, we successfully synthesized mineral-infused substrates with up to 50wt% of calcitic calcium carbonate, without incorporating any additives. The morphology, microstructure, and surface roughness of such substrates have been studied. In FDM, we have been able to fabricate mineral-infused filaments, containing up to 50wt% of calcitic calcium carbonate, also without additives. These filaments are currently undergoing characterization and will be implemented in FDM 3D-printing in the future. This research demonstrates the potential of 3D-printed substrates to advance coral conservation efforts by optimizing settlement conditions through precise control of substrate properties.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Additive Manufacturing

Degradation and Biocompatibility of 3D-Printed PLA Reinforced with WS_2 Nanotubes for Bone Scaffold Applications

Ofek Golan[1], Noa Granada[1], Lin Lemesh[1], Salome Azoulay-Ginsburg[2], Roey J. Amir[2], Francesca Netti[3], Lihi Adler-Abramovich[3], Noa Lachman[1]
[1]*Department of Materials Science and Engineering, Tel Aviv University, Israel*
[2]*Department of Organic Chemistry, Tel Aviv University, Israel*
[3]*Department of Oral Biology, Tel Aviv University, Israel*

Recent advancements in bone tissue engineering have increased interest in 3D-printed scaffolds for bone regeneration, overcoming the limitations of traditional bone grafts by allowing for patient-specific implants and customizable patterns that better support bone regeneration. A suitable scaffold should exhibit biocompatibility, degrade in alignment with bone growth rate, and possess mechanical properties at least equal to the original bone. Among the materials examined worldwide for bone scaffolds, Polylactic acid (PLA) stands out as a promising candidate. PLA is a biocompatible and biodegradable polyester with significant medical application potential. Reinforcing PLA with inorganic nanotubes of tungsten disulfide (INT-WS_2) enhances its suitability as a bone scaffold due to the chemical stability, biocompatibility, non-toxicity, and favorable mechanical and rheological properties of INT-WS_2.

This study investigates the biocompatibility of 3D-printed samples made from PLA reinforced with 0.5%wt INT-WS_2, as well as their morphological and mechanical properties under hydrolysis degradation. The samples are proposed as a concept for a 3D-printed load-bearing bone scaffold, with the femur bone (hip) chosen as an extreme example.

Controlled hydrolysis degradation of the PLA/INT-WS_2 samples was conducted over 12 weeks to simulate human-body conditions. Degradation was evaluated by weight loss, gel permeation chromatography (GPC), and differential scanning calorimetry (DSC), which was used to monitor both degradation and thermal properties. Mechanical properties were assessed via tensile strength and micro-hardness tests. Sample morphology was analyzed using scanning electron microscopy (SEM), and biocompatibility was examined by viability assays on both the PLA/INT-WS_2 and neat PLA (used as control) filaments and printed samples. Results demonstrated that the PLA/INT-WS_2 nanocomposite exhibited non-toxic behavior, promoting cell proliferation and viability. Additionally, the material underwent bulk degradation while maintaining mass and surface hardness properties. Although a slight decrease in tensile strength was observed, the ultimate tensile strength remained significantly higher than the maximum stress experienced during normal walking on the human femur bone.

Despite the need for a longer experiment to fully assess the degradation rate, this study indicates that PLA reinforced with 0.5wt% INT-WS_2 is a suitable candidate for a tailored 3D-printed bone scaffold for individual patients.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Additive Manufacturing

HfB2 Coating Fabrication Using Laser Powered Directed Energy Deposition

Shir Andreev Batat[1], Vladimir Popov[1], Zlatomir Apostolov[2], Noam Eliaz[1]
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[2]*Materials and Manufacturing Directorate, Air Force Research Laboratory, Ohio, USA*

Directed Energy Deposition (DED) is an additive manufacturing process in which concentrated high thermal energy source is used for locally melting selected powder or wire materials. The energy source can be either electron beam, plasma arc or laser. Laser Powered Directed Energy Deposition (LP-DED) combined with raw material in the form of powder enables the use of small amount of feedstock materials and thus the fabrication of coating layers. In our study, HfB2, which is an Ultra High Temperature Ceramic (UHTC) was DED'ed on different substrate materials: 316L stainless steel, pure tungsten, Ti and carbon-carbon composite. Deposition on each substrate material was performed using different and optimized process parameters, such as laser power, laser scan speed and powder mass flow rate. All coating samples were characterized using light microscopy, scanning electron microscopy, adhesion testing, microhardness testing, and X-ray photoelectron spectroscopy. For all samples, melting rather than sintering, was observed in the HfB2 coating layer. Visually, good adhesion could be seen for the tungsten and stainless steel substrates, while Ti and composite substrates example poor adhesion and lack of sufficient coating layer growth. For tungsten and stainless steel substrates, coatings were nearly void-free and clear interface could be observed, with only minor elemental mixing at an intermediate layer between the substrate and the coating layer.

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Additive Manufacturing II (Wednesday, February 26, 2025 14:30)

Oral Presentation

Bio- and Soft Materials

Sustainable 3D-Printable Ionic Eutectogels for Multifunctional Sensing

Yuchen Wang[1], Sergey Nechausov[1], Yi Jiang[1], Aslan Miriyev[1]
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Integrating sustainability and multifunctionality in soft materials is paving the way for a new type of physically intelligent soft robots for future human-robot-nature ecosystems. Creating robots for such a symbiotic environment involves co-advancing new sustainable stimuli-responsive material systems with their design and fabrication methods. The key challenge on the path to these materials is understanding the interplay between their mechanical, rheological, and electrical properties to shape the interdependent design-fabrication-functionality relations. Here, we show the gelatin/ethaline (GelEth) ionic eutectogel with high ionic conductivity, its direct ink writing (DIW) 3D-printing method and machine, and its implementation as a wearable joint motion sensor and as a part of a multifunctional pressure and location sensing mechanism. The GelEth composition, in soft robotics and making contributions to medical diagnostics and rehabilitation. combining gelatin matrix with water and the ethaline deep eutectic solvent, which consists of choline chloride and ethylene glycol, was chosen out of a variety of matrix-DES combinations due to its high ionic conductivity measured at 4.2 mS/cm. We showed that adding water decreased the material gel time and slightly increased its modulus and tensile stress at break while reducing the tensile strain. Additionally, the rheological study showed that decreasing the temperature to 5°C significantly decreased the gel time and allowed immediate solidification of the extruded GelEth, enabling the formation of stable 3D structures during DIW 3D-printing. To ensure proper extrusion of GelEth during 3D-printing, we performed thermal simulations and developed a modular print head with heated extruders. Moreover, to allow material deposition at the required temperature, we developed a coolable printing stage with precise temperature control. Furthermore, we demonstrated DIW 3D-printing of complex-shaped GelEth structures, including a hollow cylinder, a square block with vertical hollow channels measuring 0.5 x 0.5 mm in cross-section, and a porous mesh bilayer with vertical hollow channels. Additionally, we demonstrated the capability of the 3D-printed GelEth to serve as an ionic conductor under AC and DC conditions. Furthermore, we applied a 3D-printed GelEth mesh to create low-cost, quickly fabricated joint motion sensors that successfully tracked elbow and cervicothoracic movements on the human body. We also demonstrated GelEth as a part of a novel sensing pressure and location sensor mechanism. We suggest that GelEth can serve as a foundation for a broad range of sustainable robotic applications, including wearables, haptics, and medical devices. We believe that using GelEth will pave the way to a new type of human- and nature-friendly soft robotics and directly contribute to the circular robotics economy.

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Archaeometallurgy and Underwater Technologies for Cultural Heritage in the Eastern Mediterranean: Data Capture, Curation, Analyses and Dissemination (Wednesday, February 26, 2025 17:00)

Invited Lecture

Materials in Archeology

Archaeometallurgy and Underwater Technologies for Cultural Heritage in the Eastern Mediterranean: Data Capture, Curation, Analyses and Dissemination

Thomas Levy[1]
Center for Cyber-Archaeology and Sustainability, University of California, San Diego, United States

Archaeometallurgy, the study of metals and metal related artifacts from the past, provides a window on the evolution of societies. Like other technologies, in the eastern Mediterranean metals have impacted social evolution from its inception in the Chalcolithic period (ca. 4500 – 3600 BCE), to its widespread use in the Bronze Age (ca. 3600 – 1200 BCE) to the first industrial revolution in the following Iron Age (ca. 1200 – 586 BCE) and beyond. To measure the tempo of technological change during the Holocene, archaeologists employ radiometric dating tools such as radiocarbon, paleomagnetic and OSL (Optical Stimulated Luminance) methods. To understand the social context of archaeometallurgical and other cultural material, archaeologists increasingly use the tools of the current Information Technology revolution to accurately record and map the precise location of every artifact they encounter in the archaeological record. This paper presents some of the rapidly evolving digital tools used to capture, curate, analyze and disseminate cultural heritage data used to understand the role of metallurgy in coping with two major ancient civilizational collapse periods in the eastern Mediterranean: the end of the Early Bronze Age (ca. 2300 – 2000 BCE) and end of the Late Bronze Age (ca 1200 BCE). The data comes from the author's collaborative excavations and surveys in Jordan, Israel and Greece with UC San Diego (USA), the Department of Antiquities of Jordan, the University of Haifa (Israel), and the University of Patras (Greece).

Poster Presentation Abstracts

Tuesday, February 25, 2025

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Angular Emission Properties of Transition Metal Dichalcogenides under Uniaxial Strain

Lee Grimberg, Moshe Harats

ransition Metal Dichalcogenides (TMDs) are a special group of materials that are a few atoms thick, making them excellent candidates for new technologies like flexible electronics, light sensors, and quantum devices. Their unique optical and electronic properties can be changed by applying strain, offering a powerful way to fine-tune their behavior without using chemicals. Understanding how strain changes these properties is essential for creating better devices that are efficient, flexible, and responsive.

This research focuses on how uniaxial strain affects the light emission of different optical excitations in TMDs such as excitons and trions. A custom 3-point bending system is used to apply controlled uniaxial strain to TMD monolayers, and the changes in their angular and spectral photoluminescence (PL) is studied. In this work we present an experimental setup that is capable of resolving the spectral-angular emission pattern of strained TMDs. The schematic of the setup is shown in Figure 1. The setup is based on k-space imaging [1] of the PL from strained TMDs.

The samples are fabricated with PVA on PET to ensure efficient strain transfer from the 3-point bending device to the monolayers. The PVA is essential to avoid slippage of the monolayers [2].

Our results show that increasing strain causes a shift in the exciton and trion emission lines to lower energies (redshift), which indicates that the energy gap in the material decreases, as reported previously [3] (see Figure 2). In addition, the strain-related angular emission is used to explore the optical dipole orientation that may be altered while strain is applied.

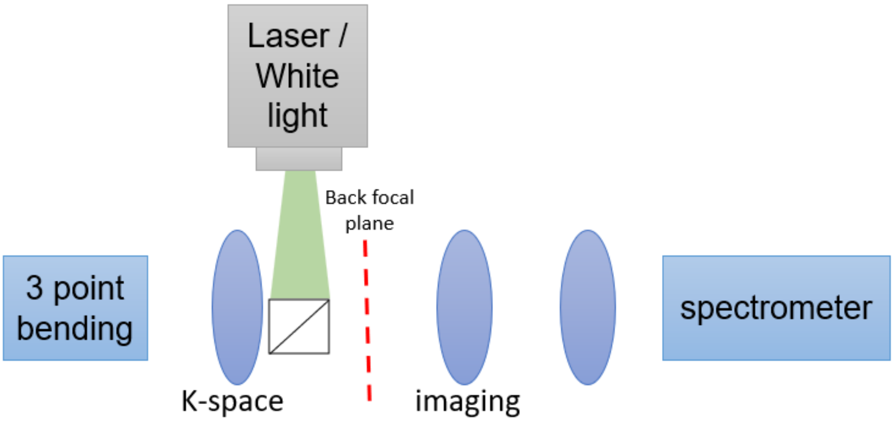

Figure 1: Schematic drawing of the spectrally resolved k-space setup

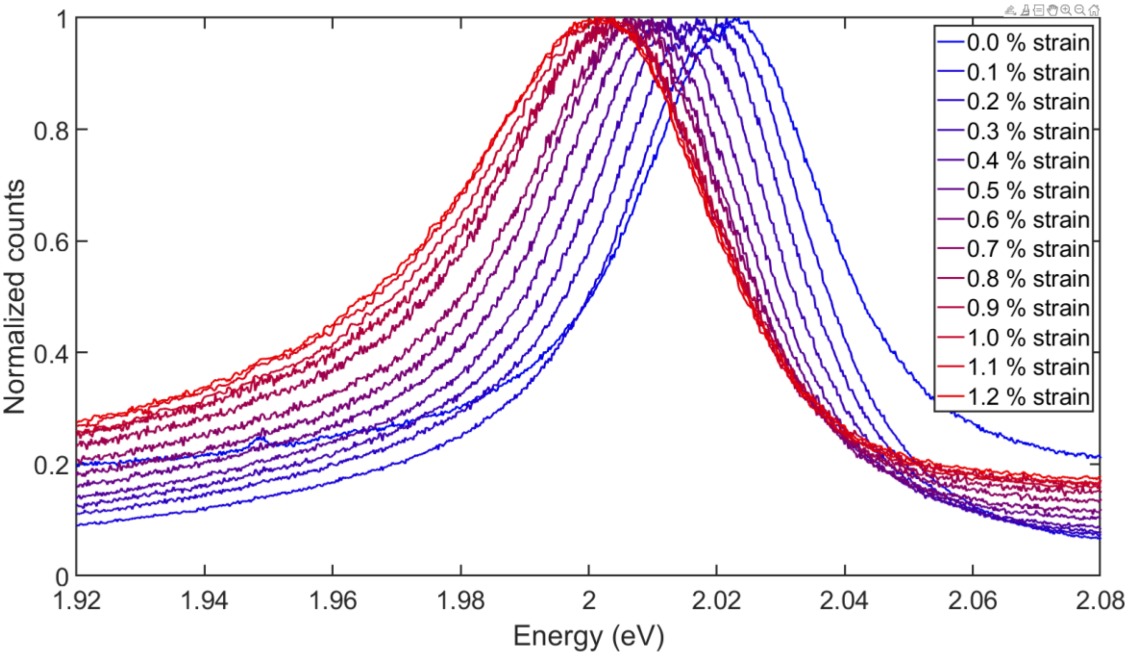

Figure 2: Normalized intensity as a function of emission energy for different uniaxial strain amplitude.

[1] M. G. Harats et al., Nano Lett 14, 5766 (2014).

[2] X. He et al., Appl Phys Lett 109, 173105 (2016).

[3] H. J. Conley et al., Nano Lett 13, 3626 (2013).

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

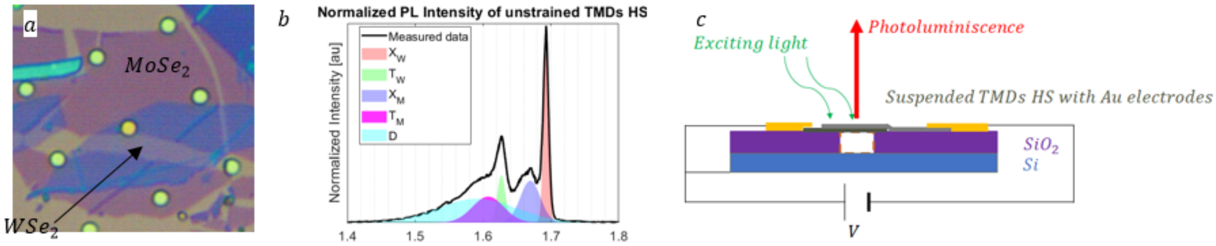
Interlayer Excitons in Non-uniformly Strained 2-Dimensional Heterostructures

Svyatoslav Kostyukovets, Moshe G. Harats

The search for efficient and flexible solar cells is an important research area with highly sought applications. Two-dimensional transition-metal dichalcogenides (2D TMDs) are natural candidates for such an approach, due to their flexibility and unique electronic properties, making them ideal for flexible photovoltaic applications1.

A single TMD monolayer is a three atoms thick layer with weak van der Waals interactions between adjacent layers. The weak interlayer coupling makes it possible to create heterostructures by stacking different TMDs layers on top of each other, leading to a plethora of novel materials with tunable electronic and optical properties2–5.

One intriguing property of TMD heterostructures is the emergence of interlayer excitons, bound electron-hole pairs where the hole and electron reside in different layers. Following the inherent charge separation of the interlayer excitons, they have a relatively long lifetime, which allows them to be transport efficiently using non-uniform strain6. In this work, we present the details of the fabrication and methodologies applied to achieve our goal - to increase the efficiency of a proof-of-concept solar cell based on heterostructures of TMDs. The non-uniform strain creates a spatial potential that transport the interlayer excitons into a small area, allowing efficient extraction of the charge carriers.



a) Suspended $MoSe_2/WSe_2$ Heterostructure (HS) on $\phi = 3\ \mu m$ hole. b) Normalized Photoluminescence of unstrained TMDs HS irradiated by 532 nm CW laser in Temperature of 5K with five visible emission lines: WSe_2 exciton (X_W) and trion (T_W), $MoSe_2$ neutral exciton (X_M) and trion (T_M), and defect-bound excitons (D). c) Schematic description of the experimental setup.

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2. Yu, H. et al. Science Advance Vol 3, Issue 11 (2017).
3. Seyler, K. L. et al. Nature 567, 66–70 (2019).
4. Rivera, P. et al. Nature Nanotechnology vol. 13 1004–1015 (2018).
5. Baek, H. et al. Science Advance vol. 6 (2020).
6. Kovalchuk, S. et al. Israel Journal of Chemistry vol. 62 (2022).

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Solubility of MoS_2 and Graphite in Molten Salt: Flowers, Faceted Crystals or Exfoliation?

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2D materials are of interest in various applications such as energy conversion, storage, and sensing. These materials are prepared by bottom-up or top-down methods that are difficult to control and suffer from low yield. Synthesis in molten salt is suggested as an alternative in which the balance between exfoliation and solubility is explored. It is demonstrated that when a pellet of 2D material is insoluble in molten salt (Graphite in any salt), it is exfoliated. For low solubility (MoS_2 in NaCl/KCl), the 2D material nucleated and grew into a small flower-like structure composed of thin MoS_2 sheets through Ostwald ripening. For high solubility in the molten salt (MoS_2 in CsCl), it formed larger flowers. Herein, the molten salt treatment of high and low surface area MoS2 (micron-size particles and a single large pellet, respectively) is compared. The particles yielded faceted MoS_2 crystals through dissolution–nucleation–recrystallization process and the pellet - flowers. This study promotes methods for synthesizing 2D materials with controllable size and shape by simple molten salt treatment that opens an avenue to the development of soluble (MoS_2) and non-soluble (Graphite) materials with different morphologies in a simple and affordable way.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Characterization of Piezoelectric Properties of 2D Perovskite Layes

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[2]*Chemistry Department, The Hebrew University, Jerusalem, Israel*
[3]*Institute of Chemistry, Casali Center for Applied Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University, Jerusalem, Israel*
[4]*Racah Institute of Physics, The Hebrew University, Jerusalem, Israel*
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A major challenge in developing perovskite-based pressure sensors is their relatively low piezoelectric coefficient. In this study, we propose the use of quasi-two-dimensional (quasi-2D) perovskite films intercalated with various spacer molecules as a promising approach to enhance the piezoelectric response. By carefully selecting these spacer molecules, it is possible to increase the material`s piezoelectric properties and improve their pressure sensing applications. We characterize the piezoelectric performance of these films using Piezoelectric Force Microscopy (PFM) and current-pressure (I-P) measurements, focusing on their sensitivity, fast response times, and overall sensor performance. Our results demonstrate that, with further optimization, quasi-2D perovskite films could offer significant advantages as a high-performance, cost-effective, and durable material for pressure sensing applications.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Enhancing Activated Carbon Adsorption for Advanced Wastewater Treatment and Effective Organic Pollutants Removal

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[2]*Technische Univesitaet Berlin – TUB, Germany*

Modern societies extensively use various organic chemicals, many of which are discharged into wastewater after use. Treated wastewater is a valuable resource, particularly for crop irrigation, but its widespread application poses risks of environmental contamination due to the accumulation of organic micropollutants (OMPs). These pollutants, often resist conventional wastewater treatment methods and present a significant challenge to water quality.

Adsorption is one of the most effective methods for OMP removal during advanced water treatment, with activated carbon being the most popular adsorbent, due to its high porosity and large surface area. While commercial activated carbon is mostly produced from coal, there is a growing interest in using organic waste biochar as raw material. Biochar is produced through pyrolysis of organic waste, transforming it into a carbon-rich material. Subsequent physical or chemical activation enhances its surface area (exceeding 1,000 m²/g) and pore structure, optimizing its adsorption properties. The performance of activated carbon is influenced by factors such as particle size, porosity, and surface functional groups, which are a function of the source material and activation process.

This research focuses on developing sustainable and efficient activated carbon adsorbents from organic waste and wastewater sludge for advanced wastewater treatment. In the initial phase, biochar from different waste sources was produced and characterized (e.g. cotton, Marrula, olives), using SEM, BET analysis for surface area determination, FTIR and XPS for chemical composition, and Zetasizer for particle size and surface potential. Subsequently, sorption tests were carried out to determine the effectiveness of the new sorbents in treating various OMPs.

Adsorption studies of three organic pollutants (carbamazepine, paracetamol, and bisphenol A) by Marrula and cotton biochar were analyzed through high-performance liquid chromatography (HPLC). Preliminary results indicated higher adsorption by powder biochar (compared to granular), with varying affinity and selectivity for different pollutants. This can be related to the biochar properties and the individual characteristics of the OMPs (e.g. kow, molecular weight, polarity, functional group).

Other sorption tests examined removing different perfluorinated compounds (PFAS) from water. The tested sorbents were based on marula seeds, wood pieces, cotton discharge, and dried wasted sludge from a municipal WWTP. In addition, we tested different mixtures of wood and sludge. All raw materials underwent pyrolysis and activation in the lab reactor. The tested PFAS were perfluorooctanoic acid – PFOA (C8), perfluorooctanesulfonic acid PFOS (C8,) and perfluorooctanoic acid – PFBA (C4), representing the two headgroups and long- and shot-chain compounds. Preliminary data showed that (i) In general, PFOS adsorbed better than PFOA, and long-chain PFAS adsorbed better than short-chain ones and (ii) of the tested materials, a mixture of wood and sludge (at 1:2 ratio) has the highest potential as PFAS sorbent.

Developing new, cost-effective, sustainable adsorbents will promote the implementation of adsorption-based treatment for water and wastewater, improving the effluent quality and OMP removal. This will ultimately prevent their leakage into the aquatic environment and their effect on human health.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Chiral Photodoping in Hybrid Graphene-$Bi_2Se_{2.5}S_{0.5}$ Photodetectors

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Graphene and inorganic two-dimensional (2D) materials hold excellent potential for developing novel future optoelectronic technologies. While graphene photodetectors are limited to low responsivity due to the low absorption cross-section, several gain mechanisms are known to enhance the photoresponse. The most common approach is the use of absorption-enhancing agents, such as quantum dots or nanocrystals (NC). The common gain mechanism of such devices is photodoping, where one photocarrier type (electron or hole) is trapped while the other type is mobile.

Here we report on incorporating sulfur-alloyed Bi_2Se_3 NCs on graphene FETs by means of laser-assisted deposition and observe a photodoping gain in the photoresponse. Interestingly, the observed photodoping is polarization-dependent, potentially revealing a spin-associated selection rule based on chirality. This optically oriented mechanism is being investigated and may be associated with the characteristic chiral spin-momentum orientations at the surface states of topological insulators.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Reactive Intercalation: A Novel Approach for Atomically Thin Heterostructures for Electronic and Optoelectronic Applications

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Department of Materials science and engineering, Tel Aviv University, Israel

In the past decade, synthesis of two-dimensional (2D) materials via chemical vapor deposition (CVD) has attracted great attention for large scale application in the fields of condensed matter physics, materials science and chemistry. 2D materials are believed to be exceptional building blocks for a wide variety of new-generation devices in nano-electronics, electro-optics, optoelectronics, nano-electromechanics, high sensitivity sensors, flexible and transparent devices, thermal management and catalysis. Despite the advances in the study of the growth strategies of such materials, controllable large-scale growth of such materials is found to be very challenging in the case of their heterostructures due to numerous reasons, such as material systems with very complex phase diagrams and polymorphism, and non-stable phases which require high-vacuum systems. Layered compounds like Transition metal dichalcogenides (TMDs) (MX2; M: Mo,W; X: S, Se, Te), having very interesting physical properties dependent on the layer number, are suitable for electronic and optoelectronic applications in a wide range of the electromagnetic spectrum. Here, we study a reactive intercalation approach, in which, first we intercalate transition metal chlorides or oxy-chlorides inside graphene sheets through chemical vapor transport (CVT) and then, we synthesize graphene-TMD heterostructures through introduction of chalcogen vapor. In the first step, we chose a mixture of MoO3 and MoCl5 for intercalating graphene sheets. Introduction of the intercalants inside graphene not only increased the van der Waals gaps in graphene to form a layered structure, but also get stabilized by charge transfer. Raman fingerprint of graphene shows significant alteration after the intercalation. Laser-induced oxidation of host-intercalant composite confirms the presence of metal chloride or metal oxy-chloride as the intercalant. High resolution microscopic imaging shows metal chloride or oxy-chloride layers in between the graphene sheets. The significance of this research is both fundamental and applied; it provides new insights into the stabilization of layered materials in confined vdW gaps, on the other hand, it may allow for the formation of very complex heterostructures and study of their properties. Moreover, the reactive intercalation in 2D materials can be expanded to a wide range of intercalants and hosts, therefore, will provide for a general strategy to study very complex and diverse material systems for a wide range of applications.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Investigating the Growth of 2D Ternary Compounds via Chemical Vapor Deposition

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Ramat Aviv, Tel Aviv 6997801,, Israel

In recent years, atomically thin two-dimensional (2D) van der Waals materials have attracted much attention due to their incredible chemical and physical properties and their potential use in modern electronic and optoelectronic devices. In particular, 2D transition metal phosphorus trichalcogenides (MPX_3, M-transition metal and X-S or Se) possess excellent optical, electronic, ferroelectric and inherent magnetic properties that can complement the performance of other 2D materials. However, most studies to date have focused on the mechanical exfoliation of bulk crystals or thin films prepared by liquid exfoliation. The synthesis of atomically thin MPX_3 by chemical vapor deposition (CVD) remains challenging due to the precise control of the molar ratio and co-volatilization of transition metal, phosphorus, and chalcogenide precursors to avoid the formation of binary byproducts. Phosphorus is extremely reactive and volatile, making its controlled incorporation into the CVD process difficult. Therefore, it is imperative to design a feasible growth process to overcome these challenges. Herein, we describe a unique and scalable synthesis approach for systematically controlling the formation of 2D antiferromagnetic $NiPS_3$ nanosheets via chemical vapor deposition under mild processing conditions, with nickel and P_2S_5 as precursors. In this work, we successfully synthesized hexagonal $NiPS_3$ nanosheets using CVD with a thickness of only a few atomic layers and a lateral size exceeding 10 µm. Raman spectroscopy revealed the unique vibrational modes of NiPS3 nanosheets, which are consistent with their crystal structure. Furthermore, EDS analysis confirmed the elemental composition and the formation of pure $NiPS_3$ nanosheets. High-resolution TEM confirmed that the nanosheets were highly crystalline. With suitable precursor selection, our synthesis method is straightforward, scalable, and adaptable to different transition metal phosphorus trichalcogenides.

Keywords: 2D Magnetic materials, $NiPS_3$, Raman spectra, Chemical vapor deposition.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Coupled Pyroelectric-photovoltaic Effect in 2D Ferroelectric α-In_2Se_3

Michael Uzhansky

The pyroelectric and photovoltaic effects play crucial roles in advanced technologies such as thermal imaging, infrared sensors, and the harvesting of thermal and solar energy. Recent developments have highlighted the significant potential of the bulk photovoltaic effect in two-dimensional (2D) semiconductor-ferroelectric materials, enabling reconfigurable p-n junction operations that may exceed the Shockley-Queisser limit. Additionally, 2D ferroelectric materials exhibit exceptional properties, including extremely low thickness, high thermal conductivity, interfaces free of dangling bonds, and stable ferroelectricity at room temperature down to a single monolayer. These characteristics contribute to a superior pyroelectric figure of merit. In our study, we conducted direct pyroelectric measurements of 2D α-In_2Se_3 in both dark and light conditions. Our findings revealed a remarkable pyroelectric coefficient of approximately 30.7 mC/m^2K and a figure of merit of around 135.9 m^2/C. We also performed temperature-dependent short-circuit photovoltaic response measurements, where the excess photocurrent was modulated in proportion to temperature variations due to induced in-plane potential changes. As a result, we discovered a combined pyroelectric-photovoltaic effect that enables both direct temperature sensing (via photovoltaic response) and temperature-derivative sensing (via pyroelectric response). Finally, we utilized the intercoupled ferroelectricity of In_2Se_3 to realize a non-volatile, self-powered photovoltaic memory operation, demonstrating a stable short-circuit current switching with a decent 10^3 ON-OFF ratio. The coupled pyroelectric-photovoltaic effect, along with the ability to reconfigure photocurrent, paves the way for innovative monolithic device technologies that integrate thermal and optical responses, in-memory logic, and energy harvesting.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

Direct Determination of Torsion in Twisted Graphite and MoS2 Interfaces

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Two dimensional (2D) materials enables stacking of individuals layers at non-equilibrium configurations, for instance via adjustment of twist angle, significantly extending the design space for heterostructures. The relative twist angle between layers modifies the crystal structure leading to a variety of intriguing physical properties such as superconductivity, ferroelectricity, moiré excitons, tunneling conductance and structural superlubricity. Researchers utilize the angular degree of freedom to manipulate material characteristics by intentional alignment of material constituents using static alignment techniques such as water assisted transfer, thermal annealing, and optical alignment of crystal edges. However, there is no available information regarding the torque required to create a dynamic misalignment from an equilibrium state and their size dependence which is essential for precise control and manipulation. In addition, the interplay between twist and sliding plays a crucial role in the mechanical alignment and actuation of 2D materials, as well as their assembly into functional devices using layer-by-layer technique.

Herein, we employ the lateral deflection of the AFM cantilever to quantitatively measure torque in graphite and MoS2 interfaces. We utilize a unique experimental technique that allows to rotate the interface, while keeping the center of rotation and contact area intact by the stabilizing adhesive line tension forces. Discrete torque peaks were observed at commensurate configurations with an angular interval of 60°, attributed to the inherent symmetry of the crystal lattices. In contrast, any measurable torque was absent in the incommensurate positions. Torque at commensurate configurations demonstrates a linear dependence as a function of interfacial area in both circular graphite and MoS2 mesostructures. Furthermore, we measured the adhesion in MoS2 and graphite mesostructures to address the interplay between sliding and rotation. Adhesion energy of graphitic interface was found to be higher than torsional energy, explaining the greater susceptibility of a commensurate interface to twist prior to sliding. Contrarily, MoS2 exhibits a higher torsional energy compared to its adhesion energy. Thus, our study indicates a fundamental difference in the interplay between sliding and twisting in MoS2 and graphite.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

2D materials

MXene-CNC Super Performing Composite Films for Flexible and Degradable Electronics

Daniel Voignac[1]
Applied physics and Plant science, Hebrew University of Jerusalem, Israel

Flexible electronics have gained significant interest due to their potential applications in wearable devices, biomedical sensors, and flexible displays. This study explores the combination of MXene and cellulose nanocrystals (CNC) for the development of flexible, conductive, and degradable materials. CNC and MXene are high-performance nanomaterials with known degradability. CNC can self-assemble into highly ordered layers and act as an ideal structural companion for enabling large surface MXene-based devices with outstanding performance. Three fabrication routes are explored in this work: self-assembly, drop casting, and dip coating. The mechanical and electrical properties of the CNC-MXene composite films were assessed. Tensile testing revealed that dip-coated films in high-loadings of MXene could exhibit enhanced toughness of up to 1.9 $\mathrm{MJ\cdot m^{-3,}}$ higher than pure MXene or CNC. The electrical conductivity of the films varied depending on MXene concentration and drying, exhibiting superior conductivity in self-assembly with higher MXene loading and rapid drying that prevents oxidation. Self-assembled MXene-CNC with a 1:3 MXene-to-CNC ratio maintained high conductivity of 2.2 × 105 $\mathrm{S\cdot m^{-1}}$. Zeta potential measurements indicate that CNC enhances the stability of MXene dispersion. These findings demonstrate good synergy between CNC and MXenes for applications in flexible, transparent, and environmentally degradable electronic.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Additive Manufacturing

Multiple Wavelength Printing in VAT Photopolymerization 3D Printing - Analyzing Solubility and Mechanical Properties of Printed Models

Yali Reuveni, Liron Ben Arush

3D printing is an innovative field that allows the printing of a wide variety of materials in different shapes, producing unique geometric models that often cannot be obtained in any other way. To achieve this, many technologies have been developed for 3D printing, one of which is Digital Light Processing (DLP). This technology uses a material containing a photo initiator, which, when exposed to light, triggers the polymerization process, thereby building layers of a 3D model on a platform. Today, many industries use the DLP printing process to create models, but in many cases, models need to be printed with support structures. After the printing process, it is necessary to manually remove these supports, as well as other parts of the model.

As part of this project, the potential to create and print printing material using a unique printer capable of operating with two different wavelengths is being examined. This method enables the use of two different materials, with different properties, where the main focus is on the solubility differences between them.

The goal of the project is to produce a printed model with desired mechanical properties at both wavelengths, so that the difference in solubility will assist in removing the supports in water without human contact.

Objectives of the project:

v Producing and Testing Various formulations suitable for 3D printing at two Different Wavelengths.

v Successfully Creating a Printed model with support structures which can be separated in water, while keeping desired mechanical properties in the final model.

So far, a large number of formulations have been tested, with changes made to the components of the formulations, including the monomers used and the different photo initiators. Additionally, various printing parameters were examined during the creation of the model, and several mechanical tests were conducted on the resulting models and their solubility.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Advanced Characterization Methods

Characterization of a Single Nano-cavity by Scanning Electrochemical Microscopy (SECM)

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[2]*Chemistry Department, The Hebrew University of Jerusalem, Israel*

Scanning electrochemical microscopy (SECM) is one of the most commonly used electrochemical SPM techniques, which enables the characterization of surfaces. SECM uses electron transfer processes to investigate and manipulate different systems locally, taking advantage of the high sensitivity of electrochemistry. The SECM offers micrometer and even nanometer resolution of the surface topography. Hence, the SECM provides local chemical and electrochemical reactivity of surface features, which add significantly to the understanding of surface functionality.

Nanoparticle-imprinted matrix (NAIM) is an approach that comprises the preparation of thin films in which nanoparticles (NPs) are imprinted as a template in this matrix. The removal of the template creates nanometric voids.

In this project, we aim at studying the NAIM systems at a single nanoparticle level. A three-dimensional SECM image will be obtained by scanning a micro and in the future nanoelectrode in the x-y plane and monitoring the tip current as a function of location. The holes should be imaged by the SECM using either the feedback or the generation-collection mode in which electroactive species, such as or as are reduced at the tip or on the surface, respectively. We have already made microelectrodes and made some approach curves to the surface, from which we can distinguish between a surface before and after imprinting as well as after the removal of the metallic nanoparticles.

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Poster Presentation

Bio- and Soft Materials

Intrinsic Mechanics and Bundled Collagen fibers Microstructure of Fetal membranes in Preterm birth

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Joshua M. Grolman

One of the main causes of morbidity and mortality of newborns worldwide is preterm birth, which also has a variety of negative effects on the relationship between the baby and his parents at the beginning of his life. Fetal membranes linked to preterm birth have historically been assumed to be mechanically weaker than full-term membranes, and evaluations using destructive mechanical testing techniques have generally agreed. However, in measuring the intrinsic mechanical characteristics of fetal membranes using nanoindentation, the results revealed a more nuanced phenomenon: fetal membranes of preterm birth were highly stiffer than those from full-term birth. To investigate the underlying structural contributors, we utilized Second Harmonic Generation (SHG) microscopy to analyze the architecture of the bundled collagen fibers. By understanding the relationship between collagen structure and mechanical properties, new insights emerged regarding the remodeling effects of Braxton Hicks contractions and the load applied as a result of fetal movements. These findings offer new perspectives on the biomechanical and structural adaptations of fetal membranes, with potential implications for understanding and managing preterm birth risks.

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Poster Presentation

Bio- and Soft Materials

Robust and Facile Methodology to Fabricate Ligand Patterns for Ex-vivo Cell Interactions

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In-vivo, cells interact with their environment, including surrounding cells, tissues, and extracellular matrix, through transmembrane receptors that bind specifically to extracellular ligands. The spatial arrangement of these ligands plays an important role in these interactions, and often determines the resulting cell response to the environmental cues. To study the role of this arrangement, various ex-vivo platforms with controlled arrangement of ligands are employed, providing the resolution of the ligand positioning down to the molecular scale. However, such platforms are usually realized by complex and expensive nanofabrication methods, which are often out of the reach of researchers in cell biology.

Here, we introduce a novel concept for ex-vivo cell stimulating platform with precise nanoscale positioning of ligands, which can be realized without any specialized equipment. The platform is based on Polymethylmethacrylate (PMMA) film imprinted with nano-topographic features, into which Polystyrene nanoparticles are inserted by mechanical rubbing. Then, the ligands of interest are selectively attached to Polystyrene, determining thereby their positioning. We demonstrated the selectivity of the ligan positioning by fluorescent imaging. We then applied this platform to control the receptor distribution in human T cells, and study the effect of this distribution on T cell immune response. This new methodology of the receptor positioning paves the way to numerous studies aimed at determining the effect of receptor-ligand interactions on the cell function.

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Poster Presentation

Bio- and Soft Materials

Aided Porous Medium Emulsification System: A Novel Method for Fabricating Microgels for Biomedical Applications

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The field of fabricating microgels is notably rich and diverse. Techniques such as batch emulsion, fragmentation, microfluidics, lithography, spraying, and centrifugation-based methods are commonly utilized in microgel synthesis. However, these methods frequently face limitations in size control, precision, scalability, and challenges may also emerge in terms of assembly, cost-effectiveness, and biocompatibility [1]. The untapped potential of using emulsification through a porous medium to create functional microgels has yet to be explored. In this work, we present an innovative method that leverages centrifugation as the driving force to emulsify two immiscible fluids within 3D heterogeneous porous media, achieving controllable droplet size and distribution. The resulting emulsified droplets can then undergo various crosslinking processes, including physical or chemical methods, to form microgels [2].

By modifying the lysine residues of bovine serum albumin with polyethylene glycol diacrylate (PEGDA) through an aza-Michael addition reaction [3,4], we have successfully synthesized responsive hybrid protein-polymer microgels using our approach. These microgels exhibit a variety of sizes, from small, monodisperse droplets to large, polydisperse ones, with diameters ranging from 5.97 ± 0.05 to 19.37 ± 0.33 µm. These microgels have a dynamic behavior, responding to changes in pH, temperature, and the presence of denaturing chemicals through unfolding and refolding mechanisms. The ability to preserve protein structural integrity and functionality has led to the synthesis of cytochrome c (cyt c) - PEGDA microgels, making them ideal for biosensing applications. Upon exposure to oxidizing agents like hydrogen peroxide (H_2O_2), the heme group of cyt c within these microgels is oxidized, resulting in variations in their absorption spectra. To evaluate the reversibility of this electron transfer, the microgels were subjected to a cycle of oxidation by H_2O_2 and subsequent reduction by ascorbic acid. This procedure highlighted the ability of cyt c to undergo reversible electron transfer between its oxidized and reduced states. This unique characteristic renders cyt c extremely valuable in biomedical applications, where changes in its absorption spectrum serve as detectable signals for the presence of H_2O_2 in various concentrations.

The adaptability of our system is highlighted by its efficiency in producing microgels using small volumes (50 µL) and concentrations (100 µM) of proteins, delivering results in minutes while preserving the proteins` structural and functional integrity. Additionally, our method generates a variety of microgel types, such as alginate-based microparticles, through physical crosslinking. This enhances the range of microgel fabrication methods, positioning our approach as a cost-effective, biocompatible, and scalable option for diverse biomedical applications, including drug delivery systems, 3D printing, and biosensing devices, with the potential for culinary innovations.

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Poster Presentation

Bio- and Soft Materials

Nanoscale Device for the Control Study of the Special Activation- Inhibitory Balance in T Cells

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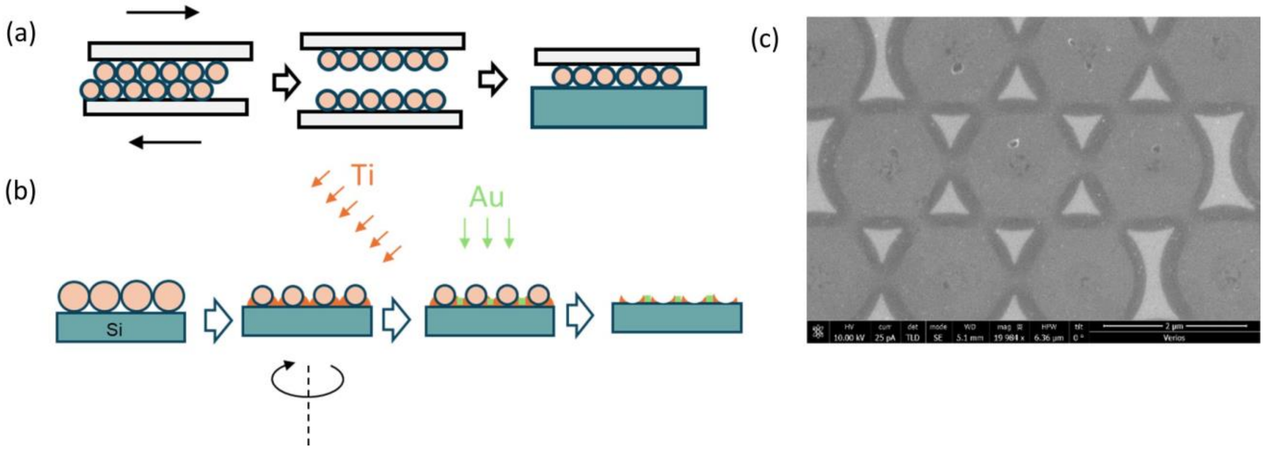
The immune system is based on innate cells, such as natural killer (NK) cells, and adaptive cells, such as T cells. These cells distinguish between healthy and diseased cells and attack tumor, virus-infected, and stressed cells. Their activity is regulated through a delicate balance between activating and inhibitory signals delivered by a multitude of activating and inhibitory receptors. The role of the juxtaposition of activating and inhibitory receptors in signal inhibition of cytotoxic lymphocytes remains intensely debated. The challenge lies in the lack of tools that allow simultaneous spatial manipulation of signaling molecules. Based on earlier research conducted in our group, the optimal spatial segregation for maximal inhibitory effect between activating and inhibitory ligands was demonstrated. However, these ligands occur in clusters naturally, and the exact nature of the impact of spatial segregation on them must be studied. This led us to develop platforms that mimic the natural clustering of these ligands.

In this study, we are developing nanoscale platforms for the controlled segregation of activating and inhibitory receptors in T cells. The platform was fabricated using colloidal lithography based on the self-assembly of polymeric nanoparticles into ordered arrays, followed by pattern transfer by angle-evaporation of Ti and Au at different angles, and liftoff, to obtain nanometric domains of Si and Au, separated by Ti strips whose dimensions will depend on the evaporation angle. These domains will then be selectively functionalized with activating and inhibitory ligands using a previously developed method. T cells will be activated on these nanofabricated surfaces, and their immune response will be evaluated through activation markers (CD69, CD107a) by flow cytometry as the function of the gap between the activating and costimulatory domains.



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Poster Presentation

Bio- and Soft Materials

Soft Robotics Actuators Based on 2D Materials

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Soft robotics bridges machines and humans and as such is based on machines made of soft and flexible materials. One of their special characteristics, unlike rigid robotics, is the ability to manipulate soft objects without damaging them. This makes them very popular in many fields such as flexible electronics, healthcare and more.

This project focuses on electrochemistry-based actuators and deals with the development of two-dimensional soft materials that will be controlled by an electrical signal. The actuator is based on an ionic polymer metal composite (IPMC), which means a charged ionic polymer containing a solvent with mobile ions and entrapped between two electrodes. The voltage difference across the electrodes produces an electric field that forces the cations to approach the cathode and the anions to the anode, changing their distribution within the solvent, and thus the actuator undergoes reversible deformation.

Today, improving the durability and strength of IPMC actuators is a major challenge. As a result, flexible, economical, high-conductive electrodes, without cracks and leaks during operation, are needed. During the project, we aim to develop actuators with large deformation ranges, high-frequency response and sufficient force to lift objects. All this while manipulating and understanding the structure of the gel, which will involve the creation of nanometric to micrometric ionic channels that will allow enhancing ion migration, to increase the displacement of the actuator and its durability. Increasing the blocking force and yet maintaining a high-frequency response will be achieved by adding CNTs or other carbon-based 1-2D materials.

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Poster Presentation

Bio- and Soft Materials

Effect of Electric Fields on Silk Proteins Self-Assembly

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B. mori silk fibroin (SF) protein is a biopolymer naturally synthesized and spun into a microfiber by the Bombyx mori silkworms. It is composed of a (GAGAGS)n backbone, that tend to self-assemble into nanofibrillar structural organization, similarly to β-sheet rich amyloid assembly, under the action of shear forces, particularly elongational flow. Due to the intrinsic characteristics of fibroin protein in its soluble state as well as a spun fibre, such as biocompatibility, biodegradability and low cytotoxicity [1], and combined with its natural mechanical properties of high tensile strength and flexibility, this substrate is of particular interest for materials for tissue engineering and regeneration applications [2]. Such usage has been registered in different forms, including films, hydrogels, scaffolds etc [3].

With a complex charge distribution on its monomers, electric fields can induce fibril orientation and even alter chain bonding. Therefore, in this work, we investigate the effect of electric fields (EF) in the context of being used as a tool for controlled self-assembly of SF proteins and films. SF was produced by the standard degumming method [4]. Briefly, B. mori cocoons were boiled in sodium carbonate, and dissolved in lithium bromide. The remaining viscous liquid solution was then dialyzed against ultrapure water for 3 days, exchanging the water several times during this period. SF films of different concentrations were made by dropcasting the solution in molds connected to platinum electrodes.

Both direct (DC) and alternate current (AC) fields were applied at different intensities. The secondary structure of the films with respect to concentration and field intensity was assessed by checking the Amide I band with Fourier Transformed Infrared Spectroscopy (FTIR), while their morphology was imaged by Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). The crystallinity of the films was probed with X-Ray Diffraction (XRD).

Preliminary results show a difference in β-sheet content regarding samples produced with an electric field from the control untreated samples, with a higher effect on more concentrated films. Furthermore, AFM analysis show an indication of fibre orientation in the EF films. SEM and AFM images of SF solutions deposited on glass clearly shows an orientation regarding the AC EF application.

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Poster Presentation

Bio- and Soft Materials

Accessible Nano Fabrication Process for Metallic Structures and Patterns for Advanced Applications

Tomer Sherf

Nano fabrication has long been a cornerstone in the development of advanced materials and electronic devices. Originally employed for microelectronics, its applications have expanded to include energy harvesting devices, biomedical research, photonics, and more. Traditional fabrication techniques rely heavily on lithography-based patterning combined with transfer methods such as etching or lift-off processes. However, these methods are often complex, require expensive equipment, and demand high levels of expertise, making them inaccessible to many researchers and industries. This limitation poses a significant challenge to the widespread adoption of nano fabrication technologies.

Here we introduce a new versatile, robust, and accessible method for fabricating metallic patterns with nano metric resolution. The process begins with creating topographical features through nanoimprinting onto a substrate of polymers (PBMA or PMMA). A metallic film is then deposited over the imprinted features via Vapor Deposition. The excess metal on the raised areas is then mechanically removed using adhesive tape, leaving behind metallic patterns embedded within the topographical features. This method circumvents the need for costly lithography equipment and expertise, offering a straightforward alternative that can be widely adopted.

Using this technique, we demonstrated the fabrication of patterns with varying feature sizes and compositions, showcasing its versatility. Additionally, the embedded metallic patterns on polymer surfaces can serve diverse applications. For instance, the polymer topography can be flattened through thermal reflow, enabling a smooth surface while retaining the metallic features. A key application of this process lies in the fabrication of bioactive nano patterns for biomedical research. Specifically, we developed patterns of adhesive ligands and activated ligands for human T cells, which play a crucial role in immune responses. These patterns enable precise spatial control over cell-ligand interactions. Allowing an opening to new avenues when studying immune cell behavior and developing advanced immunotherapies.

Overall, this work presents a highly adaptable and cost-effective nano fabrication method with potential applications in numerous fields, including photonic structures, biointerfaces, nanostructures for renewable energy, and beyond. By simplifying the fabrication process and reducing the barrier to entry, this technique paves the way for broader adoption of nanoscale engineering solutions in research and industry.

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Poster Presentation

Bio- and Soft Materials

Soft Printing of Gold Nanoislands on Flexible Polymeric Substrates

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Functionalization of polymeric substrates of artificial or biological origin is critical for many applications. Incorporation of plasmonic nanoparticles (NPs) such as gold not just onto/into solid inorganic materials, but in organic and biopolymers such as proteins and polysaccharides, to form plasmonic nanocomposites aiming to give them new properties or biological activity is promising. However, fabrication of metal NPs directly in a polymer matrix might be challenging since (1) NPs usually aggregate and hence may lose their properties and (2) polymeric substrate has peculiarities impeding direct formation of the NPs. To address existing technological challenges, we designed and developed a facile soft-printing approach to efficiently functionalize flexible polymeric materials with a series of gold nanoparticles and nanoislands (AuNIs) with tunable plasmonic characteristics. The synthetic route is based on Au nanostructures formation (ca. 2–300 nm) on a glass substrate followed by gentle hydrophobization of the functionalized surface, which in turn, allows efficient transfer of AuNIs to flexible adhesive films via soft-printing tape lithography. Owing to precise control of the gold nanostructures size, soft plasmonic films with unique spectral-selective optical properties were produced. Since the AuNIs incorporated into polymeric tape remain capping-free, their further modification is possible. We believe that the proposed method will be of interest in the development of advanced flexible (also adhesive)-polymer-based optical and functional materials.

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Poster Presentation

Bio- and Soft Materials

Magnetically Drug Release Wafer for Glioblastoma

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Local drug delivery systems (LDDS) offer significant promise in theranostics, but precise control over drug release mechanisms and rates remains challenging due to the complex interplay among system components. In this study, we propose a magnetically activated, implantable drug delivery system as a step toward a paradigm shift in personalized medicine. This system is designed to deliver drugs in a controlled manner and is demonstrated using glioblastoma multiforme (GBM) as a proof-of-concept. GBM, the most common and aggressive form of brain cancer, has a dismal 5-year survival rate of only 5.6%, even after surgical resection. Its diagnosis is often complicated by diverse symptoms that vary with tumor size and location. Due to its highly infiltrative nature, complete surgical removal of GBM without damaging healthy brain tissue is nearly impossible. Current standard treatments include surgical resection followed by radiotherapy and chemotherapy with oral temozolomide (TMZ). However, these approaches are limited by the inability of many chemotherapeutic agents to effectively cross the blood-brain barrier (BBB), leading to reduced therapeutic efficacy and increased systemic toxicity. This study focuses on the development of a novel drug delivery system capable of administering therapeutics in a personalized and localized manner. The system incorporates superparamagnetic iron oxide nanoparticles (SPIONs) coated with TMZ, embedded within a biodegradable polymer matrix, and compression-molded into a wafer form. This design aims to address the challenge of delivering systemic chemotherapeutic agents across the BBB. Drug release is triggered by an external alternating magnetic field, which induces localized heating in the SPIONs. The heat breaks the SPION coating, releasing TMZ directly into the GBM tumor residues left in the surgical cavity. The research includes the synthesis of SPIONs via a coprecipitation chemical method, functionalization and conjugation of nanoparticles with TMZ using polyethylene glycol (PEG) for stability, and folic acid (FA) to enhance cellular uptake. The SPIONs are then molded into wafers (1 mm height, 7 mm diameter) with varying concentrations (5%, 10%, 15%), and the resulting TMZ release profiles are analyzed to determine the optimal conditions for this innovative delivery system.

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Poster Presentation

Ceramics and Composite Materials

Thermal Behavior of Ablative Materials: A Study on Carbon Phenol Composites

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Thermal protection systems (TPS) are crucial in aerospace applications, shielding structures from extreme thermal environments. Carbon phenolic composites are widely used in TPS due to their ability to absorb and dissipate heat while undergoing controlled degradation. However, their complex thermal behavior and pyrolysis kinetics remain a challenge, limiting accurate predictive modeling and material optimization. The present work presents a comprehensive approach to characterizing the thermal and kinetic properties of carbon phenolic composites, emphasizing the role of fiber orientation and pyrolysis kinetics. Thermogravimetric analysis (TGA) was used to derive reaction kinetic parameters through model-free (Kissinger) and model-based methods, with measurements conducted up to 800°C. Thermal properties, including diffusivity, expansion, heat capacity, and conductivity, were measured for virgin and charred samples up to 1200°C using dilatometry, differential scanning calorimetry (DSC), and laser flash analysis (LFA). The pyrolysis process revealed overlapping reactions, reflecting complex mechanisms with three major reactions where the activation energies of the phenolic resin were changed from 237.80, 392.12, and 74.42 kJ/mol in the stand-alone to 189.69, 259.82, and 94.23 kJ/mol in the composites. The thermal conductivity ranged from 0.69 to 0.79 W/m·K (through-plane) and 2.24 to 2.79 W/m·K (in-plane), with increased values observed for charred composites due to microstructural evolution. These findings advance the understanding of carbon phenolic composites, supporting the optimization of TPS materials for aerospace applications.

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Poster Presentation

Ceramics and Composite Materials

Thermal Management: High Thermal Conductivity Low Electrical Conductivity Coating Material for Electronic Devices

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The increasing device density in modern electronics (e.g., in printed circuit boards – PCB) requires efficient thermal management solutions. PCBs are typically coated with thin film to protect them from environmental factors such as moisture and dust. However, the coating materials are usually thermally insulating, resulting in elevated device temperature and degraded performance due to poor heat dissipation. Desired properties of such coating materials for thermal management applications include Thermal Conductivity (TC 4 W m^{-1} K^{-1}) [1,2] and negligible Electrical Conductivity (EC 10^{-9} S cm^{-1} [3], green area Figure 1) to avoid short circuits. Moreover, optimal rheology properties for the coating material are required for various application methods, such as dip coating or tape casting, which typically range in shear rate between 10 and 100 s^{-1}. [4] We suggest to map these coating properties (EC, TC and rheology), which are essential for most industrial applications aiming at maintaining functionality, durability, and safety in demanding environments such as high temperatures and mechanical stress.

	Figure 1. TC vs EC map non-metallic loaded polymer composites. The green region indicates optimal conditions for thermal management coatings for the electronics industry

We demonstrate that loading polymer with boron nitride (BN) and graphite flakes (GF) fillers provide high thermal conductivity (GF, TC=3.9 W m^{-1} K^{-1}) while blocking the electrical conductivity (BN, EC= 3·10^{-10} S cm^{-1}, Figure 1), making it ideal coating for safe and effective heat management. Adjusting BN concentration also allowed control over the coating`s viscosity, offering versatile application methods.

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Poster Presentation

Ceramics and Composite Materials

Ceramic Surface as a Detection Technique for Investigating Microbe-Mineral Interactions

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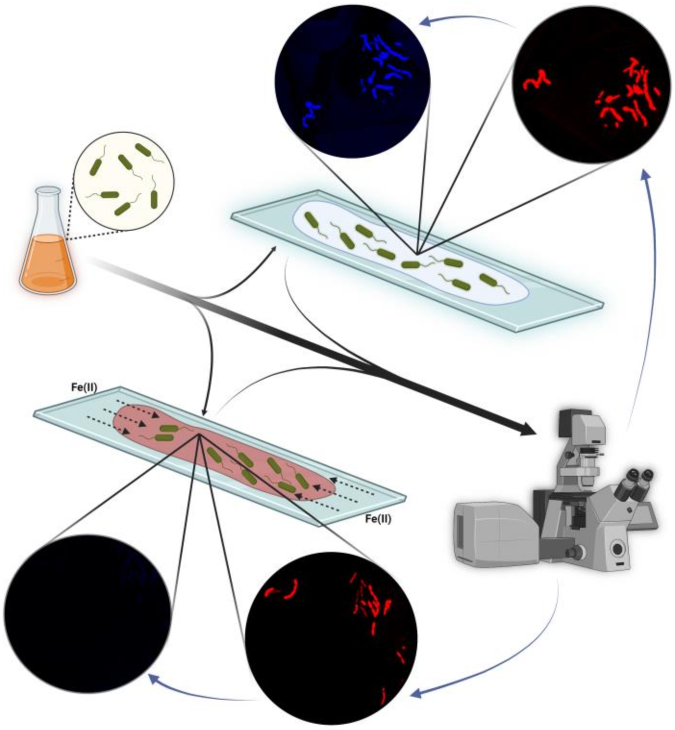
Certain soil bacteria promote direct silicate mineral weathering to obtain and benefit from caged elements. However, detection of this activity is not trivial, as the caged elements and the silicon (Si) are released in very low amounts and sometimes immediately absorbed into the extracellular bacterial polysaccharides. This study demonstrates a sensitive technique for detecting silicate weathering activity by *Paenibacillus mucilaginosus*, a bacterium known to demonstrate silicate weathering activity. We synthesized a ceramic surface through a Sol-gel process. The ceramic surface was doped with an iron and a quenched fluorescent dye. When P. *mucilaginosus* was introduced to the synthetic silicate matrix, we observed 4 to 20 times more fluorescence emission in the iron-deficient medium compared with the iron-supplemented medium, indicating iron release from the ceramic surface. The developed technique described in this study offers a new detection technique for investigating microbe-mineral interactions, particularly weathering activity.



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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Ceramics and Composite Materials

Without a Grain of Salt: Facile Micropatterning for Clean MXene Thin-Film Electronics

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Advanced 2D materials like MXenes boast exceptional electrical, mechanical, and thermal properties, offering promising alternatives in integrated circuit designs facing challenges from continuous miniaturization and power constraints. Our study presents a scalable technique for crafting sub-10 nm MXene thin-film patterns, integrating lithography and spin-coating methods. Crucially, we introduce a novel HCl spin cleaning step, effectively eliminating halide salt residues often overlooked yet detrimental to film performance and integration into device construction. Our method ensures clean and uniform formation of 6-7.5 nm-thick transparent MXene films with exceptional conductivity, resulting in precisely micropatterned films that exhibit high photosensitivity at MXene–Si junctions. This breakthrough paves the way for MXene utilization in flexible, transparent, and wearable electronics, spanning interconnects, electrodes, and sensitive photodetectors. The HCl spin cleaning elevates MXene film purity and performance, resolving a critical fabrication challenge and establishing a new standard for microelectronics applications.

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Poster Presentation

Ceramics and Composite Materials

Effect of Tantalum Carbide Stoichiometry on Densification and Mechanical Properties

Svetlana Fink Ilyasafov

Tantalum carbide (TaC) is renowned for its unique properties and is widely used in tools, gas turbines, and spacecraft due to its high melting point of 3880 °C, making it a potential candidate for thermal protection structures in hypersonic space vehicles. However, one of the challenges in TaC applications is the difficulty of densification, which requires high temperature and applied pressure. In this study, we aimed to improve the sinterability of TaC by modifying its stoichiometry. Experiments were conducted using a spark plasma sintering (SPS) apparatus at 2000°C under 50 MPa pressure for 0.5 hours. Tantalum carbide powders with carbon-to-tantalum ratios of 1 and 0.8 were tested. Nonstoichiometric $TaC_{0.8}$ was synthesized by adding tantalum powder to stoichiometric TaC. The lattice parameters of the carbides were 4.46 Å and 4.43 Å for TaC and $TaC_{0.8}$, respectively.

The density, microstructure, Young’s modulus, and hardness of the sintered samples were evaluated. The porosity of sintered TaC was approximately 6%, while that of $TaC_{0.8}$ was below 2%, leading to improved mechanical properties. Specifically, the Young’s modulus increased from 387 to 425 GPa, and the hardness rose from 750 to 1800 HV for stoichiometric and nonstoichiometric carbides, respectively. However, the nonstoichiometric $TaC_{0.8}$ sample exhibited significantly higher brittleness. Changes in the phase composition and microstructure of the sintered samples will also be discussed.

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Ceramics and Composite Materials

Three-Terminal Resistivity Switching Device Based On Reversible Oxygen Ion Migration at Room Temperature

Daniel Freidzon

Coupling between an electrochemical reaction and a functional material property has been termed electro-chemo-X (EC-X) where X refers to mechanical, optical, magnetic or thermal properties. Here, we explore this effect by presenting, as a proof-of-concept, a functioning, three-terminal, sputtered thin film-based EC-electrical switching device operating at room temperature. The stacked lamellar structure which comprises the device consists of bottom ~200nm thick Ti electrode pair ("source" and "drain") separated by 1mm wide channel. Both the electrodes and the 1mm channel are covered by a stack of Ti oxide-Ce0.8Gd0.2O1.9 nanocomposite(

I-V voltammetry revealed that following 2hr application of -/+ 6V bias between the "gate" and (temporarily shorted) "source" / "drain" electrodes under ambient conditions, the ohmic resistance of the nanocomposite in the 1mm channel changed by a factor of 4.1±0.9 upon reversal of electrode bias , with statistical uncertainty based on at least 3 cycles x 5 samples. Negative "gate" bias produced lower resistance values. The low resistance state decayed during approx. 24 hours. To complement the findings of the E-field promoted oxygen migration, we performed annealing at 633K for 23 hours in air of a device which consisted solely of the bottom electrode pair covered by the Ti oxide/$Ce_{0.8}Gd_{0.2}O_{1.9}$ nanocomposite. We observed an increase by two orders of magnitude in the conductivity of the nanocomposite in the 1mm channel, which then relaxed with time. Using XPS we found that oxidation Ce+3→Ce+4 is responsible for the observed increase in conductivity. As a control, the same thermal treatment was conducted under N_2 flow: no change was observed in channel conductivity.

A possible explanation for how oxidation may increase the nanocomposite conductivity is found in a suitable variant of the space charge model where the potential barrier for ion diffusion across a grain boundary is affected by the total real charge in the vicinity of the grain boundary. Oxidation of Ce3+ → Ce4+ lowers the total real charge, which in turn lowers the potential barrier. Reduction of Ce4+ produces the opposite effect.

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Poster Presentation

Ceramics and Composite Materials

Tungsten-Reinforced MAX Phase Composites for Structural Applications

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MAX phases are a unique class of materials that exhibit a combination of both metallic and ceramic properties, making them highly suitable for various structural applications. This study explores the integration of tungsten into MAX phase composites to enhance their mechanical properties while maintaining other key characteristics such as high temperature oxidation resistance.

Various tungsten reinforcements, including fibers, meshes, and particles, were successfully incorporated into Ti_3AlC_2 MAX phase matrices. The tungsten reinforcements exhibited good incorporation into the MAX phases through the formation of a reaction bond with the matrix, with the particle reinforcement showing the most promising results. Detailed analysis of the reaction-bonded region revealed two new M site Ti1-xWx solid solution MAX phases: a disordered 211-type $(Ti1-xWx)_2AlC$ and a near-ordered 312-type $(Ti1-xWx)_3AlC_2$.

This study highlights the potential of tungsten-reinforced MAX phase composites for applications requiring enhanced mechanical strength and durability. The findings advance the development of advanced materials that utilize the unique properties of MAX phases and tungsten reinforcements.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Ceramics and Composite Materials

Unlocking the Potential of $Y_2W_3O_{12}$ for High-Temperature Thermal Expansion Engineering

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Thermal expansion engineering promises the possibility of controlling the coefficient of thermal expansion (CTE) in a structural or functional material. In high-temperature applications, where small differences in CTE can result in major differences in physical size, CTE engineering allows greater stability and higher output by reducing strain caused by CTE mismatch between components, increasing thermal shock resistance, and increasing durability. Normally, CTE engineering is constrained to a small thermal window and is fitted to the working temperature of a device or component. $Y_2W_3O_{12}$ is distinct for having phase stability over a vast temperature range up to 1400 ^{o}C as well as high volumetric negative CTE; theoretically, $-21\times10^{-6}K^{-1}$, making it an unprecedented candidate for CTE engineering. Despite these excellent attributes, the use of $Y_2W_3O_{12}$ is very limited due to its complicated synthesis process, which continuously concludes with a higher thermal expansion than the theoretical. To fully take advantage of these unique properties, the origin of the mismatched negative CTE should be fully understood. In this presentation, the issues hindering $Y_2W_3O_{12}$ from obtaining theoretical CTE are discussed. Improvements in synthesis methods are shown, providing a way to negate some of the issues and, by that, reducing CTE. Synthesis of $Y_2W_3O_{12}$ with an optimal CTE will bring unprecedented advances in high-temperature CTE engineering.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Ceramics and Composite Materials

The Influence of Dopants and Fields on Microstructural Evolution of Alumina

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In recent years, it has become apparent that there is a direct correlation between disconnection motion and grain boundary mobility. It is known that dopants adsorbed to grain boundaries can alter the grain boundary mobility, likely via interaction with disconnections. In a similar way, external electromagnetic fields may alter the activation energy to form disconnections and/or the kinetics of disconnection motion, and thus affect grain boundary mobility. This presentation is part of an ongoing research study aimed at measuring the effective grain boundary mobility of polycrystalline alumina, as well as that of specific crystallographic planes, as a function of electric fields and dopants.

In this study the anisotropic mobility of specific grain boundaries is analyzed by measuring the rate at which an interface between specific planes of oriented sapphire moves into polycrystalline alumina as a function of an applied electromagnetic field and Ca adsorption, at a specific temperature. The grain size of the polycrystalline alumina is used as a measure of driving force so as to normalize the grain boundary velocity and determine the effective grain boundary. Oriented sapphire is then diffusion bonded to the polycrystalline alumina, and the anisotropic mobility of specific grain boundary planes is determined from measurements of the distance the interface advanced into the polycrystalline matrix, as a function of time [1,2].

The experimental system consists of a tube furnace, where the field is applied via platinum wires bonded to platinum paste applied to the back sides of sapphire diffusion bonded to polycrystalline alumina. This presentation will discuss the possible mechanisms by which an external electromagnetic field influences grain boundary mobility.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Ceramics and Composite Materials

One-pot Approach for Acoustic Directed Assembly of Metallic and Composite Microstructures by Metal Ion Reduction

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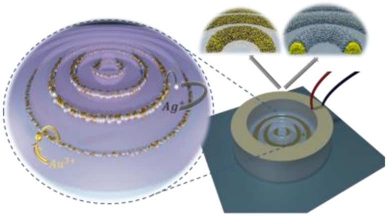
The ability to process various materials to form microstructures in the least possible number of steps is an important issue in many fields such as electronics, sensing and biology. Acoustic manipulation is a powerful technique for assembly of particles. A suspended particle that is exposed to an ultrasound standing-wave field responds to the primary acoustic radiation force by migrating to specific locations along the wave (pressure nodes or anti-nodes). Among manipulation techniques such as electric, optical, optoelectronic and magnetic tweezers, acoustic techniques have a significant advantage, as their only requirement is a difference in compressibility and density between the particles and surrounding medium (acoustic contrast), which is true for almost all dispersed systems. The power density required to manipulate particles with acoustic forces is also several orders of magnitude smaller than that of its optical counterparts and can influence a much larger area. Acoustic waves were used to manipulate and sort biological cells and particles, to selectively promote coalescence, to create ordered colloidal crystals and to form periodic arrays in a bulk matrix.



We have recently shown (*Kenigsberg et al.* Materials & Design 244, 113110, 2024) how acoustic standing waves can be used to direct products of ongoing chemical reactions and form ordered periodic metallic microstructures in a single step. By introducing metal precursor salt and reducing agent into a cylindrical piezoelectric resonator that is also used as a reservoir, we obtained concentric metallic microstructures. Furthermore, we present an innovative method to fabricate metallic multi-layer and composite structures directly by reducing different metal ions or by adding NPs to a metallic matrix during the reduction step. We fabricate these structures in a substantially reduced number of steps, and without the necessity to stabilize the participant materials or prior requirement for the chemical affinity between the metallic matrix and inorganic NPs. This method has the potential to become a new simple way to create numerous composite combinations.

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Poster Presentation

Ceramics and Composite Materials

Expanding MAX Phases: Discovery of a Double A-Layer Ti_2Bi_2C with Rhombohedral Symmetry

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MAX phases are a family of nanolayered ternary carbides and nitrides with the general formula $M_{n+1}AX_n$, where M is an early transition metal, A is typically a group 13–14 element, X is carbon or nitrogen, and n = 1–6. These materials uniquely combine metallic and ceramic properties, including high electrical and thermal conductivity, excellent machinability, thermal shock resistance, and damage tolerance. Their ability to deform plastically at high temperatures and maintain stability under extreme conditions makes them valuable for demanding applications. These exceptional properties, coupled with the fact that MAX phases serve as precursors to MXenes, an emerging class of 2D materials with remarkable properties, drive the ongoing search for new MAX phases, particularly those with novel structures and chemistries, to further expand their potential applications. The double A-layer MAX phases ($M_{n+1}A_2X_n$), A rare subset, is distinguished by two consecutive A-layers between ceramic layers and represents a particularly unique and understudied class of materials. Most known double A-layer MAX phases are formed using top-down methods involving chemical modifications of pre-existing MAX phases, with only one (Mo_2Ga_2C) previously synthesized via conventional bottom-up approaches. Here, we present the synthesis of Ti_2Bi_2C, a novel 221-type double A-layer MAX phase synthesized via a bottom-up approach by high-temperature reaction of elemental powders. Moreover, the discovered Ti_2Bi_2C is the first to adopt a rhombohedral crystal structure (space group *R*-3*m*), with its stability confirmed by density functional theory (DFT). Structural and compositional analysis was carried out by X-ray diffraction (XRD) and high-resolution scanning transmission electron microscopy (STEM). Furthermore, STEM analysis revealed a dominant orientation relationship, (102)Bi//(001)Ti_2Bi_2C and [010]Bi//[010]Ti_2Bi_2C, between Ti_2Bi_2C and Bi. The discovery of Ti_2Bi_2C expands the MAX phase family and highlights the potential of Bi as an A-site element. This work opens avenues for Bi-containing MAX phases in applications such as ammonia synthesis or durable materials for Gen-IV nuclear reactors, underscoring the potential for synthesizing novel nanolayered materials with unique properties.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Ceramics and Composite Materials

Immobilization of Cs-bearing Zeolites in Geopolymeric-zeolite Systems

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Radioactive waste streams often contain cesium radioisotopes, which may harm the environment due to their high specific activity, long half-lives and high solubility in aqueous media. In order to prevent release of cesium to the environment, it must be immobilized and encapsulated within materials that will remain stable for the long-time spans, required for radioactive decay, before being disposed in a waste repository. This study examines the ability to immobilize cesium-bearing zeolites in geopolymeric systems.

Zeolites are microporous crystalline aluminosilicates that exhibit high performance in cesium ions sorption and are used for the removal of cesium ions from the environment. Subsequent to sorption, encapsulation of the Cs-bearing zeolites becomes imperative. Geopolymers, amorphous materials with a chemical nature akin to that of zeolites, emerge as attractive candidates for this task due to their ion-binding properties and superior chemical resistance.

This work presents the structural transformations taking place following immobilization of cesium-bearing zeolites in geopolymeric-zeolite systems with varying formulation parameters (zeolite type, fraction of zeolite in the formulation, SiO_2:Al_2O_3 molar ratio) and curing conditions (time, temperature). The experimental methodology included phase analysis using X-ray diffraction (XRD) and microstructure characterization using electron microscopy (SEM). The cesium ion immobilization properties of the geopolymer-zeolite products were studied by standard leaching tests.

All tested samples exhibited evidence of Cs leaching from the Cs-bearing zeolites into the aluminosilicate gel during the geopolymerization process. Unlike cementitious systems, geopolymers effectively encapsulate the Cs ions leached from the originally introduced Cs-bearing zeolites within new zeolites and/or in the dense amorphous geopolymer matrix, preventing their release into the environment. Thus, geopolymer-zeolite composite formulations hold promise for effective encapsulation of radioactive Cs-adsorbed zeolites.

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Poster Presentation

Ceramics and Composite Materials

Ultra-fast High Temperature Sintering: Exploring Alumina

Rachel Marder

A novel sintering approach utilizing ultra-fast heating has been recently developed, wherein ceramic samples are placed within graphite felt, and heating is achieved by passing an electric current through the felt. The graphite felt serves a dual purpose, acting both as a heating element and a thermal insulator. This configuration minimizes heat loss and ensures that energy is concentrated on the ceramic sample. Known as ultra-fast high temperature sintering (UHS), this technique enables rapid heating to temperatures as high as ~3000°C within just a few seconds. Such rapid thermal processing effectively suppresses grain growth, preserving sub-micron grain sizes even at elevated temperatures.

In this study, Mg-doped alumina samples were sintered in a UHS furnace under varying parameters, including heating rate, dwell time, and peak temperature. Fully dense samples were produced using a heating rate of 800°C/min and a dwell time of 100 seconds. The sintered microstructures were characterized using scanning electron microscopy (SEM). To provide a comprehensive understanding of UHS, the sintered samples are compared to those processed using conventional furnaces and spark plasma sintering (SPS). The role of ultra-fast heating and the influence of electric fields on densification and microstructural evolution will be discussed.

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Poster Presentation

Ceramics and Composite Materials

Using Electrical Conductivity for Structural Health Monitoring in Cement-Carbon Nanofiller Composites

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Cement is a durable and strong construction material widely used in civil engineering. However, it is brittle and has a low tensile strength, which calls for monitoring its health (e.g., strain). State of the art strain sensors require the use of external, large devices that are usually of low sensitivity. It is suggested to add the cement a sensory capabilities (i.e., self-sensing) by loading it with conductive fillers such as graphene nanoplatelets (GNP). Therefore, it is expected that the conductivity of the cement changes upon deformation when the GNP concentration is close to the electrical percolation threshold. The samples demonstrate high dispersion quality of the fillers, as imaged by scanning electron microscopy Preliminary sensing results indicate a piezoresistive behavior under compressive strain, with a responsive Fractional Change in Resistivity of 0.05 (Figure 1, FCR=ΔR/R0), at this stress we find valus around 0.02-0.04[1–3].

		Figure 1 – Application of cyclic compression load (black) and FCR response (orange) for cement paste loaded with 3.5%wt GNP.

We aim at allocating the optimal GNP concentration to maximize the FCR values and plan to examine the effect of other single fillers types (e.g., carbon nanotube - CNT) or hybrid combination of fillerss (e.g., GNP-CNTs) to enhance the sensitivity of a self-sensing concrete device.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Ceramics and Composite Materials

Enhancing Oxidation Resistance in Ti3AlC2 MAX Phase With Refractory Elements Doping

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MAX phases, designated by the general formula $M_{n+1}AX_n$, constitute a class of nanolayered, hexagonal materials that combine the properties of metals and ceramics. These materials, wherein *M* denotes an early transition metal, *A* represents a group 13 or 14 element, and *X* is carbon and/or nitrogen, demonstrate remarkable characteristics that render them exceptionally appropriate for cutting-edge engineering applications. Such characteristics encompass elevated stiffness, low weight, superior thermal shock resistance, as well as notable thermal and electrical conductivities, machinability, and commendable damage tolerance. Furthermore, MAX phases are recognized for their stability at high temperatures and their resistance to creep and long-term oxidation. Among the known 342 MAX phases, compositions containing aluminum, such as Ti_3AlC_2 and Ti_2AlC, are distinguished by their outstanding continues oxidation resistance, enduring temperatures up to 1400°C in oxidizing environments. This resistance is attributed to the development of a dense, continuous, adherent α-Al_2O_3 layer at elevated temperatures, which functions as a diffusion barrier that restricts oxygen diffusion and titanium migration. The gradual formation of this protective oxide layer effectively safeguards the substrate material from subsequent oxidation. Additionally, the close correlation between the coefficient of thermal expansion (CTE) of MAX phases and α-Al_2O_3 guarantees superior adhesion of the oxide layer, even in the presence of substantial thermal stresses. This attribute renders these MAX phases particularly advantageous for applications necessitating sustained performance in high-temperature oxidative environments, such as those encountered in the aerospace, automotive, and energy sectors. To enhance the oxidation resistance of Ti_3AlC_2, our research focuses on doping the M-site with refractory elements such as Mo, W, and Zr. This aims to reduce oxygen diffusion along grain boundaries by modifying the material`s microstructure and optimizing the protective oxide layer. In the first stage of the research, we focused on improving the oxidation resistance of the pure phase for 6 hours at 1200°C by adjusting the sintering conditions and the stoichiometry of the precursors to control the material`s microstructure, including grain size, porosity, secondary phase dispersion, and more. So far, we have demonstrated a significant improvement in the material`s oxidation resistance by achieving cubic oxidation kinetics.

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Poster Presentation

Ceramics and Composite Materials

Effect of Co-doping on Non-classical Electrostriction in Zr-doped Ceria

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Many actuator technologies rely on electromechanically active materials, such as piezoelectric and electrostrictors. We have investigated the electrostriction (ES) effect, a second order electromechanical response, i.e., strain, u, is proportional to $M \cdot E^2$, where E is the applied electric field and M is the longitudinal ES strain coefficient.

Recently our group reported a non-classical electrostrictor (NCES) based on an Zirconium doped Ceria (ZCO), with the electromechanical properties comparable to the best commercial materials[1]. The mechanism behind the significant electrostrictive strain in ZCO differs markedly from previously published reports on ceria. While large electrostriction in ceria is typically attributed to oxygen vacancies, Zr is isovalent with ceria yet still presents giant ES.

The ES effect induced by oxygen vacancies is limited to frequencies bellow 1 Hz and is characterized by low saturation strain (|u_{sat}| 33|=10E-16 m^2/V^2 for x=0.1[2]. This effect persists to frequency ≥3 kHz with |u| ≥220 ppm, making Zr0.1Ce0.9O2 competitive with the best commercial electrostrictor (PMN-PT15), but with about 100 times lower dielectric constant and three-fold higher elastic modulus.

For a sample of ZrxCe1-xO2-δ before oxidation the concentration of Ce3+ ≥ 100 ppm. For charge compensation oxygen vacancies are formed, electrical conductivity is increased, and ES is suppressed. In addition, by co-doping $Zr_{0.1}Ce_{0.9}O_2$ with 0.5mol% of aliovalent cations - Ca, Sc, Yb or La - we observed that the aliovalent dopant reduces the ES strain coefficient by more than an order of magnitude and restores the values of Young’s modulus and dielectric permittivity to values close to those of undoped ceria. Since all these co-dopants, irrespective of valence and ionic radius, lead to a similar result, we concluded that the species responsible for the suppression of ES in Zr doped ceria must be the oxygen vacancies. The results are also supported by XAS, Zr K-edge EXAFS spectra reveal that, even though the molar ratio ZrCe:VO is 40:1 in the co-doped compounds, oxygen vacancies nevertheless succeed in introducing enhanced disorder into the second coordination shell.

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Poster Presentation

Ceramics and Composite Materials

The Effect of Hafnium and Tantalum on the Corrosion and Electro-Catalytic Properties of $Ti_3C_2T_z$

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MXenes, a novel family of 2D transition metal carbides, nitrides, and carbonitrides, including $Ti_3C_2T_z$, have garnered significant attention for energy and electrochemical applications such as supercapacitors, batteries, fuel cells, and electrocatalysis. Their high electrical conductivity, tunable surface chemistry, and layered structure collectively enhance ion transport, reaction kinetics, and device stability. This work investigates the impact of hafnium (Hf) doping, both individually and in combination with tantalum (Ta), on the structural and electrochemical properties of pristine $Ti_3C_2T_z$ MXene. Potentiodynamic corrosion measurements revealed that increasing Hf and Hf-Ta co-doping concentrations improves the formation of a stable passivation layer, broaden the electrochemical stability window, and enhance MXene's suitability for electrochemical application. Through accelerated stress tests, we studied the degradation mechanisms and observed that Hf-doped MXene and Hf-Ta co-doped MXene exhibit specific pathways of material breakdown under high stress. Fuel cell performance tests demonstrated that higher concentrations Hf-Ta co-doping improve performance, while Hf doping alone results in performance decline. These findings highlight the potential of tailoring dopant concentrations to enhance MXene functionality, with future work elucidating degradation mechanism and exploring other oxyphilic metals dopants to further improve MXene durability.

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Poster Presentation

Ceramics and Composite Materials

Tuning the $LaFeO_3$ Particles size by Elucidating the Molten Salt Synthesis Mechanism

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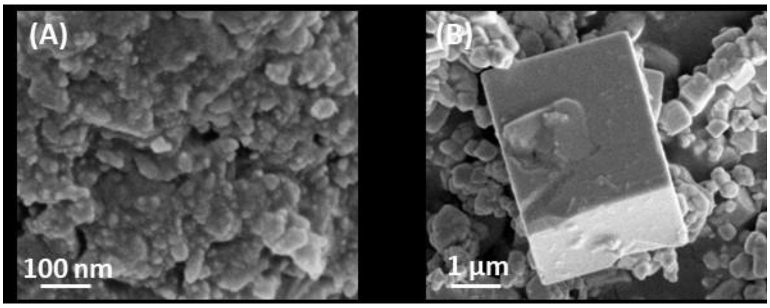
Perovskite type oxides (PTOs) such as $LaFeO_3$ are an interesting class of oxides with promising applications in solid oxide fuel cells and heterogeneous catalysis [1]. In traditional synthesis methods the formation of perovskite crystals occurs via a process in the solid phase, which limits the ability to control the product morphology and particle size. Molten salt offers a unique liquid medium for the PTOs formation, potentially enhancing control over product properties by tuning the synthesis conditions [2]. In order to fully utilize the advantage of molten salt synthesis (MSS), there is a need for deeper understanding of the mechanistic aspects and the factors affecting the perovskites formation process [2-4]. In particular, very little is known about the kinetics of PTOs particle formation during MSS [4].

In this work we synthesized $LaFeO_3$ via MSS using varying conditions to elucidate their effect on the product particles. Sampling the molten salt reaction medium throughout the synthesis facilitated detailed investigation of the MSS kinetics including evolution of PTO morphology (using HRSEM). Increasing the MSS temperature, the salt:reagents ratio, and oxides solubility (by using KF-KCl rather than LiCl-KCl) yield XRD-pure $LaFeO_3$ in only few minutes. The prevailing nucleation at these conditions result in small particles (100 nm, Fig.A), whereas conditions requiring longer durations result in much larger particles (1µm, Fig.B).



These insights into MSS kinetics and its nucleation and growth mechanism achieved by sampling the melt facilitated controlling the PTO particle size by tuning MSS conditions.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Materials for Energy Storage and Conversion

Ratchet Based Ion Pumps for Fine Tuning of Electrochemical Reactions

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Precise control of electrochemical reactions can have a tremendous effect in enhancing the performance of electrochemical energy storage and conversion systems. However, electrochemical reactions are extremely sensitive to the physical and chemical environment at which the reaction takes place. Thus, control of the electrolyte ionic content and the electrochemical potential of specific ions at the vicinity of the electrodes can enhance their selectivity towards the desired products and modify the overpotential of redox reactions. In this contribution we show that ion pumps based on a ratcheting mechanism can be used to tune the overpotential and current of electrochemical reactions.

Flashing ratchets are devices that utilize temporal modulation of a spatially asymmetric electric field to drive a non-zero-time averaged current. We have recently demonstrated experimentally first-of-their-kind ratchet-based ion pumps (RBIPs). Since the ion pumping modifies the electrochemical potential and the concentration of ions, and the reaction rates are determined by the electrochemical potential and concentration, ratchet-based ion pumping provides an additional degree of freedom in tunning electrochemical reaction rates and overpotentials.

RBIPs were fabricated by coating the two surfaces of nano-porous alumina wafers with gold and a thin layer of TiO2 forming nano-porous capacitors. The application of an input signal to the ratchet is shown to accelerate or inhibit reactions on the surface of the Pt electrodes according to the ratchet properties. The pumping direction is determined by the ratchet`s input signal and not by the potential applied to the electrodes. It is shown that proton pumping towards the cathode lowers the HER reaction overpotential, and pumping protons away from the cathode increases the HER reaction overpotential. The ratchet regulated the pH in the cathode compartment. By pumping protons towards or away from the cathode, the cathode compartment proton concentration can be maintained or depleted. The combination of selective ion pumping with the control of reaction rates may also allow tuning the electrolyte content at the vicinity of the electrodes performing the electrochemical reaction independent of their potential thus providing another degree of freedom for the electrochemical process.

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Poster Presentation

Materials for Energy Storage and Conversion

Surface vs. Bulk: Exploring Alumina Coating`s Dual Role in High Energy Cathodes

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At the forefront of today`s energy storage systems, lithium-ion batteries (LIBs) are valued for their high energy density. They are the most prominent choice in mobile electronic devices and zero-emission or hybrid electric vehicles. Owing to their significance and the need to meet growing consumer demands, extensive research is being conducted to enhance battery performance. Specifically, there is a need to develop cathode materials that provide high voltage to raise the energy density of the cell. Generally, these cathode materials are prone to degradation and structural alterations caused by interfacial chemical reactions, which lead to loss of active material, reduced ionic conductivity, and overall poor battery performance. An effective strategy for managing these complications is designing functional nanoscale cathode surface coatings that serve as a synthetic cathode electrolyte interface (CEI). By regulating the composition of the CEI, coatings can provide stability and passivity while maintaining efficient ion transfer. Alumina, Al_2O_3, is one of the most common surface treatments employed to passivate both cathode and anode materials. While it is often demonstrated to have a beneficial effect on electrodes` performance, the chemical and structural origins of this effect remain a subject of ongoing debate. Here, we present a mechanistic investigation of the beneficial effect of alumina coating on lithium cobalt oxide (LCO), a common cathode known to degrade when pushed to high potential. Combining electrochemical characterization with advanced NMR spectroscopy approaches, we provide a complete analysis of the interfacial chemistry and surface structural changes and describe their benefits to the battery performance. Additionally, we use these methods to correlate between surface treatment and cathode lithiation/delithiation reaction efficiency. We find that the coating offers increased stability and improved rate performance of LCO when cycled up to a potential of 4.5 V. Atomic scale insight into the cycled LCO cathode material is obtained from solid state NMR, revealing a more complete lithium deintercalation reaction mediated by the coating. Furthermore, we reveal the chemical transformation of the nanometric coating layer upon contact with standard $LiPF_6$-based electrolyte. These chemical transformations improve Li ion transport, likely due to Li ions incorporated into the coating upon lithiation. Tracking Li isotope exchange by NMR provides direct insight into the Li permeability of the coating artificial CEI. Interestingly, coated LCO has a quick and superficial exchange process due to its low bulk conductivity. These results further establish the affect surface treatment has on the bulk of the cathode suggesting a dual role played by alumina coating in stabilizing the surface and controlling the bulk. A comprehensive understanding of the coating reactivity will advance our ability to design precise coating compositions for specific cathode materials, thus developing stable, efficient, and well-performing batteries.

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Poster Session 1 (Tuesday, February 25, 2025 13:10)

Poster Presentation

Materials for Energy Storage and Conversion

Effect of Hydration on Electrical and Electromechanical Properties of Lanthanum-cerium Oxides

Or Ben Zion[1], Tahel Malka[1], David Ehre[1], Isaac Abrahams[2], Igor Lubomirsky[1]
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In recent years, there has been a growing interest in the pursuit of efficient, clean, and environmentally friendly energy sources. Fuel cells have emerged as a promising technology, allowing the conversion of the chemical energy present in fuel gases into electrical work. Solid oxide fuel cells, utilizing ion-conducting ceramics as electrolytes, have been at the forefront of these developments. However, a significant drawback has been the high operational temperatures typically required, ranging from 300°C to 900°C, due to the thermally activated nature of ion conduction in ceramics.

All solid oxide fuel cells (SOFCs) and electrolyzers (SOEs) operating above 300 °C demonstrate rapid electrode kinetics, especially those based on proton-conducting systems, but are limited in their long-term stability due to thermal stress. Ceramic devices operating between 150-250 °C could enjoy rapid electrode kinetics, even without Pt-based catalysts, and would avoid large thermal stress. However, proton conducting ceramics showing appreciable conductivity in this temperature range have yet to be identified. Developing such a material could revolutionize the field of renewable energy.

Hydrated rare earth oxides, known for their chemical and thermal stability, have emerged as potential low-temperature proton conducting ceramics. Our study of $La(OH)_3$, a material insoluble in water and chemically stable in the presence of carbon dioxide, revealed that the dominant contribution to the conductivity of $La(OH)_3$ below 200 °C is protonic. However, it is not sufficiently high for practical applications. The grain boundaries in $La(OH)_3$ ceramics are non-blocking for proton transport, inspiring further investigation.

We have investigated the partial substitution of La^{3+} by a tetravalent cation, like Ce^{4+}, to increase the oxygen to hydrogen ratio. We have found that ceramics of $La_xCe_{1-x}O_{2-x/2}$ (LCO) with x 0.5 decompose to $La(OH)_3$ and CeO_2 upon contact with water or water vapor, limiting the search range to $x \leq 0.5$.

We have developed a hydration protocol for LCO50 ceramics, leading to ≈7.5±1% of hydration with respect to the theoretical limit. The hydration results in a 0.17% lattice expansion due to water incorporation and a large increase in electrical conductivity. Further hydration results in the mechanical disintegration of the ceramic pellets, prompting the investigation of LCO with x 0.5.

No evidence for water incorporation for $x = 0.2$ and $x = 0.4$ compositions was found under any conditions. Hydration of LCO45 at 200 °C for 48 hours in steam causes fragmentation of the ceramic pellet. However, as determined by thermogravimetric analysis, the replacement of steam by water-saturated nitrogen (25°C) results in 17% of the oxygen vacancies being filled up, expansion of the lattice by 0.18%, an increase in electrical conductivity, and a decrease in activation energy.

We expect that further work will lead to a viable proton conducting ceramics suitable for use a bulk and micro-fabrication-compatible thin films.

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Poster Presentation

Materials for Energy Storage and Conversion

Energy Band Engineering of Charge Transfer Layers for Voltage Loses Optimization in Photovoltaic Application

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Solar energy is an unlimited green energy and for that reason there is a motivation to utilize this energy. The existing challenge in this field is the development of photovoltaic cells that enable the conversion of solar energy into electrical energy with high efficiency, long stability and at an affordable cost. One of the materials used in photovoltaic cells is halide perovskite, a crystalline structure with an ABX3 structure where A and B are cations and X is an anion. In order to effectively extract charge from the perovskite layer and minimize voltage losses, a match must be made between the energy bands of the perovskite and the layers around it that serve as charge transfer layers.

In my research I focus on the synthesis and characterization of pure metal oxides and their mixtures, for use as charge transfer layers. I currently use a solution process to form thin films, followed by a high-temperature annealing under ambient conditions. Another synthesis process makes use of thermal evaporation based on electron-beam heating, enabling the evaporation of different metals under oxygen-rich atmosphere and substrate heating. The characterization of the energy bands is done by direct measurements of the energy gap and conduction band under standard atmospheric conditions, using spectral measurements such as absorbance and photoemission yield spectroscopy in air (PYSA). These measurements will make it possible to choose the ideal charge transfer layers for a given perovskite according to their energy band.

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Poster Presentation

Materials for Energy Storage and Conversion

Structural and Electrical Properties of Metal-oxide Based Photoelectrodes for Water Splitting Devices

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Photoelectrochemical cells (PECs) that utilize sunlight and electric potential to convert water into green H_2 fuel present a promising source of alternative energy. In these cells, the semiconductor photo-absorber plays a critical role in determining overall efficiency. Metal oxides are attractive candidates for PECs due to their wide band gaps, stability in aqueous environments, low toxicity, and cost-effective processing. However, many metal oxides face challenges such as low light absorption, poor conductivity, and high recombination rates of photogenerated carriers, all of which limit their conversion efficiency. In this study, we investigate the structural and electronic properties of $CuFe_2O_4$ and $ZnFe_2O_4$ thin films, focusing on the influence of post-deposition thermal treatments on these properties. We show that annealing the films at 500°C enhances their crystallinity, improves carrier mobility, and facilitates more efficient charge transport, all without altering film stoichiometry, as confirmed by energy-dispersive X-ray (EDX) spectroscopy. Kelvin probe measurements reveal a significant reduction in the surface work function after annealing. Temperature-dependent electrical conductivity measurements indicate that annealing reduces the intrinsic defect density (e.g., cation and oxygen vacancies), as evidenced by a decrease in conductivity, which could contribute to enhanced photoelectrochemical performance. Additionally, photoemission spectroscopy provides valuable insights into the valence band position, enabling the construction of band diagrams for both materials. These results highlight the crucial role of thermal treatment in optimizing the electronic properties of $CuFe_2O_4$ and $ZnFe_2O_4$ thin films, with potential implications for improving the efficiency of PEC water splitting devices.

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Poster Presentation

Materials for Energy Storage and Conversion

Optimizing the Thermoelectric Properties of TiCoSb-based Half-Heusler Alloys

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Thermoelectric materials, are one of the most interesting methods for sustainable energy conversion. The conversion of waste heat into electricity is passive and requires slightly to no maintenance due to the solid-state conversion. Materials based on TiCoSb half-Heusler (HH) compounds show promise due to their unique crystallographic structure. Optimizing their composition and phase stability is a critical first step towards enhancing their thermoelectric performance. This study focuses on stabilizing the HH phase in TiCoSb through single and double alloying with Fe and Ni, to try and understand the doping solubility limit on the Y site of XYZ half Heuslers and the effect of double alloying. Adding either Fe or Ni on the cobalt site would violate the 18 electron rule for semiconducting half-Heusler's. However, by using both, the semiconducting nature of the Half Heusler compound should be maintained. In this study $TiCo_{1-2x}(Fe_xNi_x)Sb$ alloys with x=0,0.1,0.2,0.3,0.4 were produced by arc-melting the constituents, followed by hot-pressing at 900°C. In addition, samples of $TiCo_{0.8}Fe_{0.2}Sb$ $TiCo_{0.8}Ni_{0.2}Sb$ were prepared to understand the effect of each dopant. All samples exhibit mainly HH TiCoSb crystallographic structure with a small secondary phase of TiSb. Other HH phases such as and with traces of Co, CoSb and TiCo were detected by using electron dispersive spectroscopy (EDS) only. The sample doped with low Fe concentrations showed p-type conduction, whereas the rest of the samples showed n-type behavior. Alloying with either Fe and or Ni reduced the thermal conductivity by a factor of 2 compared to the unalloyed sample, having the lowest electronic conductivity. The double alloyed samples, exhibit low Seebeck coefficient, indicating that further optimization of the charge carrier concentration is needed. A dimensionless thermoelectric figure of merit (ZT) of 0.12 have been obtained for the composition of $TiCo_{0.8}$ $Ni_{0.2}$ Sb at 775K.

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Poster Presentation

Materials for Energy Storage and Conversion

Synthesis of Noble-metal-free Electrocatalysts as Free-standing Electrodes for Electrochemical Applications

Roni Cohen Vaza, Jonathan Tzadikov, Liel Abisdris, Menny Shalom

Electrochemical water splitting provides a sustainable and clean source of hydrogen which is considered one of the most sought green energy alternatives. Electrochemical water splitting consists of the cathodic hydrogen evolution reaction (HER) and the anodic oxygen evolution reaction (OER). Not only does OER requires more net energy spend, therefore increasing the total cost of hydrogen production, but the formation of oxygen also has no added value and the catalyst usually suffers from decomposition due to the high energy requirement of OER. On the other hand, the anodic electrochemical valorization of glycerol in aqueous media requires lower energy as well as the formation of value-added chemicals. The synthesis of the electrocatalysts involves developing novel synthetic methods for free-standing electrode preparation based on fine-tuned fabrication of transition-metal-phosphides catalysts (TMPs). These TMP materials are expected to exhibit high catalytic activity and selectivity towards the desired oxidation products without using precious metals. These catalysts will be employed for the electrochemical valorization of glycerol examining the H2 production, total products, and product selectivity. Replacing the OER in the anodic part of water splitting will pave a path toward sustainable production of hydrogen as well as value-added chemicals from glycerol. In addition, understanding the underlying principles that drive this reaction forward will help to fully comprehend the structure-activity relations of future electrocatalysts.

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Poster Presentation

Materials for Energy Storage and Conversion

Influence of O_2 on Zinc Electrodeposition in Batteries with Near-Neutral Electrolytes

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Primary Zn-based batteries have a long history of use and commercialization. However, the potential for secondary (rechargeable) Zn-based batteries has not been attained. Zinc electrode is high-energy, with theoretical capacity above 800 mAh/g, in aqueous electrolytes. Zinc, an abundant metal in the Earth`s crust, has a well-established production and supply chain. Additionally, zinc and zinc oxide can be recycled using various chemical and electrochemical methods. All of these are reasons for choosing zinc as a key candidate for replacing lithium-based batteries, which suffer from safety problems, and require relatively high production costs in a dry environment.

Reversible charging-discharging Zn metal electrode is challenged by several processes such as: non-uniform Zn deposition and stripping during cycling, passivation layer formation which integrates in anode structure. Passivation layer and morphological changes reduces the battery efficiency, while dendrite formation can impair the separator and lead to short circuit. This research is focused on the effects of atmosphere on Zn electrodeposition in Zn cells with non-alkaline electrolytes, which are considered a favorite in terms of cyclical stability. The study examined the atmospheric oxygen presence on the coulombic efficiency (CE) of Cu/Zn cells. We compares the CE under argon, ambient air and oxygen with two near-neutral electrolytes ($Zn(OAc)_2$ and $ZnSO_4$), and characterized Zn electrodes ex situ using X-ray diffraction and electron microscopy. We found an inverse correlation between oxygen concentration and CE in both electrolytes. A substantial enhancement in efficiency (above 20%) was achieved under argon conditions with $Zn(OAc)_2$, whereas the impact of oxygen on the $ZnSO_4$ electrolyte was slighter.

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Poster Presentation

Materials for Energy Storage and Conversion

Tailoring the Growth of Epitaxial Phase Pure Ilmenite Nitio3 Thin Film Photoanodes

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Efficient utilization of solar energy for sustainable green hydrogen production through photoelectrochemical (PEC) water splitting remains a significant challenge. At the heart of PEC cells is the semiconductor photoelectrode, which absorbs light and generates electrons and holes to drive water oxidation and reduction reactions. Recent studies suggest that open d-shell metal oxides, promising candidates for photoelectrode materials, exhibit a non-unity yield of photogenerated mobile charge carriers compared to metal oxides with cations possessing either empty or fully filled d-shells. The underlying mechanisms and the extent of this phenomenon across various open d-shell metal oxides remain poorly understood.

To explore these effects, we propose investigating the influence of d-orbital occupancy on non-contributive absorption processes in open d-shell materials by modulating the cation site in the ilmenite structure ($MTiO_3$; M = Ni, Mn, Co, Fe, and Zn). Achieving this goal requires first establishing epitaxial phase-pure $MTiO_3$ thin films. Here, we present the growth optimization of phase-pure $NiTiO_3$ photoanodes by pulsed laser deposition (PLD), a representative material in this series. A key challenge in growing $NiTiO_3$ thin films lies in achieving stoichiometric composition. To address this, we adopted strategies such as enriching the volume fraction of NiO in the $NiTiO_3$ target to compensate for Ti off-stoichiometry, as suggested previously.

We examined the effects of target stoichiometry and growth conditions on film composition and phase purity. Films grown from stoichiometric and off-stoichiometric Ni:Ti targets often exhibited segregation of TiO_2 in the form of nanocolumns within the NiTiO3 matrix, as confirmed by transmission electron microscopy (TEM) and Raman spectroscopy. These films demonstrated enhanced PEC performance due to the presence of the TiO_2 phase. However, the TiO_2 phase obscures the intrinsic properties of $NiTiO_3$, necessitating its suppression. Through systematic optimization of deposition parameters, we successfully eliminated TiO_2 nanocolumns, achieving single-phase epitaxial $NiTiO_3$ films.

Our findings highlight the critical importance of precise control over growth parameters to tailor the phase composition of complex oxide thin films and show that previously reported efficiency benchmarks attributed to NiTiO3 photoanodes likely stem from secondary phase formation of rutile type TiO2. This work underscores the broader challenge of phase segregation in multicomponent oxide systems and provides a framework for addressing similar challenges in future research.

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Materials for Energy Storage and Conversion

Removal of Carbon Dioxide by Its Dissolution of Calcium Carbonate

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The industrial era has seen a sharp increase in atmospheric carbon dioxide (CO_2) levels, leading to significant environmental challenges such as ocean acidification and global climate change. This study explores an innovative method for CO_2 removal by its use to dissolve calcium carbonate ($CaCO_3$) with and without carbonic anhydrase (CA) catalysis.

Objectives of the project:

❖ To evaluate how different conditions that affect the rate of calcium carbonate dissolution using both continuous flow reactor and confocal microscopy techniques.

❖ To assess the effectiveness of carbonic anhydrase as a catalyst in enhancing calcium carbonate dissolution.

The data from the continuous flow reactor for quantitative tracking of the dissolution rate determined by the calcium concentration after reaching a steady state and the flow rate. Monitoring of pH changes around the crystals was performed in the high-resolution confocal fluorescence microscopy. The collected data from the continuous flow reactor demonstrated a clear influence of CO_2 concentrations on the dissolution rate: high concentrations (5%) significantly accelerated the process due to increased proton production, while at low concentrations (420ppm), the rate was limited by proton availability in the solution .

The enzyme CA was found to be an effective catalyst from both methods for enhancing the dissolution rate by a factor of 2-4, particularly during the initial stages of the process, due to the acceleration of proton production. Additional observations showed that flow rate plays a crucial role in preventing local saturation, sustaining the dissolution process under certain conditions. In contrast, the temperature was not found to significantly impact the dissolution rate within the experimental range (11°C−35°C).

Confocal microscopy provided detailed profiles of pH distribution around calcium carbonate crystals, revealing that significant changes were concentrated near the crystal surface, with steeper gradients under high CO_2 concentrations. Over time, the system tended to approach steady state around the crystals, with solutions containing higher CO_2 concentrations taking longer to reach to this state. The findings highlight the potential of capturing CO_2 by calcium carbonate dissolution, facilitated by enzymes.

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Materials for Energy Storage and Conversion

Peptide Self-Assembly Evolution and its Effects on Proton Conductivity

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Proton transfer (PT) lies at the heart of numerous biological processes and advanced electrochemical devices. Previous studies in our group show that peptides, with their inherent biocompatibility, efficiency, and stability, are versatile candidates for engineering proton-conducting systems. In this work, we explore the dynamic conformational behaviors of self-assembling peptides and their effects on the electrical properties.

Using a self-assembling amphiphilic peptide design, we show that linear zwitterionic peptide assemblies undergo a time-dependent transformation from left-twisted ribbons to double-walled nanotubes morphologies, in the frame of one week. This transformation is accompanied by progressive change in the diameter of the fibrils from 1 nm to 7 nm. Intriguingly, these structural transitions correlate with a significant decline in proton conductivity. Specifically, we find that left twisted ribbon-like thin peptides-assembly shows one to two orders of magnitude higher conductivity than helical nanotube fibrils. This stark difference highlights the critical impact of peptide configuration on the resulting functional properties. The linear peptide’s time-dependent assembly offers complementary insights into tailoring peptide-based materials for bioelectronic applications.

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Materials for Energy Storage and Conversion

Investigation of Charge Carrier Dynamics in Spinel Ferrite Photoabsorbers by Time-Resolved Microwave Conductivity (TRMC)

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Spinel ferrites, with the general formula MFe_2O_4 (where M represents a divalent metal cation such as Co^{2+}, Ni^{2+}, Zn^{2+}, Cu^{2+}, etc.), have emerged as promising photoabsorbers for photoelectrocatalytic applications, including solar-driven water splitting. Understanding charge carrier dynamics in semiconducting materials is essential for enhancing their performance in photocatalysis and optoelectronics. In this study, we investigate the photophysical properties of polycrystalline and epitaxial spinel ferrite (MFe_2O_4) thin films using Time-Resolved Microwave Conductivity (TRMC). TRMC measures the transient, contactless change in microwave reflectivity of a semiconductor following a laser pulse, providing insights into charge carrier generation, mobility, and recombination lifetime. We conducted TRMC measurements on several spinel ferrite thin films, including $ZnFe_2O_4$, $CoFe_2O_4$, $MgFe_2O_4$, and $CuFe_2O_4$. The impact of the M^{2+} cation and film crystallinity on the optoelectronic properties of these materials is discussed.

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Materials for Energy Storage and Conversion

Operando Optical Imaging and Processing for Nickel Hydroxide Electrodes

Aleksandr Kurilovich

Nickel hydroxide-based electrodes have been widely used in various practical applications over the last century. Central to those applications is the 1e- electrochemical oxidation/reduction of Ni2+(Ni(OH)2)/Ni3+(NiOOH) redox couple in alkaline media corroborated with H+ (de)intercalation. The apparent simplicity of this process, in fact, masks its complex spatiotemporal dynamics. This is demonstrated, for example, by phase-transition and phase-boundary movement, polymorphism, strong conductivity – state of charge (SOC) dependence, hysteresis and asymmetry in oxidation/reduction. In addition, oxygen evolution reaction (OER) is thermodynamically allowed at the potentials where Ni2+/Ni3+ redox process takes place with the NiOOH being an active electrocatalyst. This could limit the columbic efficiency and cause mechanical degradation of the nickel hydroxide electrodes at operation conditions. Therefore, elucidating the mechanistic details of nickel hydroxide redox reaction with its decoupling from parallel OER is crucial to target the application-based optimization of nickel-based electrodes.

Addressing this problem could be facilitated by monitoring the electrochromic properties of nickel hydroxide electrodes during operation, leveraging on the optical contrast between the Ni(OH)2 (green) and NiOOH (grey) phases. This enables direct operando imaging of nickel hydroxide redox process and its spatiotemporal dynamics using an appropriate design of the electrochemical cell. Well defined quantitative results could be obtained by using model electrodes with minimized heterogeneity such as uniform thin film electrodes, and analyzing the results using image processing algorithms to characterize the space-resolved SOC distribution and to decouple the OER contribution.

This work focuses on the image processing and characterization details of operando digital microscopy data crucial for analyzing thin-film nickel hydroxide redox reaction. The working electrode was deposited unto indium tin oxide (ITO)-coated glass substrate by successive ionic layer adsorption and reaction (SILAR), producing dense and uniform nickel hydroxide thin films. Combined with additional microscopic characterization to be done, it could further provide valuable mechanistic insights for the redox reaction in nickel hydroxide-based electrodes.

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Materials for Energy Storage and Conversion

Thermally Conductive Molten Salt for Thermal Energy Storage: Synergistic Effect of a Hybrid Graphite-Graphene Nanoplatelet Filler

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Renewable energy technologies depend, to a large extent, on the efficiency of thermal energy storage (TES) devices. In such storage applications, molten salts constitute an attractive platform due to their thermal and environmentally friendly properties. However, the low thermal conductivity (TC) of these salts (1 W m^{-1} K^{-1}) downgrades the storage kinetics. A commonly used method to enhance TC is the addition of highly conductive carbon-based fillers that form a composite material with molten salt. However, even that enhancement is rather limited (9 W m^{-1} K^{-1}). In this study, the partial exfoliation of graphite to graphene nanoplatelets (GnP) in a molten salt matrix is explored as a means to address this problem. A novel approach of hybrid filler formation directly in the molten salt is used to produce graphite–GnP–salt hybrid composite material. The good dispersion quality of the fillers in the salt matrix facilitates bridging between large graphite particles by the smaller GnP particles, resulting in the formation of a thermally conductive network. The thermal conductivity of the hybrid composite (up to 44 W m^{-1} K^{-1}) is thus enhanced by two orders of magnitude versus that of the pristine salt (0.64 W m^{-1} K^{-1}).

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Materials for Energy Storage and Conversion

Analyzing Dendrite Formation and SEI Composition in All-Solid-State Lithium Metal Batteries under Varying Current Density using Overhauser Dynamic Nuclear Polarization (DNP)

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Lithium-ion batteries (LIBs) are the most efficient portable storage technology. Lithium metal batteries (LMBs) offer a potential tenfold increase in energy density, theoretically reaching 3860 mAh/g. However, lithium reactivity result in limited cycle life, due to the formation of the Solid Electrolyte Interphase (SEI) and lithium dendrites during cycling. The SEI is a heterogeneous nanoscale layer that forms on the anode surface upon reaction with the electrolyte. Dendrites are formed during cycling, leading eventually to short circuit. Understanding the SEI composition and dendrites formation is crucial for improving battery performance.

While traditional LIBs are made with flammable liquid organic solvents, all-solid-state batteries (ASSBs) are safer alternatives, despite their lower conductivity. However, they are still susceptible to SEI and dendrites formation. In this study we investigate dendrite formation and morphology as a function of current density in ASSLMBs. Lithium dendrites typically exhibit mossy structures at low currents and needle-like structures at higher currents1.

Conventional techniques like scanning electron microscopy (SEM) offer insights into the SEI but lack quantitative analysis. Nuclear magnetic resonance (NMR) of 7Li has already proved to be an efficient tool to investigate dendrites growth in a quantitative manner2, although having low sensitivity. Dynamic nuclear polarization (DNP) offers a promising approach to overcome this challenge; by hyperpolarizing lithium in the SEI using conduction electrons of the lithium metal (Overhauser effect3) followed by lithium exchange, DNP enhances the NMR signal, allowing us to characterize the SEI and dendritic components. Symmetric lithium metal coin cells sandwiched with Polyethylene Oxide (PEO) as a solid electrolyte were used as a model. After cycling with increasing current density, DNP of 6Li for PEO displayed a clear trend; enhancement increased with increasing current density indicating more efficient lithium exchange likely due to larger surface area which is suitable for needle-like dendrites. Dendrite quantity also rises with current density as determined from quantitative NMR. SEI peak deconvolution revealed that the SEI is composed of lithium oxide (Li2O) and lithium hydroxide, and additional unknown environments. Additionally, 2D 6Li-6Li measurement was used to determine the formation of a mosaic structure of the SEI, with mixed LiOH and Li2O phases.

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Poster Presentation

Materials for Energy Storage and Conversion

Ionic Conductivity and Phase Stability in the SrF2- Bi2O3 System

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Oxyfluoride type materials are very interesting for their potential as mixed conductors in fuel cells, batteries, thermoelectrics and other applications. Some Oxyfluorides can act as conductors for O2-, F-, e- and h+. Materials based on Bi2O3 are some of the best oxygen ion conductors known. However, ionic conductivity is obtained only above the phase transition temperature which does not allow for use in any real-life applications. One way to mitigate this is to alloy Bi2O3 with an alkali earth oxide such as SrO, CaO or BaO allowing for the formation of the β1 phase which has only slightly lower conductivity but higher stability.

One aspect that was never tested in this system is the effect of F- ion on the system and the phase stability. In this work we compared the effect of SrF2-Bi2O3 replacements for the SrO-Bi2O3 system. SrO or SrF2 powders were mixed with Bi2O3 to create compositions from 9:1 to 1:6 ratio of Bi2O3:SrO/SrF2. The different compositions were pressed into 13mm pellets under 60MPa and heat treated at 800°C for 350 hours resulting in pellets for conductivity measurements. The pellets were tested using x-ray diffraction (XRD) and then plated with platinum and measured using electrochemical impedance spectroscopy (EIS) in air and Ar to determine the ionic conductivity of the samples.

With the SrF2-Bi2O3 type compositions only β1 and SrF2 were identified as stable phases as opposed to the many phases stable in the SrO-Bi2O3 system. In addition, EIS results in air and in argon show that replacing O with F increases the bulk conductivity of the materials. However, it also lowers the overall performance due to lower catalytic activity for oxygen reduction. This might be mitigated by using a proper cathode instead of platinum paste. In this work we will describe in detail these results and show the effects of F- replacement of these materials.

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Quantification of Mobile Charge Carrier Yield and Spatial Collection Efficiency in Ultrathin Film Light-trapping $ZnFe_2O_4$ Photoanode

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The search for ideal semiconducting materials that use solar energy for photoelectrochemical (PEC) water splitting is a critical challenge. $ZnFe_2O_4$ (ZFO) has emerged as an attractive photoanode candidate material because it possesses strong absorption capability within the visible region (Eg~2.1 eV) and possesses long term photostability in aqueous solutions. However, due to poor charge transport properties, nanostructured thin films are typically used to improve charge extraction efficiency. Here, we take a different approach and fabricate compact ultrathin (8-14 nm) Ti-doped ZFO (Ti:ZFO) films by pulsed laser deposition on a specular back reflector (Ag coated Mica) to boost photoanode performance through enhanced light trapping by strong optical interference, resulting in a roughly fourfold improvement in photocurrent density as compared to similar films deposited on transparent substrates. The HR-XRD (θ-2θ, rocking curve, phi scan) studies confirm the epitaxial nature of all the samples. The PEC measurements performed on these samples shows that our 8 and 10nm films exhibit one of the highest reported photocurrents for planar thin films without a nano-structured morphology. However, the photocurrents still remain far below the theoretical maximum. To further understand this performance gap, external quantum efficiency measurements and detailed optical modelling were performed to extract the wavelength-dependent yield of photogenerated charge carriers and the spatial charge carrier collection profile in the thin films. In spite of the high photo active performance enabled by the light-trapping devices, the results showed that the Ti:ZFO films still suffer from significant charge carrier recombination in the depletion region and a non-unity photogeneration yield across the entire visible spectrum, ultimately limiting the maximal attainable performance of ZFO.

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Materials for Energy Storage and Conversion

Electrochemical Charging of MAX Phases and MXenes as Candidates for Hydrogen Storage Materials

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Hydrogen storage is a pivotal challenge in the transition to renewable energy systems, where hydrogen serves as a clean and efficient energy carrier. However, many current storage materials – such as metal hydrides, porous carbons, and metal-organic frameworks (MOFs) – not only require extreme conditions like high temperatures, but can also involve energy-intensive synthesis methods and non-sustainable raw materials. MAX phases and their two-dimensional derivatives, MXenes, offer a promising alternative due to their unique layered structures, which provide multiple hydrogen trapping sites, including interstitial spaces between carbide layers, interlayer regions between MXene sheets, and surface terminations. Their ability to store and release hydrogen under milder conditions – while retaining structural integrity – positions them as strong candidates for practical hydrogen storage applications. Although theoretical studies have suggested their potential, experimental research on MAX phases and MXenes remains in its early stages. Thus far no studies have investigated electrochemical charging of these materials, the hydrogen diffusion mechanism, and the effect of hydrogenation on their properties. Herein, we address this gap by a first demonstration of electrochemically charged MAX phases and MXenes, showcasing associated challenges and hydrogen storage capabilities. To characterize hydrogen trapping behavior and microstructural effects, a combination of advanced techniques were employed, including hydrogen charging, thermal desorption spectroscopy (TDS), Kelvin probe (KP), in-situ X-ray diffraction (XRD), and scanning electron microscopy (SEM). Gaining a deeper understanding of hydrogen permeation and trapping mechanisms can pave the way for the development of sustainable hydrogen storage technologies for future energy systems.

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Materials for Energy Storage and Conversion

The Effects of High Temperature Compression on the Physical and Mechanical Behavior of the Thermoelectric GeTe Alloy

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The shortage of mechanical characterization studies on thermoelectric (TE) materials is one of the major setbacks in achieving a higher technological readiness level for thermoelectric generators (TEGs). GeTe is a base alloy for forming a series of efficient TE materials in the 200 ÷ 500ºC temperature range, which have been intensively investigated and successfully applied in several TEGs.

This study is innovative in this respect, for focusing on the mechanical behavior of the GeTe alloy under compression tests conducted at ambient to high temperatures. This study also incorporated extensive electron microscopy and crystallographic characterization methods. It revealed a unique microstructure modification, resulting in a brittle to ductile transition and a significant reduction in the materials` mechanical properties, at temperature of ~260°C - well within the expected service temperature range of the TEG.

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Materials for Energy Storage and Conversion

Enhanced Proton Conduction in Zwitterionic Peptide Assemblies

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Proton transfer (PT) is fundamental to both biological processes and electrochemical devices. In living systems, PT powers ATP synthesis, while in devices like fuel cells, batteries, and sensors, it facilitates efficient charge transport and energy production. Inspired by natural PT mechanisms, proteins and peptides have emerged as promising candidates for preparing proton-conducting materials, offering biocompatibility, efficiency, and stability. These bioinspired materials show great potential for advancing bioelectronics and nanotechnology applications. Previous findings from our lab demonstrated that anionic functional groups enhance the water-mediated proton conductivity of self-assembled peptide structures. In the current work, we study zwitterionic peptide design, hypothesizing it will produce superior proton conductivity due to salt-bridge interactions between charged side chains. In particular, we compare the functional behavior of a zwitterionic sequence to its cationic and anionic counterparts—under both hydrated and dry conditions.

Our studies show that the zwitterionic peptide assembles into stable nanotubes under a broad concentration range between 50 µM and 2 mM in water, in contrast to a limited assembly concentration range, under 100 µM, for the cationic peptides. Differences in fibrillar diameter were found with ~ 2, 4, and 6 nm diameters for the cationic, anionic, and zwitterionic fibrils, respectively. The zwitterionic peptide achieves superior proton conductivity, particularly at high relative humidity, showing a two-orders of magnitude increase in conductivity compared to the anionic peptides. With its superior temporal stability, enhanced electrical performance, and inherent biocompatibility, the zwitterionic peptide shows great potential as a bioinspired, proton-conducting material for advanced applications in bioelectronics.

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Materials for Energy Storage and Conversion

Possible Bond Character Effect on Self-healing Properties for Sustainable Energy Conversion

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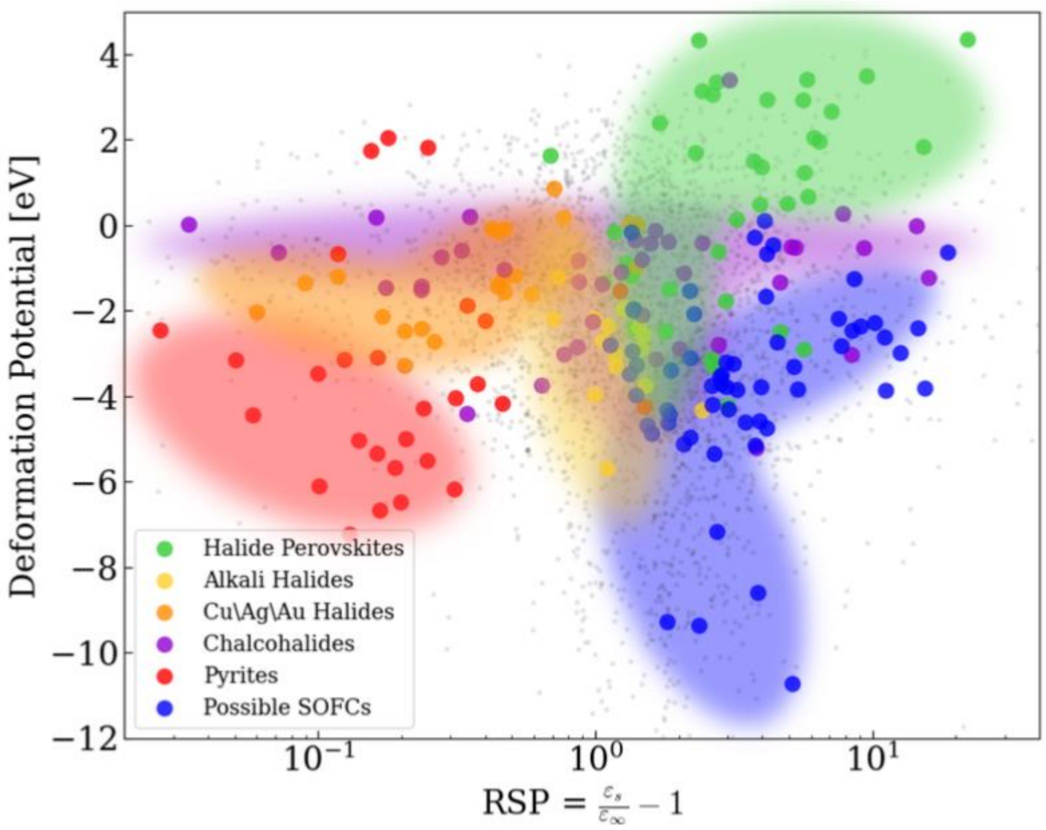
The sustainability of materials used for energy generation and storage highly depends on their ability to self-heal from mechanical and thermal damage. Self-healing of said materials occurs through a variety of different mechanisms, such as dynamic disorder in halide perovskites[1], ionic conductivity in solid oxide fuel cells (SOFCs)[2] and CIGS[3], and photo-induced pathways as found in certain chalcohalides[4]. Although this property is very important in many applications, there are no known physical or chemical rules that can be used to predict the self-healing abilities and mechanism of a material.

This work describes a data-driven approach to find parameters that affect the self-healing mechanism in different materials. We use data mining of experimental and computational data from the Materials Platform for Data Science (MPDS) database, Materials Project, and other sources to look for four bond character related parameters: (i) deformation potential, (ii) relative structural polarizability (RSP), (iii) Pauling’s ionicity and (iv) microhardness. Clusters and trends of these bond characteristics are presented for several material classes with known self-healing properties, and are thus, associated to different mechanisms.

From the trends and clusters, we derive that materials with positive deformation potential and high RSP values tend to exhibit dynamic disorder self-healing. Similar RSP values with negative deformation potentials are associated with photo-induced dynamic disorder. On the other hand, RSP values around 1 are attributed to ionic conductors such as SOFCs, and no correlation with the forming elements is observed. Microhardness can be correlated with Pauling’s ionicity and RSP values to emphasize the bond effects on the self-healing mechanism. The results shown in this work present preliminary steps in the understanding of the self-healing process, which can direct the search of sustainable self-healing materials for energy uses.



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Poster Presentation

Materials for Energy Storage and Conversion

Towards Eco-Friendly Batteries: Using Advanced Natural Polymer-Based Binders for Carbonaceous Li-Ion Anodes

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The ongoing pursuit of high-energy and high-power density batteries is driving the development of new strategies to enhance the performance of lithium-ion batteries (LIBs). LIBs are electrochemical systems, and their performance is heavily influenced by the components involved, including the electrolyte composition, active materials, separators, and, notably, the binders. The most commonly used binder in the industry is polyvinylidene fluoride (PVDF). However, the solvent used to dissolve PVDF, N-Methyl-2-pyrrolidone (NMP) is toxic and volatile[1,2]. As a result, there is a strong need for the development of more sustainable binders that enable high-capacity energy storage, while being safe and environmentally friendly.

In our research, we have explored protein-based bovine serum albumin (BSA)[3], and a combination of styrene-butadiene rubber (SBR) and sodium carboxymethyl cellulose (CMC) as potential binders for LIBs. Our goal was to develop advanced, eco-friendly, low-cost binders with strong adhesion and high stability, which could enhance performance during battery cycling. The electrode preparation using these innovative binders involved an atypical thermal treatment ("baking") that induced structural transformation.

We studied the impact of these advanced binders on battery performance using various methods, including FTIR, TGA, BET, and several electrochemical techniques such as cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic measurements. We found that thermal treatment of the binders at temperatures above 120°C removed any tightly bound water, which is detrimental to LIB performance. While new chemical bonds were formed in both MCMB-BSA and MCMB-CMC/SBR, the primary covalent structure of these binders remained intact.

The use of these "baked" advanced binders, which improve reversible and repeated Li-ion transport, can reduce irreversible capacity losses, increase energy storage capacity, and provide uniform protection. Additionally, these natural polymer-based materials offer environmental benefits, as they can be safely degraded upon disposal[4].

Acknowledgments:

This work was supported by the Israel National Institute for Energy Storage (INIES) and by the Grand Technion Energy Program (GTEP).

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The Stability and Performance of Bi2O2Te for Thermoelectric Applications

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Thermoelectric materials are a promising method for energy recovery applications drawing energy from waste heat. One of the widely applied thermoelectric materials in the field is Bi2Te3, exhibiting high thermoelectric performance. New studies on Bi2O2Te show some potential of reducing the amount of tellurium in the system and replacing most of it with Bi2O3 which is low cost, non-toxic and highly stable. Bi2OxTe3-x has emerged as an interesting compound in the field of thermoelectric materials. However, the synthesis process, phase stability and processing conditions have not been thoroughly studied yet. This research aims to enhance the stabilization of Bi2OxTe3-x through optimized thermal processing techniques and enhancing his thermoelectric properties. The major method was using CuO to stabilize the partial oxygen pressure in the system. Lower pressures reduce the concentration of bismuth oxide, while higher pressures oxidize Bi2Te3. Electronic properties characterization of the material revealed n-type semiconducting properties, with a notable transition from extrinsic to intrinsic charge carrier behavior occurring around 350°C. Surprisingly both the electrical conductivity and the thermal conductivity remained relatively stable between 100-500°C. This in contrasts with previous publications showing a highly semiconducting behavior. Previous publications have only reported thermoelectric transport properties values up -to 300°C, exhibiting maximal thermoelectric figure of merit, ZT, values of up to approximately 0.15 at this temperature. In contrast, our results have shown a maximal- ZT of 0.27 at 520°C for undoped material. In the presentation we will show thermoelectric performance of undoped and doped Bi2O2Te, aiming to optimize the thermoelectric properties.

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Solid-state Synthesis of High-entropy Oxides for Use as Electrochemical Catalysts in Electrochemical Cells

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The growing demand for renewable energy and sustainable living has spurred extensive research into green energy technologies. Among these, water splitting to produce green hydrogen is a promising method for generating clean energy. However, the process faces significant thermodynamic and kinetic challenges, particularly in the oxygen evolution reaction (OER), which is the rate-limiting step. To enhance OER efficiency, catalysts are essential. While metal oxides like ruthenium oxide and iridium oxide exhibit excellent catalytic properties, their high costs and limited availability hinder widespread adoption.

High-entropy oxides (HEOs) have emerged as a novel class of materials for catalytic applications, offering the ability to integrate five or more metals into a single crystalline structure which is thermodynamically stabilized by high entropy. This unique composition enables tunable catalytic properties due to the presence of different active sites on the surface, which can adsorb reactants, providing a cost-effective and sustainable alternative.

Our study focuses on the solid-state synthesis of a high-entropy oxide $(Cu_{0.2}Co_{0.2}Mg_{0.2}Ni_{0.2}Zn_{0.2})O$ for use as a catalyst in electrochemical cells. The research aimed to achieve a material with a single-phase structure with equal molar ratios of the constituent binary metal oxides, which can be used as electro-catalysts in electrochemical cells for water electrolysis. Two synthesis methods were explored: (1) Preparing a pellet from a homogeneous powder mixture of the oxides, then sintering in a high-temperature oven. (2) Preparing electrodes coated with the metal oxide mixture, which underwent rapid heating using photon curing. The pellet-based synthesis successfully achieved a single-phase HEO in rock-salt structure, while the photon-curing method achieved a mixture of oxide phases and the HEO phase. Nevertheless, the electrodes prepared using the latter approach were employed in an electrochemical cell for preliminary OER testing. Initial results demonstrated comparable performances as known electrodes comprising binary oxides and the HEO mixture.

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Nickel-doping Strategy for Perovskite Anodes toward High-performance Ammonia-fueled Solid Oxide Fuel Cells

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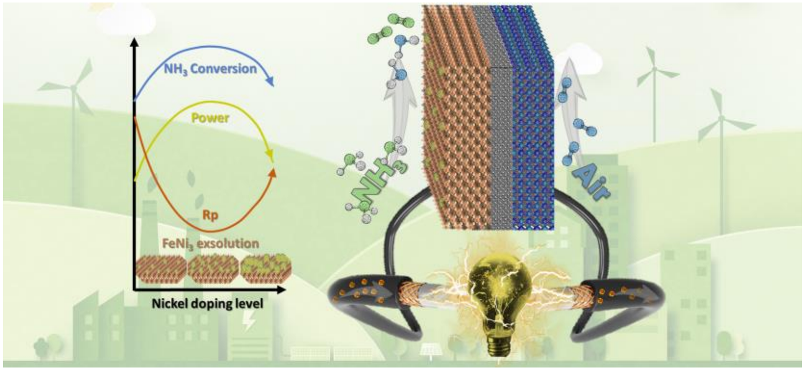
The use of ammonia as a carbon-free hydrogen carrier in solid oxide fuel cells (SOFCs) presents a sustainable pathway for energy conversion [1,2]. This research focuses on the development of Ni-doped $Sr_{1.9}Fe_{1.5-x}Ni_xMo_{0.5}O_{6-\delta}$ (SFNM) perovskite anodes with exsolved $FeNi_3$ nanoparticles to enhance catalytic performance and electrochemical properties under direct ammonia feed. Nickel doping plays a pivotal role in optimizing the structural, morphological, and catalytic properties of SFNM anodes. By varying the Ni content ($x = 0.1, 0.2, 0.3$), the study identifies an optimal doping level (SFNM2, $x = 0.2$) that achieves a balance between nanoparticle dispersion and catalytic activity. The SFNM2 anode demonstrated exceptional performance with a peak power density of 516 $mW \cdot cm^{-2}$ at 800 °C, ammonia conversion efficiency of 99.6%, and a low polarization resistance of 0.15 $\Omega \cdot cm^2$.

This success is attributed to the in-situ exsolution of $FeNi_3$ nanoparticles, which provide abundant active sites for ammonia decomposition and hydrogen oxidation [3]. Electron microscopy and X-ray diffraction analyses revealed that the uniformly dispersed nanoparticles in SFNM2 minimize particle aggregation and maintain structural integrity under operational conditions. Electrochemical impedance spectroscopy further highlighted SFNM2's superior low-temperature performance, with reduced area-specific resistance and enhanced reaction kinetics. The findings underline the effectiveness of Ni-doped SFNM anodes in overcoming challenges associated with conventional deposition techniques, such as catalyst agglomeration and deactivation. Moreover, this study provides a roadmap for tailoring electrode microstructures to optimize both performance and stability in ammonia-fueled SOFCs. The work advances the integration of Ni-doped perovskites in sustainable energy technologies, offering a practical and efficient solution for direct ammonia utilization.



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Materials for Energy Storage and Conversion

Hydrogen Release Kinetics in Thermolysis of Commercial Magnesium Hydride

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Hydrogen is a promising energy carrier for reducing carbon emissions due to its high energy density and water-only by-product.

However, effective hydrogen storage remains a significant challenge, with metal hydrides such as magnesium hydride (MgH_2) offering a viable solution.

A critical obstacle is the demand of hydrogen desorption from MgH_2 at temperatures of under 100 degrees Celsius. To address this, we investigated the hydrogen release mechanism of commercial MgH_2 powder through thermolysis, employing advanced techniques to analyse the desorption steps kinetics, in attempt to identify a rate determining step.

Our study pinpoints four distinct stages in the desorption process of the pristine MgH_2, starting with a temperature depended delayed activation step which is exclusively found in commercial MgH_2. Understanding the causes for this delayed activation step may assist in finding a possible key to the sluggish thermolysis of pristine commercial MgH_2.

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Biphasic Electrolytic Process for Generation of Green Hydrogen and Value-added Chemicals

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Generation of hydrogen gas by water electrolysis is important for the energy transition and decarbonization of various industrial processes. In water electrolysis, water is decomposed by electricity into oxygen gas at the anode ($H_2O \rightarrow O_2 + 4H^+ + 4e^-$, $E_0 = +1.23$ V at pH 0) and hydrogen gas at the cathode ($2H^+ + 2e^- \rightarrow H_2$, $E_0 = 0$ V at pH 0). However, oxygen gas is a low value product and the oxygen evolution reaction has sluggish kinetics, which decreases the electrolytic efficiency with typically 300-500 mV overpotential and results in increasing the cost of hydrogen production by water electrolysis. Another challenge of hydrogen production by water electrolysis is that this process conventionally requires the use of expensive membranes in order to separate the hydrogen gas and oxygen gas for safe operation.

The use of aqueous bromide solution can replace the oxygen evolution reaction by bromine evolution reaction for enhancing the kinetics of hydrogen gas production because it has lower driving force when converted to bromine, $2Br^- \rightarrow Br_2 + 2e^-$ ($E_0 = +1.09$ V at pH 0), compared to oxygen evolution ($E_0 = +1.23$ V at pH 0). A biphasic electrolyzer with water and immiscible organic solvent (heavier than water) is proposed to enhance the phase separation and collect the bromine for subsequent reactions with organic molecules. This leads the way to various chemical processes that use bromine, such as bromination, alcohol oxidation, hypobromous acid production for further epoxidation, and more.

Our biphasic electrolyzer produces hydrogen gas and bromine products with higher value in comparison to conventional water electrolyzers that generate hydrogen and oxygen gas products. In result of electrolysis, both hydrogen and bromine evolution reactions showcased high Faradaic efficiency of 96±5% at ampere-level current density. The subsequent bromination using toluene as substrate demonstrated 100% selectivity and 93±7% yield. These promising results provide alternatives to upgrade the use of electrolyzer for both green hydrogen fuel, as well as high-value chemicals.

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Mixed Phase TiO2 Nanowire Array Substrate to Enhance Hydrogen Evolution Activity of Ru Nanoparticles in Near-neutral Electrolyte

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Green hydrogen is a major candidate for a sustainable energy carrier and an important reagent for industrial chemicals and engineering materials such as ammonia synthesis and metals refining. Water electrolysis driven by renewable electricity offers great promises for green hydrogen production, which is expected to reach to 34 Mt per year by 2030 and ~10% of the global energy market by 2050 in order to meet governments` climate pledges.

A recent approach to address the drawbacks of highly acidic/alkaline electrolytes is the use of neutral or near-neutral electrolytes (pH = 5-9) for hydrogen evolution reaction (HER), which have significant advantages: (1) They are less corrosive, thus can minimize electrolyzer and catalyst corrosion and increase stability; (2) Electrocatalysts do not require to be stable in highly acidic/alkaline solution, which significantly expands the variety of suitable materials; (3) Cell stacks employed in neutral electrolyte are safer to use, and can be made of abundant materials; (4) It is potentially feasible to directly split seawater (pH 8) which may reduce the cost of industrial-scale hydrogen production and increase its feasibility in coastal arid zones. However, near-neutral electrolyte, due to its low proton concentration, makes a challenging environment for hydrogen evolution reaction, even for platinum-group-metal (PGM) based electrocatalysts.

Recently, electrochemical – chemical cycle for decoupled water electrolysis was developed by our group, presenting a proof of concept (POC) using a near-neutral NaBr electrolyte. In this process the bromide/bromate cycle divides the OER into two stages, without the challenges arising from the use of a membrane and the expensive construction required of conventional electrolysis that burden the production cost of green hydrogen. This approach obtained highly efficient decoupled water electrolysis in buffered NaBr electrolyte (pH=8) with continuous hydrogen and oxygen production. However, the POC employed a platinum foil as cathode material that must be replaced by a PGM-free or low-PGM cathode to make this process scalable.

In this study, we demonstrate that employing a TiO2(B)/Anatase mixed-phase nanowire array substrate enhances the catalytic activity of the Ru catalyst by up to 3x in a near-neutral electrolyte. This approach results in a highly active and durable electrode, capable of sustaining over 100 hours of electrolysis, with micro-loading of Ru metal.

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Eletrochemical Bubble Release from Tunable Porous Carbons

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Fuel cells and electrolyzers hold great promise as sustainable energy storage technologies, utilizing redox reactions at the anode and cathode for energy storage. However, they are hindered by several challenges such as low power density, costly catalysts, and bubble poisoning. Bubble poisoning, caused by gas generation during electrochemical reactions, results in bubble adhesion to electrode surfaces, reducing the active surface area, impairing mass transfer, and limiting the exposure of catalytic sites.

Porous electrode structures are a promising strategy to mitigate bubble poisoning. Their effectiveness depends on parameters such as pore size distribution, surface area, and tortuosity. Nevertheless, cracking the link between porous structure and bubble mitigation is not simple, as many variables come to play at the bubble release dynamics.

To address this, we synthesized N-doped carbons using a hard-template method with acrylonitrile as a carbon precursor, and silica spheres as template, changing only the pore sizes (40, 80, 120, and 200 nm) . By decoupling pore size from other structural parameters, we systematically investigated the relationship between pore size and bubble poisining.

The materials were characterized using scanning electron microscopy (SEM), nitrogen adsorption, and Raman spectroscopy. Bubbles were formed using hydrazine oxidatiob and hydrogen evolution reactions, with both voltammetry and amperometry methods. Bubble behavior was further analyzed via photographic imaging in three-electrode setups, revealing a clear trend between pore size and bubble release dynamics.

Our findings provide fundamental insights into the role of pore size in electrochemical gas generation, paving the way for the rational design of porous electrodes to optimize performance in fuel cells and electrolyzers.

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Cathode Composite Engineering for High-Energy Sulfide-Based All-Solid-State Lithium Batteries

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All-solid-state batteries (ASSBs) employing solid electrolytes (SEs) are considered promising candidates for next-generation energy storage systems due to their superior safety, higher energy density, and simplified packing design. Among the various types of inorganic SEs such as oxides, sulfides, and halides, sulfide SEs stand out for their exceptional ionic conductivity, easy processability, and superior formability. However, the practical application of ASSBs encounters significant obstacles, including interfacial degradation, poor electrochemical stability, and lithium dendrite penetration. Further, achieving compatibility among the cell components remains challenging. In this research, we address these challenges by careful engineering of the cathode composite structure featuring a single-crystal $LiNi_xCo_yMn_{1-x-y}O_2$ (NCM) cathode to eliminate intergranular cracking associated with volume changes and mechanical instability. We demonstrate high performance achieved on such ASSB cells incorporating a pristine single-crystal $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (SC-NCM811), a Li_6PS_5Br (LPSB) SE, and a Li-In alloy anode, delivering a high discharge capacity of ~190 mAh/g at C/5. By conducting comparative studies on polycrystalline and single-crystal NCM811 composite cathodes, we reveal the working mechanism that enables enhanced cycling stability in the latter design. This work emphasizes the critical role of optimizing cathode composite structures and provides key insights for advancing the development of better-performing ASSB cells.

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Pt Single-Atom Catalysis in Carbon Nanotubes as a Platform for Confinement Limited Electrocatalysis

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Nanoconfinement of electrocatalytic reactions offers a powerful approach to modulate reaction kinetics. The extent of confinement significantly influences electronic properties, mass transport parameters, and disrupts the scaling laws governing surface activity in electrocatalysis. In this study, we designed a highly confined system to investigate the effects of nanoconfinement on the hydrogen oxidation reaction (HOR) in an alkaline medium. Carbon nanotubes (CNTs) with an inner diameter of 14 Å were employed to encapsulate Pt single-atom catalysts (SACs). The confinement resulted in slower HOR kinetics in alkaline conditions, evidenced by a higher overpotential for Pt SAC within the CNT compared to its non-confined counterpart. This effect diminished with larger-diameter CNTs. Notably, nanoconfinement did not impact HOR kinetics in acidic media for any of the catalysts tested. The observed alkaline-specific behavior is attributed to mass transport limitations of OH^- within the 14 Å CNT, which influence the Heyrovsky rate-determining step. Density functional theory calculations further corroborated the energy barrier for OH^- diffusion inside the CNT.

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Influence of Doping on Mobile Charge Carrier Generation and Collection in Hematite Photoanodes for Solar Fuel Production

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Transition metal oxides are the leading candidates for photoelectrochemical solar hydrogen production, chief among them hematite (α-Fe_2O_3) due to its non-toxicity, abundance, stability in alkaline conditions and suitable bandgap (~2 eV). However, hematite suffers from poor charge transport properties, resulting in extremely short charge carrier diffusion lengths, lowering device efficiency. Furthermore, open d-shell materials like hematite exhibit non-unity photogeneration yield (PGY) due to the existence of ligand field states, meaning that not every absorbed photon generates a mobile electron-hole pair. Doping hematite has been shown to improve the photocurrent produced by hematite-based devices, but the nature of this effect is still under debate. In some cases, doping has been suggested to reduce transport losses and enhance the spatial collection efficiency (SCE) of charge carriers while in other cases doping has been suggested to minimize losses resulting from non-unity PGY. However, since PGY and SCE losses are coupled in conventional photoelectrochemical characterization methods, it is difficult to assess how doping affects each loss mechanism individually. In this work, we present a novel analysis technique to decouple PGY and SCE losses in planar thin films with minimal a priori assumptions to shed light on the effect of doping in hematite. Initially, hematite thin film photoanodes with varying dopant concentrations were prepared using pulsed laser deposition. The optical constants of the thin films were extracted via spectroscopic ellipsometry, and transfer matrix method simulations were then used to model their optical response. Using these optical simulations and measured incident photon-to-electron conversion efficiency (IPCE) data, an algorithm was developed to extract the PGY and SCE from the experimental inputs, leading to insight into how doping affects transport and photogeneration losses in hematite photoanodes.

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Investigation of the Surface Processes and Kinetics of the First Hydrogenation of Pure Mg Chips

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This study investigates the potential of Mg chips, produced via a mechanical chipping method in air, as hydrogen storage materials. Surface analysis of the outermost layers of the Mg chips, conducted before and after activation procedures, reveal critical insights into the surface reactions and thermal processes occurring during the first hydrogen absorption in pure Mg. X-ray photoelectron spectroscopy (XPS) analysis shows that the surface layer of the Mg chips is composed mainly by MgCO3 and some MgO. After heating the Mg chips to 300 °C for 3 hours under vacuum, the surface layer consists of MgO and metallic Mg. We show that spontaneous decomposition of MgCO3 into MgO and CO2 occurs at these conditions. We further assume, in agreement with observations by Bloch et al [1]., that surface oxygen diffuses into the metal, while metallic Mg ions migrate towards the surface. Thus, the emergence of active Mg sites on the surface enables the initiation of hydrogen absorption.

The first hydrogen absorption kinetics are characterized by a low-dimensional nucleation and growth mechanism. Apparent activation energies for hydrogen absorption and desorption, derived using the Avrami and Kissinger equations, are in accord with reported values for absorption and are notably lower than those for desorption. This work demonstrates that mechanical chipping in air offers a simpler alternative to ball milling for producing Mg chips for hydrogen storage applications, although an activation step is required prior to hydrogenation.

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Tuning the Physical Properties of Crystals via the Incorporation of Organic Molecules

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The incorporation of organic macromolecules into the lattice of inorganic hosts is one of nature's strategies for enhancing the mechanical properties of crystals. In this case, the biomacromolecules act as barriers for crack propagation.

Recently, our lab expanded the concept of amino acid incorporation into a variety of crystal hosts and investigated their effect on different materials properties. For instance, it was demonstrated that the inorganic crystal $MnCO_3$ can be synthetically synthesized with incorporated individual amino acids, enabling fine-tuning of the mineral`s magnetic properties. In this case, the incorporation of aspartic acid led to an increase of magnetic susceptibility at low temperatures and lowered the Neel's phase transformation temperature.

Our lab has also expanded the amino acid incorporation concept to hybrid organic-inorganic perovskites (HOIPs), a family of semiconducting materials that have emerged as extremely promising for solar energy applications. Lysine was successfully incorporated into lead halide perovskite $MAPbBr_3$ through a bio-inspired molecular bridging, enhancing the crystal stability under humid conditions and enabling the tuning of the optical and thermal properties. Moreover, it was recently demonstrated that lysine incorporation into $MAPbBr_3$ also hinders post-synthetic halide exchange, a process that degrades sharp interfaces of all-perovskites heterostructures needed in optoelectronic applications.

Following these findings, we will further investigate the effects of amino acid incorporation into different material systems. As a first case study, we will examine materials with contrasting magnetic properties. We will explore how amino acids influence their structural characteristics, including grain size and morphology, and how these factors affect the magnetic properties of the host lattice. Additionally, we will discuss the stabilization of different material phases in the presence of specific amino acids.

As a second case study, we will focus on the challenging synthesis of mixed-halide perovskite crystals of micrometric size and their non-trivial isolation. We will examine how amino acid incorporation impacts their stability under external stimuli and its potential role in mitigating processes that reduce efficiency in energy-related applications.

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Poster Presentation

Materials for Energy Storage and Conversion

Design and Performance of Pt_3Ni and PtCu Nanocrystals as Electrocatalysts for Oxygen Reduction Reaction in Acidic Medium

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This study explores the synthesis and performance of Pt-based nanoparticles (NPs) as electrocatalysts for the oxygen reduction reaction (ORR) in proton exchange membrane fuel cells. Pt3Ni and PtCu nanocrystals are synthesized with controlled morphologies—octahedral Pt3Ni with a Pt-enriched shell and cuboctahedral PtCu with a Pt skin—by tuning experimental parameters. Characterization techniques, including X-ray diffraction (XRD), transmission electron microscopy (TEM), and inductively coupled plasma (ICP) analysis, are used to assess particle structure and composition, while rotating disk electrode (RDE) measurements evaluate their electrocatalytic activity. The study highlights the superior ORR performance of Pt3Ni and PtCu nanocrystals with exposed Pt-rich {111} crystallographic planes, with both types of NPs exhibiting a Pt skin that enhances catalytic efficiency. Additionally, a systematic investigation of PtCu octahedral NP synthesis reveals the influence of synthesis duration on Pt-skin evolution and copper dealloying, providing valuable insights into the degradation mechanism. The optimized PtCu-48 sample (48 is synthesis time in hours) demonstrates enhanced stability after 10,000 cyclic voltammetry scans, offering important guidance for developing more stable and efficient electrocatalysts.

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Poster Presentation

Materials for Energy Storage and Conversion

Composition and Microstructure Effects on the Hydrogen Desorption Temperature and Storage Capacity of Ti_xZr_{1-x} Thin Films

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Metal hydrides (MH_x) provide a promising solution for a future hydrogen-based energy system due to their high hydrogen storage density and safety advantages compared to compressed or liquefied hydrogen. However, so far, current hydrogen storage materials lack the requirements in one or more of capacity, absorption/desorption temperature and pressure, fast kinetics or cost. Thin films were proposed to ease the absorption/desorption cycles by maximizing the surface-to-volume ratio. Moreover, thin films can be used as a model to develop new metal compositions. In this paper, we study the relationships between microstructure and composition of Ti_xZr_{1-x} thin films, in order to reduce the absorption/desorption temperature and to increase the rate and absorbed hydrogen volume. To achieve this goal, a series of Ti, Zr and Ti_xZr_{1-x} thin films were deposited, on copper and silicon substrate, using pulsed-DC co-sputtering magnetron apparatus. The microstructure was controlled by changing the substrate bias voltage, while the composition was controlled by adjusting the power ratio of the Zr and Ti targets. The thin film`s hydrogenation was conducted as follows: The samples were held at 350°C under vacuum ($5x10^{-3}$ Pa) for 1 hr for surface activation, then the chamber was filled with pure hydrogen to $9.6\pm0.1x10^4$ Pa. The samples were held under H_2 for up to 6 hours at 350°C before the chamber was evacuated and cooled down. Temperature-Programmed Desorption (TPD), Glow Discharge Spectroscopy (GDS), XRD and electron microscopy were used to study the microstructure of the films, hydrogen storage capacity, desorption temperature, and the durability for multiple absorption/desorption cycles. When deposited on copper substrate, TiHx thin films showed a desorption temperature of 320-360°C, which was lower by ~150°C and ~200ºC, compared to dense TiHx thin films and TiH2 powder, respectively. However, the puros TiH_x thin film had 25% less hydrogen stored. Moreover, this microstructure effect was not found in thin films deposited on Si substrates. The composition of Ti_xZr_{1-x} thin films had also an effect on the desorption temperature and thin films with compositions of $Ti_{50}Zr_{50}H_x$ and $Ti_{75}Zr_{25}H_x$ showed hydrogen desorption onset temperatures lowered than TiH2. These preliminary results show the ability of both microstructure and composition to control the properties of hydrogen storage materials.

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Poster Presentation

Mechanical Properties and Failure

Enhancing Fatigue Resistance and Fatigue Limit of SLM PH 15-5 Stainless Steel Using Hot Isostatic Pressing Process

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Additive Manufacturing (AM) is a transformative fabrication technology enabling the layer-by-layer construction of components via selective material deposition. This process involves slicing the desired geometry into discrete two-dimensional layers, which are sequentially deposited to build the part additively. Unlike traditional manufacturing, AM eliminates the need for material removal or mold creation, offering unparalleled design flexibility. The technology has been successfully extended to metallic materials, employing methods such as selective rastering of metal powders using laser or electron beams to form a liquid melt pool which allows for the production of fully dense parts with strong interlayer bonds.

This study focuses on AM using the Selective Laser Melting (SLM) technique applied to PH 15-5 stainless steel, a precipitation-hardened alloy known for its exceptional mechanical properties and corrosion resistance across a range of temperatures. Widely used in aerospace, medical, chemical, and other engineering applications, this alloy`s quasi-static mechanical properties produced by SLM have been extensively characterized and are comparable to those of wrought materials. However, engineering components often fail due to cyclic loading rather than quasi-static conditions, and a critical barrier to the adoption of SLM parts in structural applications is the lack of comprehensive fatigue data. Additionally, AM processes inherently introduce defects such as Lack of Fusion (LOF), porosity, inclusions, microstructural inhomogeneities, anisotropy in mechanical properties, and residual stresses, which significantly compromise fatigue performance.

This research investigates the fatigue behavior of SLM-fabricated 15-5 PH stainless steel with and without Hot Isostatic Pressing (HIP) treatment, comparing results to wrought material. The HIP process, conducted at 100 MPa and 200 MPa at 1081°C, effectively mitigates porosity and other defects, enhancing ductility, fatigue resistance, and overall material quality. Fatigue testing was performed primarily in the high-cycle fatigue regime (107 cycles), with stress amplitudes set at 50% of the ultimate tensile strength of the as-built material (700 MPa). Hourglass-shaped specimens, oriented along the Z-axis, were tested under load control using a computerized electro-resonance machine. Microstructural and fractographic analyses were conducted using scanning electron microscopy (SEM) to examine quasi-static and cyclic fracture mechanisms, including rosette-type fractures, fish-eye features associated with internal defects, and fatigue striations.

The results demonstrate a significant enhancement in fatigue resistance and an elevated fatigue limit following HIP treatment, as observed in the S-N curve. While the fatigue performance of SLM specimens remains inferior to their wrought counterparts, the gap narrows substantially with HIP.

Additionally, fatigue damage progression was monitored through changes in resonance frequency, providing insights into damage initiation and propagation phases.

This study highlights the critical role of integrating advanced mechanical testing with innovative characterization techniques to address fundamental and practical challenges in AM. The findings contribute to the broader understanding of AM alloy behavior and support the safe incorporation of AM-fabricated components into critical load-bearing applications.

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Poster Presentation

Mechanical Properties and Failure

CoCrFeNiTi0.2 High Entropy Alloy (HEA) vs CoCrFeNi Medium Entropy Alloy (MEA): Microstructure, Mechanical Properties and Hydrogen Embrittlement

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CoCrFeNi-based High Entropy Alloys (HEA) have garnered significant attention due to their potential applications as structural materials, which require high ductility, fracture toughness, and resistance to corrosion, irradiation, and hydrogen embrittlement. However, their low tensile strength limits their usage. Precipitation hardening is a mechanism that may help to address this issue. The addition of Ti promotes the precipitation of various phases which can promote the hardening. Following intermetallics can be listed as desired precipitating phases: γ` ($(Ni,Co)_3Ti$-type, Pm m, a = 0.36 nm) and/or η (Ni_3Ti-type, P63/mmc, a = 0.51 nm, c = 0.83 nm). On the other hand, the σ-phase ((Fe,Co)Cr-type, P42/mnm, a = 0.88 nm, c = 0.45 nm) can also precipitate at grain boundaries at certain temperatures, leading to brittleness. To facilitate the use of these HEAs, precise identification of the precipitate type, morphology, and precipitation sequence is required.

In the current research, the CoCrFeNiTi0.2 alloy was thoroughly characterized using electron microscopy, microhardness, and thermal analysis. It was compared to CoCrFeNi (as a γ single-phase reference alloy) that underwent the same thermo-mechanical treatments. Additionally, the mechanical behavior of these alloys, both with and without hydrogen, in different thermo-mechanical states was studied using the Small Punch Test (SPT). Significant differences in mechanical behavior were observed due to the presence of γ` and/or σ phases. Furthermore, it was found that different morphologies of γ` could alter the susceptibility to hydrogen embrittlement.

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Poster Presentation

Mechanical Properties and Failure

Failure Analysis of a Carabiner and Quench Cracking in 7xxx Aluminum Alloys

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This study presents a comprehensive failure analysis of a carabiner that catastrophically failed during a rappelling incident, resulting in serious injury to the user. Through extensive metallurgical investigation, including fracture surface examination, material characterization, reverse engineering of the manufacturing process, and computational analysis, quench cracking in the 7xxx aluminum alloy was identified as the primary failure mechanism.

This phenomenon is extremely rare in aluminum alloys and requires specific conditions for its occurrence—conditions that were unique to the failed carabiner, as demonstrated by the absence of defects in other specimens from the same production batch. By systematically ruling out alternative physical and chemical failure modes, and correlating observed material features with known cases in the literature, we established quench cracking as the most probable cause. A failure mechanism was proposed to explain why this defect manifested uniquely in the failed carabiner. Upon presenting our findings to the manufacturer, they confirmed our conclusions and initiated an internal investigation into their raw material quality control processes. This case highlights the critical implications of manufacturing-induced defects in load-bearing safety equipment and underscores the necessity of stringent quality control measures in high-risk applications.

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Poster Presentation

Nanomaterials

Insight Into the Complex Surface Chemistry of Inorganic Ligand Exchanged Nanocrystals from Solid-State NMR spectroscopy

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Colloidal quantum dot solids (CQDS) are assemblies of quantum dots coalesced into a solid. This unique class of materials offers tuneable optical and electronic properties, making them highly interesting for various applications. Challenges like inefficient charge transport and recombination at quantum dot interfaces hinder device performance, thus requiring precise control over surface ligands and QD-QD interactions. Inorganic ligands have emerged as alternatives to organic ligands, capable of improving conductivity in the resulting CQDSs up to several orders of magnitude. Elucidating the interactions of inorganic ligands with quantum dot surfaces and ligand exchange kinetics requires advanced characterization techniques.

Solid-state NMR spectroscopy provides atomic-level and isotope-specific characterization. Here we used it to investigate ligand exchange processes and surface chemistry in colloidal CdS nanocrystals (NCs). Investigating CdS NCs capped by conventional oleylamine ligands revealed two distinct core phases and two surface environments. Building on this, we explored the ligand exchange process to create CdS NCs capped with phosphoric acid ($CdS–H_3PO_4$). NMR spectra reveal that oleylammonium groups remain and interact with a variety of phosphate species on the nanocrystal surface, suggesting the formation of unexpected oleylammonium phosphate salts. This indicates complex surface chemistry that routine purification procedures and analysis miss.

We also investigated CdS NCs undergoing ligand exchange from oleylamine to selenide ions (Se^{2-}, from Na2Se). Solid-state NMR unraveled multiple ^{23}Na signals, indicating unexpected residual sodium species that reside within the NCs sample with various binding environments. Understanding ligand exchange kinetics, function and coordination of residual metal cations is key for improving synthetic routes to produce high-quality NCs with tailored properties.

This study demonstrates the use of solid-state NMR in unraveling complex surface chemistries in NCs systems and advancing control over CQDSs.

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Poster Presentation

Nanomaterials

Biocompatible Monodispersed Nanohydrogels for Drug Delivery

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Biodegradable synthetic polymeric materials have gained significant attention as promising candidates for sustained drug release, offering distinct advantages in controlled drug delivery applications. This study focuses on the development and synthesis of a novel class of biodegradable, cross-linked, monodispersed nanohydrogels (NHGs) that exhibit a broad range of sizes with low toxicity, making them well-suited for various biological applications. The NHGs were synthesized using an innovative approach, in which a thermo-responsive mixture of monomers undergoes self-assembly, followed by confined polymerization. By precisely controlling the monomer ratios, the size of the intermediate self-assemblies and the final NHGs can be finely tuned within the nanometer scale (20–500 nm). To enhance enhance biodegradability, specialized cross-linkers were introduced into the polymeric backbone. The resulting NHGs exhibit ideal properties for drug delivery, including biocompatibility, high drug loading capacity, controlled release profiles, and potential for targeted delivery. We investigated the application of NHGs as carriers for the antifungal drugs voriconazole and amphotericin B, testing the loaded NHGs against clinical isolates of molds and yeasts. Additionally, in vivo toxicity and efficacy of the drug-loaded NHGs were assessed in murine models with invasive Candida albicans infections. Overall, this study contributes to the expanding field of biodegradable materials and demonstrates the potential of NHGs as versatile platforms for controlled drug release in biomedical research and therapeutic applications.

Keywords: self-assembly; thermo-sensitivity; polymers; biodegradable; nanohydrogels; drug delivery.

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Poster Presentation

Nanomaterials

Solvent-Driven Polymorphism and Growth Dynamics in Supramolecular Crystals

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Supramolecular materials have gained significant attention due to their diverse biological, chemical, and physical properties, which stem from their precise nanoscale arrangements. Achieving control over the solid-state packing and growth dynamics of these materials remains a critical challenge in advancing supramolecular material design. In this study, we investigate solvent-mediated polymorphic transitions within peptide-based supramolecular assemblies, revealing a sharp transition between two distinct crystalline forms. Analyses demonstrate that this transition is dictated by solvent composition, which modulates monomeric conformations and their interactions with crystalline templates. Complementary microfluidics experiments and simulations further elucidate the influence of the solvent environment on assembly pathways, offering a detailed perspective on the underlying mechanisms. Our findings reveal that subtle variations in solvent conditions result in markedly different outcomes, including crystal growth, equilibrium states, or complete disassembly. This work advances the mechanistic understanding of polymorphism and crystal growth in supramolecular systems. By elucidating the role of solvent-mediated dynamics at the molecular level, we provide a framework for the rational design of hierarchical materials with tunable properties, paving the way for innovations in material science and biotechnology.

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Poster Presentation

Nanomaterials

Mechanistic Insights into the Nucleation and Growth of Bimetallic Gold Nano-Stars

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Gold nanoparticles (GNPs) are renowned for their chemical and physical stability, reproducibility, ease of modification, and biocompatibility. Their synthesis through various methods allows for the creation of a wide range of structures, morphologies, and porosities. Bimetallic nanoparticles (BMNPs) represent an advanced class of nanostructures with enhanced technological properties, which vary based on their size, shape, composition, and structure. In particular, gold and silver-based BMNPs are highly valued for their superior sensitivity as surface-enhanced Raman scattering (SERS) substrates, benefiting from the synergistic enhancement of the properties of both elements. The combination of gold with silver and silver chloride (Ag-AgCl) has demonstrated superior absorbance and localized surface plasmon resonance (LSPR) properties compared to Ag-AgCl alone, along with increased stability and reproducibility, making them ideal for use in catalysis and sensing applications.

Gold nanostars (GNSs) are extensively studied for their applications in biosensing, bioimaging, and photothermal therapy, due to their enhanced local optical and electromagnetic properties, particularly in their star-like protrusions. A simple, rapid, and efficient method to produce GNSs is a one-pot, seedless, bottom-up synthesis. This method involves the reduction of HAuCl4 and AgNO3 by ascorbic acid (AA) under acidic conditions, avoiding the use of toxic materials. The final morphology of GNSs depends on several factors, including the gold-to-silver ratio, reaction time, pH, and the AA amount. However, the exact mechanism of GNS synthesis using HAuCl4, AgNO3, and AA is not yet fully understood. It is hypothesized that gold and silver distribute evenly throughout the particles, forming an alloy composition.

In our study, we investigated the complex process of nucleation and growth of these bimetallic GNSs. We focused on the effects of temperature and the timing of silver ion introduction on the morphology, size, particle concentration, stability, and optical properties of the BMNPs. Chemical analysis was conducted using high-angle annular dark-field scanning transmission electron microscopy (HAADF STEM) in a high-resolution transmission electron microscope (HR-TEM), providing detailed insights into the synthesized GNSs. Additionally, synchrotron high-resolution powder X-ray diffraction and other experimental data helped us propose a nucleation and growth mechanism for GNSs. We developed a theoretical model and calculated the energy barriers for nucleation and particle growth.

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Poster Presentation

Nanomaterials

Achieving Polymer-like Quasi-elasticity in Gold Nanoparticles through Chemical Treatment

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Nanoparticles have been the subject of extensive research in recent decades due to their unique properties and applications. In particular, their mechanical properties differ significantly from those of bulk materials. Earlier studies indicated that nanoparticles fabricated by the solid-state dewetting method can, in some cases, reach the theoretical strength of the material they are made of.

We have studied the influence of chemical treatment on the mechanical properties of gold nanoparticles. Our findings indicate that certain treatments result in massively improved elasticity. During the initial stages of deformation the particles reach up to 50% quasi-elastic strain before the onset of plastic deformation, more than twice the strain achieved in pristine gold nanoparticles. Such behavior rivals the elasticity of many polymers while maintaining the ultrahigh strength characteristic to metal nanoparticles.

We propose a model to explain this behavior, suggesting that stacking fault tetrahedra (SFTa) are formed by the agglomeration of vacancies generated by the chemical treatment. These SFTa represent exhaustible dislocation sources which vanish after only a few dislocations are produced during the compression process. The new dislocations cause limited plastic deformation until all the SFTs vanish, after which the particle continues to deform elastically until the onset of strain burst characteristic for plasticity controlled by massive dislocation nucleation.

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Poster Presentation

Nanomaterials

The Strange Case of Ordering Transformation in FePd: A Nanomechanical Enigma

Yarden Flash

What mysteries lie within the tiny world of Iron-Palladium nanoparticles, supported by a sapphire substrate? What complexity does the presence of atomic long-range order bring to small-scale plasticity? As evidence is collected and more clues are revealed, it appears not every intermetallic system plays by the literature rules, and not every nanoparticle is confined to a single phase.

The Fe-Pd alloys exhibit shape memory behavior, unique magnetic anisotropy, high catalytic activity, and capability to absorb atomic hydrogen. These properties are closely related to crystallographic structure and can be manipulated by order-disorder phase transformations. A notable example is the cubic FCC (A1) to the tetragonal L10 (g1) phase transformation in nearly equiatomic Fe-Pd. Reliable characterization and quantification of such an ordering transformation, especially in oriented Fe-Pd nanoparticles on a substrate, proves to be a challenge.

We employed various materials characterization tools – from selected area electron diffraction (SAED), through X-ray diffraction (XRD) and electron backscatter diffraction (EBSD), and all the way to in-situ nano-compression testing – in trying to identify the suspected phases and to piece the puzzle together. We found that multiple ordering domains, tetragonality-induced orientational variants, film-substrate orientation relationships, and dewetting-induced strains can all affect the resulting properties. In particular, we linked the exceptional compressive strength of FePd nanoparticles (tens of GPa) to solid-state dewetting fabrication conditions and their crystallographic structure. Can these particles hold their secrets forever?

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Poster Presentation

Nanomaterials

Revealing the Nucleation and Growth Mechanism of Gold Nanoparticles within Mucin Glycoprotein

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A green synthesis involves the production of metal nanoparticles using natural materials such as plants, proteins, or microorganisms. Mucin, a glycoprotein found in various organisms (e.g., jellyfish), has been identified as a promising candidate for the biosynthesis of metal nanoparticles (NPs), serving as both a reducing and capping agent. However, the precise mechanism behind this green synthesis remains unclear. This study focuses on identifying and understanding the adsorptive sites in the mucin biomolecule, such as sulfur-containing species, which bind to gold ions and reduce them into nanoparticles. Additionally, the mechanism of nanoparticle growth within the protein matrix is of particular interest, including the stabilization, shape, and size determination facilitated by the mucin template. Gold NPs biosynthesis was investigated under various conditions, including a wide pH range (3–11), temperature variations, and the presence of background salts. The effects of pH on both mucin structure and the resulting nanoparticles were analysed using titration and dynamic light scattering (DLS). Advanced analytical methods, including X-ray photoelectron spectroscopy, X-ray absorbance spectroscopy, UV-visible spectroscopy, small-angle X-ray scattering, and X-ray diffraction, were employed to unravel the key pathways by which mucin binds to gold ions, reduces them, and mediates the nucleation and growth of initial nanoclusters. Overall, this research provides valuable insights into the mechanism of biosynthesizing gold nanoparticles using mucin.

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Poster Presentation

Nanomaterials

Exploring Halide Perovskite Nanocrystal Decomposition: Insight by In-Situ Electron Paramagnetic Resonance Spectroscopy

Philip Immanuel, Anastasiya Sedova, Lena Yadgarov

Zero-dimensional (0D) and three-dimensional (3D) halide perovskite nanocrystals (HP-NCs), owing to their unique optoelectronic properties, are extensively studied for photocatalytic activity. However, HPs are highly sensitive to light, humidity, and other environmental factors, which accelerate their decomposition. Understanding the decomposition process is crucial for gaining insights into how to stabilize HP-NCs. Here, we investigate the radical-driven decomposition process and dynamics of the 0D C_4PbBr_6 and 3D $CsPbBr_3$ NCs under the influence of visible light and a polar solvent by electron paramagnetic resonance (EPR) spectroscopy. Our findings indicate that light accelerates radical formation over time, making the decomposition of HP-NCs a self-sustaining process. Upon illumination of the NCs, hydroperoxyl radicals are formed first, followed by unconventional Br, Cs, and Pb-related radicals, indicating the initiation of NC decomposition. The decomposition of $CsPbBr_3$ NCs starts after 3 min of light exposure, while Cs_4PbBr_6 NCs take 18 min, indicating the greater stability of the latter. Additionally, we evaluated the photocatalytic activity of the HPs toward degrading organic dyes. The 3D $CsPbBr_3$ NCs performed as superior photocatalysts compared to their 0D Cs_4PbBr_6 NCs counterparts. Yet, linking the results of EPR measurements with the photocatalytic efficacy suggests that the $CsPbBr_3$ NCs undergo degradation during the photocatalytic process, thereby serving as a sacrificial agent to enhance photocatalytic activity. The understanding derived from EPR spectroscopy in tracking radical formation and dynamics can be extended to enhance the stability and efficiency of various nanomaterials in optoelectronic and photocatalytic applications, thus contrib-uting to advancements beyond the HP family.

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Poster Presentation

Nanomaterials

Enantioselective Solid-State Synthesis of Guided Chiral Nanowires

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The enantioselective synthesis of chiral materials has always been interesting in pharmaceutical, biological, and physics, as two enantiomers could have different chemical and physical properties. For physical applications such as circularly polarized photodetectors, having ordered and uniform chiral crystals with the same handedness is crucial for realizing their full potential. Although there are several solution-phase-based methods for growing chiral crystals with controlled handedness, there have been limited attempts to control the handedness of chiral crystals using solid-state methods. Here, we present the enantioselective synthesis of chiral nanowire arrays by guided growth on low-symmetry substrates. Using scanning and transmission electron microscopy (SEM, TEM), we determine the morphology and handedness of the nanowires array. We elucidate that the growth mechanism of the nanowires is studied by advanced in-situ- electron microscopy, revealing how the nanowires nucleate and grow while maintaining their handedness during growth. Based on the experimental results, we developed a kinetic model that explained the enantioselective growth mechanism. Density functional theory (DFT) and molecular dynamics (MD) simulations support our suggested mechanism for enantioselective growth. A circularly polarized photodetector based on the array of nanowires, demonstrates their potential for advanced optoelectronics and future spintronic devices.

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Nanomaterials

Order-Disorder Transition in Nickel-Platinum Nanoparticles

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Nanoparticles of Ni-Pt alloys attract great attention due to their potential to substitute the more expensive Pt in various catalysis-related applications. The shape, size, and distribution of these nanoparticles play a crucial role in determining their functional performance.

In this work we studied the disorder – order phase transformation in Ni-Pt nanoparticles synthesized by solid-state dewetting of the Ni-Pt bilayers deposited on a sapphire substrate. The dewetting annealing at the temperature of 1000 °C resulted in disordered solid solution Ni-Pt nanoparticles exhibiting (111) and (100) out of plane orientations. The subsequent annealing in the stability region of the ordered phase has resulted in partial ordering of the particles and oscillatory cyclic-type changes in the fraction of disordered (100)-oriented nanoparticles. This unusual cyclic behavior during isothermal annealing was correlated with particle rotation and re-orientation. Our microstructural studies revealed that the change in the degree of long-range order in the particles and their rotation are closely associated with twinning that occurs during the ordering annealing. This twinning is promoted by a combination of residual stresses, and the stress associated with ordering transformation strain in the particles. The discovery of ordering-induced particle rotation and reorientation introduces a novel approach to engineering the functional properties of supported metal nanoparticles.

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Nanomaterials

Collective Interactions of Excitons in Halide Perovskite Nanocrystal Superlattices

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The collective optoelectronic properties emerging from highly ordered nanocrystal superlattices hold significant interest in the field of nanomaterials. Self-assembled superlattices of cesium lead halide (CsPbX3, X=Cl/Br/I) perovskite nanocrystals are particularly promising for future implementation in various applications ranging from bright and efficient emitters to high energy ultrafast detectors. Halide perovskite nanocrystal superlattices exhibit collective emission, due to dipole-dipole interactions between several simultaneously excited emitters. This coupling, enabled below a critical temperature of 180-200K, changes both the transition energy and emission rate compared with emission of individual uncoupled nanocrystals. We demonstrate how quantum confinement governs the type of coupling through synthetical control over nanocrystal size, and by compositional control over the Bohr radius via anion exchange. In superlattices made of weakly confined nanocrystals, the collective emission is red-shifted with a faster emission rate, showing characteristics of superfluorescence. In contrast, the collective emission of superlattices made of strongly confined nanocrystals is blue-shifted with a slower emission rate. The confinement modifies the preferred alignment of transition dipoles in the nanocrystals, shown by analysis of angular-dependent emission patterns, thereby changing the relative dipole orientation between neighboring nanocrystals, and dictating the resulting optical behavior of the ensemble. These findings showcase the rich landscape of collective emission behaviors presented by perovskite nanocrystal superlattices, and the ability to tune their specific collective behavior.

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Poster Presentation

Nanomaterials

Periodic Edge-sharing/Corner-sharing Perovskite Heterostructures Nanocrystals

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Heterostructure nanoparticles challenge our common understanding of interfaces due to quantum confinement and size effects, giving rise to synergistic properties. An alternating heterostructure in which reoccurring interfaces appear in a single nanocrystal is hypothesized to accentuate such properties. Following the study by Aubrey et al.[1], which first introduced the layered heterostructure in bulk form, we developed for the first time a colloidal synthesis for perovskite layered heterostructure nanoparticles2 to prove the concept and advance our understanding of perovskite heterostructures. We produce a layered heterostructure containing two repeating layers of ($PbBr_4$) octahedra akin to perovskite structure and a non-perovskite layer of ($Pb_2Br_2(AMTP)_2$) where AMTP is the organic molecule 4-(ammoniomethyl)-Tetrahydropyran.

By varying the synthetic parameters and selection of precursors, we control particle size, shape, and product priority. For example, as the synthesis temperature increases, the particle size decreases, in agreement with classic nucleation theory. This variation in particle size, in turn, leads to a blue shift in optical properties.

Furthermore, our recent publication on perovskite monolayers3, along with the advancement of heterostructure development, will contribute to the engineering of future heterostructures. We aim to engineer and utilize new colloidal perovskite nanoparticle heterostructures and use their unique interfacial properties for applications that exploit such internal potentials as photovoltaics, photocatalysis, and optoelectronics. The heterostructure interfaces can facilitate faster charge carrier transfer, separation, tuneable recombination rate, and higher efficiencies.

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(2) Massasa, E. H.; Kortstee, L. T. J.; Lifer, R.; Shaek, S.; Pokroy, B.; Castelli, I. E.; Bekenstein, Y. Colloidal Synthesis of (PbBr2)2(AMTP)2PbBr4 a Periodic Perovskite “Heterostructured” Nanocrystal. Cryst Growth Des 2023.

(3) Massasa, E. H.; Strassberg, R.; Shechter, R.; Dror, S.; Khalfin, S.; Shaek, S.; Khristosov, M. K.; Hadar, I.; Bekenstein, Y. Entropic Ligand Mixing for Engineering 2D Layered Perovskite from Colloidal Monolayer Building Blocks. Adv Funct Mater 2024, 34 (2).

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Poster Presentation

Nanomaterials

Simple and Scalable Wet Chemical Synthesis of Nanomaterials: the Cases of High-Concentration Metal Oxide Nanocolloids and Two-Dimensional Chalcogenide-Hydroxide Materials

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Syntheses of nanoparticulate materials usually involve multistep procedures and expensive reagents; one of the main reasons behind this is the tendency of nanoparticles (NPs) to aggregate because of high surface activity, losing their unique characteristics. The problem is commonly overcome by using stabilizing agents, which cap nanocrystals, keeping their distinctiveness. Steric organic surfactants in a wet chemical synthesis also provide colloidal stability of nanoparticle dispersions; however, they block the NP surface and make it hydrophobic, and then should be removed for many applications. We propose simple manufacturing of high, up to ~1 kg/L, concentrations of nanoparticles of magnetite/maghemite $Fe_{3-x}O_4$, 3d metal ferrites, including high-entropy ones, CuO nanorods, nanosilver, etc. Stability and low viscosity of the dispersions are achieved by removing electrolyte and tuning the surface charge and hydrophilicity via utilization of citrate anions or some other small molecules, which allow (electro)chemical reactions of the particle cores. Solvent (water) molecules in conjunction with the capping ligands and counter-cations are believed to be crucial for the production of nanoparticles and the dense colloids, and their special properties.

Another example is a family of two-dimensional materials inspired by valleriite group minerals, which are composed of alternating “incompatible” molecular sheets of 3d metal sulfides and hydroxides of Mg, Al, Fe, Li, etc., stacked by means electrostatic, rather than van der Waals, forces. The simple one-spot hydrothermal synthesis of $[Fe_{1-x}S_n]^{\delta+}\cdot[(Mg,Fe)(OH)_2]^{\delta-}$, $[Cu,Fe_{1-x}S_n]^{\delta+}\cdot[(Mg,Fe)(OH)_2]^{\delta-}$, $[(Cu_{1-x}S)]^{\delta-}\cdot[(Mg,Al)(OH)_2]^{\delta+}$ and their derivatives was performed in reactions between aqueous salts of the transition metals, sodium sulfide and magnesium (Al, Li) hydroxides. Typically, the flakes of the lateral size of 100–200 nm and thickness of 10-20 nm are formed through self-assembly of the sulfide and hydroxide entities driven by their opposite electric charges. The hydroxide layers contain Fe^{3+} cations (10 to 40% of total iron) and can be doped with Al, Li, Na; Co, Ni, Cr, etc. enter both the sulfide and hydroxide parts, tailoring the electronic, magnetic, optical, and thermophysical properties of the 2D sheets and the whole material. Easy large-scale production and engineering of nanomaterials could be game changers for many fields.

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Poster Presentation

Nanomaterials

Shuttle Peptide-Modified Doubly Self-Assembled Polymeric Nanoparticles for the Targeted Delivery of an Anticancer Antibody in Glioblastoma

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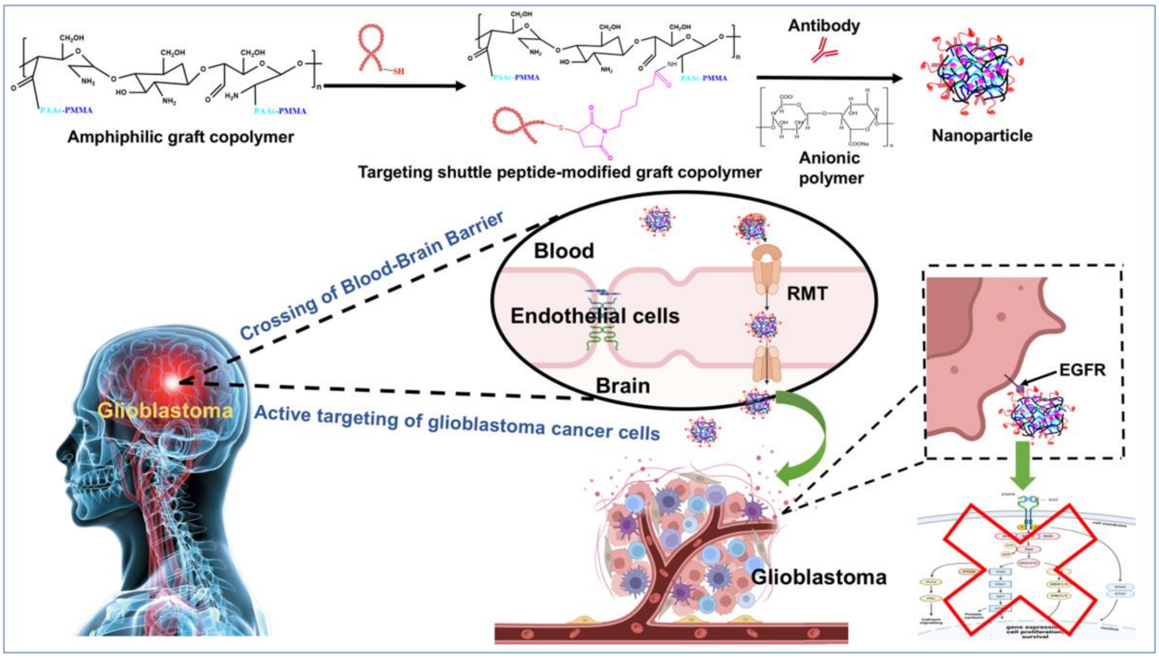
Glioblastoma multiforme (GBM) is the most common and aggressive primary brain tumor, characterized by a poor prognosis and limited treatment options. The blood-brain barrier (BBB) presents a significant challenge in delivering therapeutic agents to the brain, limiting the efficacy of conventional treatments. In this work, we synthesized and characterized chitosan-graft-poly(methyl methacrylate)-poly(acrylic acid) (CPMA)/alginate nanoparticles by a double self-assembly mechanism for the encapsulation of a monoclonal antibody targeting the epidermal growth factor receptor (EGFR) in GBM. To enhance the targeting and delivery efficiency to GBM across the BBB, the nanoparticles are functionalized with a cyclic shuttle peptide, known to bind integrin receptors overexpressed on BBB and GBM cells. The synthesis of the CPMA copolymer is conducted via free radical graft copolymerization, with careful control over reaction parameters to ensure optimal grafting efficiency. The conjugation of the peptide, modified with a poly(ethylene glycol) spacer and a terminal thiol group, is performed using 1-ethyl-3-diaminopropyl carbodiimide/N-hydroxysuccinimide chemistry and a thiol-maleimide click reaction. This conjugation is confirmed using proton-nuclear magnetic resonance and quantified by the Ellman`s reaction. Then, the nanoparticles were prepared using a microfluidics setup to form a polyelectrolyte complex between the polycationic chitosan backbone with polyanionic alginate, optimizing encapsulation of a high molecular weight drug. Characterization of the nanoparticles included size, polydispersity index and zeta-potential by dynamic light scattering and nanoparticle tracking analysis, while the antibody encapsulation and loading was quantified by sodium dodecyl-sulfate polyacrylamide gel electrophoresis and the Bradford assay, respectively. In vitro studies were conducted to evaluate cell compatibility and uptake of the antibody-loaded nanoparticles in the GBM cell line U87. The ability of these nanoparticles to cross an in vitro BBB model is assessed using human endothelial cells in semipermeable inserts. Advanced imaging techniques, such as confocal microscopy and imaging flow cytometry, monitor the internalization and therapeutic effects of the nanoparticles on GBM cells. Hemocompatibility is evaluated using a hemolysis assay with freshly isolated rat red blood cells. The efficacy of the nanoparticles is tested using the MTT assay on the U87 cell line, and uptake studies are performed with confocal microscopy.

Acknowledgements-This work is supported by TheraTools (Ref. 101073404) under the project Innovative Tools to Treat and Model Complex Cancer Environments, funded by the HORIZON-MSCA-2021-DN-01



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Poster Presentation

Nanomaterials

Electrochemical Reduction-Oxidation Processes for the Removal of Perfluoroalkyl Substances from Water

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Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals used in various industries, such as fire-fighting foams, non-stick cookware, food packaging, and water-repellent coatings. PFAS are characterized by high chemical and thermal stability and a tendency for bioaccumulation. They are linked to several human health issues caused by exposure from various sources, specifically drinking water, leading to their emergence as environmental concerns. Due to their chemical persistence, PFAS are extremely hard to degrade using conventional water treatments. So far, there is no efficient full-scale method to remove and decompose PFAS from drinking water using environmentally friendly conditions. This research aims to design, synthesize, and demonstrate the use of a Janus membrane, made of a palladium anode, a platinum cathode, and a ceramic core, to perform an electrochemical reduction-oxidation process to degrade four PFAS compounds efficiently. This work presents the synthesis and characterization of the membrane reactive surfaces using E-beam evaporation. Alongside, preliminary work was done using a microfluidic device, as a membrane analog, showing promising degradation of the strong carbon-fluorine bonds in the PFAS compounds under ambient conditions, which was best performed using the palladium as a cathode. Moving forward, we aim to optimize the operation conditions of the membranal reactor, followed by removal mechanism analysis and demonstration of the operation with real water matrices.

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Nanomaterials

Shuttle Peptide Modified Polymeric/Ceramic Hybrid Nanoparticles for Sonodynamic Therapy of Brain Cancer

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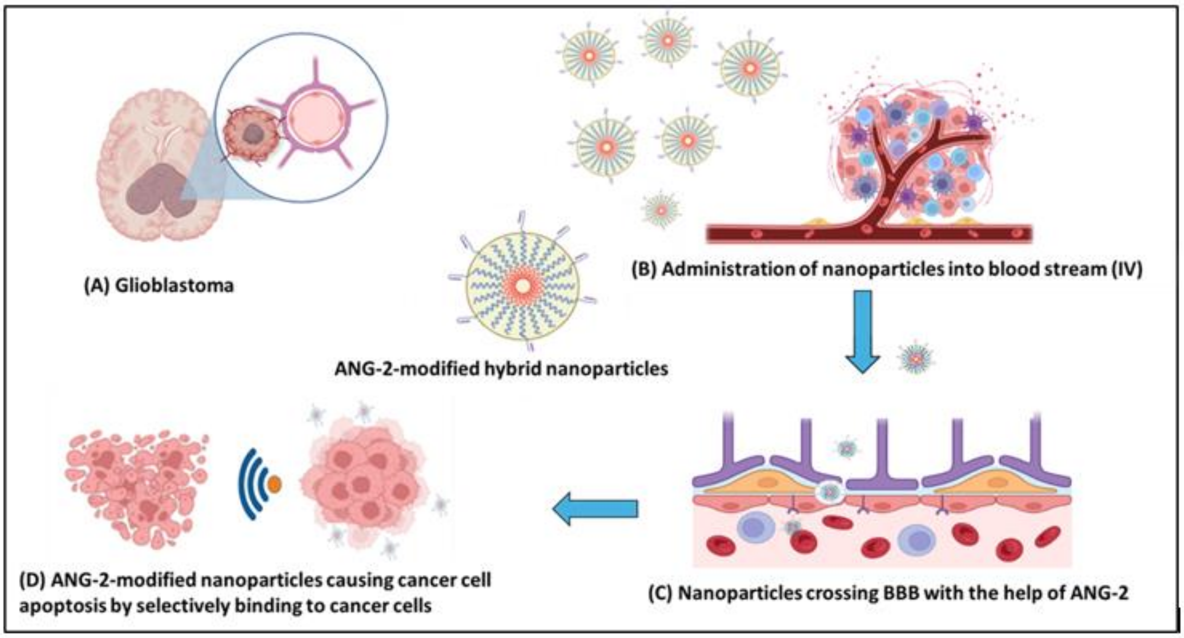
Glioblastoma multiforme (GBM) is one of the most aggressive and fatal brain cancers, characterized by limited treatment options and a grim prognosis. Current modalities, including surgical resection, radiotherapy, and immunotherapy, yield modest survival benefits, with a median survival of only 12 to 15 months. Despite advances in therapy, the blood-brain barrier (BBB) remains a significant obstacle, hindering therapeutic delivery to tumor sites. This challenge underscores the urgent need for innovative strategies that can traverse the BBB, selectively target GBM cells, and minimize systemic off-target effects. Cancer cells, with their heightened metabolic activity, overexpress surface receptors exploitable for receptor-mediated drug delivery. One such receptor, the low-density lipoprotein receptor-related protein-1 (LRP-1), is overexpressed on the BBB and GBM cells. Angiopep-2 (ANG-2), a 19-amino acid shuttle peptide, exhibits high affinity for these receptors, enabling selective binding and reduced systemic toxicity. An ANG-2-based formulation, ANG1005, in Phase II clinical trials, highlighted its therapeutic promise. Conventional treatments struggle to differentiate between malignant and healthy cells, leading to significant collateral damage. Addressing this, sonodynamic therapy (SDT) has emerged as a promising alternative. SDT uses sonosensitizers activated locally by low-intensity ultrasound to generate reactive oxygen species (ROS), inducing cancer cell apoptosis. In this work, we investigate hybrid amorphous titanium dioxide (aTiO_2)/polymer sono-sensitizer nanoparticles synthesized via a Ti (IV) oxo-organo complex. The block copolymer used in the synthesis is the four-arm amphiphilic poly(ethylene oxide)-b-poly(propylene oxide) block copolymer Tetronic® 1107 (T1107) that is conjugated to ANG-2 via the 1-ethyl-3-diaminopropyl carbodiimide/N-hydroxysuccinimide chemistry and confers double targeting features to cross the BBB and bind GBM cells. Attenuated total reflectance-Fourier transform infrared spectroscopy analysis and proton-nuclear magnetic resonance confirmed the successful conjugation of ~3 shuttle peptide molecules per block copolymer molecule. Nanoparticle characterization by via dynamic light scattering and high-resolution scanning electron microscopy reveals a monomodal size distribution, and spherical morphology. Doppler micro-electrophoresis confirms changes in the surface charge between unmodified to ANG-2-modified nanoparticles, suggesting the exposure of the shuttle peptide on the nanoparticle surface. In vitro studies on the U87 glioblastoma cell line using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay demonstrated acceptable cell compatibility before ultrasound irradiation, while hemolysis assays with rat red blood cells suggested their compatibility for intravenous injection. Confocal microscopy shows efficient cellular internalization of fluorescently labeled nanoparticles, with ANG-2-modified nanoparticles under ultrasound significantly reducing cancer cell viability compared to unmodified counterparts.



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Poster Presentation

Nanomaterials

Phase Stability and Mechanical Properties of Cobalt Nanoparticles

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Cobalt nanoparticles have attracted high interest due to their unique combination of functional and magnetic properties, making them highly relevant in fields such as energy storage, catalysis, and biomedicine. A unique feature of metallic cobalt is reversible phase transformation between hexagonal close-packed (HCP) and face-centered cubic (FCC) structures. This martensitic transformation occurs because the difference of Gibbs energies between the two phases is very small. The transformation temperature can be tuned by pressure and alloying elements. Most previous studies of metallic cobalt focused on bulk samples, leaving the understanding of cobalt nanoparticles incomplete. This study aimed at determining the mechanical properties of cobalt nanoparticles and correlating them with their phase transformation behavior.

Defect-free Co nanoparticles were fabricated via solid-state dewetting of Co thin films deposited on sapphire substrates. Although at room temperature the HCP phase is thermodynamically more stable than its FCC counterpart, obtaining the HCP nanoparticles has proven difficult, as most employed synthesis methods favored the formation of FCC phase due to kinetic and size-related constraints. A combination of atomic force microscopy, scanning electron microscopy, and X-ray diffraction was employed to systematically investigate the equilibrium crystal shape of cobalt and to identify the phase composition of the nanoparticles. In-situ micro compression tests of the nanoparticles were performed using Hysitron PI85 picoindenter. Our results demonstrated that defect-free, FCC cobalt nanoparticles with equilibrium crystal shape were obtained after dewetting. This state of the nanoparticles was preserved after prolonged thermal treatments in the stability region of the HCP phase. The stress-strain curves obtained in micro compression tests indicated ultrahigh strength of the FCC nanoparticles in the range of tens of GPa. Finally, we correlated the ultrahigh strength of the FCC nanoparticles with their exceptional phase stability.

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Nanomaterials

Parameter Optimization of High-energy Ball Milling Process for TiO_2 Powder using the Taguchi Method

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The Taguchi method`s robust design was applied to investigate the effect of main high-energy ball milling (HEBM) parameters – milling time (MT), ball-to-powder weight ratio (BPWR), and milling speed (MS) – on the TiO_2 crystallite size (CS). The experiment used the $L_{16}(4^3)$ orthogonal array (OA). The as-received and milled powders were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The CS of TiO_2 varied between 3.48 and 73.70 nm depending on the HEBM conditions. The optimum milling parameter combination was determined by using the analysis of signal-to-noise (S/N) ratios. Based on the S/N ratio analysis, optimal HEBM conditions were found to be MT 100h, MS 400rpm, BPWR 50:1. The analysis of variance (ANOVA) was used for indicating the significance of each milling parameter and their effect on CS. Statistical analysis by S/N and ANOVA established that the MT is the most influential parameter, followed by MS and BPWR. The results of the parameter optimization experiment were validated by a confirmation test at a 90% confidence level. The confirmation test showed that there is a good agreement between the experimental and statistical data

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Nanomaterials

Mapping Stability and Efficiency for Anion Mixtures of Sodium Indium Double Perovskites Applying a High-Throughput Approach

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Lead-free double perovskites are candidates for optoelectronic applications; however, suffering from low photoluminescence quantum yield (PLQY) due to forbidden transition, indirect band-gap, and energy traps. The mechanism by which many double perovskites emit includes the transfer of free exciton into self-trapped exciton. Exploring the role of dopant and B site alloying highlighted Sb-doped in $Cs_2NaInCl_6$ to be a promising double perovskite candidate with notable PLQY(Shaek et al., 2023). However, the role of anion compositions and the extent of mixtures possible under thermodynamic and kinetic consideration is still at large.

Here, we employ two distinct approaches of halide mixing. Firstly, a direct synthesis method was employed, involving varying halide ratios (Cl, Br, I). Secondly, a high-throughput post-synthesis technique was introduced employing an automated robotic system. The rationale for using a robot is the vast experimental parameters space we want to explore. For example, various compositions, including mixtures of X-site halides and the contribution of the nature of passivating ligands, affect the exchange kinetics. Automated experiments also allow for the variation of the temperature of the exchange reaction. We hypothesize that such high-throughput data will shed light on the kinetic impact of temperature on halide exchange rates and the thermodynamic stability of halide-mixture phases. We hypothesize that the stability of halide mixture phases could be extended to higher bromide and iodide concentrations, compared to the bulk counterparts. The high surface-to-volume ratio and the effect of passivating ligands can lead to kinetic trapping, in which, more stable phases are not accessible and the double perovskite structure remains, similar to ideas that redemonstrated for the silver Bismuth system. (Kluherz et al. 2023).

In our experiments, we see that exchanging chloride to larger halide species induces redshifts in excitation and emission wavelengths while enlarging the perovskite lattice spacing. The excitation wavelength was redshifted about ~45nm, while the emission was redshifted about 180nm. According to our X-ray diffraction measurements, the halide-mixture phase was stable at up to 90% of the bromide content in the X-site. The resultant product was not a double perovskite when we used only bromide as an X-site halide. Nevertheless, the resultant product (Cs_3InBr_6) exhibited emissive properties and maintained the observed redshift trend.

The vision is that similar implementation of high throughput methodologies in future research will create comprehensive datasets to solve challenges in material stability and toxicity.

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Nanomaterials

Synthesis of Copper Nanowires for Fabrication of Stretchable Electrodes

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Electrical circuits based on metallic nanowires have been intensely studied and developed as they enable the formation of electrodes with high stretchability, flexibility, and transparency. This technology is used for advanced applications such as touchscreen displays, photovoltaics, sensors, and wearable electronics. Copper Nanowires (CuNWs) synthesis has drawn much interest due to its substantial potential to replace the expensive silver-based nano inks that are mainly used in printed electronics. A significant challenge in utilizing CuNWs is the coppers` tendency to oxidize at ambient conditions. Additionally, the synthesis of CuNWs is usually an expensive process and requires high-pressure or dangerous reagents. Recently, several approaches for copper nanoparticles oxidation protection were reported. One promising approach is the core-shell process in which the CuNWs are coated with a thin layer of less reactive metal, such as silver, by a simple galvanic replacement process. Core-Shell nanoparticles can resist oxidation under ambient conditions and keep their desired properties of conductivity, transparency, and stretchability.

In this research, we aim to develop oxidation resistant CuNWs at mild synthesis conditions for the fabrication of stretchable electrodes and thus to lower the price of electronic devices. So far, we have successfully synthesized thin (~60nm) and long copper nanowires by a simple synthesis at mild conditions. The optimized synthesis resulted in obtaining NWs at a lower temperature than is reported in the literature. In a later stage, the Cu NWS were coated with silver to form Cu@Ag core-shell which stabilized the particles upon oxidation. So far, preliminary results showed that embedding the nanowires in organic polymers has not shown any conductivity.

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Nanomaterials

Enhancing Water Treatment Efficiency: MXenes as an Energy-Efficient Catalyst

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Israel`s crowded demographic, arid nature, and limited water sources, coupled with climate changes and water pollution, demand more effective and reliable water treatment technologies. Nanotechnology-based approaches have been increasingly explored to enhance or replace traditional remediation methods due to high reactivity and tunable properties of nanomaterials. This research focuses on MXenes— an emerging family of two-dimensional (2D) materials composed of transition metal carbides, nitrides or carbonitrides —use for water decontamination. MXenes` are renowned for their unique atomically thin structure, which imparts exceptional mechanical, electrical, and chemical properties, leading to diverse applications. Lately, titanium-based transition-metal carbide MXenes have been suggested as candidates for effectively removing diverse water impurities, owing to their hydrophilic properties, catalytic properties, high surface-to-volume ratio, and tunable surface functionality. However, their practical application remains limited due to their primary use as co-catalysts rather than primary catalysts and the challenges in recovering these hydrophilic nano-scaled materials from treated water following use. This research aims to create a selective catalyst using MXene, which can also function later on as a sensor for water contaminants.

Initially, focus was given to securing MXene nanosheets onto a larger matrix for easy retrieval that minimally disrupts the process while emphasizing sustainability and scalability. Potential solutions tested include a microporous ceramic composite of Al_2O_3 and MXene and a bulk pellet of multilayer MXene. These materials were then used to activate peroxymonosulfate (PMS) to generate sulfate radicals which degrade contaminants effectively. The MXene-based materials demonstrated decomposition of the organic dye Rhodamine B (Rh-B) which varied depending material properties (e.g., presence of molybdenum in the MXene composition). Lastly, we investigate the catalytic mechanism as well as the differences between the MXene surface and edges activity. In conclusion, this research holds significant importance for global well-being, with particular relevance to Israel, advocating the use of MXene as a promising water treatment catalyst.

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Nanomaterials

Development of High Efficiency Nano-Structured Ratchets for Selective Ion Pumps

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Membrane-based selective ion separation is a longstanding challenge in science and technology. The introduction of such a technology can lead to significant breakthroughs in water treatment, green fuels generation and other applications. In a previous work we have shown theoretically that by modulating a spatially asymmetric electric field, flashing ratchets can drive ions of the same charge in opposite directions according to the difference in their diffusion coefficients.

Ratchet based ion pumps (RBIPs) were fabricated by coating the two surfaces of anodized aluminum oxide (AAO) membranes with thin layers of gold resulting in a porous capacitor-like structure. Although these devices show a ratcheting behavior, their performance is not repeatable, and their spatial asymmetry is not defined in the fabrication process.

Here we report on the demonstration of a RBIPs with a controlled asymmetry, fabricated by coating one surface of the AAO with a thin layer of platinum, and the other with a thin layer of gold. The induced asymmetry resulted in a significant increase in the output voltage. Conductance measurements have shown the ability of the RBIP to desalinate water by driving both cations and anions in the same direction. We also report on the development of RBIPs in which the asymmetry is defined by their geometry and can potentially lead to a further enhanced performance. Using conventional nanofabrication techniques, alternating thin layers of metal and dielectric materials with different thicknesses were deposited on commercially available AAO membranes. This structure allows a better control of the ratchet properties, as its geometry defines a saw-tooth potential distribution, and therefore is expected to exhibit a better performance than the current devices. Structural characterization shows that the pores of the membrane remained unclogged after the fabrication process. The resistance between the metal layers in the stack reaches up to ~700Ω demonstrating that the optimized deposition process results in conformal and compact layers with minimal pinholes. The optimization of this process is the first step towards the realization of high performance RBIPs for selective ion separation.

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Poster Presentation

Nanomaterials

Water Decontamination through Sulfate-Radical Oxidation in a Nano-Enabled Catalytic Filtration Process for Water Reuse

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Effective removal of the multitude of microbial and chemical contaminations in treated wastewater is challenging and energy-intensive. In this study, we engineer, optimize and upscale an alternative treatment concept with a novel nano-enabled catalytic filtration process as the core element applicable for non-potable and potable water reuse applications. The nano-enabled catalytic filtration process generates sulfate radicals ($SO_4^{\cdot-}$) through catalytic decomposition of peroxymonosulfate (PMS) via MnO_2-based nanomaterials. Integration of such nanocatalysts in water reuse holds promise in inactivation of pathogens, removal of a variety of trace organic chemicals (TOrCs), and mitigating the spread of antibiotic microbial resistance (AMR) from municipal wastewater with high durability in long-term operation. Through immobilization of the nanomaterial onto a granular media and packaging of the resultant nanocomposite in a filtration unit, we allow efficient, sustainable, and practical use in reuse schemes at comparable costs to established processes.

This poster will focus on the synthesis, characterization, and catalytic activity of MnO_2 on various substrates, with an emphasis on activated carbon (AC) for its high adsorption capacity for water contaminants. Challenges in achieving uniform MnO_2 coverage and the catalyst-substrate adhesion will be discussed alongside alternative synthesis approaches to improve catalyst stability and minimize MnO_2 leaching. This study demonstrates the efficiency of MnO_2@substrate in activating peroxymonosulfate (PMS) to generate sulfate radicals ($SO_4^{\cdot-}$) for degrading pollutants, including dyes and TOrCs. Results confirm the superior catalytic performance of MnO_2-activated PMS over adsorption or direct oxidation mechanisms.

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Poster Presentation

Polymers and Colloids

Hydration Effects Driving Network Remodeling in Hydrogels During Cyclic Loading

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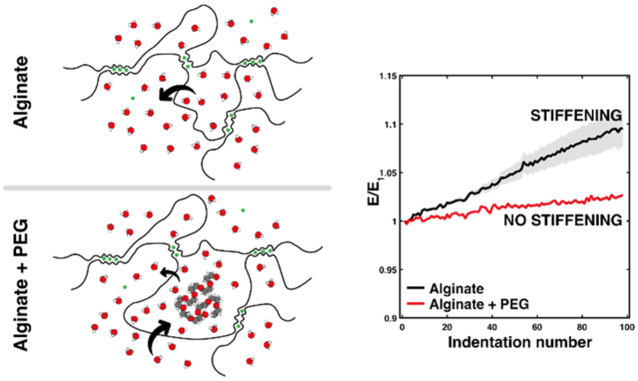
The mechanical properties of complex networks, such as the extracellular matrix (ECM), are profoundly influenced by the movement of both constituent and entrapped polymers. Given that many cells respond sensitively to the mechanical remodelling of their microenvironment, understanding how these entrapped polymers affect network dynamics is critical. In this study, we investigate the molecular mechanisms of network remodelling in a calcium-crosslinked alginate hydrogel, used as an ECM model, loaded with hydrophilic PEG nanoparticles to mimic non-interacting proteins embedded in the ECM. Our findings reveal that the hydrophilicity of these non-interacting polymers significantly enhances the bulk properties of the hydrogel, by linearly increasing stiffness and water retention of the ECM-like polymer. Under dynamic stimulation, the presence of hydrophilic polymers stabilizes the hydrogel matrix by altering its mechanical response: water displacement driven by the polymers' hydrophilic nature transforms the hydrogel from a strain-stiffening to a non-strain-stiffening material. This localized, time-dependent remodelling mechanism underscores the role of water movement as a key driver and provides a broader understanding of hydrogel behaviour, with implications for tissue engineering, disease modelling, biomaterial development, and food science.



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Poster Presentation

Quantum Materials

Magneto-optical and Transport Measurements of Magnetic Weyl Semimetals

Dima Cheskis

Weyl semimetals display remarkable quantum phenomena, such as the anomalous Hall effect and the chiral anomaly, manifesting as significant macroscopic effects. These phenomena arise from breaking inversion or time-reversal symmetry, leading to the separation of Weyl points based on momentum or energy. Around these points, fermionic quasiparticles exhibit opposing chirality, resulting in non-trivial topological phases that remain stable even at temperatures exceeding 77 Kelvin.

Experimental evidence for these effects includes observations of anomalous Hall conductivity in materials like Co3Sn2S2 and magneto-optical responses in Cd3As2. Our work focuses on the magneto-optically induced chiral anomaly effect in Co3Sn2S2, with potential applications in chiral-sensitive devices similar to field-effect transistors (FETs). Unlike traditional ARPES techniques, our approach operates at elevated temperatures and monitors behavioral changes under external magnetic fields.

Additionally, Weyl semimetals show a broad response to low-energy photons, particularly in the infrared spectrum, facilitating the excitation of electrons within the Weyl cone structure.

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Poster Presentation

Quantum Materials

Metal-Insulator Transition Dynamics in Boron-Doped VO_2 Thin Films

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Abstract

Mott insulators are a unique class of materials where strong electron-electron interactions lead to an insulating state, despite predictions of metallic behavior based on band theory. Among these, VO_2 stands out due to its reversible metal-insulator transition (MIT) at ~340K. In VO_2 powders, Boron (B) doping decreases the MIT temperature in a history-dependent manner, driven by thermally activated transitions of B interstitials between metastable to stable states[1]. The dynamic modulation in the MIT temperature of B-doped VO_2 may provide a mechanism for developing resistive switching devices that mimic neural adaptation, offering potential for neuromorphic computing and memory devices. Although demonstrated in VO_2 powders, this memory effect has yet to be investigated in thin films, which are essential for device applications.

To bridge this gap, we sputter B-doped VO_2 thin films and perform electrical, structural and elemental analysis to examine their quality and uniformity. Preliminary results indicate that Boron doping reduces the MIT temperature in thin films, mirroring the behavior observed in powders. We then study the influence of B doping on the dynamical electrical properties of VO_2 thin films as a function of temperature, electric field and time, paving the way towards possible device applications.

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Poster Presentation

Quantum Materials

Effect of Ion Irradiation on the Resistive Switching properties of Mott Insulators

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Mott insulators are materials in which strong electron–electron interactions induce an insulating state even though they are expected to be metallic according to conventional band theory. In some Mott insulators, an insulator-to-metal transition (IMT) can be induced by changing temperature or applying an electric field. These interactions also lead to coupled structural, magnetic and electronic phase transitions. This IMT can be harnessed for resistive switching (RS), a phenomenon in which the resistance of a device can be modified electrically, with vast applications in various fields and especially neuromorphic computation.

In this work we aim to understand the effect of ion irradiation on the RS process, based on previous results which showed a drastic reduction of the voltage and power required for switching in irradiated Mott insulators. Control over this process may enable a large enhancement in the energy efficiency of Mott-insulator based devices but requires an in-depth understanding of its underlying mechanism. To shed light on this phenomenon we use various Mott insulators (VO_2, V_2O_3 and NiO) which exhibit significantly different IMT properties to examine the applicability of ion-irradiation assisted RS to Mott insulators in general. We also examine the nature of this effect in devices irradiated with Ga and Xe ions which have very different implantation characteristics to study the importance of ion implantation for RS properties.

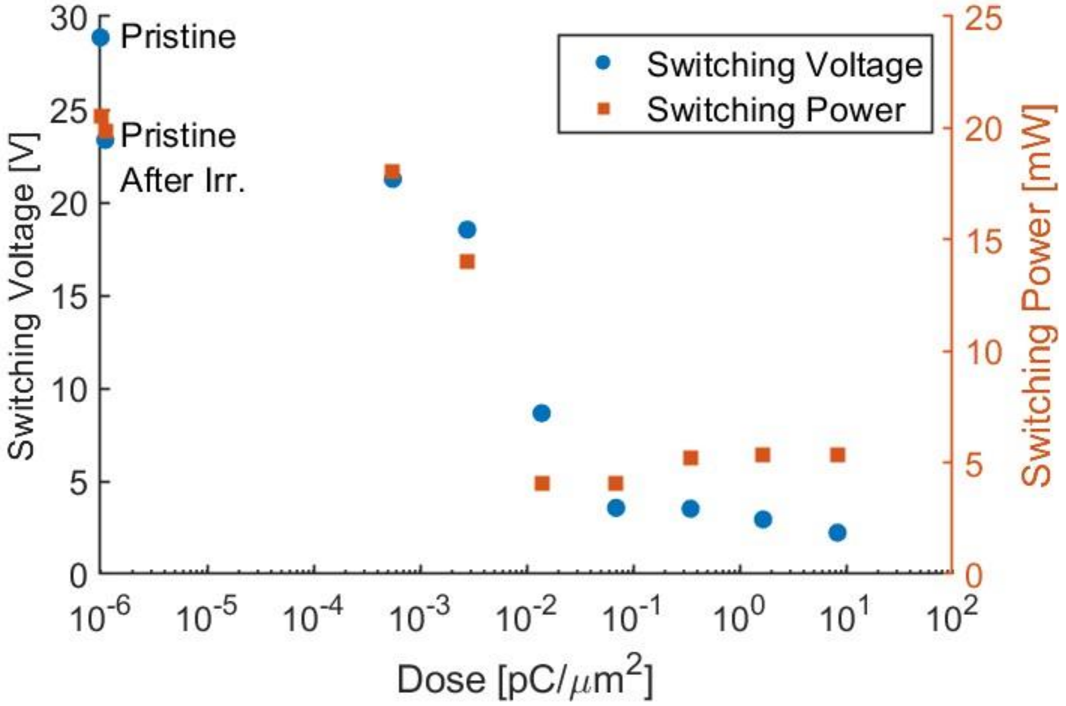

Figure 1: Switching Voltage and Switching Power of a VO_2 thin film as a function of dose of Xe irradiation with energy of 30KV

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Poster Presentation

Quantum Materials

High-Temperature Superconductor-Based Photon Detector

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Abstract: High-temperature superconductors enable SNSPD operation at significantly higher temperatures (77 K), allowing for the use of liquid nitrogen cooling. This translates to reduced operational costs and increased system portability compared to conventional low-temperature superconductor-based detectors.

We report on the development and characterization of high-temperature superconducting micro/nanowire detectors based on YBa2Cu3O7-δ (YBCO). Our devices exhibit ultrafast optical response times, with rise times of ~850 ps and fall times of ~1250 ps, and an upper limit of timing jitter of ~100 ps [1]. Utilizing high-quality YBa2Cu3O7-δ (YBCO) thin films and advanced nanofabrication techniques, including hard oxide (Al2O3) masking, we have successfully fabricated miniaturized microwires with widths approaching 100 nm [2]. Our investigations demonstrate a strong correlation between the optical response and the critical parameters of the superconductor, such as critical temperature (Tc) and critical current density (Jc). Peak optical responses are observed near these critical values, indicating a sensitive dependence on the superconducting state. Furthermore, we have observed a pronounced absorption maximum at wavelengths from visible to near-infrared for temperatures below Tc. We have extended the operational range of these detectors to the mid-infrared spectrum (3.25 and 4.25 μm), achieving photoresponse at temperatures nearly ten times higher than conventional low-temperature superconducting detectors [3]. This significant advancement opens up new possibilities for a wide range of applications, including environmental monitoring, medical diagnostics, and space exploration. These findings provide crucial insights into the fundamental physics of high-Tc superconductor nanowires and pave the way for the development of highly sensitive and versatile single-photon detectors. The ability to operate at elevated temperatures significantly enhances the practicality and affordability of these devices, bringing us closer to the widespread adoption of ultrafast quantum technologies.

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Poster Presentation

Quantum Materials

Single Crystal Diamond Growth by Chemical Vapor Deposition for Nano-scale Sensing

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The nitrogen-vacancy (NV) center is a prominent point defect in diamond that exhibits spin-dependent photoluminescence properties. Its spin state features a relatively long coherence time (in the order of milliseconds) and can be measured using optically detected magnetic resonance. As its spin state can be read out optically, one can infer information about external perturbations, including temperature, strain, and electric or magnetic fields, making it a valuable tool for room-temperature quantum sensing. However, for nano-scale sensing applications using a single NV center, achieving improved sensing performance and extended NV spin coherence time is essential. Noise caused by nearby spin defects in the diamond lattice, collectively referred to as the spin bath, degrades NV center optical measurement sensitivity. To address this, diamond crystals must be carefully engineered with optimized properties, including a low concentration of NV centers (to eliminate NV-NV interactions), minimal substitutional nitrogen impurities, and a reduced abundance of ^{13}C carbon isotopes.

Since the 1980s, chemical vapor deposition (CVD) has been extensively studied as a method for growing diamond, offering precise control over material properties in a repeatable manner. In this work, we demonstrate the growth of single-crystal diamond with exceptionally low concentration of NV centers, making it well-suited for engineering single NV-based quantum sensors. The low NV content of the diamond is confirmed through electron paramagnetic resonance and fluorescence measurements. Future efforts will focus on further enhancing NV spin coherence by reducing the ^{13}C spin contribution through the growth of single-crystal diamond using isotopically purified $^{12}CH_4$ as the carbon source.

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Poster Presentation

Quantum Materials

Observation of Three-Photon Cascaded Emission from Triexcitons in Giant $CsPbBr_3$ Quantum Dots at Room Temperature and Multiexciton Dependence on Blinking State

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Colloidal semiconductor nanocrystals are a candidate source of time-correlated and entangled photons through the cascaded radiative relaxation of multiexcitonic states (multiple excitons within the same nanocrystal). However, the efficient nonradiative Auger-Meitner decay of multiexcitons renders them mostly nonemissive. This limits not only potential uses but also their investigation, particularly their spectroscopy. I will present the heralded spectroscopy of three-photon cascades from triexcitons in giant $CsPbBr_3$ nanocrystals at room temperature.[1] Heralded spectroscopy, realized previously in our group,[2] is a single-particle technique using a single-photon sensitive, 180-picosecond time-resolved spectrometer based on a single-photon avalanche diode (SPAD) array. By post-selecting events of triple photon detections following a single laser pulse, we isolate the triexciton relaxation cascades. This allows us to resolve the weak binding energies associated with the triexciton and the biexciton emissions in the cascade (1.13 ± 0.27 and 0.46 ± 0.28 meV, respectively). Simultaneously, we measure the lifetime of each relaxation step individually, despite their high similarity (triexciton: 0.51 ± 0.08 ns, biexciton: 0.82 ± 0.11 ns, and exciton: 2.21 ± 0.17 ns). These nanocrystals also exhibit near unity values of the second- and third-order correlation functions, $g^{(2)}(0) = 0.97 \pm 0.01$ and $g^{(3)}(0,0) = 0.94 \pm 0.02$. Those weak exciton–exciton interactions can be explained by the nanocrystals' diameter of 26 nm, more than four times the exciton Bohr diameter in CsPbBr3 (7 nm),[3] whereas stronger interaction and binding were previously found in smaller-size (6 nm edge) $CsPbBr_3$ nanocrystals by our group, studying biexcitons using the same technique.[4] Our work also combines fluorescence lifetime analysis, photon statistics, and spectroscopy, to verify emission from a single emitter despite the high emission quantum yields of multiply excited states and the comparable emission lifetimes and energies of singly and multiply excited states. We further compared the biexciton and exciton emission properties during fluctuations in the nanocrystal's emissivity ("blinking" between on, gray, and off states). Such blinking is typically attributed to Auger-Meitner recombination with excess charges or to surface-trap recombination. Finally, I will present indications that blinking can change the multiexciton-to-exciton emission rate ratio, which could be a potential pathway toward control of the photon number statistics of multiexcitonic emission cascades.

Figure: TEM image of the quantum dots and a scheme of the triexciton relaxation cascade.

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Poster Presentation

Quantum Materials

Mechanisms Driving Defects–induced Resistive Switching in V2O3 Mott Insulator Thin Films

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The archetypal Mott insulator V_2O_3 shows a reversible insulator–to–metal transition (IMT) from an antiferromagnetic monoclinic insulator phase (at low temperatures) to paramagnetic rhombohedral metallic phase (at high temperatures) at a temperature of 160 K. Resistive switching (RS) in V_2O_3 can be achieved by driving a voltage⁄current in the insulating phase whereby metallic domains form a conducting filament across the insulating matrix. This type of RS is volatile with no permanent change in the V_2O_3 device, and is promising for applications, such as hardware level artificial neurons. Additionally, non–volatile RS can occur in many transition metal oxides due to electrically induced defects such as oxygen vacancies⁄ions or metallic cations. In the present work, a comprehensive study has been undertaken to generate⁄incorporate defects in the purely insulating phase of V_2O_3 and thereupon study its effect on the volatile IMT–driven RS phenomenon. We show various ways of generating sub–stoichiometric V_2O_{3-x} by electroforming processes, manifesting decreasing activation energies of the insulating state, but with no effect on the transition temperature. We find that in these defective V_2O_{3-x} devices, the voltage⁄power required to induce the volatile (IMT–driven) RS diminishes considerably. These results pave the way towards enhancing RS energy efficiency by controlled electroforming process in Mott–insulator based devices.

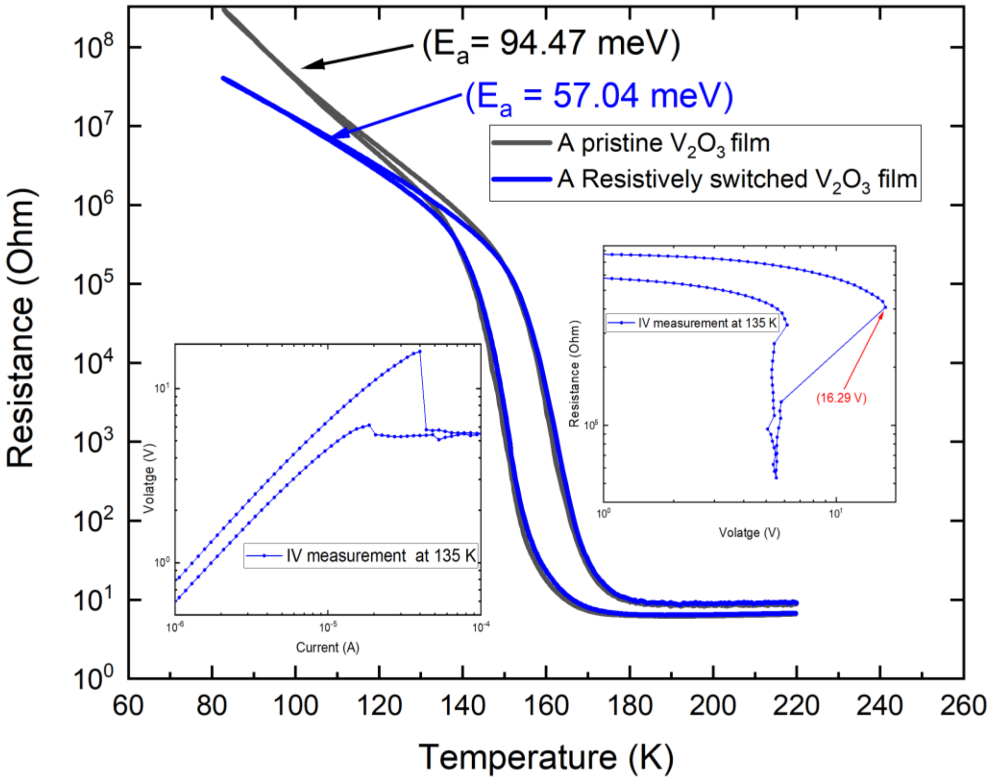

Figure 1: Resistance vs. Temperature measurements of a pristine V2O3 film (black curve) and after current–voltage (IV) measurements at 135 K (blue curve). Inset depicts the IV done at 135 K and also shows that the film underwent a permanent resistive switching at 16.29 V. This non–volatile RS decreased the activation energy from 94.47 meV to 57.04 meV.

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Poster Presentation

Quantum Materials

Light-Matter Interactions and Trion Dynamics in WS_2 Nanotubes

Hila Shalom

Strong light-matter interactions are crucial for the development of advanced optoelectronic devices. Light-matter interaction occurs through the coupling between material excitations and optical cavity modes. Transition metal dichalcogenides (TMDCs) are remarkable semiconductors that feature A, B, and C exciton transitions in the visible light range. [1,2] Due to their strong Coulomb interactions, monolayers of TMDCs exhibit pronounced excitonic effects with binding energies in the range of several hundred meV, facilitating thereby the formation of charged excitons (trions). [3] WS2 nanotubes (NTs) possess a unique structure that allows the control of light-matter interactions as a function of the NT radius. [4] In such nanostructures, the confinement of light into small volumes enhances the electric field strength, promoting nonlinear effects and increasing emission and absorption probabilities. This enhanced electric field increases the presence of residual free electrons, facilitating interactions between excitons and surrounding charges. Eventually, this leads to the formation of charged excitons called trions. Dispersion of WS_2 NTs in dilute potassium iodide solutions leads to an increase in free electron concentration through surface adsorption of iodide ions on the WS_2 NTs, which is conductive for the formation of trions and trion-polaritons. This approach opens the door for a more detailed investigation of trion-polaritons through absorption, extinction, and transient absorption measurements as well as finite domain time difference (FDTD) simulation.

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Oral Presentation

Quantum Materials

Single Photon Emitter from Hexagonal Boron Nitride Nano-Bubbles

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Single Photon emitters (SPE) made by defects hexagonal-Boron-Nitride (hBN) are promising components for integrated quantum information processing and could be useful for quantum calculation and photonics. The point defects result in color centers that show features of 2-states or 3-states systems, emitting single photons. We report on bright SPEs that are highly correlated at room-temperature. As a piezoelectric material, hBN allows for emission wavelength tuning via the Stark effect. This study focuses on unique phenomena arising from strained bubble-shaped structures of hBN, observable through AFM and s-SNOM measurements, as well as by investigating the quantum emission as affected by funneling.

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Poster Presentation

Quantum Materials

Self-Induced Strain: A Tool for Modulating Phase Transitions in Mott insulators

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Vanadium sesquioxide (V_2O_3), a prototypical Mott insulator, exhibits magnetic and electronic phase transitions driven by temperature and pressure, and doping. Due to the coupling to a structural transition, strain induced by the substrate can have large effects on the phase transition. Indeed, strain engineering by lattice mismatch and differential thermal contraction between the substrate and film have been intensively explored in Mott insulators. Here, we suggest a novel way for strain engineering using geometrical confinement of thin films by the substrate as they undergo a structural phase transition[1]. Upon cooling across the transition temperature, the structural transition tends to increase in-plane lattice parameters while the substrate clamps the film. This induces in-plane strain and changes the transition trajectory from isobaric to isochoric, following the phase equilibrium line between the metallic and insulating phases. A useful analogy for this effect is the isochoric freezing of water where freezing increases pressure, thereby decreasing its freezing point and maintaining thermodynamic equilibrium between water and ice. In this work we reveal a surprisingly large effect of small modifications of substrate morphology on the confinement effect, leading to changes of over 8 orders of magnitude in resistance at low temperatures (as shown in the figure below). This unique state of matter where the insulating and metallic phases are in thermodynamic equilibrium across a broad temperature regime is promising for the development of novel resistive switching applications.

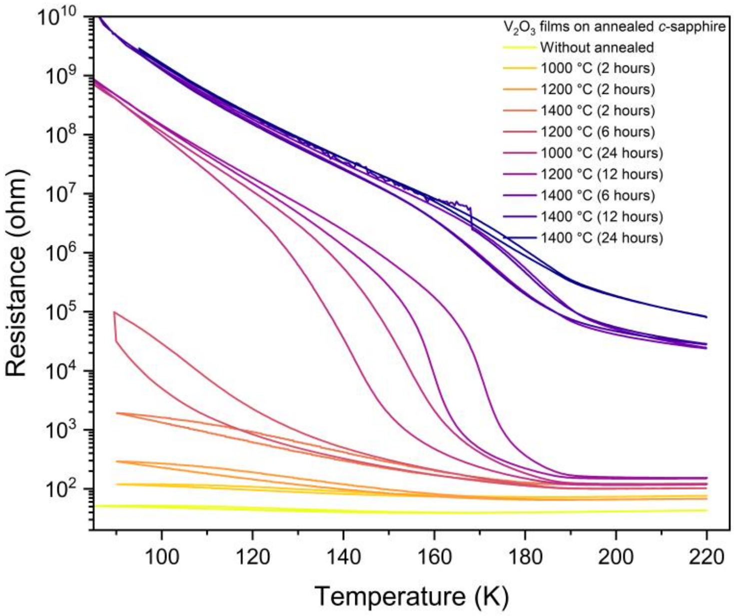

Figure: Resistance versus temperature for a 100 nm V_2O_3 film grown on c-sapphire showing different evolution of metal-insulator transition.

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Poster Presentation

Quantum Materials

Unveiling the Structure of Electrons and Photons: a Lattice-based Theory for Quantum Materials

Roy Winter

Introduction:

Electrons and photons are cornerstones of quantum materials, yet their fundamental behaviors often defy intuitive understanding. This work introduces a deterministic framework that redefines these particles through a Planck-scale lattice, describing the electron as a stable knot and the photon as a spiral disturbance. By addressing the origin of mass, charge, and polarization through this model, we offer a fresh perspective that bridges quantum mechanics and relativistic physics.

Objective:

The aim is to present a unified theoretical framework that explains the mass and charge of electrons and the polarization of photons as emergent properties of a discrete lattice structure. This approach challenges traditional probabilistic interpretations, providing a deterministic basis for quantum phenomena.

Theoretical Framework:

Electron Model:

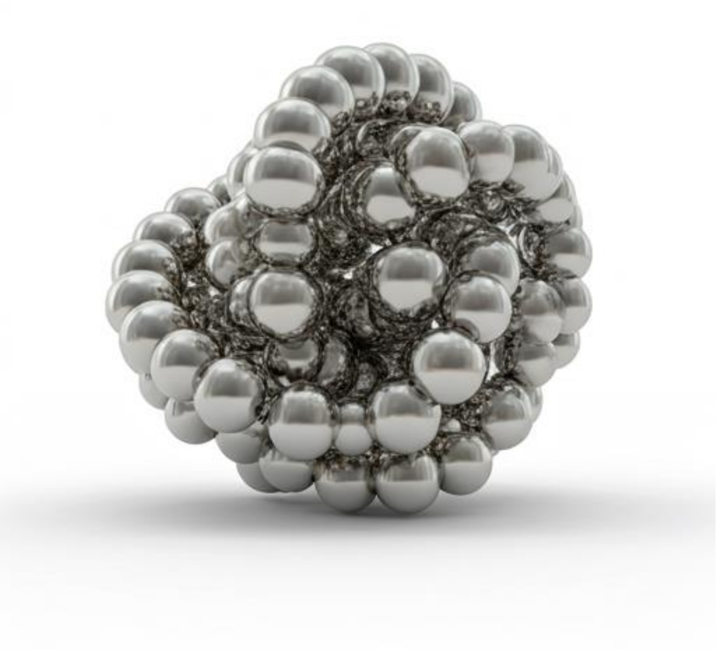
The electron is conceptualized as a knot formed by Planck-scale spheres oscillating within a lattice. The motion of these spheres generates a defined charge and mass:

Charge: The electron’s negative charge arises from the directional motion of spheres within the knot, creating a net imbalance in elastic collisions that propagates outward. This explains the interaction of the electron with the surrounding lattice and the consistent negative electric field.

Mass: The electron`s mass is the result of harmonic motion within the lattice and the surrounding disturbance created by elastic collisions. The total mass is calculated as the cumulative effect of these interactions, aligning with experimental observations.

Photon Model:

Photons are described as spiral disturbances propagating through the lattice. Their polarization is determined by the orientation of this spiral motion relative to lattice symmetry. This deterministic view of polarization offers insights into classical phenomena like light propagation and interference.



Key Equations:

The framework introduces velocity as a variable, with discrete time steps corresponding to Planck-scale collisions. The uncertainty principle is naturally derived as , unifying non-relativistic and relativistic cases.

Key Outcomes

1. Electron Properties:

Demonstrates how electron charge emerges as a macroscopic result of directional sphere movement.

Provides a deterministic basis for electron mass, with elastic collisions through the lattice.

Spin states (up and down) arise naturally from the knot structure, consistent with the lattice symmetry.

2. Photon Properties:

Polarization is explained as the orientation of spiral disturbances in the lattice.

Predicts directional dependencies in photon-material interactions, offering new insights into optical phenomena.

3. Unifying Quantum and Relativity:

The model bridges gaps between quantum mechanics and relativity, redefining key principles like the uncertainty relation through lattice-based physics.

Conclusions:

This deterministic framework reinterprets electron and photon properties, offering explanations for mass, charge, and polarization within a Planck-scale lattice. While theoretical, the model sets the stage for future experimental validation and applications in quantum materials.

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Poster Presentation

Semiconductors and Electronic Materials

Electrochromic Materials: P-Type Semiconductor Polymers Based on Furans for Smart Windows

Hila Friedlander

Compared to inorganic semiconductors, organic semiconductors have many advantages such as simple preparation conditions, processing of organic semiconductors is usually much less strict and sensitive than the inorganic ones. In addition, they are flexible, corrosion resistant, and they usually have low specific weight etc. Organic semiconductors have many applications that are currently under development in the industry such as OLED's (Circularly polarized-organic light emitting diodes), OFET's (Organic field effect transistors), Spintronic devices and more. The application we will focus on is electrochromic devices. My project deals with electrochromic materials examining the effectiveness of the polymers as an active layer for smart windows was tested. The structure and optical properties of the P(Bifuranimide)Fu2, a unique monomer, semiconducting polymer based on furans are investigated in the project. The polymerization method for obtaining a semiconducting polymer used as an electrochromic device was electrochemical polymerization, with the help of cyclic voltammetry. In addition, various measurements were performed to find the optical properties of the polymer such as absorption measurements and spectroelectrochemistry. In addition, various methods were conducted on the polymer to test and define its electrochemical and photochemical stability. We saw that the photochemical stability of the P(BFI-H)Fu2 is significantly higher than the stability of PFu3, while the opposite results were obtained for the electrochemical stability.

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Poster Presentation

Semiconductors and Electronic Materials

Validation of Integrated UV Filtering System for Treating Mikvas Water

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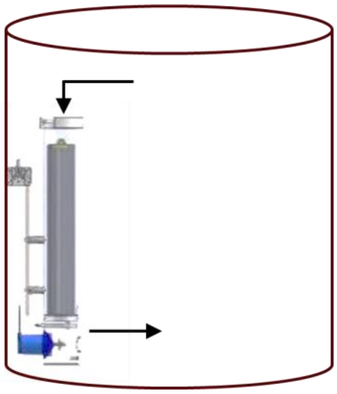
Using contaminated water is a common cause for diseases spread by pathogens like bacteria, viruses, and protozoa. Notably, common bating places such as municipal swimming pools are potential exposure hotspots. Other examples for popular bating locations are Mikveh places, i.e. Jewish ritual baths. To maintain water quality and prevent disease in the Mikveh, chlorine is typically used as a disinfectant. However, chlorine has limitations, such as the need for constant monitoring and its ineffectiveness against certain pathogens, especially protozoa like Cryptosporidium.

In recent years, UV disinfection has gained popularity as an effective alternative to chlorine. UV radiation, particularly in the 200-280 nm range, can damage microorganisms DNA, inactivating them and preventing their reproducing. A significant advantage of UV over chlorine is its high efficacy against protozoa. This study focused on validating a new water treatment system for mikvehs that combines filtration with UV exposure, using 280 nm wavelength light emitting diodes (LED) lamps. UV LEDs are relatively new technology for water treatment, with advantages such small footprint and long lifetime. The specific goal was to determine the system`s effectiveness and reliability under various conditions.



The intensity of the UV radiation was measured using a collimated beam reactor and biodosimetry, with E. coli bacteria and MS2 viruses as model microorganisms. The results were plotted as dose-response curves to correlate radiation dose with microbial inactivation.

E. coli inactivation in the collimated beam was highly effective, with more than 2-log reduction (99% removal) at a radiation dose of 5.36 mJ/cm2. The MS2 viruses were much more resistant, required a dose of 75 mJ/cm2 to reach an almost 2-log reduction.

Inactivation in the pilot system was examined under different water qualities. The water quality changed by varying turbidity with fulvic acid - increasing fulvic acid concentrations, simulating decreasing water quality (UV transmittance %UVT). The results showed that lowering the UVT of the water decreased the inactivation rate of microorganisms. Nevertheless, the system could inactivate both microorganisms at sufficient effectiveness, even at the lowest UVT of 65%. Altogether the study showed that combining UV LEDs into a Mikvah treatment system can improve the quality of the water, preventing the exposure of bathers to pathogenic microorganisms and protecting their health.

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Poster Presentation

Surfaces and Interfaces

Enhancing Tribological Performance Through Nanoscale Coating and Interfacial Modification

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Controlling interfacial properties at the nanoscale is critical for enhancing device functionality across diverse technological fields, including microelectronics, optoelectronics, and tribology. This project focuses on the synthesis and characterization of nanolayers constructed via self assembly method on hydroxylated substrates, such as glass and silicon. These nanolayers were fabricated using 1H,1H,2H,2H-Perfluorooctyltriethoxysilane (POTS) as the coupling agent.

The nanolayers were characterized using contact angle measurements to evaluate hydrophobic properties and ellipsometry to determine thickness. Additionally, tribological properties, including adhesion and friction, were analyzed using a custom-designed tribometer developed in the Tribology Laboratory of the department of Mechanical Engineering at Azrieli college of engineering. Static and dynamic friction coefficients were measured on bare and modified substrates to comprehensively assess the layer′s tribological behavior.

Preliminary findings demonstrate the successful formation of uniform POTS nanolayers, as confirmed by ellipsometry. Major change in the contact angle was observed (90°) upon POTS monolayer formation, as expected for hydrophobic coupling agent. Adhesion forces showed notable changes, reflecting the impact of the modified surface properties. Future research will explore how these surface modifications influence the frictional behavior of the nanolayers, aiming to optimize their performance for applications where friction is a critical factor.

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Poster Presentation

Surfaces and Interfaces

Impact of Coating Structure on Reaction Rates of Coupled Dissolution–Precipitation Reactions

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Dissolution–precipitation coupled reactions, in which primary minerals dissolve and new phases precipitate, are very common in the Earth`s crust and significantly influence natural systems. Carbonate minerals, such as calcite, dissolve in the presence of acidic solutions, releasing cations that subsequently re-precipitate as new phases like gypsum. These reactions not only alter the mineral composition of rocks or soils but also lead to changes in their chemical composition.

The coupled dissolution-precipitation reactions are not simply the sum of the individual mechanisms, making it more challenging to understand their processes. One of the main reasons for this complexity is the accumulation of secondary minerals on the surface of the dissolving primary phases. This reduces the reactive surface area and limits solution transport to and from the dissolving mineral surface. Consequently, this can affect reaction rates, and weathered minerals that form coatings under natural conditions dissolve much more slowly than unweathered minerals. Understanding the mechanisms and reaction rates of these processes is crucial for advancing knowledge and management of geochemical processes.

Project Objectives:

- To investigate the structure of the coating formed on calcite samples as a result of dissolution-precipitation reactions.
- To develop a new model for the process.

Throughout the year, calcite stones were immersed in sulfuric acid for specific durations. Samples were periodically extracted to study the structure of the coating and its changes over time. Using optical microscopy and SEM (Scanning Electron Microscopy), results were obtained that contributed to the development of a new model.

It was found that the thickness of the coating increased over time, porosity changed, and there was a certain cyclicity observed in the coating.

A new model describing the formation of the gypsum layer was developed: the new layer consists of two sub-layers — an outer porous layer and an inner layer containing cracks.

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Poster Presentation

Surfaces and Interfaces

Investigation of the Growth Kinetics of Hydroxyapatite on CP-Ti and Ti65Zr Alloys Treated by Plasma Electrolytic Oxidation

Elinor Zadkani Nahum[1], Svetlana Lugovskoy[1], Alex Lugovskoy[1], Barbara Kazanski[2], Alexander Sobolev[1]
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A study was conducted to examine the growth kinetics of hydroxyapatite on titanium alloys, specifically CP-Ti and Ti65Zr. The specimens underwent Plasma Electrolytic Oxidation (PEO) treatment and were immersed in Hanks` solution. PEO treatment was carried out using an AC mode with a current density of 4 A/dm^2. The electrolyte used during PEO treatment contained calcium acetate and calcium glycerophosphate, facilitating the inclusion of calcium and phosphorus in the resulting oxide layer. This incorporation is known to promote osseointegration when applied to bone tissue. The treated specimens were subjected to different immersion times in the Hanks` solution, and subsequent analyses were performed to evaluate changes in morphology, chemical composition, and phase composition. Surface wettability was also tested, and the corrosion behavior of the treated samples was investigated. Observation of the CP-Ti samples treated with PEO for 5 and 30 minutes revealed the presence of small hydroxyapatite crystals on their surfaces.

In contrast, the Ti65Zr sample exhibited a distinct layer of hydroxyapatite morphology after a 5-minute PEO treatment. When considering the immersion times, the Ti65Zr samples treated with PEO for 5 minutes and immersed for 14 days displayed the highest crystal growth velocity. This finding was confirmed through morphology changes and electrochemical analysis. Furthermore, X-ray diffraction (XRD) analysis of the Ti65Zr samples treated with PEO for 5 minutes indicated that the Srilankite phase, accounting for 60% of the crystal growth, played a crucial role in achieving the highest crystal growth velocity and demonstrating favorable corrosion properties.

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Poster Presentation

Additive Manufacturing

Novel Hydrothermal Surface Modification Process for Powder Manufacturing of Al.

Maria Atamna, Michael zingrad, alexander sobolev

This research examined the impact of the hydrothermal coating technique on the modification process of Al powder. Commercial pure aluminum powders were coated with a silica nano-layer via a single-step hydrothermal treatment. This study investigates the effect of incorporating surface-modified particles on the properties of aluminum powder manufactured using the powder metallurgy method. The samples were analyzed using scanning electron microscopy (SEM) with an EDS detector, optical microscopy, image analysis software, X-ray phase analysis (XRD), and tensile test machine measurements. The findings showed that the sample`s structural characterizations revealed a silica nano-coating on aluminum particles, as depicted in the SEM micrographs with the cross-sectional results of the EDS-mapping analysis of the coating aluminium particles by HTT technology. The EDS-mapping analysis confirmed the presence of a silica layer that is continuously coated on the core particle surface of aluminum. Furthermore, the incorporation of surface-modified particles by powder metallurgy resulted in improved grain structures and a decrease in grain size. Mechanical testing proved that the modified samples displayed superior tensile strength and elongation in comparison to pure aluminium samples. This research highlights the potential of surface modification of aluminum powder in advancing the powder manufacturing of aluminium alloys for nanotechnology applications, offering insights into the fabrication and characterization of nanostructured materials for industrial applications.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Additive Manufacturing

The Effect of 3D Printing Process (PBF vs. DED) on Properties of 15-5 PH Stainless Steel

Maxim Bassis[1], Amnon Shirizly[1], Eli Aghion[1]
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Additive manufacturing (AM), often referred to as 3D printing, has transformed the production of complex geometries and high-performance materials by enabling layer-by-layer construction directly from digital models. This innovative manufacturing approach provides unparalleled design flexibility, material efficiency, and customization potential, making it extremely valuable in various industries. Among the different AM methodologies, Powder Bed Fusion (PBF) and Direct Energy Deposition (DED) stand out for their ability to process advanced alloys with tailored properties. Each of those methods possess opposing advantage and disadvantages. Moreover, the intricate relationships between process parameters, material microstructure, and mechanical performance remain critical areas of study to fully exploit the potential of AM.

In this study, 15-5 PH stainless steel, a precipitation-hardenable martensitic alloy renowned for its excellent strength, toughness, and corrosion resistance, was fabricated using both PBF and DED techniques. Both alloys underwent identical H1150M heat treatment, establishing a consistent thermal framework for comparative analysis. The DED process was conducted in a nitrogen atmosphere, whereas the PBF process utilized an argon atmosphere. This deliberate choice of shielding gases was informed by processing challenges encountered during DED, aiming to optimize the microstructure and enhance the material's environmental and mechanical properties. The comprehensive characterization was performed using optical and electron microscopy to study microstructural properties and inherent defects present in the alloys. Tensile testing and hardness testing was applied to understand the mechanical properties of the two alloys. Potentiodynamic polarization and impedance spectroscopy were utilized to study the environmental behavior of the alloys. The obtained results clearly highlighted the different effect of the 3D printing methods on the material characteristics.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Additive Manufacturing

The Influence of Hip and Heat Secondary Treatments on the Hydrogen Embrittlement, Microstructural and Mechanical Behavior of Electron Beam Melted (EBM) Ti–6Al–4V Alloy

Noa Bitton, Nissim Navi

The α(hcp) + β(bcc) Ti–6Al–4V alloy is the workhorse among all titanium alloys. Additive manufacturing (AM) has become attractive for processing of Ti–6Al–4V (and other alloys). Secondary (complementary) thermal or thermo-mechanical processes typically change the microstructure of the alloy, and therefore – its properties, including susceptibility to hydrogen embrittlement (HE).

This study investigates the influence of hot isostatic pressing (HIP) and heat treatment (HT) on the microstructure, mechanical behavior, and susceptibility to HE of electron beam-melted (EBM) Ti–6Al–4V, before and after electrochemical hydrogenation (EC). Scanning electron microscopy (SEM), X-ray diffraction (XRD), thermal desorption analysis, and small punch testing (SPT) were used for characterization.

In the as-built condition, the β-phase exhibited a discontinuous Widmanstätten structure. The secondary HIP and HT processes altered the β-phase morphology from discontinuous lamellae to a more continuous structure. After EC, a hydride layer formed on the surface of the as-built alloy, but not on the HIP or HT alloys. Higher hydrogen content was observed in the HIP and HT alloys compared to the as-built alloy, followed by a pronounced mechanical degradation. It is suggested that the continuous β-phase pathways that resulted from the secondary treatments facilitated hydrogen diffusion into the bulk, thus increasing the susceptibility to HE. On the other hand, the discontinuous β-phase in the as-built alloy reduced hydrogen penetration and promoted a surface hydride layer that further inhibited hydrogen diffusion into the bulk, thus resulting in higher sustainability to HE. This study emphasize the critical role of secondary processes in tailoring the continuance of the β-phase in EBM'ed Ti–6Al–4V when EC hydrogenation is involved.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Additive Manufacturing

Poly-Tungsten - 3D Printing

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Poly –Tungsten (also known as Tungsten-filled Polymer) is a definition for Polymer- Tungsten composites which are substitutes for Lead or sintered Tungsten base heavy alloys. The composite systems are a combination of two components: A polymer which is acting as filler and combines high weight percent of tungsten powder. It is possible to introduce, for example, 97.5wt% of tungsten powder to nylon filler and to reach to density of up to 13 g/cm3. High density Tungsten-Polymer is a composite of rigid or soft material in the range of densities of 10 to 13 g / cm3 . Each of the specific gravities will be customized and formulated for the specific application. The Polymer- Tungsten will not require sintering as tungsten base heavy metals, since it is usually processed similar to a regular polymer by injection molding. The new age for those high density composites provides us with technological opportunities in the design for medical machinery, mobile phones, fishing, balancing and radiation shielding. The option for additive manufacturing of Poly –Tungsten was initially tested through regular fused filament fabrication (FFF). A self-made filament with low content of tungsten powder is achievable. However, the filament is not producible when the tungsten content is higher than 50Vol.%. The filament will be brittle and can`t function in regular 3D printer. Next step was to mold 2.85mm dia. rods and feed them to a regular fused deposition modeling (FDM) printer .It may be technically possible but too expensive and requires additional development of a new printing technology. The practical state of art came out to print our Poly-Tungsten from regular pellets with the same injection molding feedstock which is being used for Poly-Tungsten (Fig.1) . Fused pellets fabrication (FPF) is an extrusion-based printing technique (Fig.2) . The printing process is as follows: 1. Plastic pellets are loaded into a hopper 2. A motor starts to turn the rotary screw, moving the pellets towards the heater. 3. As the pellets make their way through the extruder, the heater melts them into a semi-liquid state. 4. The molten plastic is then pushed out through a heated nozzle in thin layers direct onto a heated build plate. 5. The nozzle moves in predefined paths based on the 3D model data. The FPF technology will open a new cheaper approach as a substitute to the FFF technology.

Fig. 1: Poly-Tungsten Pellets

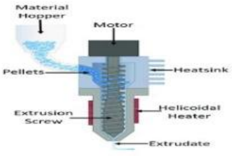

Fig. 2: FPF Extruding System

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Poster Presentation

Additive Manufacturing

Zirconium Oxide Coatings on TI-6AL-4V Alloy via Electrophoretic Deposition for Improved Orthopedic Implants

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Department of Chemical Engineering, Ariel University, Israel

This study investigates the use of electrophoretic deposition (EPD) to coat Ti-6Al-4V alloy particles with zirconium oxide (ZrO_2) for enhanced orthopedic implant performance. Ti-6Al-4V is widely used in biomedical applications for its mechanical strength and biocompatibility, though surface modifications are necessary to improve wear resistance and reduce metal ion release [1]. A zirconia nanoparticle suspension was prepared and applied using a DC power source and rotating reactor to ensure uniform coating. Key EPD parameters, including suspension composition, electric field strength, and deposition time, were optimized to achieve a dense, defect-free zirconium oxide layer. This coating significantly enhanced the alloy's mechanical properties, biocompatibility, and corrosion resistance, making it more suitable for durable orthopedic implants [2]. Analytical methods such as SEM, EDS, and mechanical testing confirmed the coating's uniformity, adhesion, and structural integrity. This work presents an innovative surface modification approach for 3D-printed biomedical materials, with further potential in oxide dispersion strengthening (ODS) coatings to improve implant longevity and functionality. The findings provide a pathway for developing next-generation orthopedic implants with improved biocompatibility and durability.

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Poster Presentation

Additive Manufacturing

3D-printed Patient-specific Metallic Lattice Bone Reconstruction Implants

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Biomedical Engineering, Ben Gurion University of the Negev, Israel

Critical-sized bone defects, commonly arising from traumatic injuries, tumors, or bone diseases, present significant challenges in orthopedic surgeries. Effective bone regeneration, essential for addressing these defects, remains a major hurdle due to the complexity of designing an ideal scaffold capable of replacing or restoring the damaged bone section. An optimal scaffold must exhibit physical, mechanical, and biological compatibility while mimicking the structure and properties of natural bone. In this field, physical compatibility involves resistance to corrosion, ensuring the scaffold maintains its functionality without surface degradation or substantial mass loss. Mechanical compatibility refers to the scaffold`s ability to endure the expected loads and stresses, functioning mechanically like the target bone. Biocompatibility denotes integration with biological tissues in the target area without adverse effects such as infections or immune responses. Biological bone grafts, including autografts and allografts, are commonly used for bone defect reconstruction due to their inherent mechanical and physical properties. However, these approaches have significant limitations: autografts are associated with severe donor site pain and limited availability, while allografts, although more readily available, often exhibit poor biocompatibility and a higher risk of immune rejection. In recent years, substantial advancements have been achieved in the field of additive manufacturing (AM), allowing the design of customized implants that perfectly meet the specific clinical needs associated with critical-sized bone defects. 3D-printed metal implants have emerged as a promising alternative, offering high strength, excellent corrosion resistance, biocompatibility, and customization. Laser powder bed fusion (LPBF) techniques, such as selective laser melting (SLM) and electron beam melting (EBM), are widely employed for 3D printing metals. These methods provide material versatility and the ability to produce parts with excellent mechanical properties. However, challenges such as limited geometric complexity, safety concerns with metal powder handling, and intricate post-processing remain significant drawbacks. Tritone^{TM} MoldJet technology is a novel powder-free AM technique that addresses these limitations by enabling large-scale, high-speed production of geometrically complex metal parts with excellent mechanical properties and simplified post-processing. This research presents a characterization process aimed at evaluating the physical, mechanical, and biological properties of 3D-printed scaffolds fabricated using the MoldJet technology to examine their potential to be used as bone reconstruction implants. The research focuses on the 316L stainless steel alloy for its superior strength, corrosion resistance, and biocompatibility. Microstructure analysis was conducted using X-ray diffraction and optical microscopy, while physical properties were assessed through density measurements and corrosion tests. Mechanical characterization included tensile and fractographic testing. Finally, in vitro evaluations were employed in indirect and direct cytotoxicity tests to validate biocompatibility. The obtained results demonstrated isotropy, high corrosion resistance, enhanced mechanical properties, and promising biocompatibility. These results demonstrate that 316L scaffolds 3D-printed using Tritone^{TM} MoldJet technology have promising potential to be used as bone reconstruction implants.

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Poster Presentation

Additive Manufacturing

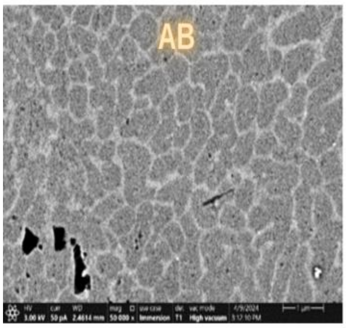
The Effect of Heat Treatments on the Microstructure, Properties, and Residual Stress in 3D Printed AlSi10Mg

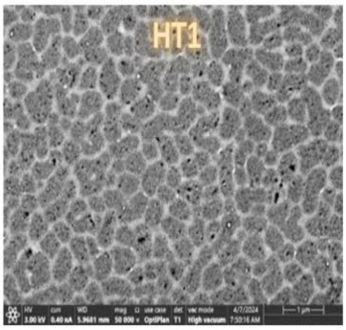
Chen Erlich

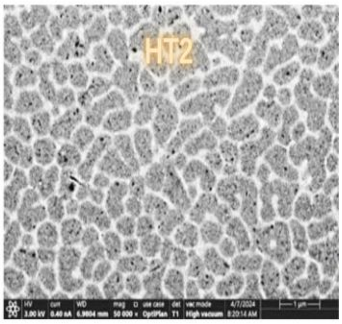
Al10SiMg is the most widely used material in additive manufacturing worldwide due to its lightweight, high strength, and favorable thermal properties. These attributes make it ideal for a range of industrial applications, particularly in the aerospace and automotive sectors.

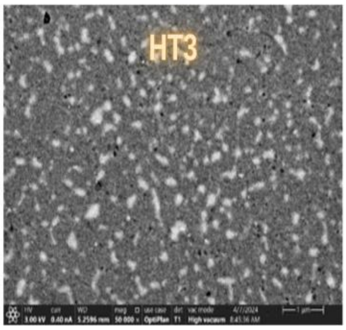
The standard heat treatment for this alloy is full stress relief. This study investigates the effect of heat treatment time and temperature on the material's microstructure, mechanical properties, electrical conductivity, residual stress and fracture surfaces. It was found that as the temperature increases, the Silicon continuous network at the grain boundaries microstructure changes to scattered Silicon agglomerates. It was also found that this process enhances the material's ductility while concurrently reducing both its strength and the residual stress.

The findings provide engineers with a comprehensive design framework, enabling the optimization of various properties from the same alloy.









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Additive Manufacturing

The Effect of HIP on the Dynamic Properties of SS316L Made by EB-PBF

Gleb Gil Goviazin[1], Dor Braun, Eithan Tiferet, Shmuel Samuha, Shmuel Hayun,
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Investigation of the effects of various hot isostatic pressing (HIP) treatments on the dynamic mechanical behavior and thermomechanical coupling of 316L stainless steel produced by electron beam powder bed fusion (EB-PBF) was carried out. The tests were carried out using a Split Hopkinson pressure bar (SHPB) synchronized with high-speed infrared camera. All samples showed similar mechanical properties to annealed bulk material, except for a higher Taylor-Quinney coefficient (~0.7) in the EB-PBF material. The density remained unchanged through all HIP treatments.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Additive Manufacturing

Additively Manufactured PEI-Based Patient-specific Bone Replacement Implants

Sahar Halevi[1], Itamar Tulpan[1], Amnon Shirizly
Biomedical Engineering, Ben Gurion University of the Negev, Israel

Recent advancements in additive manufacturing have significantly advanced medical applications, particularly in the production of personalized implants for bone repair and reconstruction. Although metals like titanium and its alloys are still the most widely used materials for such purposes, they are hindered by limitations such as stress shielding, high density, and complications in radiographic imaging. Polyetherimide (PEI, Ultem 1010), an amorphous high-performance thermoplastic polymer, has gained attention as a promising alternative due to its excellent mechanical strength, thermal resistance, and biocompatibility. However, issues such as brittleness and poor interlayer bonding in 3D-printed parts have posed challenges for its use in load-bearing applications. This research aims to optimize the 3D printing parameters to enhance the manufacturability and mechanical performance of PEI as a material for bone replacement implants. Samples fabricated using an FDM printer were assessed through compression and tensile testing, fractographic analysis, μ-computed tomography, and benchmarked against parts produced with an industrial-grade printer. Additionally, in vitro biocompatibility and cytotoxicity tests were conducted. The findings demonstrated substantial improvements in the mechanical properties and dimensional precision of 3D-printed PEI, along with excellent biocompatibility. These results underscore the potential of PEI as a robust material for bone replacement implants, effectively addressing several drawbacks of conventional metallic alternatives.

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Poster Presentation

Additive Manufacturing

Novel Hybrid Patient-specific 3D-printed Garment for Hypertrophic and Keloid Scar Treatment

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Hypertrophic and keloid scars (H/KSs) pose significant challenges to wound recovery, impacting both physical mobility and psychological well-being. Despite advancements in scar therapy, issues such as patient discomfort and low compliance remain challenges. This study presents an innovative hybrid solution: a patient-specific 3D-printed garment that integrates pressure and silicone therapies to optimize treatment outcomes. Utilizing advanced 3D scanning and printing technologies, the garment is precisely customized to the scar's dimensions and the patient's unique anatomical proportions. The design incorporates a dual-layer structure: an inner layer for hydration and enhanced scar remodeling, and an outer layer that delivers optimal therapeutic pressure of 24 mmHg directly to the scar. Thermoplastic polyurethane (TPU), selected for its durability, biocompatibility, and flexibility, was used for the pressure layer with varying shore hardness levels. The garment's fabrication was optimized through extensive mechanical testing, cytotoxicity assays, and iterative design modifications to ensure efficacy and patient comfort. Preliminary findings demonstrate the feasibility and effectiveness of this approach. The garment exhibited high dimensional accuracy, patient comfort, and therapeutic potential while minimizing unnecessary pressure on healthy skin. Cytotoxicity assays confirmed material biocompatibility and 3D scanning evaluations validated the precision in capturing scar morphology and progression. Future work will involve clinical trials to further validate therapeutic efficacy and patient satisfaction. This research marks a significant advancement in personalized medicine for scar treatment, offering a scalable, patient-centered solution that could transform recovery and improve the quality of life for individuals with hypertrophic and keloid scars.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Additive Manufacturing

3D-printed Silica-phosphate Glass

Daria Savraeva[1], Shlomo Magdassi[1]
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In recent years 3D printing of glass has become a promising technology, enabling layer-by-layer fabrication of objects with complex shapes. Among the various 3D printing techniques, digital light processing (DLP) is one of the most effective methods for producing optical-quality glass [1, 2].

This study combines DLP printing with a sol-gel process to create high-quality glass structures. We developed a hybrid ink composed of an aqueous solution of silica and phosphate precursors combined with photopolymerizable materials. This approach enables 3D printing of objects with complex shapes and allows to easily adjust the glass composition, and therefore its properties, by changing the components of the liquid mixture.

The 3D printed objects undergo an aging and post-printing thermal processes to remove the organic components and, upon densification, are transformed into glass. The amorphous state of densified material was examined using X-ray diffraction (XRD), and the glass composition was analyzed through energy-dispersive X-ray spectroscopy (EDS). The optical properties of the resulting glass were evaluated using spectrophotometry in UV, visible, and near-infrared ranges, as well as their refractive indices.

The developed method is general for making multicomponent glasses, with a simple control of the composition which is achieved by proper selection of the soluble precursors.

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Poster Presentation

Advanced Characterization Methods

Electrochemically Controlled X-Ray Spectroscopies of Solid-liquid Interfaces

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X-Ray photoelectron spectroscopy (XPS) is arguably one of the most powerful techniques for probing solid-liquid interfaces. However, this element-specific and surface-sensitive technique requires high vacuum conditions. Over the last two decades, ambient pressure XPS (AP-XPS) has been developed extending the operating range to the mbar region. Still, this technique alone is not sufficient to allow working with liquids and gases. To this end, a few approaches have been developed, including the dip-pull method and graphene-capping approach. The first requires hard X-rays and synchrotron radiation, whereas the latter can be used in lab X-ray sources, making it more versatile. Moreover, the graphene-capping approach can also be easily used under operando conditions: graphene is strong enough to sustain the large pressure difference but still thin enough to allow sufficient photoelectrons to pass through.

Our group uses a very unique approach, where microelectrochemical reactors are capped with perforated silicon nitride grids containing a few layers of graphene. Graphene acts as a catalyst bed for the model catalyst NPs while it is transparent enough to allow access to spectroscopies using X-rays as a probe. In this contribution, we demonstrate the succesful application of the graphene-capping approach to study the redox behaviour of transition metal NPs in a mildly alkaline aqueous solution under electrochemical control. For this purpose, we used X-Ray Photoelectron Spectroscopy (XPS) in conjunction with Near Edge X-Ray Absorption Fine Structure (NEXAFS) to investigate Ni NPs under operando conditions in alkaline media. While XPS gives access to the oxidation state, NEXAFS is also sensitive to the bonding environment, so it can provide information about the geometry, bonding distances and neighboring atoms. Our approach showed similar or better signal-to-noise ratios in contrast to other studies in the literature that use synchrotron radiation and/or more complex setups. This tandem XPS/NEXAFS approach can be extended to other reactions as well, revealing insights into the working mechanism and efficiency of the electrocatalyst NPs.

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Poster Presentation

Advanced Characterization Methods

Structural Phase Transitions in $K(Ta_{1-x}Nb_x)O_3$: Insights from High-Resolution single crystal X-Ray Diffraction

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$K(Ta_{1-x}Nb_x)O_3$ (KTN) is a ferroelectric material well known for electro-optical properties, enabling its applications in various optical devices, such as beam deflectors, Q-switches, high-speed optical shutters [1]. These properties are related to its perovskite-based structural flexibility and phase transitions, which are influenced by factors such as composition, temperature, and electric field. KTN exhibits a cubic paraelectric phase above the Curie temperature, transforming into ferroelectric phases of tetragonal, orthorhombic, or rhombohedral symmetries at lower temperatures. Studying the mechanisms driving the structural phase transitions of KTN is crucial, as it not only enhances the understanding of its properties but also provides insights into the behavior of other perovskite-based materials.

In this study, we investigate the influence of temperature and electric field on the structural phase transitions of KTN. Using in-situ high-resolution single-crystal X-ray diffraction [2], we collect 3D reciprocal space maps that represent the diffraction intensity distributions around Bragg peaks. A fine temperature step of approximately 1 K enables accurate tracking of the phase transitions. Figure 1 illustrates the diffraction intensity distribution during a heating-cooling cycle, showing the splitting of a Bragg peak near the phase transition into sub-peaks. This splitting, caused by the formation of ferroelastic domains, underscores the high-resolution of our method. Detailed analysis of these features provides insights into the structure of the ferroelastic domains and the phase evolution of KTN. These findings improve the understanding of the relationship between the phase transitions of KTN and its functional properties, while also shedding light on the mechanisms driving phase transitions in perovskite-based materials.

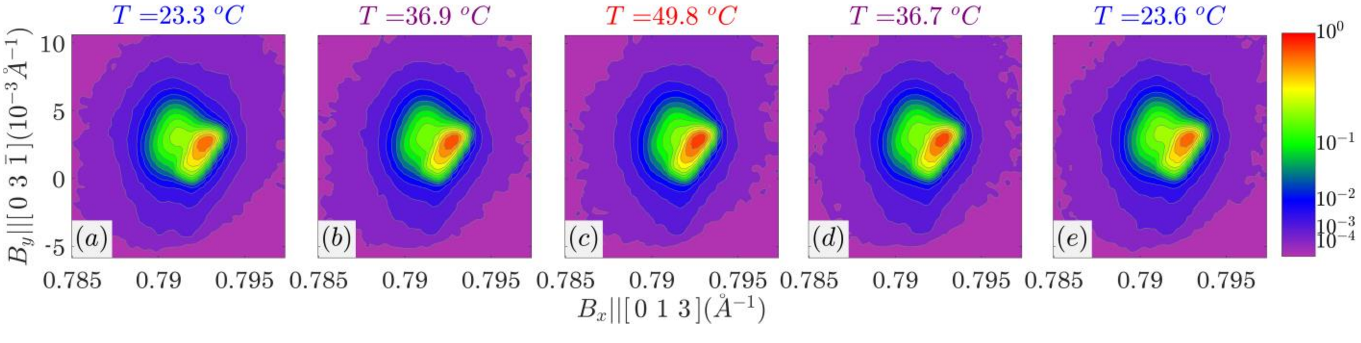

Figure1: Projection of the diffraction intensity distribution around the 0 1 3 Bragg peak during a heating-cooling cycle. The Cartesian x-axis is parallel to [0 1 3]*. Near room temperature (a, e), the

Bragg peak shows noticeable splitting, indicating the presence of sub-peaks. At higher temperatures (b–d), these sub-peaks merge into a single cubic peak.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Advanced Characterization Methods

Chemical Tomography of Cancer Organoids and Proteo-genomic Development Stages through Chemical Communication Signals

Vivian Darsa Maidantchik[1], Arnab Maity[1], Keren Weidenfeld[2], Dalit Barkan[2], Sarit Larisch[2], Hossam Haick[1]
[1]*Department of Chemical Engineering, Technion, Israel*
[2]*Department of Human Biology and Medical Sciences, University of Haifa, Israel*

Organoids are 3-dimensional (3D) structures with complex cellular interactions, and therefore may provide deep insights into physiological pathways that may lead to disease development, in comparison to 2D cell culturing. Continuous and real-time monitoring of organoids might offer a profound understanding of mechanisms of disease development and possible treatments.[1-4] However, traditional methods for disease diagnosis and follow-up do not provide real-time data, are in majority destructive and costly.

Herein, a novel hierarchical stacked geometrical configuration (HSGC) graphene oxide-based nanosensor array printed on free-standing cellulose films was used to detect Volatile Organic Compounds (VOCs) from cellular samples. Tailored ligands, composed of thiols and amines, functionalized the graphene oxide-based nanosensors. After synthesis, the functionalized dried sensor powder was redispersed in dimethylformamide (DMF) and sonicated for 1-2 minutes for better dispersion, before its use in inkjet printing on paper substrate, in a dispersing system with piezoelectric nozzle. The ready nanosensor array was utilized to generate volatilomic fingerprints of MCF-10 human breast cell line-based organoid samples, from healthy through the premalignant state, until reaching the malignant state.

The device operates in a time-space model through the separation of compounds within a gaseous-phase mixture from the sample, followed by their detection by the sensors. Consequently, a mass spectrogram of the VOCs is obtained. An Artificial Intelligence (AI)-driven analysis of the data provided by the sensor array enables the obtention of the VOC spatiotemporal distribution, generating digital patterns of morphological and proteogenomic features of organoids in different cancerous stages from 2D tomographic inputs.

The method successfully differentiated between organoids in the healthy, transitory and cancerous states, during epithelial-mesenchymal transition (EMT) process. The AI-powered spatiotemporal VOC tomographic analysis, and its validation using the traditional Gas Chromatography-Mass Spectrometry (GC-MS) technique, helps in the understanding of important biochemical pathways responsible for the VOC production, and present in the EMT process.

The volatilomic analysis enables the identification of biochemical processes such as aromatic acid degradation, carbohydrate and lipid metabolisms, that can be associated with cancerous progression, in a non-destructive way and with real-time and continuous monitoring. The novel method presented offers multiple omics integration using AI-powered analysis of data provided by nanosensors, advancing the field of oncological-related biomarkers.

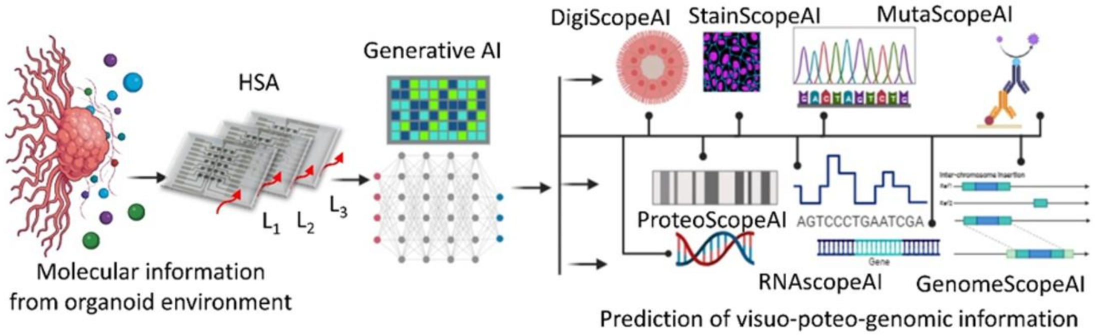

Figure 1: Schematic representation of bridging volatilomics with multi-dimensional imaging as well as proteo-genomics using generative AI.

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Poster Presentation

Advanced Characterization Methods

Quench Rate Effects on the Boson Peak in Orthoterphenyl

Shachar Keren, Omer Yaffe, Matan Menahem, Nimrod Benshalom

Glasses exhibit properties distinct from their crystalline counterparts. Unlike crystals, which have long-range periodic order, glasses lack translational symmetry, resulting in a disordered atomic arrangement. This structural difference gives rise to unique mechanical, thermal, and vibrational behaviors that cannot be explained using models designed for crystalline solids.

These distinctions are particularly evident in the low-frequency region of the vibrational density of states (VDOS). According to the Debye model, the VDOS of crystals is proportional to ω2 at low frequencies. However, this relationship does not hold for glasses, which exhibit an excess intensity in the low-frequency region of the VDOS. This phenomenon, known as the boson peak, is highly dependent on the thermal history of the glass.

Traditionally, neutron scattering has been the primary method for investigating the boson peak. However, this technique presents challenges, including the requirement for large sample volumes, limited resolution, and complex data reduction procedures, which hinder rigorous analysis.

To overcome these limitations, we employ Raman spectroscopy, which provides rapid, high-resolution measurements. Using our custom-built Raman system and an novel cryostat setup designed to control thermal history—specifically quench rates.

We systematically investigate how quench rate affects the boson peak. Orthoterphenyl (OTP), a model molecular glass former, was selected for this study due to its low glass transition temperature of 244 K. This feature enables repeated quench cycles in the cryostat.

Our findings reveal a clear dependence of boson peak intensity on quench rate, with faster quench rates leading to more pronounced boson peaks. These results highlight how thermal history directly influences vibrational dynamics in glasses, providing deeper insights into the microscopic origins of disorder-related vibrational modes.

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Poster Presentation

Advanced Characterization Methods

Nonlinear Orthotropic CMC Modelling with Abaqus

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The technology of Ceramic Matrix Composites (CMC) constantly grows and has been improved through the recent decades, primarily due to their high compatibility to extreme heat flow rate conditions. Developing a computational base for this material group is critical for reliable design of functional parts, like leading edges, TVC vanes, etc.

The current work shows the process of material characterization through a set of tensile tests, constitutive law for the material, its implementation on Abaqus UMAT and, finally, a comparison of the FEA prediction and a test of two complexly loaded parts.

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Poster Presentation

Advanced Characterization Methods

Revisiting Asymmetric Raman Lineshapes in Silicon Using Green`s Function Analysis

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I am developing a time-resolved Raman spectroscopy system to probe electron-phonon interactions (EPI) and dynamics in semiconductors. To demonstrate its utility, we investigated photoexcited silicon, where coupling between intervalence band electronic transitions and optical phonons creates an asymmetric Raman lineshape.

Traditionally, this asymmetry is analyzed using the Fano model, which describes the interference between a discrete vibrational state (the optical phonon) and a continuum of electronic transitions, resulting in an asymmetric lineshape. However, the Fano model fails to explain the transient evolution from an asymmetric lineshape in photoexcited silicon to a symmetric Lorentzian as photogenerated carriers decay. This limitation arises from the Fano model`s exclusion of intrinsic phonon lifetimes and anharmonic effects, which are significant at finite temperatures. We developed a Green`s function-based coupled-modes model to address these shortcomings. By explicitly incorporating phonon-phonon interactions through intrinsic phonon lifetimes, this framework separates the contributions of EPI and anharmonic lattice dynamics, offering a clearer understanding of the processes governing Raman lineshape evolution.

Temperature-dependent Raman measurements validated this approach, demonstrating its ability to capture full spectral lineshapes and provide deeper insights into the interplay between EPI and anharmonic lattice effects.

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Poster Presentation

Advanced Characterization Methods

Crystallographic Laws of Easy Polishing Directions in Diamond Single Crystals

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Diamond, one of the hardest known natural materials, exhibits anisotropic hardness, meaning its resistance to polishing and abrasion varies depending on the crystallographic orientation. This unique property has been exploited by diamond polishers for centuries, using empirical techniques to determine optimal polishing directions. However, despite advances in diamond processing, the polishing process remains labor-intensive and highly dependent on skill, making it difficult to scale. Additionally, existing theories mainly address the polishing of surfaces parallel to the crystal's primary axes, leaving a significant gap in the understanding of how facets not parallel to any of these axes react to the polishing process.

The purpose of this research is to validate and extend the existing theories on diamond polishing by conducting experiments using X-ray diffraction on diamond single crystals. The study focused on investigating the preferred polishing directions for various crystal planes, with particular attention to surfaces that are not parallel to the primary crystallographic axes of the diamond. By analyzing the polishing rates of these facets, the research aimed to identify more efficient polishing directions.

The results confirmed aspects of traditional theories for facets where the angle between the surface and the crystal primary axes tends to zero, usually referred to as facets aligned with primary axes. The results also revealed important insights about the polishing of surfaces with a larger angle to the axes, usually referred to as non-aligned facets. The findings suggest that the polishing mechanism is very complex, especially for facets that deviate from the primary axes. The study's conclusions, while not definitive, are especially relevant for the development of automated diamond polishing systems, which are essential for meeting the growing demand in both gemquality and industrial applications.

This work contributes to the theoretical understanding of diamond polishing and provides a foundation for improving both traditional manual polishing techniques and the emerging field of automation in diamond processing.

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Poster Presentation

Advanced Characterization Methods

Interfacial Electric-Field Inhomogeneities in Hafnia-Film, Studied by 4D-STEM

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Ferroelectricity in hafnia films has been discovered only ten years ago, but has already attracted huge interest dues to possibility for integrating ferroelectric properties in the semiconducting silicon industry. Contrary to conventional bulk ferroelectrics, thin-film hafnia exhibits mainly short-range ordering, which can be further be turned into long-range ordering under the action of applied electric field. The fundamental mechanism of ferroelectricity and ordering in such heterogeneous material is still not fully understood, and a major reason for this knowledge gap is the limited observations of both short-range ordering and local heterogeneities. Here, we used advanced electron-microscopy techniques, mainly 4D-STEM, for revealing and mapping intrinsic variations in the internal electric field. We found that the electric-field variations are substantial near the interface, paving the way to interface-engineered hafnia samples with augmented functional properties.

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Poster Presentation

Advanced Characterization Methods

Qualitative and Quantitative Micro-CT Studies on Metal-Organic Framework (MOF) Single Crystals

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Micro-computed tomography (micro-CT) is a non-destructive 3D imaging technique based on the x-ray attenuation of materials. It gives not only reconstructed 3D structures but also material density. In this talk, I will present the applications of micro-CT on the multi-domain metal-organic framework (MOF) single crystals. The micro-CT reveals unique symmetrical structures of the MOF crystals, and the quantitative study shows non-uniform density distribution. To understand the growth mechanism, samples from different reaction durations were subjected to micro-CT scans, and the results were correlated to other material characterization methods, such as single crystal XRD and FIB-SEM. We proposed a growth model for these unique MOF structures based on the correlative study.

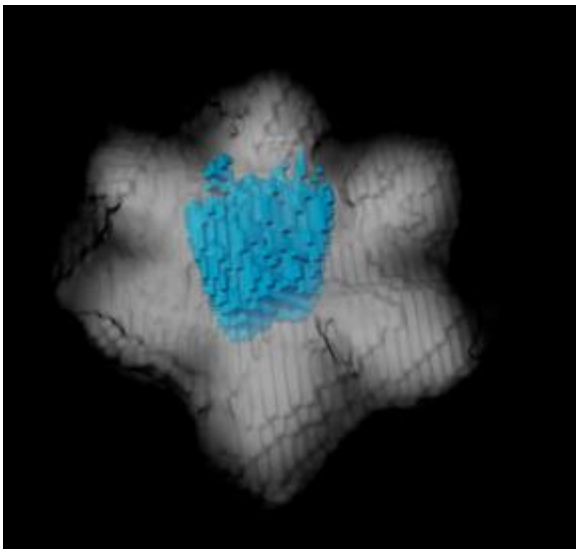

Figure 1. Micro-CT reconstruction of the Cu-AdDB MOF crystal. The less-dense region is highlighted in blue.

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Poster Presentation

Advanced Characterization Methods

Characterization of the Structure of an $Al_{81}Fe_{10}Pt_9$ Phase Using 3D Electron Diffraction Method

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The Al-Fe-Pt alloy system belongs to the Al-T-T1 group, where T and T1 are transition metals. These systems exhibit complex periodic and quasiperiodic intermetallic phases, which are of significant interest for both fundamental and applied research. Periodic crystal structures, consisting of the same atomic clusters as quasicrystals, are defined as approximants. Approximants can be categorized into "families," such as the ε phases, which can be either binary Al-T or ternary Al-T-T1, typically forming within compositional ranges of 60 to 85 at% Al. The crystallographic structures of the ε phases are orthorhombic, with consistent a and b lattice parameters ($a \approx 23$ Å, $b \approx 16$ Å), while their c lattice parameters follow the sequence $1:(1 + \tau):(2 + \tau):(3 + \tau):(4 + \tau)$, where τ is the golden mean. The index i represents the number of the strong (0 0 l) reflection, corresponding to an interplanar spacing of approximately 2 Å. The reported ε phases include i = 6, 16, 22, 28, 34, etc. (see Ref. [1] and references therein).

In addition, an orthorhombic phase with the lattice parameters $a = 23.4$ Å, $b = 16.2$ Å, and $c = 20.0$ Å has been identified in the Al-Rh-Ru alloy system. This so-called E phase can be considered as belonging to the above-mentioned group with i = 10, bridging the gap between i = 6 and i = 16 reported earlier.

During an investigation of the Al-Fe-Pt alloy system, a new complex ternary phase of unknown structure, forming in a compositional region around ~$Al_{79}Fe_{12}Pt_9$, was revealed [2]. Powder X-ray diffraction was ineffective in determining its structure due to significant peak overlapping. Similarly, transmission electron microscopy (TEM) applied to powdered material could not resolve the structure, as all broken fragments were oriented identically due to their preferential cleavage. However, initial TEM investigations of an $Al_{81}Fe_{10}Pt_9$ sample indicated that this phase is probably orthorhombic, with $a \approx 23$ Å and $b \approx 16$ Å lattice parameters, suggesting a possible relation to the ε family of phases.

Using the 3D electron diffraction methods, the geometry of this phase was determined, linking its structure to the E phase and the ε family of approximant phases.

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Poster Presentation

Advanced Characterization Methods

Optical Microscopy Based Prediction of Nanoparticle Height Distribution in Pt Nanogrates Using Artificial Intelligence

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Interest in nanoscale particles is growing at a staggering pace. Nanoparticles dimensions impact them with enhanced optical, electronic, catalytic and mechanical properties sparking worldwide research and development of nanodevices and materials. Nanoparticle characterization is often cumbersome and slow. Typically, atomic force microscopy (AFM) is used for determining the height of particles; yet it is slow, labor-intensive and therefore not suitable for large scale space variable characterization. Arrays of substrate-supported nanoparticles or nanogrates tend to reflect specific colors due to short range correlation of size and position which causes resonance of certain wavelengths. In this work we have taken advantage of this phenomenon. We trained a neural network to predict the height distribution of Pt nanoparticles using optical microscope images of the surface. The goal of presented work is to create a fast and scalable method for characterizing nanoparticle ensembles. We demonstrate the capability to extract spectrum information from the optical microscope images which could be useful for analysis of physical properties of nanogrates beyond the standard optical microscopy applications.

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Poster Presentation

Bio- and Soft Materials

Monodispersed Nanohydrogels for Drug Delivery

Gerardo Byk[1], Eswaran Lakshmanan[1], Sinyal Abu-Rabyah[1], Danit Zegal[1], Gila Kazimirsky[1], Nir Osherov[2], Yana Shadkhan[2], Maria Lujan Cuestas[3], Shaul Deniz Cemal[1]
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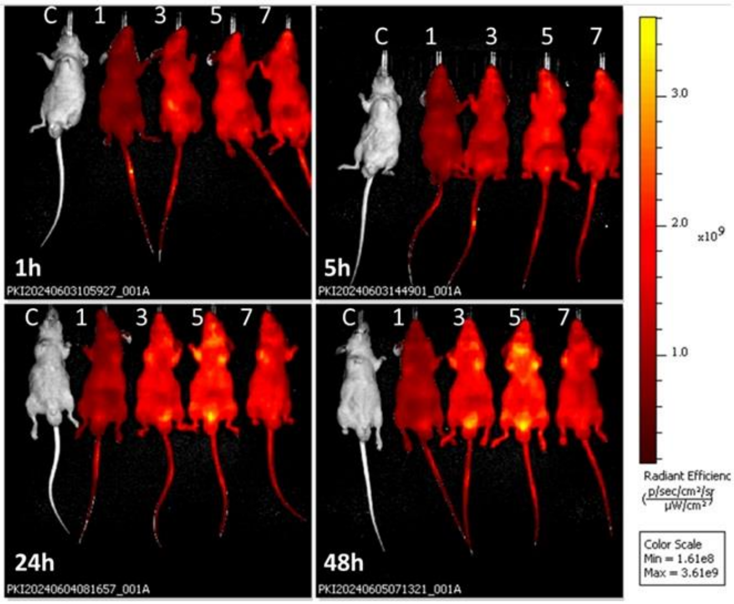
Biodegradable synthetic polymeric materials have emerged as promising candidates for the sustained drug release, offering significant benefits in controlled drug delivery. This research project focuses on the design and synthesis of a novel class of bio-degradable cross-linked monodispersed nanohydrogels (NHGs) encompassing a wide range of sizes with no significant toxicity suitable for diverse biological applications. These monodispersed NHGs were prepared via a recently developed synthesis whereby a thermo-responsive mixture of monomers undergoes self-assembly followed by confined polymerization. By carefully adjusting the monomer ratios, the size of intermediate self-assemblies and produced NHGs can be precisely tailored in the nanometric range (20–500 nm). To enhance biodegradability, special cross-linkers were introduced into the polymeric backbone. The obtained NHGs represent ideal candidates for drug delivery due to their exceptional properties, including biocompatibility, high drug loading capacity, controlled release mechanisms, and potential for targeted delivery. We explored the potential of NHGs as carriers for the antifungal drugs voriconazole (VRC) and amphotericin B (AmB). The loaded NHG's were evaluated in clinical isolates of molds and yeasts. Furthermore, the in vivo toxicity and efficacy of loaded NHGs were also tested in murine models with invasive Candida albicans infections. Overall, this study contributes to the expanding field of biodegradable materials and showcases the potential of NHGs as versatile *platforms for*

controlled drug release in biomedical research and applications.



Cy7 Nanohydrogels of different sizes administered IV to mice. 1= 400nm, 3and 7 =200nm, 5= 30 nm

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Poster Presentation

Bio- and Soft Materials

A Self-healing Multispectral Transparent Adhesive Peptide Glass

Gal Finkelstein-Zuta, Ehud Gazit

Despite its disordered liquid-like structure, glass exhibits solid-like mechanical properties. The formation of glassy material occurs by vitrification, preventing crystallization and promoting an amorphous structure. Glass is fundamental in diverse fields of materials science, owing to its unique optical, chemical, and mechanical properties as well as durability, versatility, and environmental sustainability. However, engineering a glassy material without compromising its properties is a major challenge. Here, we report the discovery of a supramolecular amorphous glass formed by the spontaneous self-organization of the short aromatic tri-peptide YYY initiated via noncovalent cross-linking with structural water. This system uniquely combines often contradictory sets of properties; it is highly rigid yet can undergo complete self-healing at room temperature. In addition, the supramolecular glass is an extremely strong adhesive yet it is transparent in a wide spectral range from visible to mid-infrared. This exceptional set of characteristics is observed in a simple bioorganic peptide glass composed of natural amino acids, presenting a multi-functional material that could be highly advantageous for various applications in science and engineering.

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Poster Presentation

Bio- and Soft Materials

In-vitro Behavior of Zn-Nd Base Alloy as Structural Material for Biodegradable Implants

Efrat Hazan Paikin

The potential of Zn-based alloy with up to 3%Nd, as structural material for biodegradable implants was evaluated in in-vitro conditions. The selection of Zn as a matrix metal related to its inherent excellent biocompatibility and essential role in many physiological reactions. The advantage of Nd as an alloying element was attributed to its relatively adequate biocompatibility and strengthening effect capabilities. Optical and scanning electron microscopy combined with X-ray diffraction analysis were used to examine the microstructure while the mechanical properties were evaluated in terms of hardness and tensile strength. The corrosion behavior in simulated physiological environment in the form of phosphate-buffered saline (PBS) solution was examined by immersion tests and potentiodynamic polarization analysis. Mus musculus 4T1 cells were used for cytotoxicity assessment in terms of direct and in-direct cell viability analysis. The results of this study displayed the strengthening effect of Nd via a secondary phase formation ($NdZn_5$), which did not have any significant deteriorating effect on the corrosion resistance. The cytotoxicity assessment has suggested that the tested alloys have a strong favorable effect on cell viability. In addition, it was demonstrated that the cell viability tendency was amplified as the Nd content was increased.

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Poster Presentation

Bio- and Soft Materials

Electrically Conductive Peptide/MXene Hydrogel Scaffold for Tissue Regeneration

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Advances in tissue engineering requires the development of biomaterials that mimic the extracellular matrix (ECM) while offering additional functionalities to support cell growth and tissue regeneration. This research focuses on the fabrication of an electrically conductive hydrogel scaffold composed of self-assembling peptide hydrogels and MXene nanosheets, specifically designed for wound healing applications. The scaffold integrates the unique properties of the peptide hydrogels with the exceptional electrical conductivity of MXene, forming a multifunctional platform to enhance tissue repair through applied voltage stimulation.

MXenes are two-dimensional materials known for their high electrical conductivity, hydrophilicity, and ease of surface modification. Incorporating MXene nanosheets into the hydrogel matrix introduces significant functionality by enhancing electrical conductivity. The conductive MXene network facilitates the delivery of electrical stimulation to cells, which is particularly beneficial for electrically responsive cell types such as fibroblasts—key players in wound healing. Under applied voltage, the scaffold promotes cellular activities by modulating ion exchange, membrane potential, and intracellular signaling pathways. It was previously demonstrated that a conductive environment significantly enhances cell proliferation, migration, and viability, accelerating the wound-healing process. Here, we demonstrated fibroblast accelerated growth, with significant increases in proliferation observed under physiologically relevant electrical stimulation.

Additionally, continued development could expand its use to chronic wound treatment, further establishing its role as a versatile platform for regenerative medicine.

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Poster Presentation

Bio- and Soft Materials

Innovative Lithographic Platform For Reference-free Traction Force Microscopy

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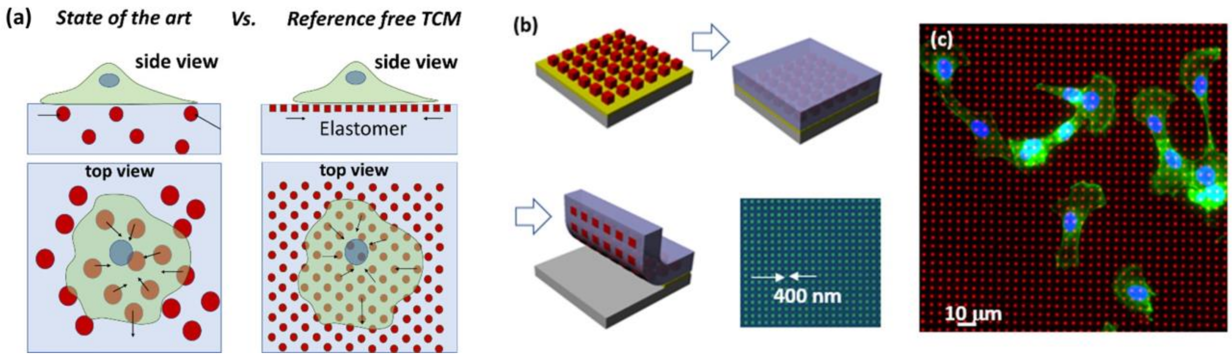
The mechanical communications between cells and their surroundings, such as other cells and extracellular matrix, is fundamental to regulating complex biological processes during tissue development, repair, or pathology. Quantifying the forces cells produce and sense is essential for understanding cellular function. The most common way to identify these forces is Traction Force Microscopy, by which cells are placed on an elastomer surface with embedded fluorescent nanoparticles, whose displacement indicates the force direction and magnitude. However, traditional traction force microscopy has three main limitations: (i) The initial position of randomly distributed nanoparticles must be recorded before the cell experiment to detect their displacement, (ii) The random nanoparticle location in z direction makes some of them out of focus, and produce uncertainty in their lateral displacement, and (iii) the nanoparticle displacement can be track with limited resolution, usually above 1 micron.

To circumvent these limitations, we engineered a novel platform for traction force microscopy, in which the fluorescent markers with arbitrary size and distribution are controllably positioned in ordered arrays, with the resolution down to the nanometric scale. To fabricate such a platform, we coated the Silicon wafer with a sacrificial film of Au. We patterned it on top of fluorescently colored epoxy resin (SU-8) by either negative-tone photo- or e-beam lithography. Then, we cast PDMS, a biocompatible elastomer, over this and separated it from Si by etching the Au. This way, we produced elastomer surfaces with arrays of various fluorescent markers sized down to 300 nm. We functionalized the surface with fibronectin, a vital component of the ECM (extracellular matrix), to allow cell adhesion. To verify the feasibility of the platform, we seeded NIH 3T3 mouse fibroblast cells, demonstrating that the fluorescent arrays indicate the force distribution within and around the individual cells. The new platform paves the way for numerous studies to understand cells` mechanical activities, focusing on the nanoscale force distribution at the cell-matrix interface.



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Poster Presentation

Bio- and Soft Materials

Artificial Silk Fibers with Tunable Mechanical Performance

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The silk industry significantly contributes to global pollution, producing up to 11 million tons of defective cocoons and other silk fibrous waste annually.Our research addresses this problem by developing a sustainable method for the reconstitution of silk fibroin from defective cocoons and reconstructing the protein into a morphology mimicking natural silk fiber in its appearance and mechanical properties. A wet-spinning artificial silk fibers platform was developed to achieve this scientific goal. The research results further contribute to a better understanding the fundamental mechanisms of spinning fibrillar proteins into continuous solid fibers with controllable mechanical characteristics.

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Poster Presentation

Bio- and Soft Materials

Copper Oxide Nanoparticle Embedded Super Absorbing Biopolymers to Enhance Nutrient Supply and Water Retention in Agriculture

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The combination of superabsorbent polymers (SAP) and nano-fertilizers offers a promising solution to address critical challenges in agriculture. SAPs enhance water retention in soil, improving water use efficiency, and supporting higher crop yields. Integrating nano-fertilizers with SAPs will enable both controlled release and precise delivery of essential nutrients. This synergy not only improves plant health and productivity but also optimizes resource use and minimizes environmental impacts, offering a sustainable approach to modern agricultural challenges. In this study, we synthesized biodegradable alginate-jellyfish-based hydrogels with embedded copper oxide nanoparticles (NPs). Cu is an active nanomaterial with antifungal and micronutrient properties that improve nutrient utilization efficiency and help manage disease and crop loss. The chemical structure of the composite was characterized, and drying methods were explored to choose the optimal method in terms of subsequent Cu release efficiency and water uptake. Two drying methods of the SAP were explored: air drying and freeze drying. Freeze drying exhibited 900% water uptake compared to 170% when air dried. The release of the freeze-dried beads over a period of 2 weeks was an order of magnitude higher than that of the air-dried ones. Release was measured over a period of 2 months, where only 3.5% of the total CuO NPs were released, indicating slow release suitable for irrigation. Overall, this work offers a new composite for slow release of fertilizers based on alginate-jellyfish hydrogels with high potential for contribution to crop yield and water retention in soil.

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Poster Presentation

Computational Materials Science and Machine Learning

Monte Carlo Simulated Annealing and Machine Learning Interatomic Potentials for High-Entropy Materials Design

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High-entropy materials form a class of new advanced functional materials with multi-element compositions that offer exciting opportunities in a variety of fields, including cathodes for energy storage applications [1-3]. However, determining the atomic arrangements in these complex, solid-solution systems is challenging, and density functional theory (DFT) calculations for large numbers of configurations are not practically feasible due to high computational costs. To facilitate generation of low-energy configurations for such complex systems, we developed a Monte Carlo Simulated Annealing (MCSA) code within the Atomic Simulation Environment (ASE) framework, which can utilize any potential energy models with an ASE interface, including various machine learning interatomic potentials (MLIPs).

As a case study, we applied this code to high-entropy oxyfluoride cathodes (HEOFs) for Na-ion batterie. We compared the energies of a large number of HEOFs configurations obtained from various general-use MLIPs, including MACE, ORB, SevenNet, FAIR-Chem, and CHGNet, with DFT results. We also benchmarked the optimized HEOFs lattice parameters for different desodiated states obtained from MLIPs against DFT results. Our analysis evaluates how well the MLIPs reproduce DFT energy and lattice constant trends as a function of desodiation, and we identify the most reliable MLIP models for modelling HEOFs.

Building on the framework presented here, we aim to calculate voltage profiles, lattice distortions, and other structural properties across varying compositions to identify promising cathode materials. The current methodology lays the groundwork for future efforts in screening and optimizing *complex high-entropy and other materials for next-generation energy storage applications.*

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Poster Presentation

Computational Materials Science and Machine Learning

Computational Studies of Liquid Potassium Under Pressure Using First Principles and Machine Learning Methods

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The high-pressure behavior of the alkali metals remains a “hot topic” in both experimental and theoretical physics. Despite the apparent simplicity of these metals (a single valence s electron), they exhibit quite surprising and interesting properties at high pressure. At ambient temperature, they all undergo a series of phase transformations into complex, low-symmetry open-packed, crystallographic structures at elevated pressures. Another common feature of the alkali metals is an anomalous melting behavior. Transitions in the liquid phase should affect the shape of the melting curve and may explain its complex nature.

To investigate the structural and electronic properties of compressed liquid potassium, we employ first-principles molecular dynamics (FPMD) simulations of potassium in the liquid state up to 30 GPa along the 600 K isotherm. Our simulations indicate structural and electronic changes in liquid potassium under pressure. At pressures below 15 GPa, liquid potassium has a bcc-like short-range order (SRO). In higher pressures, the SRO of liquid potassium deviates from the bcc-like, as reflected in the reduction of the coordination number and the changes in the radial distribution function. Moreover, at high pressure, liquid potassium exhibits a lowering of the electronic density of states near the Fermi level (this phenomenon is known as a pseudogap), indicating some localization of the valence electrons.

To overcome the limitations on the system size and the simulation duration due to the computational cost of FPMD, we apply machine learning methods to generate interatomic potentials optimized to reproduce the first principles data. Our machine-learned force field (MLFF) fully captures the pressure-induced structural changes in the liquid phase observed in the FPMD simulations. Using our MLFF, we conduct large-scale molecular dynamics simulation to calculate the melting curve of potassium using the two-phase coexistence method.

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Poster Presentation

Computational Materials Science and Machine Learning

In-gap States and Carrier Recombination in Quasi-2D Perovskite Films

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In-gap states and their effect on recombination rates in quasi-2D lead–iodide- based perovskites, intercalated with various spacer molecules, are studied using a combination of scanning tunneling spectroscopy and temperature-dependent photoconductivity measurements. The results are further analyzed by a Shockley–Read–Hall model. Indications for shallow in-gap states, positioned at about 0.15–0.2 eV below the bottom of the conduction band, are found. These states are identified as dominating the recombination route of photogenerated carriers in these systems, with a relatively large capture coefficient of about $10^{-5} – 10^{-6}$ at room temperature. First-principles calculations based on density functional theory imply that these states are not an intrinsic effect of the inclusion of the spacer molecules, but rather one that arises from chemical defect formation or structural deformation of the perovskite layers. The results suggest that further improvement of the performance of solar cells that are based on quasi-2D perovskites requires, along with enhancing carrier mobility, efforts to suppress the concentration of these detrimental defect states.

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Poster Presentation

Computational Materials Science and Machine Learning

Evaluation of Mn Doped Perovskite-type Oxides as Electrolyte Materials for Hydrogen Conversion

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The conversion of hydrogen gas from chemical form to electrical form can be achieved in a proton ceramic fuel cell where the proton conducts through the electrolyte. During this process, the dissolution of hydrogen under hydrogen atmosphere may be coupled to the creation of oxygen vacancies in the electrolyte material $AZrO_{3-x}$, where A=Ba, Sr, Ca. The energy required to create these oxygen vacancies plays a role in proton conductivity. First-principles calculations based on density functional theory reveal that by substitutional doping of Zr with ~5% Mn reduces the oxygen vacancy formation energy by more than two-fold in $SrZrO_3$ and $CaZrO_3$. The partial density of states after doping shows that the Fermi level shifts towards the valence band edge and mid-gap states arising from Mn. Bader charge analysis confirmed a reduction of Mn ions due to the creation of oxygen vacancies. Such variations in the oxygen vacancy formation energies and the electronic structure of perovskite-type oxides by the addition of Mn may lead to efficient conversion of hydrogen from chemical to electrical energy.

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Poster Presentation

Computational Materials Science and Machine Learning

The Effect of Oxygen Terminations on Charge Transport Across Mos$_2$ Monolayers

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Two-dimensional materials, like MoS$_2$ monolayers, are gaining a lot of interest in the field of nano-electronics due to their relatively high charge mobility, tunable bandgaps, high optical transparency, exceptional mechanical properties, good chemical stability, and atomically thin structures with large surface area. These properties position MoS$_2$ as an ideal candidate for next-generation applications, including photo-devices, nano-transistors, and flexible ultra small devices, where the traditional materials face scaling and performance limitations.

The electronic properties of MoS$_2$ monolayers can be significantly tuned by intrinsic sulfur vacancies that may be substituted by terminating oxygen atoms from the gaseous environment. The relationship between these defects and the resulting electronic properties is complex and not fully understood. In this study, we aim to investigate how the distribution and concentration of these defects affect the electronic conductivity of MoS$_2$ monolayers. We examined MoS$_2$ structures with sulfur vacancies substituted with oxygen defects at various concentrations and distributions, using the following methodologies: density functional theory (DFT) for calculation of electronic structure properties, tight-binding theory for building the tight-binding Hamiltonian, non-equilibrium Green's function (NEGF) formalism for transmission function calculations, Landauer-Büttiker formalism for calculating charge transport, and a design of experiment (DOE) method for identifying what are the most important structural features that influence the electric current. We found that substitution of sulfur vacancies with oxygen atoms resulted in a degradation of the charge permeability to levels comparable to pristine MoS$_2$ monolayers. These findings provide valuable insights into the relationship between structural defects across MoS$_2$ monolayers and charge permeability, enabling the rational design of functional materials through targeted defect engineering.

Keywords:
MoS$_2$ monolayers, atomic defects, sulfur vacancies, oxygen substitution, defects concentration and distribution, electronic properties and conductivity, design of experiments.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Computational Materials Science and Machine Learning

Uniaxial Strain-Induced Multiferroicity in $EuTiO_3$ Membranes: Insights from DFT Simulations

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Strain control in free-standing membranes opens new avenues for manipulating lattice deformations, offering access to a broader range of strain values compared to epitaxial films. The present study investigates the effects of uniaxial tensile strain of up to 10% on the multiferroic properties of $EuTiO_3$ membranes. Using Density Functional Theory (DFT) simulations, we explored the phase diagrams of $EuTiO_3$. We demonstrate that strain induces a variety of phases associated with the rotation of oxygen octahedra, potentially contributing to the stabilization of polarizable phases. The multiferroic properties of $EuTiO_3$ were investigated under strain, with notable coupling between its ferroelectric and magnetic properties. Our results show that tensile strain alters the electronic structure, leading to the emergence of functional instabilities that are absent in the unstrained state. Furthermore, strain probably enhances magnetoelectric coupling by generating spontaneous polarization and modifying magnetic ordering, which could have implications for future applications. The analysis reveals the presence of soft phonon modes, indicating structural instabilities accompanying phase transitions. These findings provide deeper insight into the potential of strain engineering as a versatile tool for tailoring the physical properties of materials, particularly in multiferroics where coupling effects play a central role.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Computational Materials Science and Machine Learning

Adsorption and Intermediate Reactants Study of Nitrogen Reduction Reaction on Bi Surface Using Machine Learning Based on DFT Calculated Database

Sean Pachmanov Dvir, Maytal Caspary Toroker

Heterogenous catalysis is a widely research filed, aiming to utilize solar energy in an efficient way. Within a variety of reactions that received high interest, nitrogen reduction is very noticeable in latest research works. Both bismuth and Bi-based alloys have been shown to be promising catalysts for the nitrogen reduction reaction. When performing a theoretical study of electrochemical process, one of the first and most important steps is finding the adsorption site on the catalytic surface, followed by a mechanistic study of the reaction. The time limitations of DFT doesn’t enable the researcher to achieve full confidence in the adsorption site determined only by a few initial guesses and DFT geometry optimization. In this work, we demonstrate combining machine learning algorithms with DFT calculations-based data as a method for finding an initial guess for an adsorption site. Using the method, several intermediate reactants of nitrogen reduction reaction will be studied in bismuth-based systems.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Computational Materials Science and Machine Learning

First Principles Calculations of the Magnetic Structure of the RE-based -MAX Phases – a Family of Nanolaminated Magnetic Materials

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The recently discovered in-plane ordered MAX phases (henceforth -MAX) with the chemical formula $(Mo_{2/3}RE_{1/3})_2AlC$ (RE = lanthanide), have opened the possibility to manufacture magnetically ordered 2D derivatives. Neutron diffraction (ND) and muon spin rotation (µSR) studies revealed that the -MAX phases order magnetically as spin density waves with ordering temperatures between 3.5 K and 29 K. However, many open questions remain regarding the nature of these magnetic structures. Particularly, µSR revealed that for RE heavier than Gd, the magnetic structure fluctuates on a time scale of µs, short-range order was observed for RE = Ho and Er in ND and field dependent magnetization measurements show a rich phase diagram under an applied magnetic field. To help explain the experimental observations, a first-principles approach is used to construct an effective spin Hamiltonian for the RE--MAX system. The exchange interactions are calculated from perturbation theory using the Liechtenstein formula. The existence of spin density waves is explained from competing antiferromagnetic interactions in the RE layer, and the experimentally observed trend in the magnetic transition temperatures is well reproduced by a mean field calculation based on the computed exchange interactions. Moreover, the calculated magnetic exchange interactions are compared with experimental values obtained using magnetic neutron diffuse scattering. Good agreement is observed with experiments, thus validating the first principles calculation. The strongest exchange interaction for RE = Nd, Gd, Tb and Dy is found to be between RE atoms separated by the Al layer. This result has strong implications on the possibility to retain magnetism in the 2D derivative.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Computational Materials Science and Machine Learning

MD Calculations of High Pressure Pb-Sn Alloy

Daniel Rabin[1], Guy Makov[2]
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We investigated the Pb-Sn alloy system under dynamic pressure using molecular dynamics (MD) focusing on the eutectic composition compared with pure Pb. A Modified-Embedded-Atom-Method (MEAM) potential with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software were used. We applied shock loading using the Piston method to calculate the alloy Hugoniot. The results were transformed into the P-T plane to identify the melting. In addition, we examined the change in the phase diagram at high pressure, by calculating the binary interatomic parameters as a function of pressure.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Computational Materials Science and Machine Learning

Ab Initio Study Of Point Defects In Tungsten Metal

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Point defects generated from radiation damage in tungsten (W) metal were studied using density functional theory (DFT). The energetics of vacancy defects, including single, di-, and tri-vacancies, and interstitial defects at tetrahedral and octahedral sites were calculated in W. We found that the adjacent di-vacancies were energetically preferred over separated vacancies, with a binding energy of 0.35 eV. Additionally, the interstitial defect at the tetrahedral site was energetically more stable than at the octahedral site. The material properties, including cell parameters, cohesive, and binding energies, were determined using two approximation methods: Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). The results obtained from the GGA method were relatively close to the experimentally reported values.

We calculated the formation energy for tri-vacancies in three configurations, including collinear vacancies along the diagonal and two non-collinear cases. We found that the collinear tri-vacancies were energetically preferred over other configurations.

Moreover, migration energies of point defects were calculated using the constrained relaxation method along the (001) direction. The migration energy of the vacancy defect was found to be a few meV and shows good agreement with experimental and previous theoretical results. Therefore, we conclude that vacancy defects can accumulate and form vacancy clusters in W during the radiation damage.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Corrosion and Protection of Materials

The Effect of TiO2 Particles in Zinc Coating on Corrosion of Low Carbon Steel ST 37

Harel Cohen, Svetlana Lugovskoy, Alex Lugovskoy

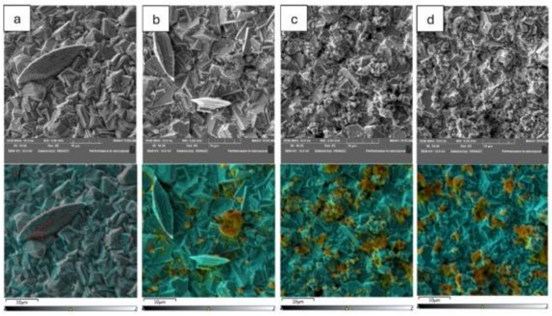
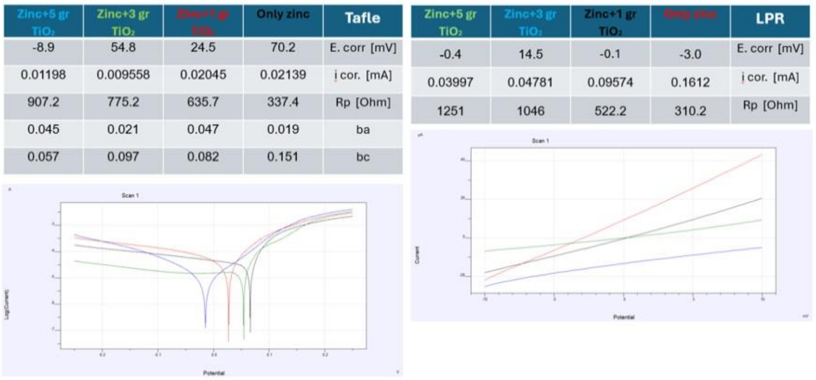


Fig 1. SEM images of ST 37 with (a) Zinc coating, (b) Zinc coating with 1 g/L TiO_2 nanoparticles (c) Zinc coating with 3 g/L TiO_2 nanoparticles, and (d) Zinc coating with 5 g/L TiO_2 nanoparticles.



Zinc+5 gr TiO_2	Zinc+3 gr TiO_2	Zinc+1 gr TiO_2	Only zinc	Tafle
-8.9	54.8	24.5	70.2	E. corr [mV]
0.01198	0.009558	0.02045	0.02139	i cor. [mA]
907.2	775.2	635.7	337.4	Rp [Ohm]
0.045	0.021	0.047	0.019	ba
0.057	0.097	0.082	0.151	bc

Zinc+5 gr TiO_2	Zinc+3 gr TiO_2	Zinc+1 gr TiO_2	Only zinc	LPR
-0.4	14.5	-0.1	-3.0	E. corr [mV]
0.03997	0.04781	0.09574	0.1612	i cor. [mA]
1251	1046	522.2	310.2	Rp [Ohm]

Fig 2. Corrosion analysis results from LPR and Tafel measurements for ST37 steel with zinc coating and varying concentrations of TiO_2 nanoparticles (1, 3, and 5 g/L).

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Corrosion and Protection of Materials

Enhanced Corrosion Protection and Electrochemical Activity for Aluminum Fluoride Surface

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NRCN, israel

This work deals with the passivation of aluminum surfaces by controlled reactions of fluoride ions from different salts such as KF or NH_4F. Aluminum is important metal because of its great technological value in many industries. Despite its high reactivity, it has high resistance to corrosion achieved by a passivity natural oxide layer (alumina) formed immediately upon exposure to air.

Fluorine has special properties like high electro negativity and a small relative size of its anion. Fluorine is very reactive and reacts almost with all the elements. In aqueous solution the chemistry of fluoride is interesting. On the one hand, the fluoride creates an insoluble precipitate with different cations depending on the oxidation state of the metal. On the other hand, fluoride causes dissolution of insoluble salts especially oxides.

In this study indicate that the exposure of aluminum surfaces to concentrated fluoride salts aqueous solutions increases the weight of the aluminum samples. A new layer is formed on the surface that combines the Al-F-O atoms and the salt cation depending on the type of salt used. The new layer creates an insoluble compound on the surface that appears as a coating on the metal. Under Certain conditions, the coating can be seen visually. Its color is white and is firmly attached to the surface. The coating is not removed by smearing tests performed.

Morphological characterization of layer indicates the kinetics and compositions obtained. As expected, the thickness of the coating depends on the time of soaking in the solution. The thickness can range from several microns after several hours in solution and develop up to tens of microns after several days in solution.

The advantages of passivation in this method were examined later in the work compared to natural aluminum surfaces (without treatment). It has been found that aluminum fluoride coating improves resistance to corrosion both in basic NaOH media and in acidic HCl media, which are known to accelerate the corrosion of aluminum.

An electro-chemical study was carried out using Cyclic Voltammetry and Impedance methods. The results indicated that aluminum with Al-F coatings has different electro-chemical properties compared to standard aluminum surfaces. This phenomenon can be applied for Al-air fuel cell.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Experimental Apparatus for SMA Springs Analysis: Design and Results

Israel Alexandron[1], Gal deBotton[1,2]
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[2]*Department of Mechanical Engineering, Ben-Gurion University of the Negev, Israel*

Shape Memory Alloys (SMAs) are well known for their ability to recover their original shape from significant, seemingly plastic deformations upon heating, a phenomenon known as the Shape Memory Effect (SME). This unique characteristic arises from the thermoelastic reverse martensitic phase transformation between the cold martensite phase and the hot austenite phase. The associated large strain, force, and high energy density make SMAs highly attractive as thermally stimulated actuators in aerial, industrial, and biomedical applications. Despite their potential, limited research has focused on springs made from SMAs, even though they hold significant promise for various applications. To advance research on SMA springs, particularly in the cold martensite phase, a novel experimental apparatus was designed and constructed. This apparatus enables extensive testing of different SMA springs under diverse boundary conditions, while accurately measuring and controlling the three parameters governing the state of SMA springs: temperature, elongation, and force. The apparatus is composed of four main components: a bath, a thermal unit, a mechanical unit and a control. The SMA sample is immersed in a water bath with the temperature controlled by a specialized thermoelectric Peltier device. The low temperature gradient, combined with the SMA sample’s low heat capacity and high thermal conductivity, ensures that its temperature closely matches the water temperature. The mechanical components of the apparatus include a tension-compression motorized unit to set the spring`s elongation and a force gauge to measure the applied force. A custom-designed LabVIEW program continuously monitors and controls all experimental parameters. To demonstrate the apparatus`s capabilities, experiments were conducted where temperature was varied while either elongation or force was held constant, and the other variable was monitored. These experiments highlighted the role of thermal phase transformations. Isothermal experiments characterized the force-elongation relationship at various temperatures. Additional experiments explored combinations of elongation, force, and temperature profiles altered simultaneously, revealing the complex, history-dependent behavior of SMA springs, particularly in the cold martensite phase. In conclusion, the experimental apparatus is capable of conducting highly precise experiments, enabling detailed investigation of the complex, history-dependent behavior of shape memory springs.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Material Coefficient Extraction Through Design and Modeling of Magnetoelectric Devices in Higher Bending Modes

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The Internet of Things is driving advancements in sensors, communication components, and power sources. Ideally, these components should be powered by sustainable energy readily available in the environment [1].

A magnetoelectric (ME) composite, comprised of piezoelectric and magnetostrictive layers, enables magnetic-to-electric energy transduction through functional materials properties. Through operation in mechanical resonance, ME devices appear to be one of the most promising technologies for wireless power transfer (WPT), when small device sizes (or low frequencies) are required.

Previous work focused on various ME devices modelling, of which the magneto-mechano-electric equivalent circuit method is very common [2]. In this study, we expand the model to account for ME operation in higher bending modes of the cantilever by incorporating the Euler-Bernoulli cantilever equation. The accuracy of our model will be compared with experimental results for Ni/PVDF composite cantilever devices.

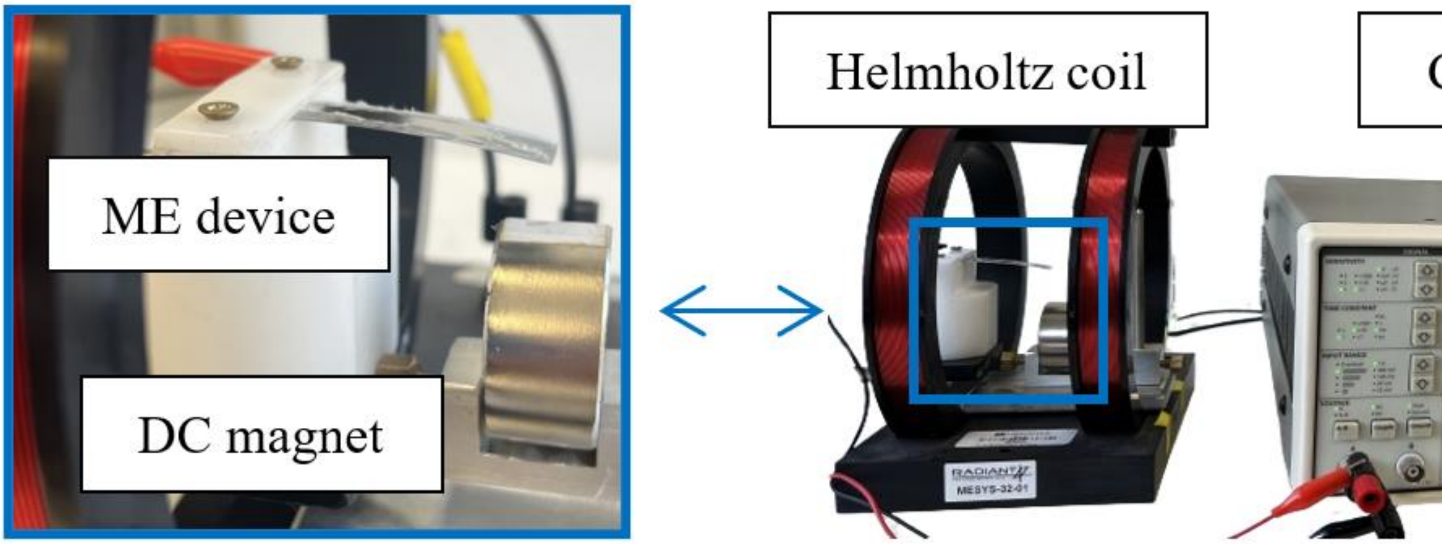

Figure 1: ME measurement set-up.

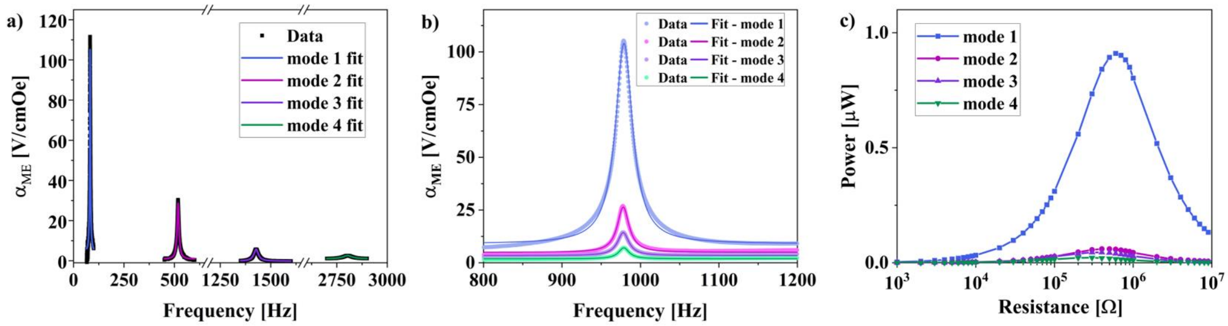

Figure 2: ME measurements with low AC magnetic field drive (Hac=0.13 [mT]). a) α_{ME} (dE/dH -ME voltage coefficient) vs. frequency in different modes in the same ME device. b) α_{ME} vs. frequency in different devices, designed to have the same resonance frequency, in different modes. c) the power of the different devices.

Our results suggest a good agreement between the derived models and ME output (both open circuit and power), up to the 4th operating mode. From the fitting to the model, we can extract material coefficients such as the piezoelectric or the piezomagnetic constant. We will discuss the usage the higher modes for device and application design (accounting for e.g., frequency requirements) as well as performance and materials analysis.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Functional Materials

Conductive Peptide-Based MXene Hydrogel as a Piezoresistive Sensor

Dana Cohen-Gerassi[1], Or Messer[1], Gal Finkelstein-Zuta[1], Moran Aviv[1], Bar Favelukis[1], Yosi Shacham-Diamand[1,2], Maxim Sokol[1], Lihi Adler-Abramovich[1]
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[2]*Reichman University, Israel*

Wearable pressure sensors have become increasingly popular for personal healthcare and motion detection applications due to recent advances in materials science and functional nanomaterials. In this study, a novel composite hydrogel is presented as a sensitive piezoresistive sensor that can be utilized for various biomedical applications, such as wearable skin patches and integrated artificial skin that can measure pulse and blood pressure, as well as monitor sound as a self-powered microphone. The hydrogel is composed of self-assembled short peptides containing aromatic, positively- or negatively charged amino acids combined with 2D $Ti_3C_2T_z$ MXene nanosheets. This material is low-cost, facile, reliable, and scalable for large areas while maintaining high sensitivity, a wide detection range, durability, oxidation stability, and biocompatibility. The bioinspired nanostructure, strong mechanical stability, and ease of functionalization make the assembled peptide-based composite MXene-hydrogel a promising and widely applicable material for use in bio-related wearable electronics.

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Poster Presentation

Functional Materials

Controlling Independently the Pyroelectricity and Piezoelectricity of Doped Mixed Crystals

Shiri Dishon Ben Ami[1], David Ehre[1], Meir Lahav[1], Igor Lubomirsky[1]
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Generally, symmetry dictates that mono-component polar crystals are expected to be both pyroelectric and piezoelectric at least along their polar directions. In this work we investigate the nature of polarity in doped mixed organic crystals resulting from lattice symmetry reduction, using pyroelectric and piezoelectric measurements as a probe. The method is based on doping of centrosymmetric crystals, with “tailor-made” guest molecules that convert them into polar mixed crystals. The polarization of such crystals has two distinct contributions, one arising from the difference in dipole moments between guest and host molecules and the other one originating from the displacement of host molecules residing neighboring to the guests, from their symmetry-related positions.[1] Based on the chirality, structure, and concentration of the guest molecules, we can separate and investigate the different contributions to the polarization and therefore, to the pyroelectric and piezoelectric response. This enables the design of pyroelectric crystals with minimal or no piezoelectricity.[2] Thus, in such mixed molecular crystals, the link between pyroelectricity and piezoelectricity can be broken.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Bio-Inspired Core-Shell Crystalline Guanine Spherulites

Lotem Alus[1,2], Lothar Houben[3], Noy Shaked[2], Angelica Niazov-Elkan[1], Iddo Pinkas[3], Dan Oron[1], Lia Addadi[2]
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The study of photonic crystals in different organisms unveiled the use of common purines, pterins, and pteridines, molecules that are known to participate in biochemical metabolic pathways, as highly birefringent crystalline materials with unique optical functions. A combination between the molecular structure and the crystal structure, together with their assembly into controlled architectures, creates complex photonic crystals used for efficient light scattering and reflectance, even in aqueous environments. One example are the highly birefringent ($\Delta n \sim 30\%$) organic core-shell nanometric spherulites found in the vision system of decapod crustaceans that pack into ultra-thin reflectors. The shell of each spherulite is composed of nanoplatelets of single-crystal isoxanthopterin that are radially stacked in a manner which imposes birefringence on the spherulite, with a distinct difference between the tangential (nt=1.88) and radial (nr=1.4) refractive indices.[2-3] The resulting optical anisotropy increases light backscattering from single particles and reduces optical crowding across the aggregate, thus enhancing light scattering in a broad wavelength range.[4] This spherulitic metastructure and its optical properties have no synthetic equivalent to date.

In this work, we demonstrate the synthesis of bio-inspired core-shell guanine spherulites ($\Delta n=25\%$) using a two-step emulsification process and an acid-base crystallization reaction. Raman spectroscopy and 4D-STEM analysis confirm that the spherulites consist of single, radially stacked ß-guanine platelets, oriented tangentially to the spherulite surface. Mie theory calculations and forward scattering measurements from single spherulites reveal that due to the single-crystal properties and orientation, the synthetic spherulites possess a high tangential refractive index (nt=1.84), comparable to their biogenic isoxanthopterin counterparts. We explore the impact of varying parameters, such as the choice of the acids used to neutralize guanine toward crystallization, on the crystallization process in the ternary emulsion and its influence on the resulting spherulitic structures. These synthetic, wavelength-scale spherulites pave the way for novel applications in artificial structural coloration and as highly efficient light-scattering media.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Nitridochromates as Potential Functional Materials

Natalia Gloriozova[1,2], Yurii Prots[1], Franziska Jach[1], Mitja Krnel[1], Alim Ormeci[1],
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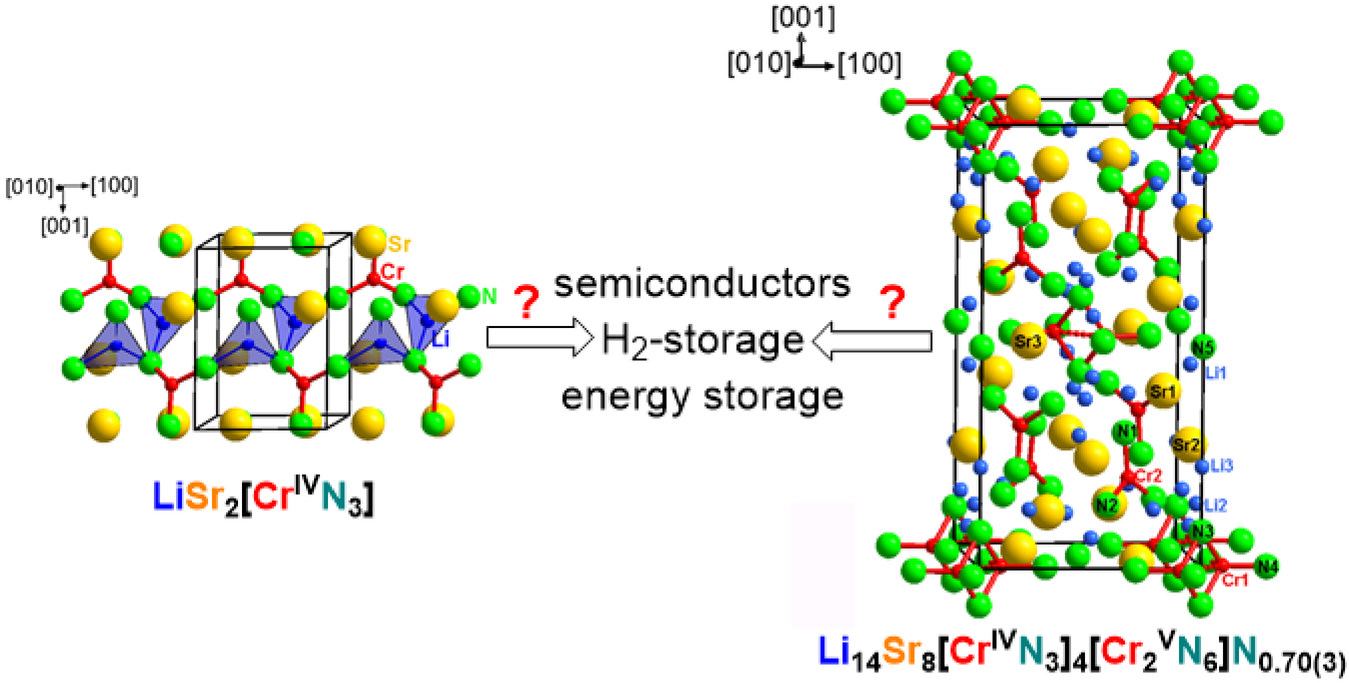
Nitridometalates are a unique class of nitrogen-containing compounds, consisting of $[T_x\mathrm{N}_y]_{z-}$ anions (T is a transition metal), stabilized by cations alkali, alkaline-earth, or rare-earth metals.[1] While initially studied for their diverse crystal structures, compositions and chemical bonding, lithium-containing nitridometalates have recently attracted interest as potential functional materials, however, the knowledge about them remains limited.

Chromium-containing nitridometalates, or nitridochromates, are particularly intriguing due to a wide variety of oxidation states of chromium, ranging from III to VI. To date, only a few lithium-containing nitridochromates with chromium in high oxidation states, such as $\mathrm{Li_4Sr_2[Cr_2^{V}N_6]}$, $\mathrm{Li_6[Cr^{VI}N_4]}$, $\mathrm{Li_{15}[Cr^{VI}N_4]_2N}$, $\mathrm{Li_{14}[Cr^{VI}N_4]_2O}$, and $\mathrm{Li_{10}[Cr^{VI}N_4]O_2}$, have been reported.[1,3] Lithium-containing nitridochromates with chromium in lower oxidation states remain elusive.

An investigation of the Li–Sr–Cr–N systems reveals two new quaternary phases with different Li content: $\mathrm{LiSr_2[Cr^{IV}N_3]}$ and $\mathrm{Li_{14}Sr_8[Cr^{IV}N_3]_4[Cr_2^{V}N_6]N_{0.70(3)}}$.[4] Both compounds crystallize in unique structure types with space groups $P2_1$ and $P4_2/mnm$, respectively. The lithium substructures exhibit notably different arrangements. In $\mathrm{LiSr_2[Cr^{IV}N_3]}$, lithium atoms are threefold coordinated by nitrogen, forming slabs along the (001) plane. The Li-substructure in $\mathrm{Li_{14}Sr_8[Cr^{IV}N_3]_4[Cr_2^{V}N_6]N_{0.70(3)}}$ is significantly more complex, comprising a combination of tetrahedrally coordinated $[\mathrm{LiN_4}]$ and trigonally coordinated $[\mathrm{LiN_3}]$ units. These units form a two-dimensional network, with voids within the layers occupied by double $[\mathrm{Cr_2N_6}]$ tetrahedra, while adjacent layers are interconnected by $[\mathrm{CrN_3}]$ units. Increasing lithium content leads to greater structural complexity.

Detailed investigations of crystal and electronic structures, as well as magnetic and vibrational properties, provide insights into the nature of $[\mathrm{CrN_3}]$ and $[\mathrm{Cr_2N_6}]$ units as well as Li-substructures. This research contributes to the broader understanding of nitridochromates and their potential as functional materials.



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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Characterization of Electro-mechanical Performance of Soft Ionic Materials

Yi Jiang, Yuchen Wang, Sergey Nechausov, Aslan Miriyev

Realizing the potential of soft functional ionic gels implies the characterization of their electrical and mechanical properties and their interplay. Electrical performance at rest and under deformation directly affects the response accuracy and the speed and stability of the signal transmission within the functional material. This includes dynamic measurement of parameters such as resistance, impedance and conductivity at rest and under various deformation modalities. However, there is scarce knowledge of systematic methods for the characterization of the electromechanical performance of ionic gels. The current work introduces a method for assessing the electrical and mechanical properties of ionogels and ionic eutectogels under mechanical deformation. Specifically, it covers the electromechanical performance of ionogel and ionic eutectogel wires (i-wi), sustainable gelatin/ethaline ionic eutectogel wearable sensors (GelETh), and dual capacitive and resistive response mechanism of ionic eutectogel/perforated mesh (Perf-iGel) pressure value and location sensors. We suggest that our systematic property testing method can provide a basis for material selection and structural and functional optimization of ionic materials, and improve their reliability and applicability in soft robotics and intelligent devices.

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Poster Presentation

Functional Materials

Development and Characterization of Bovine Serum Albumin-based Sponges for Efficient Removal of Perfluorooctane Sulfonate

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Perfluorooctane sulfonate (PFOS; $C_8F_{17}SO^{-3}$), are infamously known as "forever chemicals" due to their extreme persistence in the environment. PFOS has garnered particular attention due to its widespread use in consumer products, including textiles, polymers, and food packaging. Their resistance to breakdown and potential health impacts, such as cancer, immune dysfunction, and hypertension, contribute to their environmental threat [1,2]. As a result, considerable efforts have been directed towards developing technologies for PFOS removal. However, existing methods often suffer from inefficiency, high costs, and environmental concerns, largely due to the strong C-F bond in PFOS, which resists degradation and leads to bioaccumulation [3,4]. Unlike many other substances, PFOS accumulates in protein-rich tissues such as the liver, kidneys, and blood serum albumin, which is the primary binding target for PFOS under physiological conditions [5]. Drawing from this, we introduce a novel approach utilizing bovine serum albumin (BSA)-based sponges designed with an optimized microstructure for enhanced PFOS removal. By fine-tuning key factors like mixing speed, surfactant concentration, and foaming duration, we created highly porous sponges that are both mechanically stable and effective at adsorbing PFOS. Advanced characterization techniques, including micro-computed tomography and cryo-scanning electron microscopy, confirmed the structural robustness of these sponges. Their natural affinity for PFOS led to a removal efficiency of approximately 80% under physiological conditions of pH of ~7.4, similar to conditions found in natural water sources [6]. The adsorption process was well-described by Langmuir and Freundlich models, indicating strong surface interactions and high adsorption capacity. Additionally, mechanical testing verified their durability, making them suitable for practical use. This sustainable and cost-effective approach surpasses traditional PFOS removal technologies and shows promise for various applications, including drug delivery, tissue engineering, and catalysis.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

THZ-Raman Spectroscopy Probes Lattice Dynamics of Metal-Organic-Frameworks

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Metal-organic frameworks (MOFs) are exciting materials to study due to their unparalleled structural tunability, high surface area, and versatility, enabling applications in gas storage and separation to catalysis, sensing, and drug delivery. The dynamic behavior of MOF lattices can influence these applications by affecting properties such as adsorption and diffusion of small molecules, and mechanical stability.[1] Despite its importance, experimental studies of MOF lattice dynamics are rare.[2] In this work, we demonstrate that THz-range (below 200 cm^{-1}) Raman scattering is a powerful technique to probe the structural fluctuations of MOFs.[34] Two nickel-based MOFs with identical ligands and similar coordination chemistry were used. The MOFs have different metal-to-ligand ratios, space groups and porosity (Pnna, 13%; P-421C, 51%).

Our study reveals that the MOF with space group Pnna exhibits a Raman spectrum with distinct, well-defined peaks, suggesting that the Raman selection rules are preserved due to longer coherence lengths of lattice vibrations. In contrast, the MOF with space group $P^{-}42_1C$ displays a broad and diffuse Raman spectrum, indicative of a breakdown in selection rules caused by a very short coherence length of lattice vibrations, reflecting strong anharmonicity. The MOFs were chemically modified by embedding sodium resorufin into their channels to affect the vibrational properties. Our results indicate that the more porous MOF ($P^{-}42_1C$, 51%) accommodates a larger amount of guest molecules and strongly influence the Raman spectrum, leading to the appearance of sharp, distinct peaks. The Raman spectrum of the less porous MOF (Pnna, 13%;) also shows noticeable peak shifts reflecting interactions between the cationic host framework and the negatively charged chromophore. These findings demonstrate that lattice dynamics and long range order in MOFs is highly dependent on the crystallographic structure. The lattice dynamics are affected by host-guest interactions as demonstrated by Raman spectroscopy.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Studying the Involvement of Cells and the Interplay of Mineral and Silk Protein Gel in Mollusk Shell Formation

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Biomineralization is a fundamental biological process that enables organisms to form hard tissues such as shells, bones, and teeth. Mollusk shells are remarkable materials comprising mineral-organic matrix composites. Many bivalve shells comprise an outer calcitic prismatic layer and an inner aragonite nacre layer, each with distinct geometries. This unique structure contributes to the shell`s exceptional mechanical stability, even under high pressure.

In mollusks, biomineralization is orchestrated by the mantle tissue, which deposits minerals in an extracellular organic matrix. This matrix comprises a sophisticated network of β-chitin, hydrophilic proteins, and silk fibroin1. The silk fibroin phase forms a hydrated gel2 enriched with glycosaminoglycans, playing a critical role in shell formation. While the composition of mollusk silk fibroin has been characterized3, significant gaps remain in understanding how mantle cells synthesize the organic matrix and whether initial mineral deposition occurs intracellularly. We study the complex interactions between organic and inorganic components in mollusk shell biomineralization, highlighting the role of mantle cells and offering insights into biomaterials` development and materials science.

Environmental scanning electron microscopy (E-SEM) revealed a compressed gel, embedded between nacre plates, that leaks out upon nacre fracture. We also detected channels within the mineral that may facilitate communication between the growing mineral layers, enabling the transport of amorphous calcium carbonate (ACC) and organic matrix components. Using cryo-SEM on whole very young mollusks, we observed mantle cells intimately juxtaposed to growing prisms, directly contributing to prism formation. However, it remains unclear whether silk fibroin and ACC are formed synergistically within the cell or ACC is formed in a different stage, possibly in the extracellular matrix.

These findings shed light on the intricate interplay between cells, organic and inorganic components during mollusk shell biomineralization, providing new insights into the evolution of biomaterials and advancing materials science.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Influence of SrTiO3(001) Substrate Temperature on the Structure and Magnetic Properties of FePd Films

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Ferromagnetic films of chemically-ordered L10 tetragonal alloys attract attention for spin-electronic applications due to their high magneto-crystalline anisotropy [1-5]. However, the required L10 ordered phase is reported to appear only following thermal annealing [6]. Here, we examine FePd films deposited on SrTiO3(001) (STO) substrates using high frequency magnetron sputtering. The choice of an STO substrate is due to the relatively small lattice mismatch with L10 FePd compared to other technologically relevant single-crystal oxide substrates. Therefore, we investigate the effect of substrate temperature (150°C - 600°C) on the structure and magnetic properties of the FePd films. Reciprocal space mapping by X-ray diffraction, along with transmission electron microscopy (TEM) and electron diffraction reveal that long-range chemical order increases with substrate temperature. Films deposited at low substrate temperatures exhibit a disordered FCC structure, whereas those deposited at higher substrate temperatures show the ordered L10 structure with an epitaxial relation of STO(001)[100]||FePd(001)[110].

The microstructure of the films, as examined by TEM, reveals an island-like morphology following deposition at higher substrate temperatures, in contrast to continuous films observed at low substrate temperatures, Fig.1(a),(b), respectively. Room-temperature magnetic measurements indicate that the easy axis of magnetization lies in-plane for films deposited at low temperatures (150°C) but changes to out-of-plane for films deposited at high temperatures (600°C) along with a substantial increase of coercivity to ∼1.2kOe, Fig.1(c),(d), respectively.

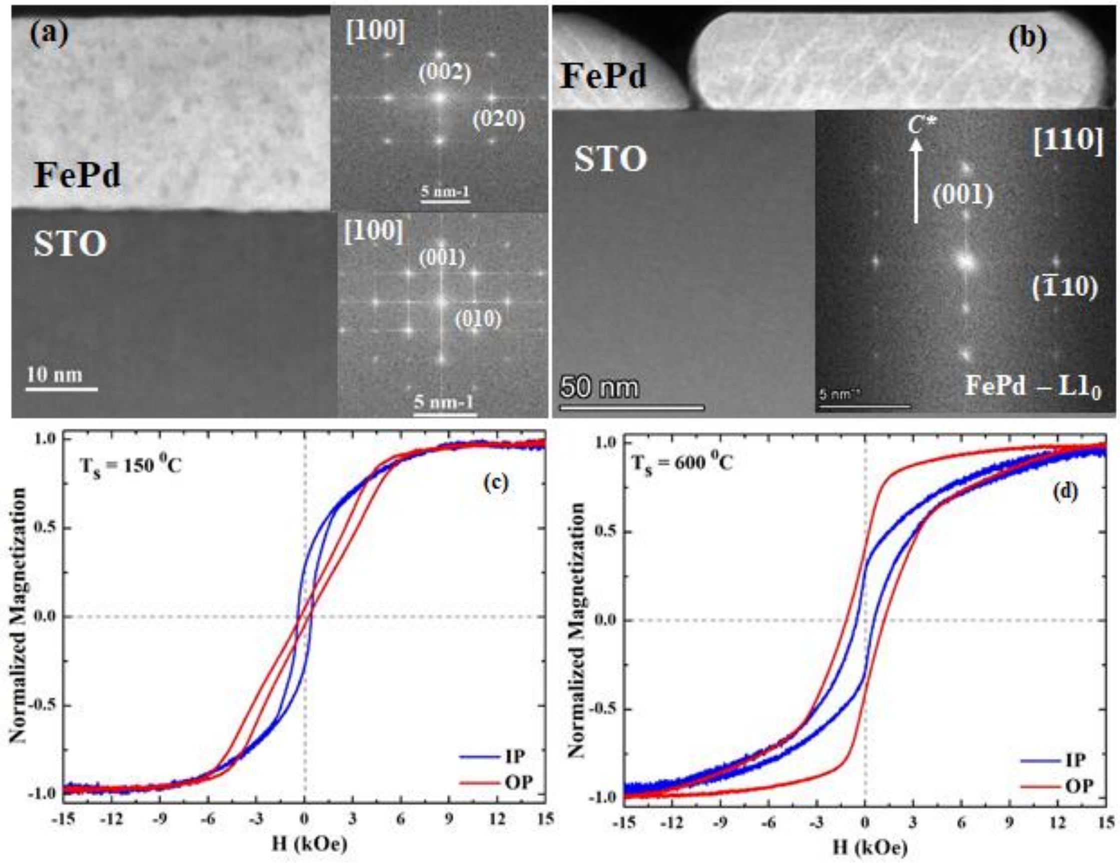

Figure 1. (a),(b) Cross-sectional high-angle annular dark-field STEM images, and (c),(d) normalized magnetization curves (measured at room-temperature) for the in-plane (IP) and out-of-plane (OP) orientations of FePd films deposited on STO at substrate temperatures of 150°C and 600°C, respectively. Power spectra of the STO and FePd images are shown as insets in (a) and (b).

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Porous Galfenol Films on Porous Silicon: Magnetic and Magnetostrictive Properties

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Magnetostriction, the property of magnetic materials to change shape under a magnetic field, plays a crucial role in magnetoelectric (ME) composite structures. Among such materials, Galfenol (FeGa) stands out as a promising candidate due to its exceptional mechanical and physical properties. Its rare earth-free composition offers advantages like lower production costs, a wider operational range, reduced saturation field, and low coercivity [1].

However, when Galfenol thin films are grown on rigid substrates, the clamping effect restricts the propagation of magnetic field-induced strain. To overcome this limitation, porous silicon (pSi) substrates, fabricated via anodization, are employed for sputtering Galfenol thin films. These films are then analyzed for their morphology and magnetic properties. By combining image analysis with magnetic characterization, the influence of substrate porosity on film properties can be systematically evaluated.

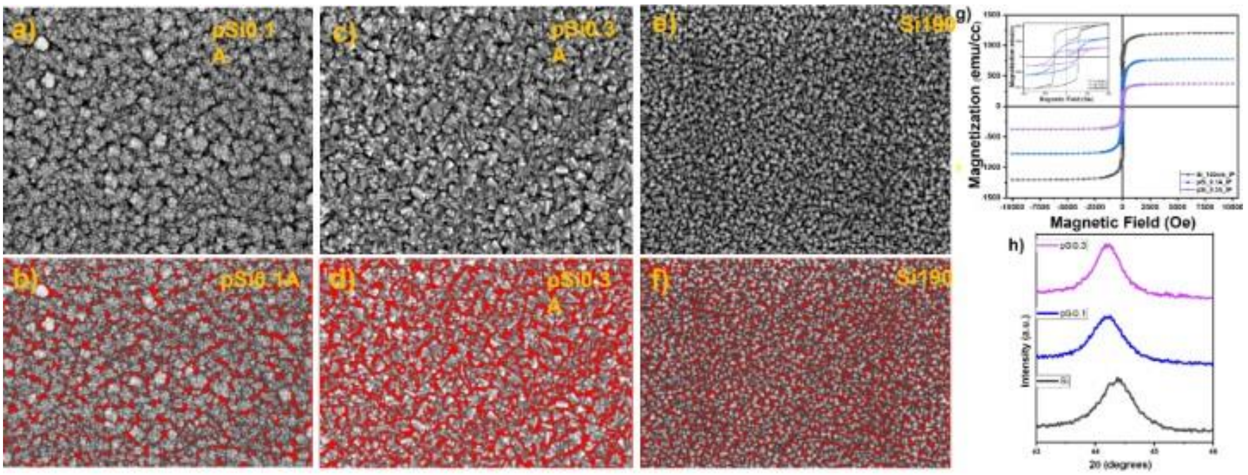

Figure 1: a-f : SEM top view images of the FeGa thin films sputtered on varying porosity Si substrates and their corresponding porosity analysis g: hysteresis loops and h: XRD patterns of the samples

The use of pSi substrates significantly impacts the porosity of the deposited FeGa thin films, which inherently exhibit some nanoporosity between columnar grains. Substrate porosity affects the film growth, leading to increased film porosity relative to the substrate. This increase in porosity is associated with reduced magnetization and higher coercivity. High-Resolution X-ray Diffraction (HR-XRD) measurements reveal a shift to lower 2θ values, indicative of lattice relaxation.

The magnetostrictive behavior of the FeGa films is further examined through in-situ XRD under an applied magnetic field [2]. These findings highlight how porous FeGa films can be tailored for advanced applications, paving the way for the development of strain-engineered nanomaterials and devices such as high-performance microelectromechanical systems (MEMS), energy transducers, and ME composites.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Post–Functional Integration of Mechanophores into Heterogeneous Biologically Derived Materials via "Dip–Conjugation"

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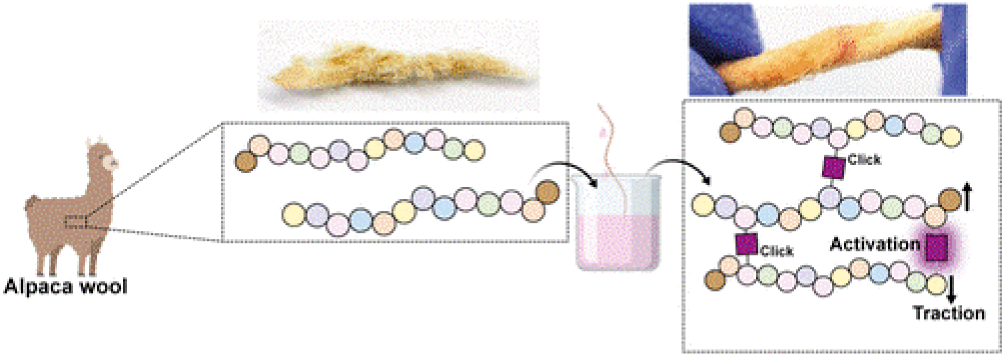
Mechanical force plays a crucial role in numerous biological processes. However, the complex structure of biomaterials makes it challenging to directly quantify mechanical forces and nearly impossible to synthesize them artificially. In this study, we utilize Click chemistry to functionalize alginate and alpaca wool fibers with mechanophores(force-responsive molecules). This conjugation enables these materials to function as chemical–level force sensors, exhibiting scalable force–responsive capabilities detectable via optical signals. Our findings expand the potential applications of mechanophores, extending their use from conventional synthetic materials to complex, heterogeneous biological systems to direct and quantitative 3D force measurements in mechanobiology.



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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Trypsin-Induced BSA-PEGDA Hydrogel as an Extendable Soft Robotic Drug Carrier

Yuchen Liu

The development of hybrid protein-polymer hydrogels with programmable shape-morphing abilities, extended site retention, tunable mechanical properties, high biocompatibility, and sustained drug release continues to present significant challenges. Here, we introduce a novel enzyme-triggered hydrogel system based on bovine serum albumin (BSA) and polyethylene glycol diacrylate (PEGDA), offering dual functionalities of controlled drug release and unfolding actuation. This design leverages the biological versatility of proteins and the structural flexibility of synthetic polymers, enabling enhanced responsiveness and functionality (1). Our study demonstrates that tuning the hydrogel composition and its interaction with trypsin enables precise customization of physical and microstructural properties. Notably, BSA-PEGDA hydrogels treated with trypsin exhibited significant transformations, including a reduction in stiffness from ~100 kPa to ~10 kPa and enhanced swelling capacity. These changes allowed the hydrogels to autonomously untie knots and transition from curved shapes to straight configurations in response to enzymatic stimuli. Utilizing the biochemical versatility of BSA, we conjugated Fluorescein Isothiocyanate (FITC) as a drug model, to its surface to form BSA(FITC)-PEGDA hydrogels. We found that the drug release rate is significantly influenced by the trypsin concentration (0.25% and 0.01% w/v) and the crosslinking degree of the hydrogel matrix, controlled by BSA/PEGDA concentrations ratio. In addition, we found that the drug release mechanism is governed by erosion and diffusion mechanisms, as validated by the Korsmeyer-Peppas model (2). Finally, by integrating shape morphing with controlled release, we developed a soft robotic drug carrier, where enzymatic stimulation by trypsin (0.01% w/v) not only triggered shape morphing but also significantly influenced the drug release rate. This work underscores the potential of enzyme-responsive hydrogels for innovative applications in targeted drug delivery and bioinspired actuation systems.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Unique Pathway of Metal to Halide Perovskites Conversion

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Bromide based perovskites are always under focus due to their high open circuit voltage in perovskite solar cells. Here we introduce a new strategy for the conversion of metals to bromide-based perovskite using Polybromide melt. We discovered a new solvent free unique approach using a MABr: Br2: HBr composition named as Polybromide melt (PBM) which converts metallic lead and non-lead metals like Cu, Au into their Halide Perovskite Counterpart. Research groups have reported conversion metallic Pb and Au into their iodide based perovskite compositions. The corrosive nature of the melt which contained Brn- characterized by Raman studies helps to overcome the thermodynamic barrier of the conversion. We converted metallic powder and sputtered metals into perovskites thin films, generated large single crystals using PBM. We also understood the insitu conversion of Bromide based Perovskite in transmission XRD mode. UV-Vis, PL and SEM, XPS studies were also performed on the fabricated thin films. Different bromide-based amine salts can also be used in place of methylammonium bromide as a precursor solution. This work will add a new dimension in the field of Halide Perovskite based research.

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Poster Presentation

Functional Materials

Dry Etched Periodic Nanopores in GaN and Their Effect on Electromechanical Properties

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Gallium nitride (GaN), of the III-N family, is a wide bandgap, high electron mobility and high breakdown field semiconductor material. Moreover, due to its Wurtzite structure, it has a permanent polarization along the c-axis ([0001]) and is similarly piezoelectric.

Nano-porosity is a known way of controlling both optical and mechanical properties of GaN and other materials based on specific needs. Recent findings suggest that nano-porosity could boost GaN`s electromechanical coupling, potentially enhancing its piezoelectric capabilities[1]. To accurately characterize the effect of porosity on piezoelectric and electric properties, the nanopores` geometry—diameter, depth, and spacing—must be precisely controlled.

A specialized process was developed to create a hexagonal array of nanopores with diameters and distances ranging from 110 nm to 30 nm in 20 nm steps. This process involves Electron Beam Lithography (EBL) for patterning and afterwards, dry etching with plasma in ICP-RIE is applied while using the altered resist as a protective mask carving the nanopores as per pattern. CSAR-62 is used as a positive tone resist due to his high resolution and selectivity[2]. To further enhance the selectivity, chemical etching approach using $Cl2$ plasma gases are applied, increasing the GaN etching rate[3]. Furthermore, in order to control the pores` depth, a protective mask was put between the resist and the GaN in a certain thickness because its selectivity with respect to GaN to $Cl2$ plasma in the during the ICP dry etching is well known and higher than the resist itself.

After the samples are prepared, the pores` geometry was examined by SEM and the properties of the nanopores` influence on GaN`s piezoelectricity was evaluated using Piezoresponse Force Microscopy (PFM). Scans of different Voltages were aligned together in order to create a d33 map and analyze from it the change in d33 in porous and nonporous areas. The results obtained so far suggest a distinction between the porous and non-porous area, and as a function of pore size. This shows the potential of structured porosification as an engineering tool for GaN functional properties.

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Poster Presentation

Functional Materials

Magnetron Sputtered Fe_3Si Full Heusler Compound Thin Films: the Effect of Microstructural Evolution on Physical Properties

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Heusler compounds constitute a large family of ternary intermetallics with highly tunable magnetic, topological, electronic and thermoelectric properties. Fe_3Si is the only binary exception to this family, attracting attention as a potential spin injector due to its predicted half-metallicity and spin polarization properties[1–6].

Given that both structural ordering and chemical composition strongly affect magnetic properties in Heusler alloys[7], understanding their evolution during growth and processing is essential. We study structural properties of Fe_3Si thin films prepared by single-target magnetron sputtering on thermally oxidized SiO_2/Si(100) substrates at different deposition temperatures (RT-300°C), followed by annealing at 500°C for 2 hours. Magnetometry confirmed that all films were ferromagnetic both before and after annealing.

Selected area electron diffraction (SAED) patterns (e.g. Fig. 1(a)), corroborated by x-ray diffraction (XRD) measurements, showed a single cubic phase with a lattice parameter close to bulk Fe_3Si. Energy dispersive x-ray spectroscopy (EDS) mapping by scanning transmission electron microscopy (STEM) (Fig. 1(b)) revealed significant oxygen content (20 at%) with inhomogeneous distribution throughout the film, in the form of Fe-rich and more oxidized Si-rich patches. However, phase contrast TEM showed that the crystal structure was maintained across the film. Post-deposition annealing enhanced the {220} peak intensity in XRD patterns, Fig. 1(c). This peak also shifted to a higher angle, which is closer to the expected $D0_3$ d-spacing, thus suggesting increased ordering in the film. Annealing also affected strongly the electronic properties of the films, most notably the temperature coefficient of resistance.

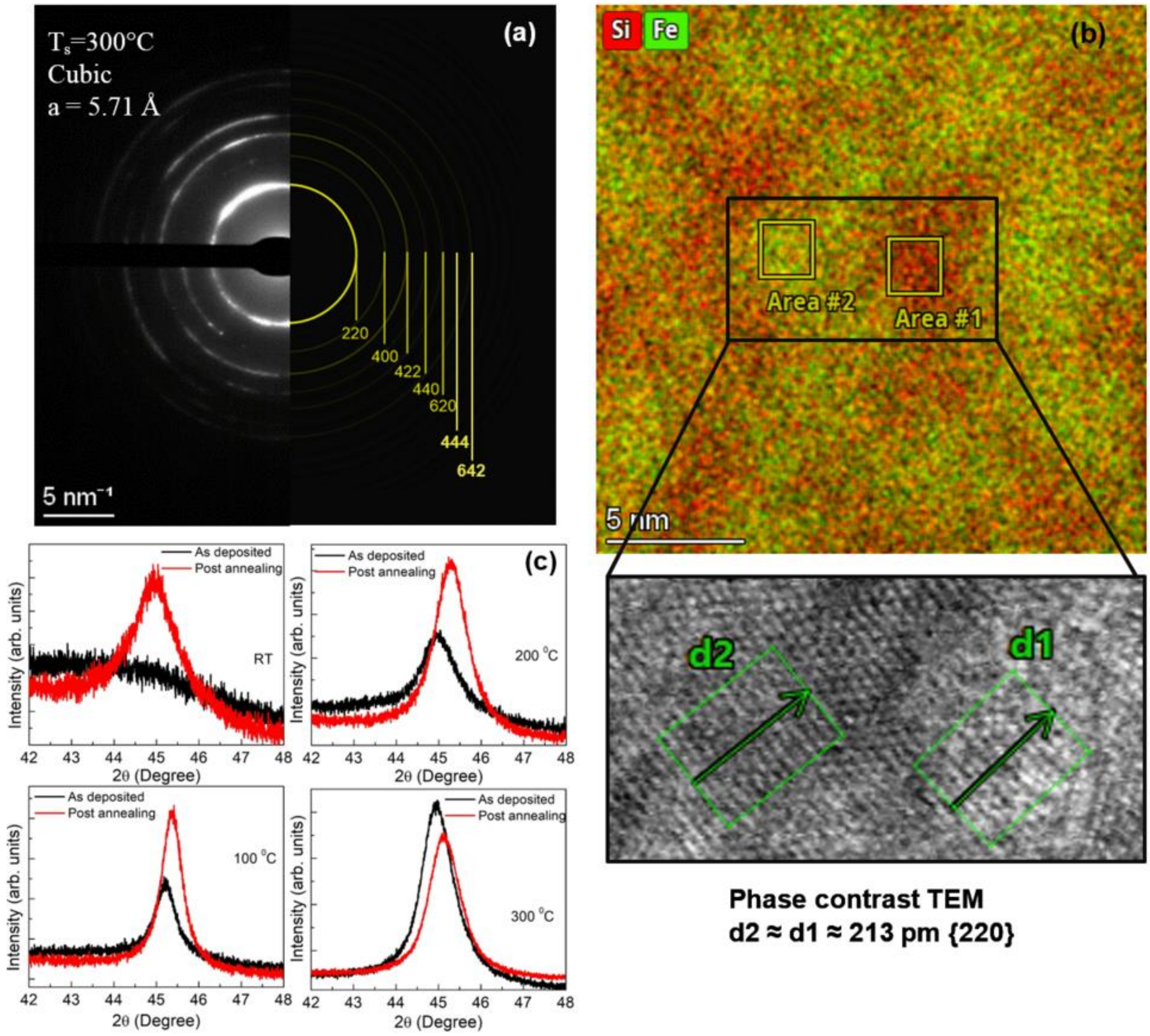

Fig. 1. Film deposited at 300°C substrate temperature: (a) Experimental (left) and simulated (right) SAED pattern of the D0$_3$ Fe$_3$Si phase (b) STEM-EDS qualitative mapping of Fe K and Si L characteristic x-ray photons (top) revealing inhomogeneous oxygen distribution along with the phase-contrast TEM image of the same area (bottom) showing a similar crystal structure across Fe-rich and Si-rich regions, (c) XRD patterns before and after annealing demonstrating enhanced {220} peak intensity in most samples.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Tuning Electrochemical Doping and Charge Transport in OECTs by Controlling Microstructure through Blends

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Organic mixed ionic electronic materials (OMIECs) show promise for bioelectronics due to their ability to translate ionic bio-induced signals to electronic signals. The primary device for such translation is the organic electrochemical transistor (OECT), where ions injected from an electrolyte dope the channel material and lead to charge transport through the channel. The OMIEC materials often comprise a conjugated backbone and polar sidechains that allow the transport of electronic charges through the π-conjugated system and the uptake and transport of ions through the sidechains. However, when processed into thin films, there is usually a structural trade-off between ionic transport and charge transport. Typically, the highest electron mobility requires significant crystallinity, while polymers that exhibit high ion conductivity are often amorphous. Thus, understanding the microstructure`s impact on ion injection, doping, and charge transport is key to optimizing OECTs. Here, we suggest harnessing tunable phase separation in OMIEC blends for more precise control over the electrochemical doping and charge transport processes in OECTs.

We selected P3MEEET, a promising p-type OMIEC derived from P3HT, with good ionic and electronic transport, and $PC_{60}BM$, a fullerene-based small molecule n-type organic semiconductor used for OFETs and OPVs. Based on the established phase evolution of the P3HT:$PC_{60}BM$ blend, we expect the P3MEEET:$PC_{60}BM$ blends to provide a plethora of tunable morphologies that will allow us to identify preferred microstructure details for OECTs. We chose several blend compositions, varying from polymer-rich to fullerene-rich blends, and applied thermal treatments. The microstructure was analyzed using High-Resolution Scanning Electron Microscopy (HRSEM) and X-ray scattering. We then correlated the microstructure with the electrochemical properties through cyclic voltammetry (CV) and spectroelectrochemistry (SEC).

In agreement with the P3HT:$PC_{60}BM$ system, we received a wide range of morphologies for the P3MEEET:$PC_{60}BM$, moving from bulk heterojunction (BHJ) in the 50:50 (w:w) as-cast film, to a bilayer in the 10:90 (w:w) polymer:fullerene as-cast film. After thermal annealing, all compositions undergo extensive phase separation. Interestingly, the SEC results show that increasing the polymer content in the blend increases the fullerene`s doping in KCl solutions. When comparing the as-cast films to the thermally annealed films, we observed a decrease in fullerene doping after thermal treatment. We hypothesize that the doping of the fullerene depends not only on the polymer`s content in the blend, but also on the presence of multiple P3MEEET:$PC_{60}BM$ interfaces that are directed by morphology. In addition, despite evidence of n-type fullerene doping in CV and SEC measurements, the n-type performance of corresponding OECTs is poor or completely absent. We attribute this low performance to the amorphous nature of PC60BM in as-cast film, limiting the electrons` mobility.

Thermal treatment increased the fullerene`s crystallinity, but led to no n-type performance in the devices, which is associated with the discontinuity of the phase-separated crystalline fullerene domains. Namely, the limiting factor in utilizing $PC_{60}BM$ in OECTs is the charge transport, not the volumetric doping. Therefore, when developing new materials for OECTs, emphasis should be placed on achieving high electron/hole mobility, as solutions for the barrier to ion injection are already available.

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Poster Presentation

Functional Materials

Challenges in Synthesizing Tungsten-Based Refractory Multi-Principal Element Alloys

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Tungsten-based refractory multi-principal element alloys (MPEAs) are becoming promising candidates for structural plasma-facing materials (PFMs) in future fusion power plants (FPPs). This is largely due to their outstanding resistance to primary radiation damage, which is a result of their intricate atomic structures. However, accurately assessing phase stability—a critical factor in designing high-performance MPEAs—remains a significant challenge due to the limitations of current experimental methods.

Most studies on these materials have primarily examined as-cast conditions or high-temperature annealing. While these approaches can reduce compositional segregation, they do not eliminate it. Only a limited number of alloys have experienced deformation processing along with annealing to further decrease chemical inhomogeneities. Achieving a single-phase material continues to be particularly challenging due to the high melting points of refractory elements and the tendency for phase segregation.

In this study, we utilized a combined processing method that involved spark plasma sintering (SPS) followed by hot isostatic pressing (HIP). This approach helps reduce compositional segregation and eliminates both micro- and macro-porosities, resulting in a dense and homogeneous microstructure. It is important to differentiate between single solid solution phases and single crystalline structures. For this study, a single-phase material is defined as one that possesses a uniform crystallographic structure and chemical composition, which can exist either as a solid solution or as a compound.

The research aims to understand the relationships between phase composition and microstructure in tungsten-based multi-principal element alloys (MPEAs). It specifically focuses on optimizing the stoichiometry of ternary and quaternary compositions to achieve single-phase structures. The W-Ta-V-Cr-Ti compositional space was investigated using advanced techniques for crystallographic and microstructural characterization. The single-phase materials identified within this compositional space will be utilized in a novel calorimetric method based on oxide melt solution calorimetry (OMSC) to determine the enthalpy of formation of the refractory MPEA system. This study will contribute to assessing their suitability as potential functional materials (PFMs) in fusion power plants (FPPs).

Three ternary tungsten-based alloys—WTaV, WTaCr, WTaTi, and WTaCrTi—along with one quaternary alloy were studied to achieve single-phase body-centered cubic (BCC) structures. X-ray diffraction confirmed that these compositions were the closest to achieving a single-phase BCC structure, with minimal secondary phases present (less than 10% by volume). Heat treatments and hot isostatic pressing (HIP) of the sintered samples further improved phase homogeneity and alignment with the multi-principal composition. To minimize evaporation and mass loss during heat treatments, the samples were encapsulated in tantalum tubes and placed in a pure argon atmosphere, supplemented with low-melting-point metals. This method effectively reduced element volatilization.

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Poster Presentation

Functional Materials

Ferroelasticity in Halide Perovskites Affects Electro-Optical Properties through Facet Stability

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Advancements in ferroic materials center upon understanding domain structures and their boundaries. This study innovates by directing the growth of lead halide perovskite microcrystals from the gas phase onto pre-chosen substrates, thereby inducing an interfacial strain that prompts ferroelasticity-driven structural transformation. A method of ferroelastic engineering in vapor-grown perovskite heterostructures is thus unveiled, revealing ordered domain patterns of bright crystals with contrasting electrooptical properties. In the case of the frustrated halide perovskite crystals, the strain is relaxed by the formation of alternating crystallographic twin domains. In the demonstrated orthorhombic system, these domains alternate between (110) and (002) orientation, with a (112) domain boundary. Perovskite ferroelastic effect with facet stability is correlated, attributed to the exposure of lower surface energy terminations, promoting the material's stability and efficiency. This findings result from direct electrical measurements, which pave the way for the tailored design of ferroic materials, optimizing their optoelectronic characteristics for enhanced device performance.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

Influence of Magnetic Field on Longitudinal and Transverse Wave Propagation in Magneto-active Polymers

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Magneto-active polymers (MAPs) possess tunable mechanical properties under external magnetic fields, making them ideal for advanced functional material applications. This study investigates the influence of magnetic fields on the propagation of longitudinal (P-wave) and transverse (S-wave) waves in isotropic MAPs. An enriched magnetoelastic energy function was formulated to characterize MAP behavior, leading to the derivation of explicit expressions for P- and S-wave speeds as functions of deformation, magnetic field, and enriched material constants. Analytical results revealed that, for an undeformed body, the in-plane S-wave (polarized in the direction of the magnetic field) speed depends on the applied magnetic field and the enriched material constant. To validate these theoretical findings, MAP samples were fabricated using fused filament fabrication (FFF) with commercially available IronPLA filament. P- and S-wave speeds were measured using the pulse-echo technique, wherein a pulser-receiver device was connected to ultrasonic transducers. Wave echo arrival times were determined using a threshold-based algorithm applied to consecutive signals. During testing, an electromagnet generated controlled magnetic fields to examine their influence on wave speeds. Experimental results demonstrated a significant dependence of the in-plane S-wave speed on the applied magnetic field. This dependence is attributed to variations in the material's elastic modulus under the field. Notably, the in-plane S-wave exhibited greater sensitivity to magnetic fields than the P-wave and out-of-plane S-wave (polarized perpendicular to the magnetic field), revealing anisotropy induced by the magnetic field. These findings enhance our understanding of MAPs, highlighting their potential in adaptive vibration control, waveguiding, and sensor applications.

Keywords: Magneto-active polymers, longitudinal wave, transverse wave, magnetic field, IronPLA, elastic modulus, anisotropy.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Functional Materials

High Entropy Rare Earth Oxides

Sapir Yail

High-entropy rare earth oxides (HEROs) represent a groundbreaking class of materials characterized by exceptional thermal stability and functional properties, stemming from their unique compositional design that incorporates five or more rare earth elements in near-equimolar proportions. These materials also show significant potential as thermal barrier coatings (TBCs) for high-temperature applications, offering robust protection against thermal degradation and enhancing efficiency under extreme conditions.

In this study, HEROs containing five rare earth oxides (Sc, Y, La, Lu, and an additional element) were successfully synthesized via a combustion synthesis method. Comprehensive characterization was conducted to examine the structural, thermal, and surface properties of the synthesized HEROs. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) confirmed remarkable thermal stability. Microstructural investigations using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) revealed a homogeneous and well-defined grain structure. Thermal performance was further assessed through specific heat capacity (Cp) and thermal diffusivity measurements—key indicators of high-temperature functionality. The results highlighted a synergistic effect among the rare earth elements, yielding enhanced thermal conductivity and heat storage capacity compared to conventional single-element oxides.

These findings position HEROs as a versatile and high-performance material for advanced thermal management, energy-related applications, and as an effective solution in thermal barrier systems, expanding their potential in both scientific and industrial domains.

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Poster Presentation

Materials under Extreme Conditions

Pressure-dependent Phase Behavior of Metallic Alloys: Thermodynamic Modeling and Experimental Insights into Binary and Ternary Systems

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The effect of pressure on the phase behavior of metallic alloys has garnered significant attention due to its implications for both fundamental understanding and practical applications. This work presents a study of the pressure-dependent phase diagrams across various binary and ternary alloy systems, revealing the profound influence of pressure on phase transitions, invariant points, structural transformations, and even on the shape of the phase diagram. The high-pressure states of the elements can significantly impact the phase diagrams of their alloys due to polymorphism in the solid state and anomalies and slope changes in the melting curve. Thus, we focused on systems that include elements that exhibit these properties: the eutectic Ga-In system [1], the isomorphous Bi-Sb system [2], the monotectic Bi-Ga system [3], and the ternary Bi-Sb-Pb system [4].

We constructed a thermodynamic model for calculating high-pressure binary and ternary phase diagrams based on ambient pressure properties of the density of sound velocity. Additionally, the model was validated by electrical resistance measurements of alloys under high pressure and temperature conditions in a `Paris- Edinburgh` (PE) large-volume press.

These studies highlight the effect of pressure on the thermodynamic behavior of alloys, indicating the need for advanced modeling and experimental techniques to understand and predict phase transitions in metallic systems under pressure.

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Poster Presentation

Materials under Extreme Conditions

Pressure Effect on Ternary Phase Diagrams: Bi-Sb-Pb as a Case Study

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Ternary phase diagrams are widely studied across various scientific and technological domains. The CALPHAD (CALculation of PHAse Diagrams) method is one of the most prominent approaches for the thermodynamic calculation of phase diagrams, specifically for multi-component systems. Pressure can affect phase diagrams significantly, as previously demonstrated on several binary systems. However, only a few studies have been conducted on the effect of pressure on metallic ternary systems.

In this study, we introduce a thermodynamic model for calculating ternary phase diagrams under high pressure across the entire composition range using only binary thermodynamic parameters and the effect of pressure on them. The model was applied to calculate the ternary Bi-Sb-Pb phase diagram up to a pressure of 2 GPa at selected temperatures as a case study, as this system involves three different types of binary phase diagrams: isomorphous, eutectic, and peritectic [1]. The results show that pressure affects the composition and temperature of the stabilization of multi-phase areas, leading to changes in the three-phase triangles and the four-phase equilibrium quadrilateral. This study provides insights into the pressure-dependent behavior of ternary systems and contributes to the thermodynamic understanding of ternary phase diagrams under high-pressure conditions.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Materials under Extreme Conditions

The Structure of Liquid Bismuth Along the Melting Curve

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Bismuth (Bi), as an elemental material, holds significant scientific interest and has been the subject of extensive research. The Bi P-T phase diagram is well-established and exhibits an anomalous melting curve and multiple solid allotropes, which may be associated with liquid transitions. Extensive research has been conducted on liquid Bi structure at ambient pressure. However, the structure of liquid Bi at high pressures remains unexplored, leading to uncertainty in the interpretation of these findings. In this study, we investigate the structure of liquid Bi in the pressure range from 1 to 4 GPa, just above the melting line, with energy-dispersive X-ray diffraction measurements (EDXRD). The measured data was treated to obtain the structure factor, S(Q), and radial distribution function, g(r), at each pressure point. The results confirm the presence of abnormal liquid characteristics in Bi, characterised by a distinct `shoulder` between the first and second peaks, high Q2/Q1 and r2/r1 ratios, and a low coordination number. The short-range order (SRO) was analysed in the Quasi Crystalline Model (QCM) framework, demonstrating that despite several transitions in the solid phases of Bi adjacent to the melt from Bi I to Bi V, the SRO of the liquid near the melting curve remains distorted Bi I A7 rhombohedral-like symmetry with only a small variation in the parameters with pressure. This suggests that while, in some cases, there may be a correlation between the structure of the solid phase and the near-melting liquid phase, this relationship does not hold for bismuth.

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Poster Presentation

Materials under Extreme Conditions

MeV Proton Irradiation Effect on Li Ion Anodes

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Lithium-ion batteries (LIBs) are known for their high energy density, large specific capacity, lightweight design, long cycle life, and high durability.

LIBs are required in automated devices in nuclear environments, and their stability under neutron radiation is of great importance. LIBs are also being considered for their potential contribution in aerospace applications where they are subject also to proton irradiation. The integrity and stability of LIB under radiation are crucial to its operation in these environments. Understanding the mechanisms of Li-battery degradation under irradiation is essential for its lifetime and durability assessments. In normal operation degradation mechanisms have been identified for LIBs, notably Li plating of the anode.

Several studies were conducted on the effect of gamma radiation on Li-ion batteries performance, while fewer studies were done on the effect of neutron radiation. E.g., proton irradiation was used to enhance defect concentrations at a titanium dioxide anode; it was shown that enhanced defects in Li metal oxide electrodes increase electrochemical charge storage.

However, the effect of protons and helium ions radiation on Li-graphite anode structure, performances, and battery functionality has not been addressed yet, to the best of our knowledge. This is desirable both to understand their direct effect and as a surrogate for more challenging neutron irradiation experiments. In this study, we will use protons and helium ions radiation as a trigger to enhance defect concentrations at the graphite anode. Proton radiation is expected to activate different mechanisms than helium ions due to the effect of lithium hydride formation.

In this study, several graphitic anodes were irradiated by 3MeV protons at -100C at Jannus Saclay. The irradiated anodes were characterized via Raman, XRD, optical profilometry and SEM. Electrochemistry study was done by unique neutron analysis at PSI. Pristine and irradiated anodes were assembled to a battery cell under the neutron beam line. The kinetics of Li insertion and extraction of pristine anodes versus irradiated anodes was studied, together with a 2D in situ mapping of Li. The effect of irradiation on graphitic anode degradation mechanisms and SEI buildup was studied.

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Poster Presentation

Materials under Extreme Conditions

Silver-Antimony-Telluride Compounds: Phase Content, Crystallography, Thermoelectric Performance, and High-Pressure Analysis

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Thermoelectric (TE) materials and devices, which enable direct conversion of heat into electrical energy and vice-versa, are considered promising candidates for sustainable, eco-friendly, and efficient energy solutions. Achieving optimal TE performance involves enhancing electron transport while minimizing thermal conductivity. Key electron transport properties include charge carrier concentration, mobility, and Seebeck coefficients, whereas thermal transport is influenced by vibrational properties.

$AgSbTe_2$ (AST) is a promising TE material for mid-range temperatures (400–700 K). While previous attempts to improve its TE performance through alkali doping proved to be success, the associated experimental complexities and the lack of consensus regarding its crystal structure remain significant challenges. In this study, we seek to clarify how the coexistence of AST polymorphs within a single matrix influences TE properties and to explore the impact of co-doping of AST with K and Te, using Na-Te co-doped material as a reference. We hypothesize that these dopants enhance electron transport by affecting the concentration of vacancies and introducing acceptor levels within the band gap, while the presence of multiple polymorphs provides additional phonon scattering mechanisms.

To test this hypothesis, we synthesized $Na_xAg_{1-x}SbTe_{2+x}$ (NAST) and $K_xAg_{1-x}SbTe_{2+x}$ (KAST) compounds with x=0 and 0.005. We conducted comprehensive characterization procedures, including electron microscopy, X-ray diffraction (XRD), neutron diffraction (ND), and TE property measurements. Both XRD and ND analysis confirmed that doping did not alter the fundamental structure of AST; however, they enable us identifying the α-Ag_2Te impurity phase in all samples, which proved to have positive effects on TE performance [1]. Whereas XRD and ND are inadequate for unequivocal identification of the four optional polymorphs of AST (two cubic, rhombohedral and tetragonal), the ordered rhombohedral structure could be clearly identified owing to its two Raman-active modes ($\Gamma=A_{1g} + E_g$), matching the experimental Raman spectrum. Additionally, high-pressure studies were done by compression of all samples in a diamond anvil cell (DAC) using Ne gas as a pressure transmission medium, and equipped with a gold pressure marker, thereby enabling us to accurately measure the bulk moduli from the equation of state. We revealed a phase transition from Fm-3m to Pm-3m at different pressures depending on composition; e.g. between 20 and 37 GPa for AST.

Analysis of the TE transport coefficients reveals that alkali doping remarkably improves the electrical conductivity, e.g. 450 for KAST and NAST vs. 350 S/cm for AST at 300 °C, respectively. Furthermore, the KAST samples exhibit thermal conductivity values as low as 0.55–0.65 W/m·K, resulting in a good *figure of merit* (*ZT*) of ca. 0.82 at 300 °C, which surpasses that of NAST, ca. 0.77.

In conclusion, our newly developed KAST compound exhibits good TE performance, for which high-pressure experiments can reveal unknown structural properties.

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Poster Presentation

Materials under Extreme Conditions

Electrochemical Properties and Pressure-Induced Phase Transformations of LiC_4N_3 and NaC_4N_3

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The growing need for sustainable energy solutions and environmental challenges requires significant advancements in alkali metal (Lithium- (LIBs) and sodium-(SIBs)) ion batteries. Recently, Li/Na-based anodic materials have gained significant attention, due to their exceptionally high capacity when combined with non-metallic cathodes. This, in turn, triggered intense research efforts on synthesizing novel alkali-metal-rich compounds with non-metallic elements. In this context, recent studies point towards carbon-nitride-based materials, that are expected to be suitable for lithiation, and they possess high capacitance with low volumetric expansion.

Previous studies provide compelling evidence that the properties of materials can undergo significant alterations when subjected to high pressure. Under such thermodynamic conditions, the structure, chemical bonding, and electrical properties of materials are modified, and thus, new materials are produced. Motivated by these findings, we aim to investigate whether compressing LiC4N3 and NaC4N3 under moderate pressure of a few tenths of gigapascal (GPa) can yield materials that are applicable as new battery materials with better efficiency. We note that both the LiC4N3 and NaC4N3 compounds, that are the subject of this study, are molecular solids and distinct from the conventional Li- and Na-intercalated g-C4N3.

LiC4N3, as the starting material, was synthesized in-house and characterized at ambient conditions, confirming the successful synthesis. At ambient conditions, cyclic voltammetry and galvanostatic charging and discharging measurements were conducted to measure the specific capacity and examine its stability over multiple cycles. A series of measurements were implemented viewing LiC4N3 as either anode or cathode material. Subsequently, we performed a high-pressure Raman spectroscopy study up to 20 GPa, and an in-situ Wide-Angle X-ray Scattering (WAXS) measurements up to 30 GPa using a diamond anvil cell (DAC). The results documented a pressure-induced polymerization above 15 GPa, concomitant with a crystalline-to-crystalline phase transformation and a possible metallization, as observed under the microscope. The quenched material remained metastable and metallic after fully releasing the pressure and survived for a couple of hours after exposing to atmospheric conditions, while remaining stable for prolonged time when stored under inert atmosphere conditions.
A similar alkali-metal battery material NaC4N3 has also been studied under high pressure using Raman spectroscopy and WAXS at DESY synchrotron source up to 32 GPa. At around 6 GPa and 20 GPa, two crystalline-to-crystalline phase transformations were observed, and the sample seemed to be metalized under the microscope. The new material was stable upon decompression and could stay in the air for a short time.

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Poster Presentation

Materials under Extreme Conditions

Mitigation of Irradiation-Assisted Stress Corrosion Cracking by Laser Annealing

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Currently, mitigation against irradiation-assisted stress corrosion cracking (IASCC) in stainless steel surfaces is primarily achieved through the use of hydrogenated water chemistry in Pressurized Water Reactors (PWRs) and Boiling Water Reactors (BWRs), known as Hydrogen Water Chemistry and its variants. Despite these measures, instances of IASCC continue to occur and are expected to increase with long-term reactor operation. This study proposes an economically viable mitigation method utilizing laser-induced lattice strain annealing.

Cold-worked 316L stainless steel with 10%-30% axial deformation was employed as a surrogate for irradiated samples. Various laser setups were tested to eliminate near-surface defects that could potentially propagate into IASCC during future service. The effects of cold work and laser treatment on the microstructure, lattice strain, and mechanical properties were assessed using nanoindentation and Electron Backscatter Diffraction (EBSD). The results demonstrate that laser annealing effectively reduced lattice strain and improved the material`s resistance to IASCC.

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Poster Presentation

Materials under Extreme Conditions

An Analysis of Modelling and Self-Consistent Calculations for Properties at High Pressure using DFT: For Rare-Earth Elements

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General results of self-consistent calculations, based on Density Functional Theory (DFT) with the ultrasoft and projector augmented wave formulations were found to be invalid in some cases. With an application of recent upgradation included in the newer version of Quantum ESPRESSO and with modified modules for some rare-earth elements, it can successfully generate various predicted properties of materials at High Pressure.

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Poster Presentation

Materials under Extreme Conditions

Ultra-low doping of Silver Thin Films with 228Th: Deposition and Radiative Emission Characterization

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This study introduces a novel method for simulating self-irradiation damage in FCC metals thin films, utilizing a small volume electroless deposition bath to achieve a controlled, homogenously distribution of ultra-low amounts of 228Th ions within Ag films. We have explored 228Th incorporation, chemical state and location in the films and its effect on film morphology. The resulted films were characterized using unique techniques due to the sub-ppm to sub-ppb 228Th content, where conventional characterization methods fail due to their limit of detection. We found that higher 228Th concentration in the bath resulted in lower film activity. This is attributed to accumulation of thorium in grain boundaries and its gradual impact on film morphology. The explanation for this phenomenon lies in the deposition process being hindered by the 228Th ions. This leads to an increase in grain size along with a decrease in film coverage, resulting in films with fewer, larger grains. Therefore, less 228Th is incorporated overall in the film, leading to a decrease in the film`s activity. In summary, incorporation of 228Th alters the grain size and film coverage, with a tendency to accumulate at grain boundaries rather than within the Ag FCC lattice. This study enhances our understanding of the role of Th in Ag thin film deposition, and lays a foundation for future research on self-irradiation damage in materials, particularly focusing on the effects of recoil atoms in the films during α-emission events.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

Effects of Grain Boundary Types and Precipitates on the Electrical Properties of DED-printed Aluminum

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Aluminum alloys are widely employed in electricity transmission lines due to their optimal balance of conductivity and mechanical strength. While precipitate formation is crucial for achieving desired mechanical properties, it suppresses the electrical conductivity. The contribution of these precipitates to electrical resistivity has not been directly quantified so far. This study investigates the impact of individual precipitates at different grain boundary types on the electrical properties in aluminum printed by Directed Energy Deposition (DED). The research focuses on characterizing the effects of different grain boundary angles, particularly low-angle (20°) and high-angle (20°) boundaries. The research methodology combines electron backscatter diffraction (EBSD) for comprehensive grain boundary analysis with in-situ four-point-probe measurements using scanning electron microscopy (SEM) to analyze local electrical properties. The study examines the correlation between grain boundary misorientation and electrical behavior, considering the unique solidification conditions and thermal history inherent in the DED process. The results are compared to similar alloys prepared by solidification. This research seeks to provide insights into the role of grain boundaries in determining the electrical properties of DED-printed aluminum, with potential implications for optimizing the electrical performance of the specific alloy.

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Physical Metallurgy

Study of the Microstructural Changes of AlCoCrFeNi System as Function of Cr and Al Variation Applying Pseudo-binary Diffusion Couple Approach

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Novel metallurgical approach of High Entropy Alloys (HEAs) involves using multiple elements in nearly equiatomic proportions to form solid solutions, which exhibit unique physical properties [1]. Among the most extensively researched systems in the HEA field is AlCoCrFeNi. Although a complete phase diagram of this system was not constructed, several researchers published partial phase diagrams which often contradicted each other, and some were experimentally disputed [2-4]. To study complex systems, one effective method is to isolate and understand the effect of each individual element. Previous studies of this system although shed light on the subject but were conducted in a nonlinear fashion, sampling specific compositions and leading to incomplete, contradictory, and inconsistent findings. In current study, two systems were studied applying pseudo-binary diffusion couple approach [5-6]: Cr joined with single phase B2 (ordered Body Centred Cubic (BCC)) AlCoFeNi and Al joined with single phase Face Centred Cubic (FCC) CoCrFeNi, using scanning and transmission electron microscopies, along with Electron Backscatter Diffraction (EBSD) methods.

The microstructure of the Al/CoCrFeNi diffusion couple changes with Al content. Below 8 at% Al (x=0.35), it remains a single-phase FCC region. As the Al content increases up to 16 at% (x=0.76), the structure transitions to an intertwined BCC-B2 morphology. Further increasing the Al content up to 36 at% (x=2.25) results in fine BCC spherical particles distributed within the B2 matrix.

Similarly, the microstructure of the Cr/AlCoFeNi diffusion couple evolves with Cr content. Below 15 at% Cr (x=0.7), it is a single-phase B2 region. With Cr content up to 20 at% (x=1.0), fine spherical BCC particles are distributed in the B2 matrix. At 21-24 at% Cr (x=1.1-1.2), the structure becomes an intertwined BCC-B2 morphology. Curved "snake-like" BCC particles appear in the B2 matrix at 25-30 at% Cr (x=1.3-1.7). At 33 at% Cr (x=1.97) and above, phase inversion occurs, revealing cuboidal B2 particles dispersed within the BCC matrix.

It is interesting to note that Al seems to diffuse out concomitantly with the diffusion of Cr. A similar pattern was observed in the Al/CoCrFeNi diffusion couple: while Al diffused in, Cr diffused out.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

Room-temperature Recrystallization of Mo Induced by Nanoindentation

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We performed nanoindentation studies on molybdenum (Mo) single-crystals (SCs) utilizing a conical indenter with a spherical tip. The samples were produced by electron beam floating zone melting method, and three different surfaces, (100)20°, (110) and (111) were tested. The load-displacement curves of all SC samples exhibited characteristic pop-in (displacement burst) indicating an abrupt transition from elastic to plastic deformation regime. The maximum elastic shear stress below the indenter in SC samples estimated with the aid of Hertzian contact theory was in the range of 12-16 GPa, which is close to the theoretical shear stress strength of Mo (~17 GPa). On the contrary, much weaker pop-ins or no pop-ins at all were observed during nanoindentation tests of polycrystalline (PC) sample prepared by powder metallurgy method (the corresponding maximum shear strength was below 0.5 GPa). This difference in nanoindentation behavior of SC and PC Mo samples indicates much lower density of pre-existing dislocations in the former. The cross-sectional transmission electron microscopy of the indented area in all SC samples revealed the formation of new near-surface grains when the loading was terminated manually immediately after the pop-in event. By contrast, no new grains could be observed in the PC sample, indicating that the pop-in and recrystallization are correlated. We propose that the dislocations nucleated during singular pop-in event are driven by high elastic stress and self-organize into a low-angle grain boundary. We estimated the density of geometrically necessary dislocations generated by the nanoindentation using the Nix-Gao model and demonstrated that misorientation of 3-4° could be achieved when all the dislocations assemble in a grain boundary, resulting in the formation of new grains. When the SC sample was continuously indented to the loads significantly exceeding the first pop-in, no visible new grains were formed. Our results shed new light on the deformation mechanisms during the nanoindentation of defect-free Mo. The room-temperature recrystallization is unprecedented for Mo which usually recrystallizes at temperatures above 1000 °C.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

Spontaneous Formation of a Eutectic Au-Co Interface via a-Low Temperature Reduction Process

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We prepared the equi-atomic Au-Co alloys through a low-temperature solid-gas phase reduction of i) the bi-metallic complex salt [Co(NH3)6][AuCl4]Cl2, and ii) an equimolar mixture of H[AuCl4] and pre-reduced cobalt. Complete reduction was achieved at 350 °C resulting in the formation of a close-to-equilibrium two-phase composition of fcc gold and hcp cobalt. The structure of the fully reduced metallic materials was composed of a free-standing single-phase Co and a two-phase bi-metallic Au-Co particles closely resembling a typical eutectic microstructure. This spontaneously formed microstructure featured fcc cobalt islands interfacing with fcc gold at a specific orientation relationship. At heating, the fully reduced Au-Co started to melt at the equilibrium eutectic melting point of 996.5 ºC. These results imply spontaneous lattice self-adjustment can occur in eutectic-type systems below melting. Hence, we show that a typical eutectic microstructure may be obtained without a melting-solidification metallurgical cycle.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

The Spinodal Decomposition Impact on Electrical Resistivity Stability of CuMn Alloys.

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Cu-Mn alloys are utilized in electrical-resistivity sensors due to their temperature-stable resistivity. Yet, the phase stability in the Cu-rich diagram is controversial, where two ordered phases (Cu5Mn, Cu3Mn) are predicted but have never been experimentally resolved. This study reports a spinodal phase decomposition of Cu-10Mn alloy at elevated temperatures and its impact on the alloy's physical properties. Alloys with the desired composition were prepared by induction melting furnace and homogenized at 700 °C. Annealing at 450-600 °C for different durations leads to periodic chemical fluctuations in the alloy. The microstructure is characterized by x-ray diffraction (XRD) and energy dispersive x-ray spectroscopy (EDS). Temperature-dependent resistivity measurements of the entire samples reveal a change in temperature coefficient of resistivity due to the phase decomposition. The findings were further studied by SEM in-situ local electrical measurements of the decomposed regions. Moreover, the effect of spinodal decomposition on mechanical properties is assessed with Nanoindentation experiments. Finally, defective 9R structure at incoherent Σ3 grain boundaries of the alloy are resolved by high-resolution transmission electron microscopy (TEM).

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

The Effect of the Elastic Energy on the Microstructure of Nano $TiNi_2Sn$ Precipitates in a Half-Heusler TiNiSn Matrix

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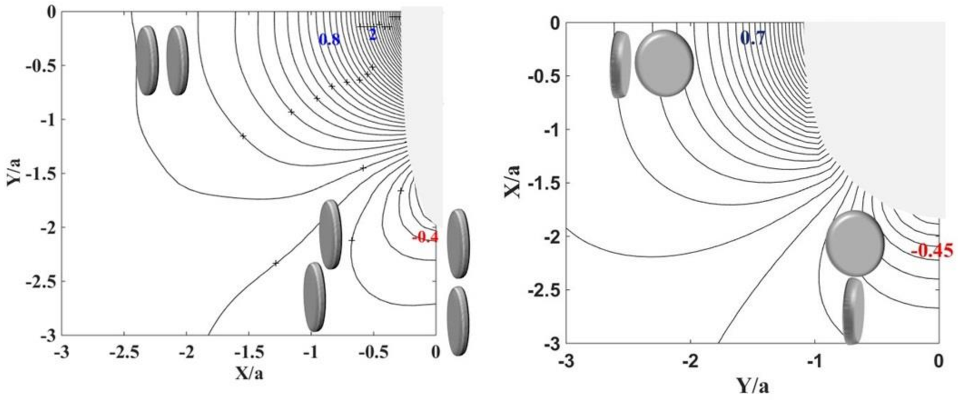
TiNiSn-based alloys have been extensively studied due their thermoelectric (TE) applications at high temperatures (700-1000K), environmentally friendly and low-cost. The crystallographic structure of this alloy is a cubic half-Heusler (HH) matrix with embedded cubic full-Heusler (FH) $TiNi_2Sn$ nano precipitates that nucleate during the aging treatment of the alloys. The appearance of the nano $TiNi_2Sn$ precipitates and other defects reduces the thermal conductivity and enhances the TE figure of merit, ZT, through phonon scattering.

Understanding the relation between the precipitates may assist in controlling their distribution and help in the design of advanced alloys. Importing practice of the Fourier transform method from the field of micromechanics of metals, role of elastic energy on the evolution of the precipitate microstructure in these alloys was estimated and compared to experimental observations [1]. The role of the elastic heterogeneity of the $TiNi_2Sn$ precipitates in the NiTiSn matrix was also evaluated.

$TiNi_2Sn$ precipitates have a minimal elastic energy while exhibiting a disk-like geometry with a low aspect ratio with {100} habit plane. Experimentally, disk-shaped precipitates with $c/a \sim 1/9$ at different {100} orientations, are observed at the peak-aged condition. The restriction on coherent thin precipitates requires a tetragonal deviation from the cubic structure. The calculated tetragonality for $TiNi_2Sn$ precipitates is 1.07, which is in good agreement with the experimental observation. Like the precipitates in many metals, the precipitates in TiNiSn are partially ordered due to elastic interactions. Pair elastic interaction favors thin face to thin face configurations both in perpendicular and parallel orientations (Fig. 1 a,b). All these configurations were assessed in experimental observations, and in particular, the parallel ‘head to tail’ arrangement that is an outcome of the elastic inhomogeneity.



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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

The Strong Effect of NiCr Adhesion Layers in Surface Micromachined MEMS Sensors

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We demonstrate that post-fabrication processes involving a very thin NiCr adhesion layer may have a strong effect on the deformation of released structures. We consider MEMS switch sensors that are constructed from suspended perforated disks. The switches are fabricated by depositing a NiCr adhesion layer over a sacrificial layer, followed by deposition of a seed gold layer. This thin seed assembly is then thickened by electrodeposition of a second gold layer. The last process step before releasing the structure is wet etching of the adhesion layer. We measured the curvature of many disk structures that are identical in all geometry and process parameters, except for the level of NiCr overetch (Fig. 1). The level of NiCr overetch was evidently related to the curvature of the released structures, but the exact physical mechanism was not clear. We found that much of the residual deformation occurs during post-fabrication packaging (Fig. 2), which requires a relatively long exposure to elevated temperature. We conjecture that interdiffusion during packaging determines the residual curvature. This interdiffusion should be different in regions where the adhesion layer has been overetched, which may explain the dependency of disk curvature on the level of NiCr overetch. Current work focuses on finding evidence of such diffusion, using comparative nanoindentation, composition depth profile and sheet resistance measurements, before and after packaging-simulating heat treatments. It is suggested that careful attention should be given to the adhesion layer, which is often neglected as it is very thin. Such attention may help to improve the reliability and functionality of surface-micromachined metallic

devices.

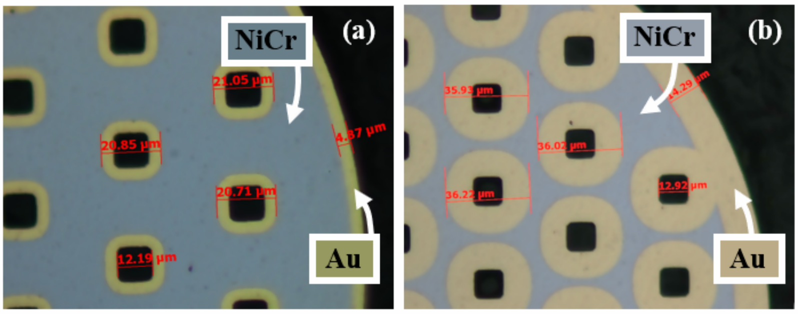

Fig. 1. Two different levels of NiCr overetch. The released disks were peeled-off and flipped to expose their bottom surface, enabling measurement of the NiCr overetch. (a) NiCr overetch of ~4.5 µm, (b) NiCr overetch of ~12 µm.

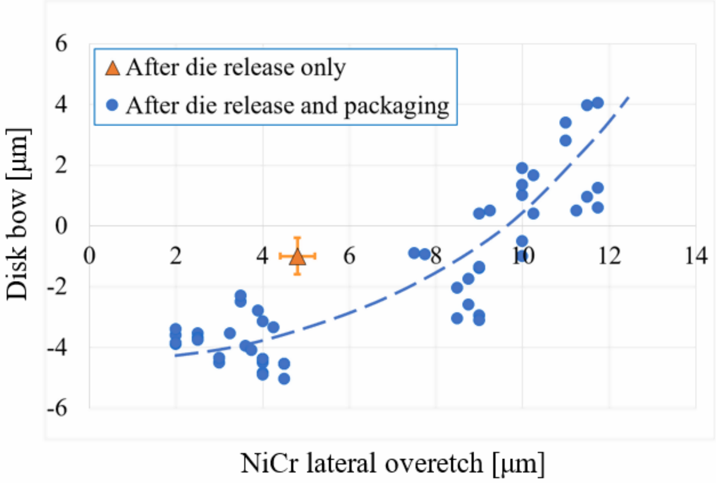

Fig. 2. Disk bows as function of NiCr overetch. The blue dots are disk bows that were measured on post-packaged devices. The orange triangle represents bows of 30 disks that were measured after release, but before packaging. The dashed line is qualitative.

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Poster Presentation

Physical Metallurgy

Characterization of Microstructure, Surface Morphology and Electrical Properties of Si-Ti-Pt-Au Contacts

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This work focuses on the effect of microstructure on the electrical contact of Ti-Pt-Au metallization to highly doped P-type (Boron) Silicon (001) substrates. This metallization is designed to be used in MEMS components, with the goal of achieving a low electrical resistance, Ohmic-like contact, where the contact electrical resistance is independent of the working voltage.

The metallization pads were evaporated on the silicon substrate using a lift-off technique, which dictates a relatively low deposition temperature (100C). The wafers with the lift-off lithography were dipped into buffered HF solution to remove the native oxide before deposition. Various post-deposition anneal treatments were examined to later reach a low electrical resistance, Ohmic-like contact to the silicon substrate. The anneals were performed in air atmosphere. Blanket samples were also evaporated together with the lift-off patterned pads, to allow more material volume for a microstructure characterization by X-ray diffraction.

It was found that after annealing at 360°C for 20 minutes, a low electrical contact resistance was established, but with a strong dependence on the applied voltage (a Schottky type contact). Increasing the anneal temperature to 450C, and extending the anneal time to 60 minutes, achieved a relatively low electrical resistance, with an ohmic-like contact. Increasing the anneal temperature beyond 400C was also accompanied by a surface texture formation, formed most likely due to inter-diffusion between the layers. X-ray diffraction (XRD), Focused Ion Beam (FIB), and Electron Back Scattered Diffraction (EBSD) investigations showed that various silicides were formed, such as PtSi, $TiSi_2$, and Ti_2Si, due to the heat treatments. A direct physical contact between a titanium disilicide and the silicon substrate was observed at specific sites when an ohomic electrical contact was measured, indicating their correlation.

In a parallel study, using a new evaporation tool with ion gun pre-deposition cleaning, an ohmic-like electrical contact was already achieved after annealing at 360°C for 20 minutes. This might suggest that a residual native oxide remained on the current wafers, acting as a diffusion barrier, preventing the formation of silicides and causing an electrical Schottky contact after the same annealing treatment. This diffusion barrier is only surpassed at higher annealing temperatures.

This work correlates between the electrical contact behavior and the microstructure of thin films, subjected to various heat treatments and evaporation systems. It shows the formation of different silicides depending on the anneal treatment, and surface morphology changes due to inter-diffusion between the layers. This study suggests how to improve electrical contact behavior by improving the deposition process.

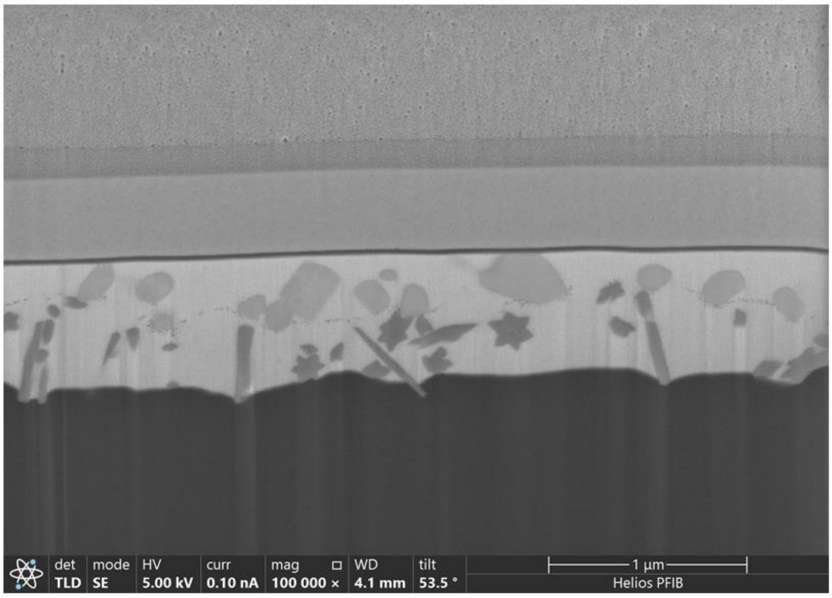

Figure 1: SEM vertical cross-section view of a blanket sample after annealing for 1hour @ 450C, showing Ti-silicide in contact with the silicon substrate, explaining the Ohmic-like electrical contact behavior.

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Poster Presentation

Physical Metallurgy

Towards Understanding the Effect of Increased Configurational Entropy on Structure and Stability of Quasicrystals and their Approximants

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Since the discovery of the first icosahedral quasicrystal (IQC) [1], these complex structural phases have attracted significant interest. One common approach to assess the stability of quasicrystals (QCs) in metallic alloys is by estimation of the electron per atom (e/a) ratio [2]. However, there is some debate among researchers regarding the specific calculation method of the e/a ratio and its application in stability assessment. For instance, it has been suggested that an e/a ratio of approximately 1.75 is necessary to achieve thermodynamically stable aluminum based decagonal quasicrystals (DQCs) [3].

In the 1990s, the concept of multicomponent alloys (MCAs) was proposed, suggesting that increasing configurational entropy by adding atoms capable of forming solid solutions could enhance materials properties. In the current research, this concept is employed to evaluate the effect of increased configurational entropy on the formation and stability of QCs and their approximants [4,5]. For this purpose, Al-Mn-Ni system was chosen as a starting point, as it contains metastable decagonal quasicrystal (DQC) [6] and several approximant phases, such as hexagonal κ [7] and ϕ [7] phases. The latter phase was numerously studied regarding its intriguing electrical and magnetic properties [8,9].

In the current research, a novel MCA with the composition Al-(TM1,TM2)-(TM3,TM4) (where TM are Fe, Ni, Co, and Mn) was prepared by arc melting and characterized applying various electron microscopy techniques. It is expected that an increase in configurational entropy (which dramatically influences the e/a ratio) will affect the formation and stability of QCs in this complex system.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Physical Metallurgy

Mechanical Properties of Ni-NiO Core-Shell Nanoparticles Prepared by Solid-State Dewetting and Oxidation

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Metals at the micron- and nano-scale often exhibit significantly higher strength compared to their macro-scale sized counterparts. For example, Ni nanoparticles fabricated by solid state dewetting have demonstrated exceptional compressive strength of up to 34 GPa. It was conjectured that this extraordinary strength may be caused by the presence of thin native NiO layer on the particle surface [1].

In the present work, we studied the effect of oxidation on the microstructure and the mechanical properties of Ni-NiO core-shell nanoparticles. Defect-free single-crystalline Ni nanoparticles were fabricated via solid-state dewetting of Ni thin films on sapphire substrates, followed by oxidation in air at elevated temperatures to produce Ni-NiO core-shell nanoparticles with varying degrees of oxidation. A combination of atomic force microscopy, scanning electron microscopy, X-ray diffraction, and in-situ microcompression tests was employed to systematically investigate the effects of oxidation on the microstructure and mechanical properties of Ni nanoparticles. Our results demonstrated a strong correlation between particle size and compressive strength across different oxidation levels. Remarkably, despite the smooth edges of the particles, increasing oxidation results in a gradual decrease of compressive strength of the core-shell particles. These findings offer valuable insights and establish a framework for designing high-performance metal nanoparticles through precise control of oxide layer thickness.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

Recombinaiton Dynamics in Chalcogenide-based Perovskite

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$BaZrS_3$ (BZS), a chalcogenide perovskite, has gained interest as a promising photovoltaic material due to its direct band-gap (~1.9 eV), high dielectric constant, and distinct optoelectronic behavior, that is more closely resembling that of materials like silicon or GaAs, despite having a structure similar to traditional perovskites. In my research, I will explore BZS`s behavior in the excited state, focusing on two primary objectives. First, I aim to map and compare the trap states in thin films and single crystals of BZS and analyze the nature of those defects. This analysis will provide insights into the optimal type and quantity of defects required in BZS thin films to create the most efficient material for photovoltaic applications. To achieve this, I will perform Time-Resolved Photoluminescence (TRPL) measurements to study the recombination processes of these materials, which are influenced by the existing defects. Second, we hypothesize that vibrations highly contribute to BZS`s dielectric constant, indicating strong electron-phonon interactions. I will examine this hypothesis using Time-Resolved Raman measurements. I anticipate observing a pronounced effect in the Raman spectra caused by these interactions, which would be minimal in materials like GaAs, where electron-phonon interactions are much weaker.

This poster will present my preliminary results comparing the chalcogenide BZS and the halide CsPbBr3 (CPB) perovskites. Despite BZS`s structural similarity to halide perovskite CPB, the emission intensity of PL of CPB is over four orders of magnitude higher, suggesting a significantly greater concentration of low-barrier or barrierless non-radiative recombination centers in BZS. To investigate the different recombination processes, I employed TRPL, an effective technique for analyzing defect-related effects and recombination dynamics.

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Poster Presentation

Semiconductors and Electronic Materials

Epitaxial MoS_2 Nanofin-Nanoribbon Hybrids for Electronic Devices

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2D materials are a versatile platform for optoelectronics, memory and energy-harvesting devices owing to their high-carrier mobility and strong light-matter interaction. Scientific efforts were invested during the last decade to tailor the physical properties of these materials by gaining control over their dimensionality. The synthesis of new structures with mixed dimensionalities, such as nanoribbons or nanofins, with controlled orientations, can give rise to a change of physical behavior and has many potential applications in electronics and optoelectronics. However, efficient synthetic methods for the bottom-up creation of aligned single-crystal nanoribbons and nanofins are still lacking.

Our group gained substantial knowledge regarding the aligned growth of 1D nanowires of different semiconductors, guided by different crystalline substrates, as part of the general guided-growth approach. This work aims to implement the guided growth approach to induce 1D growth of MoS_2 nanofins-nanoribbons with controlled orientations. Synthesized in a CVD system by epitaxy on sapphire, the formation of these unique hybrid structures is discussed in terms of crystal structure and morphology. Optical properties such as photoluminescence and Raman spectroscopy are also presented. The MoS_2 nanoribbons-nanofins were integrated into arrays of visible-light photodetectors, showing high responsivity and short response times with respect to previously reported MoS_2-based photodetectors. Such growth of nanofins-nanoribbons can be generalized to other 2D materials, suggesting new structures that enable various device architectures with improved performance.

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Poster Presentation

Semiconductors and Electronic Materials

All Optical Controlled Neuromorphic FET based on vdW Ferroelectric/Semiconductor Heterostructure

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In recent years, substantial advancements in artificial intelligence (AI) have led to a growing demand for high-speed, low-power computational system. The traditional von Neumann architecture is inadequate to fulfill these demands due to the physical separation between the memory and processor units, leading to data transfer delays and increased power consumption. Neuromorphic solid-state devices that can sense, store and process simultaneously, could play a pivotal role to overcome the von Neumann bottleneck. In the last few years there has been extensive research going on for the development of 2D materials based neuromorphic FET, especially for visual synaptic operation to emulate human visual perception and memory in a single device level. However, most 2D synapses need to be controlled using hybrid approaches involving both optical and electrical stimuli. It still remains a challenge to achieve both learning and forgetting behavior by using only optical stimuli. In the present research we have proposed a simple three terminal FET architecture based on $PdSe_2$ / α-In_2Se_3 vdW heterostructure applicable for all optical controlled synaptic device. The device is capable of demonstrating both excitatory synapse under red light (642 nm) and inhibitory synapse under green and blue light (532nm/406 nm) without any electrical input. Higher intensities of blue light (406 nm) can be employed to implement the RESET process, enabling the device to be used in a reconfigurable manner. In addition, the optically induced excitatory and inhibitory synapse can be modulated by electrical gate pulse, utilizing the dipolar field from ferroelectric α-In_2Se_3. This study provides an effective strategy to develop all optical controlled neuromorphic device as a building block for artificial neural network (ANN).

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

Ultrafast Dynamics of VO_2 Switching Devices for Neuromorphic Applications

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Resistive switching devices are integral to emerging electronic applications, from sensors to neuromorphic computing, where they mimic the dynamics of biological neurons. Among these, vanadium dioxide (VO_2) switching devices are particularly compelling due to their insulator-metal transition (IMT). This transition is characterized by sharp, orders-of-magnitude resistance changes near room temperature, enabling energy-efficient operation.

In this work, VO_2 switches were fabricated by sputtering a thin film of VO_2 and forming two metallic electrodes atop it, separated by a ~100 nm gap. Voltage pulses applied across the gap trigger an IMT followed by the reverse process when the pulse ends. This switching occurs on ultrafast timescales of tens to hundreds of nanoseconds. Using an advanced measurement platform with an ultrafast current compliance mechanism, we successfully characterized key switching dynamics: 1. incubation time, defined as the delay between the start of the voltage pulse and the onset of current rise; 2. rise time, representing the current increase during switching; and 3. retention time, describing the duration before reverting to the insulating state. Notably, the retention time increases with increasing pulse lengths, but plateaus for pulse lengths of the order of hundreds of nanoseconds, establishing the time required for reaching steady-state conditions. Understanding the ultrafast dynamics of VO_2 device dynamics, contributes to the development of robust, energy-efficient VO_2-based neuromorphic devices for high-speed computing applications and sensors.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

Influence of Kinetic Parameters and Effusion Cell Configuration on the Compositional Uniformity of InAsSb Films via Molecular Beam Epitaxy

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Epitaxial Growth Group, SCD, Israel

The composition of InAsSb films grown on GaSb(001) substrates via Molecular Beam Epitaxy (MBE) is strongly influenced by kinetic factors. This study examines how substrate rotation direction and speed affect the compositional uniformity of InAs(1-x)Sb(x) films, considering the positional arrangement of effusion cells. The findings indicate that to achieve the less thermodynamically favored In-Sb interaction more efficiently, Indium adatoms should first interact with Sb species rather than As species. The duration of Indium adatoms` exposure to Antimony before encountering Arsenic is also crucial. These results highlight the importance of optimizing kinetic parameters and effusion cell configurations to improve the MBE growth process for high-quality InAsSb films.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

Effects of Sb Alloying on the Microstructure and Thermoelectric Properties of 5 at. % In-doped Bi_2Te_3

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In recent decades, thermoelectric (TE) technology has proved to be useful for recovering waste heat into electrical energy in various applications, ranging from the automobile industry to space missions. Bismuth-telluride (Bi_2Te_3) is one of the prominent materials for TE applications near room temperature. Whereas much efforts have focused on enhancing the TE performance of single-phase Bi_2Te_3, dual-phase systems such as Bi_2Te_3-In_2Te_3 have rarely been explored. Herein, we synthesize 5 at. % In doped $Bi_{2-x}Sb_xTe_3$ compounds with x =0.05 and 0.1 to form second-phase In_2Te_3 precipitates dispersed in the Bi_2Te_3-based matrix. We, furthermore, alloy these materials with Sb to control the precipitates' morphology, thereby manipulating the TE transport properties of the composite. We perform scanning electron microscopy (SEM) observations combined with energy dispersive spectroscopy (EDS) analysis and electron backscatter diffraction (EBSD), together with X-ray diffraction (XRD) and TE property measurements for each composition. We observe that In-alloying forms elongated lamellar In_2Te_3-precipitates aligned along the Bi_2Te_3 {0001} basal planes. Upon Sb-alloying, Sb atoms tend to partition to the In_2Te_3-phase, presumably substituting for the In-atoms, which is expected to slightly reduce its lattice parameter, thereby increasing the Bi_2Te_3/In_2Te_3 interfacial energy. For this reason, the precipitates morphology gradually transforms into a more equiaxed shape with increasing Sb concentration. This affects the TE properties positively by slightly increasing both the electrical conductivity and the absolute values of Seebeck coefficients. Moreover, the lattice thermal conductivity has been significantly reduced, which is primarily attributed to phonon scattering by the Sb-atoms dissolved in the Bi_2Te_3-based matrix. Overall, this study outlines the potential for further enhancements of the TE performance in dual-phase systems.

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Poster Presentation

Semiconductors and Electronic Materials

Fully Balanced Ambipolar OECTs through Tunability of Blend Microstructure

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Organic electrochemical transistors (OECTs) are versatile devices where the electrical conductivity of an organic semiconductor is modulated by ionic interactions with an electrolyte. They are made from Organic Mixed Ionic Electronic Conductors (OMIECs), enabling efficient coupling between ionic and electronic signals. Operating at low voltages, high transconductance, and exceptional sensitivity to various stimuli, makes OECTs ideal candidates for biosensing, bioelectronics, and neural interfacing applications.

While most OECTs are unipolar, it was shown that ambipolar OECTs, i.e., operation as both n-type and p-type, can simplify circuit fabrication and offer sensing of both positive and negative ions in a single device. Conventional approaches to achieving ambipolar OECTs rely on the complex synthesis of ambipolar OMIECs, often producing imbalanced performance between polarities. Recently, we demonstrated that ambipolarity can be achieved by blending judiciously selected unipolar p-type and n-type OMIECs, offering simpler synthesis and facile fabrication with tunable performance through blend composition.[1] However, achieving fully balanced ambipolar OECTs, in which both polarities exhibit similar overall performances, remains a challenge.

We propose that microstructure, in addition to composition, can be leveraged to attain fully balanced ambipolar OECTs. For that, we selected two blends based on polythiophene:fullerene mixed conductors: the polythiophene, P3MEEET, is a benchmark p-type polymer, while the fullerene, either PTEG-1 or PrC60MA, are n-type small molecules. By controlling blend composition and thermal processing, we direct the microstructure to achieve balanced ambipolarity with near-equal n-type and p-type performances, both in the figure-of-merit transconductance and in symmetrical threshold voltages.

By coupling comprehensive electrochemical analysis (spectroelectrochemistry (SEC), cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and OECT measurements) with microstructural characterization (grazing incidence wide-angle X-ray scattering (GIWAXS) and high-resolution scanning electron microscopy (HRSEM)), we underscore the pivotal role of microstructure in OECT performance, reveal synergistic effects, and draw design rules for fully balanced ambipolar OECTs based on controlled and tuned blend microstructure.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

Stabilization of Cubic Phase of SnS using Cation Impurities

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Tin monosulfide (SnS), characterized by its low toxicity, abundant availability, and affordability, holds promise as an important material in future devices. It also showcases high absorption properties (10^4 cm^{-1}) and hole mobility. Therefore, potential uses of SnS encompass solar cells, field-effect transistors, photodetectors, as well as Li-ion and Na-ion batteries, and gas sensors. SnS exhibits two primary polymorphic phases at room temperature: the familiar and thermodynamically stable orthorhombic (α-SnS) phase and the metastable cubic (π-SnS) phase, first reported in 2015 by our group. This novel cubic phase is potentially easier to incorporate into technological layers and manifests intriguing properties, such as a wider band gap suitable for solar photovoltaic applications.

Recently, we reported controlled cation-assisted phase transformation of α-SnS to π-SnS [1]. Pb^{2+} cations added to the chemical deposition (CD) solution were demonstrated to enhance the compactness, phase purity, and growth rate of π-SnS. Furthermore, deposition under conditions favoring the formation of α- phase resulted in a gradual transition from the α-phase to the π -phase as the concentration of Pb^{2+} increased. The findings were validated through density functional theory simulations of substitutional Pb defects in SnS phases, highlighting the concentration of Pb substitutions (10 at%) needed to stabilize π-SnS, consistent with experimental observations.

Nevertheless, the hazardous nature of Pb metal requires a search for less toxic cations which can stabilize the π-phase. In the present work, we have studied the effect of Ca^{2+} cation doping in SnS and found that the free energy of the π-SnS system relatively decreased. Consequently, after sufficient Ca^{2+} doping, we found π-SnS polymorph became the ground state phase of SnS. We demonstrated the theoretical prediction of phase transitions using CD methods and found that Ca^{2+} cation doping can lead to a phase transition from α-SnS to π-SnS. Experimental characterization techniques like SEM, XRD and Raman measurements confirmed the phase transition. Interestingly, a small concentration of Ca^{2+} cation (~2 at%), obtained from XPS measurements, stabilized the π-SnS phase and favoured the phase transition. Moreover, small concentrations of Ca^{2+} doping did not significantly change the electronic structure of π-SnS material.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

Optimizing Thermoelectric Performance of $(GeTe)_{0.962}(Bi_2Te_3)_{0.038}$ Alloy Through Anisotropic Texturing

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In an attempt to reduce our reliance on fossil fuels, which are associated with severe environmental effects, the current research focuses on identifying the thermoelectric potential of the *p*-type $(GeTe)_{0.962}(Bi_2Te_3)_{0.038}$ semiconducting alloy. The thermoelectric properties of this material were systematically evaluated to investigate the effects of processing conditions, specifically melt-spinning at wheel speeds of 240 and 2400 RPM, and sample orientation relative to the hot-pressing direction. The Seebeck coefficient (α) remained stable across all samples, demonstrating minimal sensitivity to texture and processing speed, while electrical resistivity (ρ) exhibited clear anisotropy. Perpendicular to hot-pressing direction samples showed higher electrical resistivity due to alignment along the (001) crystallographic plane, characterized by weaker van-der-Waals bonds and reduced carrier mobility. Parallel samples to the hot-pressing direction, oriented along the (110) plane, exhibited lower electrical resistivity, benefiting from enhanced carrier transport through stronger covalent bonds. Thermal conductivity (κ) showed an inverse relationship with resistivity, consistent with the Wiedemann-Franz law. The electronic thermal conductivity (κ_e) was lower in the perpendicular samples due to their higher electrical resistivity, while lattice thermal conductivity (κ_l) decreased significantly at 2400 RPM. Microstructural analysis revealed smaller grains' size and increased grain boundary density at higher wheel speed, enhancing phonon scattering and effectively reducing κ_l. This microstructural refinement was confirmed by a reduction in flake thickness and columnar grain width observed in scanning electron microscopy (SEM) measurements.

The thermoelectric figure of merit ($ZT=\alpha^2T/\kappa/\rho$, where T- temperature) reached a maximum value of ~1.4 for fine-grained perpendicular samples produced at 2400 RPM over a broad temperature range of 310–500°C. This performance was attributed to optimized carrier concentration and grain boundary effects, which suppressed thermal conductivity while maintaining favorable electrical properties.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Semiconductors and Electronic Materials

A Blending Approach for Dual Surface and Bulk Functionality in Organic Transistors

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Organic transistors play a key role in semiconductor research, offering diverse functionalities based on different operational mechanisms, such as surface interactions with electrolytes or volumetric ion injection into the channel. This study investigates the development of dual-mode organic transistors that combine the functionalities of Organic Electrochemical Transistors (OECTs) and Electrolyte-Gated Organic Field-Effect Transistors (EGOFETs), achieved through blends of the p-type conjugated polymer P3HT and the n-type Organic Mixed Ionic Electronic Conductor (OMIEC) PrC60MA.

By correlating blend morphology with charge transport mechanisms, we identify the distinct roles of surface and volumetric processes in device performance. Surface hydrophobicity, driven by polymer-rich domains, facilitates effective p-type surface charge accumulation, while fullerene-rich domains enhance ionic transport for n-type behavior. Morphological analyses reveal the critical impact of blend composition on phase distribution and charge transport continuity. Time response measurements distinguish between rapid surface charging in EGOFET-dominated devices and slower volumetric doping in OECT-dominated devices, highlighting the dual contributions of surface and bulk mechanisms. This research establishes guiding principles for fine-tuning material compositions and blend microstructures to optimize device functionalities, advancing the design of efficient, multifunctional organic transistors with potential applications in sensors and bioelectronics.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Order-Disorder Transitions in Cerium and Praseodymium Hydrides, Manifested in Temperature-Dependent Raman Scattering Spectroscopy

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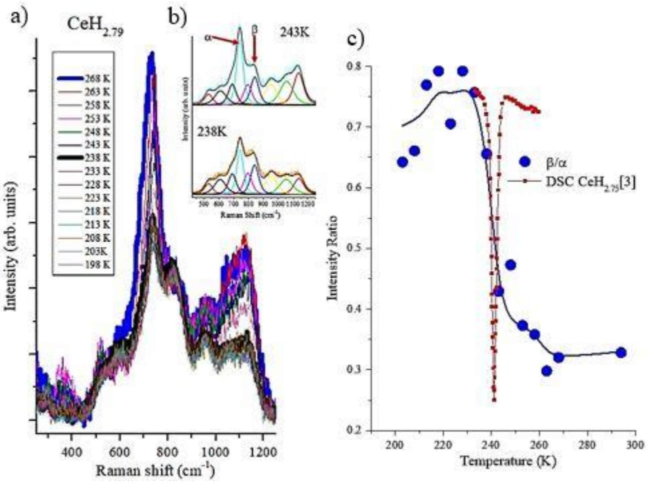
Lanthanides form a wide range of non-stoichiometric hydrides ($LnH_{2\leq x\leq 3}$). They are extensively studied due to their potential usage in devices as a result of their tunable electronic/optical properties; “switchable mirror” devices and fast ionic conductors are two well-known applications [1].

Cerium hydrides are characterized by a series of electronic and structural transitions, both composition and temperature-dependent. The high sensitivity of Raman spectroscopy to structural aspects and to the length scale of its order motivated us to extensive study and elucidate their temperature-dependent (77-353 K) spectra. Order-disorder transitions, driven by octahedral H^- sublattice rearrangements, which, as temperature decreases, give rise to a tetragonal distortion of the cubic unit cell, was the mechanism previously proposed for the metal-semiconductor transition at ~245 K in the $CeH_{\sim 2.7}$ [2]. In this study, we demonstrate for the first time that the highly accessible experimental method of Raman scattering can closely track the phase transition in $CeH_{2.79}$ (Fig. a-c) and $PrH_{2.77}$. This method allows for temperature resolution of just a few degrees by monitoring phonons attributed to the tetrahedral H^- sublattice. Quite remarkably, this phase transition is also clearly manifested in electronic Raman scattering, which is also sensitive to the crystal-field scheme around the Ce^{3+} ions.



a) Temperature-dependent Raman of $CeH_{2.79}$ in the range of 198-268 K.

b) Spectra measured before (243K-cubic) and after (238K-tetragonal) the phase transition.

c) The intensity ratio of two characteristic bands that follow the phase transition, compared to DSC measured in [3].

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

The Influence of Time, Atmosphere and Surface Roughness on the Interface Strength and Microstructure of AA6061–AA1050
Diffusion Bonded Components

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Cylindrical pairs of AA6061–AA1050 aluminum alloys were subjected to diffusion bonding experiments followed by tensile testing to evaluate the interface strength under varying conditions. The effects of bonding time, atmospheric environment, and surface roughness on interface strength were systematically investigated. Metallurgical characterization was performed to assess the quality of the bonded interface under different process conditions and to analyze oxide formation on the specimen surfaces.

Finite element analysis was employed to study the thermo-mechanical fields generated during the bonding process. A cohesive zone modeling approach was used to quantify the bond strength for various process parameters. The findings indicate that high bond strength can be achieved even in air furnace bonding, provided the surface roughness is minimal. However, increased surface roughness in air furnace bonding leads to a reduction in interface strength, an effect not observed in vacuum-bonded specimens.

Analysis of the bonded interfaces revealed that the reduction in strength is primarily due to oxidation and air entrapment between surface asperities, which impede diffusion and plastic deformation.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Surfaces and Interfaces

Development of Bioinspired Fatty Acid-Based Coatings for Advancing Sustainable Agricultural Practices

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This research investigates the development of sustainable, superhydrophobic coatings based on fatty acids tailored for agricultural applications. Recently, we have developed a facile solvent-based deposition method using a spraying technique. The choice of solvent is critical in the development of coatings due to its profound impact on the environment, health and safety, and the final properties of the coating. Solvents influence the drying speed, the formation of the coating`s microstructure, and the potential toxicity of the process. In this research, we selected ethyl acetate as it is a good alternative, offering a balance between environmental friendliness, effective evaporation rate that aids in forming superhydrophobic surfaces, and poses fewer health risks compared to more toxic alternatives. These characteristics make ethyl acetate a well-suited choice for achieving sustainable and safe agricultural coatings.

Herein, we demonstrate that we successfully formulated fatty acids-based coatings demonstrating contact angles exceeding 150° and low contact angle hysteresis, which are indicative of pronounced hydrophobic properties. These coatings also exhibit excellent thermal and UV stability, ensuring their durability and effective performance under various environmental conditions. To gain a deeper understanding of the relationship between structure and properties that supports the coating`s mechanism of action and to further optimize its performance, we are conducting comprehensive characterization studies using techniques such as scanning electron microscopy (SEM), nano-indentation, high-resolution synchrotron X-ray diffraction (HR-XRD), confocal and optical microscopy, and optical tensiometer. These analyses provide insights into the coatings` surface morphology, mechanical properties, crystal structure, and chemical composition.

Overall, this study provides a foundation for developing innovative, eco-friendly superhydrophobic coatings that could significantly improve crop yield and quality, reduce pesticide inputs, and contribute to the transition toward more sustainable agricultural practices.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Effect of ZrO_2 Nanoparticles and Electrical Parameters on PEO Coatings for MRI 230D Magnesium Alloy

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This study investigates the impact of synthesized zirconia nanoparticles (ZNP) on the composition, structure, and properties of plasma electrolytic oxidation (PEO) coatings on MRI230D magnesium alloy under varying current and voltage frequencies. ZNP suspensions, prepared via a sol-gel method, were incorporated into base electrolytes at 0, 1, 2, and 3 ml/L concentrations. The PEO coatings were characterized using SEM, EDS, XRD, and electrochemical techniques, focusing on morphology, chemical composition, and corrosion properties.

Results reveal that higher frequencies and increased zirconia concentration enhance coating uniformity, reduce pore size, and stabilize current and voltage profiles. Optimal coating properties were achieved at 600 Hz and 2 ml/L zirconium suspension, including dense microstructure and high corrosion resistance. Elemental analysis highlights consistent composition across coatings, with zirconium contributing to improved surface properties. Corrosion tests confirm the significant role of ZNP in enhancing durability and reducing degradation rates. The findings establish the synergistic influence of frequency and ZNP concentration on PEO-coated magnesium alloys.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Determination of the Diffusion Coefficients of Silver in Selected Thermoelectric Chalcogenide Compounds

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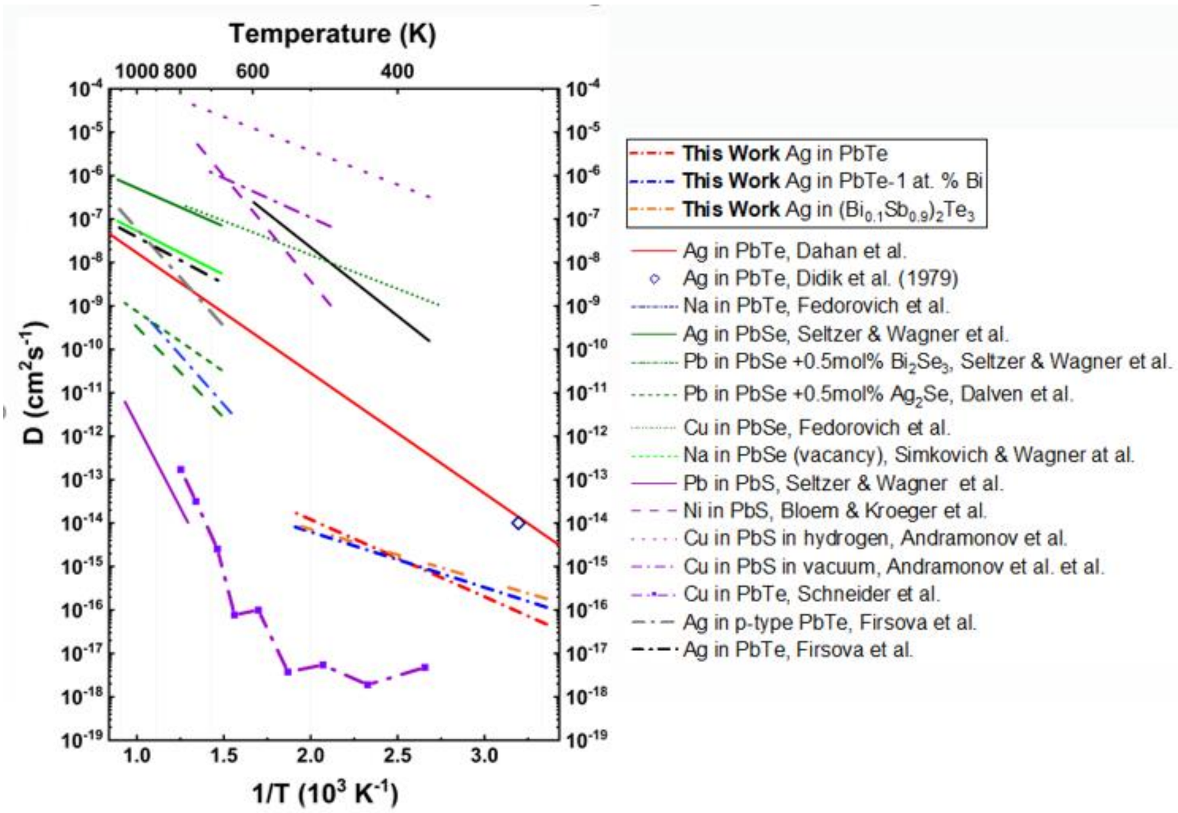
The increasing energy consumption is depleting our planet`s energy reserves. Energy harvesting involves capturing useful energy from various sources, such as mechanical, solar, or other environmental sources, and converting it into useful forms. Heat is an abundant but often wasted source of energy. Thus, harvesting even a portion of wasted heat holds great promise, e.g. applying thermoelectric (TE) technology, which enables direct heat-to-electricity conversion. TE compounds based on bismuth-antimony-telluride, $(Bi_{1-x}Sb_x)_2Te_3$ [1], and lead-telluride, PbTe [2], attract much attention due to their high conversion efficiency at ambient and elevated temperatures, respectively. Alloying PbTe with Ag above its solubility limit encourages the formation of Ag-rich second-phase precipitates, affecting electron transport and reducing thermal conductivity due to phonon scattering [2]. The evolution of these Ag-rich precipitates, particularly their nucleation, growth, and coarsening stages, is strongly determined by the diffusion rate of Ag in these compounds. Herein, we quantify the temperature dependent diffusion of Ag by deposition of thin (600 nm) Ag layers on the surfaces of polycrystalline PbTe-based and $(Bi_{1-x}Sb_x)_2Te_3$ substrates, and annealing at temperatures ranging from 100 to 250 ^{o}C for 1 h. We, first, characterized the morphology of the Ag-layers and their evolution with temperature utilizing scanning electron microscopy (SEM). We found that at adequately high annealing temperatures the Ag-layers undergo de-wetting, which limits the working temperature range. Then, we applied time-of-flight secondary ion mass spectroscopy (TOF-SIMS) to analyze Ag diffusion profiles in the undoped and 1 at. % Bi-doped PbTe samples, as well as in the $(Bi_{0.1}Sb_{0.9})_2Te_3$ samples. This enables us to derive the Ag bulk diffusion coefficients, which are $D^{Ag} = (1.55 \pm 0.04) \times 10^{-15}$, $(2.36 \pm 0.09) \times 10^{-15}$, and $(2.88 \pm 0.06) \times 10^{-15}$ cm^2/s at 150 ^{o}C, respectively. These temperature-dependent values appear in the figure below, together with corresponding values of different diffusants in similar compounds, for comparison. Most importantly, the respective diffusion activation energies were evaluated as: 34.0 ± 3.5, 24.5 ± 1.2, and 22.6 ± 0.5 kJ/mol, respectively. Bi additions seem to reduce the activation energy of Ag diffusion in PbTe, possibly due to the particular nature of point defects in PbTe, where Bi may either substitute for the Pb-atoms or form interstitial defects. This information is valuable for developing thermally stable TE devices based on multiphase PbTe and Bi_2Te_3-based compounds.



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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Effects of Grain Size and Misorientation on Thermoelectric Properties of Antimony Telluride-based Compounds

Guy Feldus[1], Yaron Amouyal[1], Zegeng Su[1], Muhamed-Khalid Dawod[1]
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Thermoelectric (TE) materials are attractive for waste heat recovery and cooling applications since they can convert heat into electrical energy and vice-versa. Notably, several TE compounds for near room temperature (RT) applications, such as Bi_2Te_3, Sb_2Te_3, and Bi_2Se_3, are well-known topological insulators (TIs), as well. Combination between both properties may be instructive for studying their charge carrier transport mechanisms. Herein, we are interested in the effects of internal interfaces, particularly grain boundaries (GBs), on TE transport properties. The $(Bi_{1-x}Sb_x)_2Te_3$ series, with x = 0, 0.2, 0.5, 0.8, 0.9, and 1, is synthesized through a process involving vacuum melting of pure ingredients to form ingots, followed by hot-pressing (HP) of hand-ground (HG) powders. Among these, the $(Bi_{0.1}Sb_{0.9})_2Te_3$ (BST0.9) compound demonstrates the most promising TE performance. Additionally, we investigate the Sb_2Te_3 (ST) compound for the sake of comparison. To further investigate the effects of grain size and grain boundary (GB) misorientation, BST0.9 and ST undergo additional processing through ball-milling (BM) for 30, 45, 90, and 120 min. followed by HP to form pellets. Characterization is performed using X-ray diffraction (XRD) and electron microscopy equipped with electron backscatter diffraction (EBSD), along with TE transport property measurements. Our EBSD analysis reveals several key trends. We observe a progressive decrease in grain size from as-grown (AG) to HG samples, with further reduction corresponding to increased BM durations. The misorientation distribution shows significant changes: as grain size decreases and saturates for the BM samples, we observe increase of highly-misoriented GBs and twin boundaries. Comparison between the TE properties of BST0.9 and ST reveals that the electrical conductivity decreases with reducing grain size, while the Seebeck coefficients increase. This effect is more pronounced for ST than for BST0.9. Both materials exhibit their highest TE power factors for the HG samples, with AG samples showing the lowest, and 45 min. BM samples display the best performance among the BM procedures, possibly due to an increased presence of twin boundaries. Interestingly, the lattice components of thermal conductivity of BST0.9 exhibit the largest values for the AG state and the lowest values for HG, with nearly identical intermediate values for all BM ones. We elucidate these findings in terms of preferred orientations, considering that the Te-Te van der Waals (vdW) bonds parallel to the {0001} basal planes reduce thermal conductivity along the c-axis. We hypothesize that grinding of the powder particles apply shear stresses that expose the basal planes and form twin GBs during HP, so that compaction of the larger, flake-like HG powder particles results in preferred [0001] orientation, whereas the pelletized BM finer powders show more isotropic behavior. This study provides an original viewpoint on microstructure-property relationships in TE compounds.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Design and Realization of a Hot Embossing Setup for Surface Engineering of Metal-plated PVDF

Basma Haj Yahya

Piezoelectric materials are unique dielectrics that can polarize in response to both electric fields and mechanical stress due to their non-centrosymmetric crystal structure. This property enables them to generate an electric charge when stressed and to deform mechanically when an electric field is applied[1]. Previous work in our group predicted through finite element simulations that altering the geometry of the surface of the piezoelectric layer improves its applicability in composite devices. Here we present the route for experimental verification of this prediction.

To modify the geometry of piezoelectric surfaces, we developed a hot embossing process[2]. The setup includes a controlled hot plate, silicon (Si) molds, and a steel weight applying 20 N of force. Seven Si molds with grating line patterns were fabricated using photolithography and dry etching, featuring a uniform depth of 25 µm, variable widths (10–40 µm), and differing periodicities. By varying the width, the number of grating lines changes as well, allowing us to investigate the influence of these parameters on the piezoelectric response.

For the molding process, the piezoelectric material, polyvinylidene fluoride (PVDF) was heated to 55°C, above its glass transition temperature (T_g) but below its Curie temperature (T_c). The patterned Si mold was placed on the heating plate, followed by the PVDF layer, a flat Si layer, and the weight. After one minute of heating, the system was cooled to room temperature for over 30 minutes before removing the weight.

To measure changes in the piezoelectric properties, a piezometer is used to evaluate the d_{33} piezoelectric coefficient before and after the hot embossing process. The results show an increase in the d_{33} coefficient after heating and applying pressure. Furthermore, as the line width becomes smaller, the periodicity decreases, and the number of lines increases, the d_{33} coefficient increases as well.

To characterize the silicon mold and the piezoelectric layers before and after the hot embossing process, optical microscopy and scanning electron microscopy (SEM) were used.

Our initial results indicate that changing the geometry of the piezoelectric layer improves its piezoelectric properties, making it possible to integrate these layers into composite materials, such as magnetoelectric composites, and enhance their output performance through changes in the interface geometry.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Invited Lecture

Surfaces and Interfaces

Defining the Surface Properties of Aerogels by their Drying Media

Guy Lazovski[1], Murial E. Layani Tzadka[1], Adira Marcus[1], Shilat Ashush[1], Pechersky Savich[2], Galit Bar[1], Igor Lubomirsky[2]
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Aerogels are a large family of porous materials, which can be synthesized from a wide variety of building blocks (ceramics, metals and organic components) predominantly through sol-gel chemistry. Aerogels are distinguished from other porous materials, not only by their production method, but also by their bulk density, being below 250 mg/cm³.

While there are several methods for drying aerogels from their wet gel state, super critical drying (SCD) is the most common. As it allows for the extraction of the gel's liquid content, with limited to negligible structural deformation. We utilized hot SCD (a sub-branch of the SCD methodology), not only as a means to dry the gels but also as a tool for controlling the surface properties of the resulting aerogel.

By carefully choosing the drying media (solvent mixture or additives), we were able to produce aerogels ranging from being hygroscopic to super hydrophobic, while originating from the same gel batch, and without the need for any pre- or post- treatment. This tool makes aerogels an even more versatile family of materials and could potentially accelerate their implementation in a wide variety of applications (selective absorbing material, long lasting thermal insulator and low dielectric permittivity material, to mention but a few).

Keywords:

Aerogels; Silicon-alkoxides; Hot supercritical drying; Surface chemistry; Process optimization.

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Quantitative Model for Low Temperature Sputter Deposition on Porous Substrates

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Ester Segal[2], Yonatan Calahorra1[1]
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Sputtering is a PVD technique used in the semiconductor industry to deposit thin films by bombarding a target with energy to transfer atoms onto a substrate. Qualitative structure zone models (SZMs) describe how the sputtered material`s morphology depends on parameters like temperature and sputtered gas pressure [1]. At low temperatures ($T0.3T_m$), the material typically shows columnar grain growth with a certain porosity level due to limited surface diffusion. While there are quantitative models for higher temperatures [2], to the best of our knowledge, no comprehensive model exists for low-temperature grain growth.

We base our model on a phenomenological model proposed by yang et. Al [3]. In this model, the grains grow as parabolic cones. Initially, N seeds are randomized on the surface. Then, a thin layer grows on the seeds according to the geometric constraints. After that places are randomized again and new seeds are placed in each chosen place that isn't on an existing grain and the process repeats. In our model, we introduced pores in the substrate that contribute two things: seeds cannot form on them and the amount of exposed surface pores increases the thickness of the layer added in each time step due to ricocheting from the pores. We simulated the growth in this model, and its results show that the higher the substrate porosity was the higher the sputtered layer porosity was and it was formed at a faster pace. These predictions agree with recent experiments of sputtering of iron-gallium thin films on porous silicon.

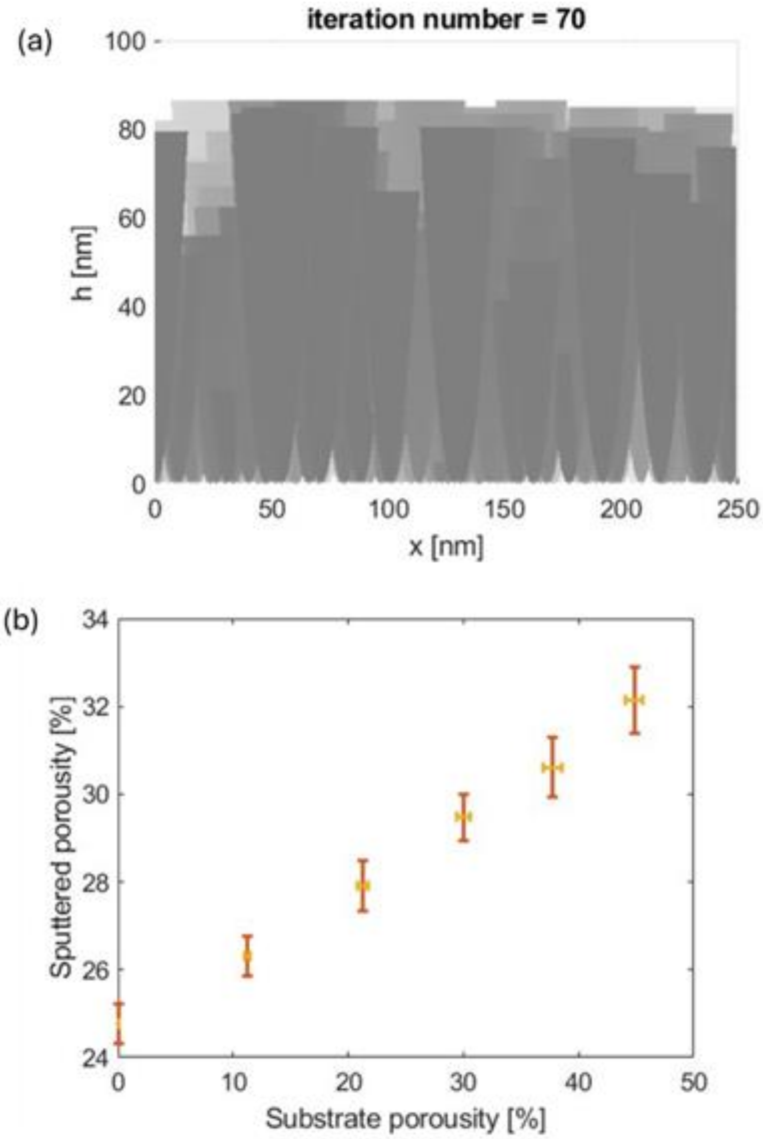

Fig. 1 (a) Cross-section of the simulated layer; brightness indicates cross-sectional depth and hence visualizes porosity; (b) Sputtered film porosity as a function of the substrate porosity

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Poster Session 2 (Wednesday, February 26, 2025 13:00)

Poster Presentation

Surfaces and Interfaces

Insights into the Oxidation Pathways of Nickel Nanoparticles Under Oxygen Evolution Reaction (OER) Conditions

Bat-Or Shalom, Miguel A. Andres, Ashley R. Head, Olga Brontvein, Alex S. Walton, Kacper Polus, Boruch Z. Epstein, Robert S. Weatherup, Baran Eren

The oxygen evolution reaction (OER) is a critical step in electrochemical water splitting, enabling the production of green hydrogen—a key component of renewable energy systems. However, its sluggish kinetics reduce the efficiency of this process [1], leaving hydrogen production heavily reliant on fossil fuel-based methods that significantly contribute to environmental pollution.

Nickel-based catalysts, widely used for OER in alkaline systems, play a key role in addressing these challenges. The chemical state of Ni during OER is particularly important, as it directly influences both the catalytic activity and stability of the material. Understanding the mechanism that takes place on the surface of Ni, under operational conditions, is essential for providing fundamental insights that can guide the development of catalysts that are more efficient, durable, and scalable, advancing water electrolysis technology.

In this study, we employ advanced techniques like ambient pressure X-ray photoelectron spectroscopy (AP-XPS) and near-edge X-ray absorption fine structure spectroscopy (NEXAFS) to investigate the chemical transformations of Ni nanoparticles under reaction conditions [2]. Using a custom-designed microelectrochemical cell, we capture real-time changes in the chemical state of Ni and map the oxidation pathways of Ni nanoparticles.

At the OER onset potential, Ni nanoparticles oxidize completely, forming a mixture of Ni^{2+} and Ni^{3+}, with no detectable metallic Ni remaining. Moreover, the initial formation of NiO precedes its conversion into other Ni^{2+} and Ni^{3+} species, accompanied by significant water incorporation. *Ex situ* transmission electron microscopy (TEM) further reveals morphological changes consistent with water incorporation, leading to structural amorphization. This study also highlights the unique role of carbonate-bicarbonate electrolyte in facilitating the formation of Ni^{3+} species and promoting water incorporation into the catalyst structure. Interestingly, thick Ni film retains a metallic core under identical conditions highlighting the influence of morphology on oxidation behavior.

Our findings provide valuable insights into the interplay between catalyst morphology, chemical state, and electrochemical performance under operating conditions, offering a foundation for the design of next-generation nickel-based OER catalysts.

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Poster Presentation

Surfaces and Interfaces

Influence of the PEO Process Parameters on the Coating Microstructure of Ti Alloy

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This study focuses on optimizing Plasma Electrolyte Oxidation (PEO) parameters by examining the effects of key variables such as current and voltage at different frequencies on the microstructure and corrosion resistance of coatings applied to the Ti-6Al-7Nb alloy. To enhance the bioactive properties of the surface, cellulose gel was incorporated into the electrolyte. The specimens underwent PEO treatment, Hydrothermal Treatment (HTT), and immersion in Hanks` solution.

The PEO process was conducted at 200 V and 9.6 A/dm² with unipolar current. The electrolyte comprised cellulose gel, calcium glycerophosphate, and calcium acetate to promote the formation of hydroxyapatite (HAp), a structure conducive to effective osseointegration with bone tissue. Experiments were carried out at six different frequencies—50 - 1200 Hz.

Following PEO treatment, the samples underwent hydrothermal treatment to facilitate the development of a crystalline hydroxyapatite structure. Subsequently, they were immersed in Hanks` solution for varying durations. Changes in surface morphology, characteristics, and composition were analyzed using X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). Additional evaluations included surface wettability, corrosion resistance, toxicity, dispersion, and pore size analysis.

The results demonstrate that the frequency of the PEO process significantly influences pore formation. Frequencies of 150 Hz, 450 Hz, and 1200 Hz produced smaller pores (less than 2 μm), while 300 Hz and 600 Hz resulted in larger pores (approximately 4 μm). Notably, optimal hydroxyapatite crystal growth was achieved at 1200 Hz after seven days of immersion in Hanks` solution. This condition yielded complete amorphous HAp coverage, indicating improved potential for osseointegration.

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Surfaces and Interfaces

Effect of Methylcellulose Concentration in PEO Process on Coating Properties for Titanium Dental Implants

Boris Shmukler[1], Alexander Sobolev[1]
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Titanium alloys are widely used for dental implants due to their exceptional mechanical properties and biocompatibility combination. Titanium`s high strength-to-weight ratio, outstanding corrosion resistance, and excellent biocompatibility make it an ideal implant material. However, challenges remain in achieving effective biological integration, particularly osseointegration, which refers to the direct bond between the implant and bone.

To enhance biocompatibility and promote osseointegration, plasma electrolytic oxidation (PEO) coatings containing hydroxyapatite with methyl cellulose additives were developed. This study investigates the properties of coatings formed with varying concentrations of methylcellulose (0.1, 2, and 3 g/L) in the PEO process. Additionally, the growth kinetics of hydroxyapatite crystals on the coated surface were examined during immersion in Hanks` solution, a body fluid simulator.

The coatings were characterized by surface morphology, chemical composition, and phase structure to evaluate their potential for improved osseointegration and overall performance in dental applications.

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Surfaces and Interfaces

The Influence of Crystal Orientation and Thermal State of a Pure Cu on the Formation of Helium Blisters

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The study investigated the factors influencing helium blister formation in copper, focusing on crystallographic grain orientation and thermomechanical conditions. Helium implantation was carried out at 40 keV with a dose of 5×10^{17} ions/cm2, followed by post-implantation heat treatments at 450 °C for varying durations. The samples were analyzed using a scanning electron microscope (SEM) equipped with an electron backscatter diffraction (EBSD) detector. The results showed that the extent and progression of blistering erosion differed based on the crystallographic plane of the free surface, with distinct behaviors observed in annealed and cold-rolled copper. Among the examined states, cold-rolled copper with a (111) free surface exhibited the highest resistance to helium blistering. This finding can be attributed to the interplay of dislocations and vacancies in the material. For the development of plasma-facing components (PFCs), further research is essential to identify the optimal combination of material properties for helium blistering resistance. If copper is chosen as a PFC material, achieving the preferred (111) orientation can be realized through cold rolling or thin-layer technologies.

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Surfaces and Interfaces

Ceramic-Metal Interface: Relationships between Residual Stress, Microstructure, and Mechanical Properties of Brazed Alumina-aluminum Composite Joints

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The proposed additive manufacturing (AM) brazing approach affirms its suitability for fabricating alumina-aluminum composites at lower joining temperatures, based on the effect of active metal titanium on interfacial bonding characteristics. This was realized through plasma-assisted physical vapor deposition (PVD) of titanium over an alumina surface, brazed with an aluminum alloy substrate using aluminum filler, which was conducted in a vacuum environment. The brazed interfacial microstructure was characterized by scanning electron microscopy (SEM) equipped with energy dispersive spectrometry and X-ray diffraction (XRD) techniques. The goal of microstructure characterization, specifically on the interface between the Al_2O_3 coating and the metal, is to explain how the ceramic is securely bonded to the metal and how vapor deposition and a vacuum atmosphere are very important in making this possible. The TiO_2 and Ti_3Al reaction compounds were identified at the interface. At the alumina-titanium interface, a reaction layer of 0.340 µm thickness is observed at a brazing temperature of 625 °C held for 40 minutes. The characterization revealed beneficial elements, including a detailed look at how titanium affects the wetting behavior of the alumina surface using the SEM method, a study of the Ti-rich intermetallic compound development and its structure using the XRD method adjoined to the alumina surface with titanium deposition, and a radiograph that checked the degree of joint quality of the brazed part to examine any flaws. The test results showed a shear strength of 36 MPa, and the fracture happened not on the brazed interface. This proved that the parameters used were effective and yielded rewarding results. Investigation on the residual stress distribution of the brazed joint interface, the results of D-spacing vs. Sin2ψ shows that prior to the brazing process, the titanium-coated surface exhibits +130.9 MPa, indicating compressive stress due to decreasing d-spacing. Upon post-joining process, the interface unveils with -3.4 MPa, indicating tensile stress due to increasing d-spacing. The degree of crystallinity at the interface is 54.46%, with an average crystalline size of 64.91 nm, evaluated from the XRD crystalline peaks. The effects conclude that the volumetric increase in intermetallics experiences negative tensile stress. The Ti-rich intermetallic compounds arrest the crack propagation about to happen due to the thermal expansion coefficient mismatch of the materials. The additive manufacturing (AM) brazing technology for fabricating ceramic-metal composites has expanded its prospects, predominantly in sensor feedthroughs. This joining technology is extensively integrated into ultra-high vacuum modules, which support manifold requirements in power electronics, biomedical engineering, and the energy sector.

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Surfaces and Interfaces

Fabrication of Vertically Aligned Nanocolumns for Advance Electrolyte Applications

Yuliy Yuferov[1], Ilia Rozenblium[1], Konstantin Borodianskiy[1]
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Ordered arrays of vertically aligned nanocolumns (VAN) on oxide templates attract great interest as functional nanomaterial composites due to their advantageous conductivity, mechanical properties, and potential applications in solid oxide electrolysis and fuel cells (SOECs and, SOFCs) and other devices. VAN arrays can serve as enhanced electrolytes, offering highly conductive pathways and operating with lower electrical losses than traditional compact layer electrolytes [1]. Such VAN can be created within nanoporous anodic aluminum oxide (AAO). However, creating these arrays is challenging due to the difficulties associated with materials deposition into the AAO pores. Some of these challenges are the complexity of the deposition of thick oxide materials, separation of the AAO membrane, opening of pore bottoms through etching, and the high cost of conductive layer sputtering required for electrodeposition. In the current study, gadolinium doped ceria (GDC) nanocolumns were successfully grown within 100 µm thick AAO templates on the initial Al-substrate, achieving a high filling ratio over 1 cm^2. The AAO templates were produced through hard anodizing in oxalic acid followed by barrier layer thinning and chemical etching[2]. This thorough process ensures the uniform opening of nanochannels, further facilitating GDC electrodeposition into nanopores.

So far, we have successfully deposited GDC nanocolumns with a length of ~ 35±5 µm (diameter ~100 nm) within AAO templates. A comprehensive study on the pore bottom opening and material deposition has revealed that this is a crucial factor affecting electrochemical deposition processes. The proposed approach could be adapted to develop extensive area VAN membranes and further advance research on functional nanocomposite materials.

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Poster Presentation

Surfaces and Interfaces

Development of Dispersion-Strengthened Coatings for Aluminum Powders via Hydrothermal Process

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Additive manufacturing is unlocking new opportunities for material innovation that remain largely unexplored. This research demonstrates how additive manufacturing can create dispersion-strengthened (DS) coatings on aluminum powder without relying on conventional mechanical alloying techniques. The proposed process involves a hydrothermal treatment that coats aluminum powder with nanoscale zirconium oxides. Incorporating these nanoscale zirconium oxides into the metal matrix during 3D printing enhances mechanical properties, particularly under high-temperature conditions. A zirconium dioxide suspension was employed as the coating material, and a series of experiments were conducted to determine the optimal deposition parameters, including reactant concentration, temperature, and processing time. The coated aluminum particles` surface morphology was analyzed using a scanning electron microscope (SEM) integrated with an energy-dispersive X-ray spectroscopy (EDS) system to assess coating quality and distribution.

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Surfaces and Interfaces

Pattern Formation through the Oriented Growth of Au-Si Thin Films on Si Single Crystals

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The fabrication of patterned surfaces is integral to various device manufacturing processes and requires precise manipulation of surface properties. This study[1] introduces a self-driven approach for patterning metal and semiconductor surfaces by solidifying eutectic Au-Si thin films on Si(001) substrates. The resulting pattern encompasses meticulously aligned Au-Si eutectic structures and Si islands attributed to the epitaxial growth of Si(001), Au(001), and Au(011) within the films. This was corroborated through electron diffraction and synchrotron radiation grazing-incidence wide-angle X-ray scattering (GIWAXS). We propose a 4:3 coincident site lattice model to elucidate the Au-Si interface, explaining the dominant $(001)[110]_{Au}||(001)[110]_{Si}$ orientation relationship that minimizes the lattice mismatch to 0.2%. Another observed orientation relationship, $(110)[001]_{Au}||(001)[110]_{Si}$, entails a 6.3% mismatch in one direction, leading to contrasting elastic strains in the Au and Si lattices. This study underscores the practicality of substrate-oriented pattern formation, with potential applications in other phase-separated systems.

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