

THE 89TH ANNUAL MEETING

OF THE ISRAEL
CHEMICAL
SOCIETY



BOOK OF ABSTRACTS

FEBRUARY 10-11, 2026

SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY

האוניברסיטה הפתוחה
THE OPEN UNIVERSITY OF ISRAEL
الجامعة المفتوحة



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International Chemical Sciences Chapter
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האוניברסיטה העברית בירושלים
THE HEBREW UNIVERSITY OF JERUSALEM

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DAY 1 FEBRUARY 10, 2026

8:30-9:30	Registration Light Breakfast, Exhibition & Poster Mounting	
09:30-10:00	Opening	Ehud Keinan, ICS President Roey J. Amir and Yuval Ebenstein, Co-Chairs
10:00-10:30	Plenary	Roderich Süßmuth, TU Berlin Peptide Antibiotics that Matter: Linking Structure to Biological Effect
10:30-11:00	ICS Excellent Scientist Prize	Gilad Haran, WIS Single-Molecule Fluorescence Deciphers the Translocation Mechanism of a Nanomachine
11:00-11:30	ICS Excellent Scientist Prize	Milko van der Boom, WIS Complex Shapes of Chiral and Colorful Crystals
11:30-12:00	Coffee Break	
12:00-12:20	Tenne Prize for a Young Scientist Award	Idan Hod, BGU MOF-based Tandem Schemes for Electrochemical Small Molecule Activations
12:20-12:40	ICS-Adama Prize for Technological Innovation	Boris Rybtchinski, WIS Self-assembled Nanomaterials
12:40-13:00	ICS-Adama Prize for Technological Innovation	Dario Dekel, Technion Anion-Exchange Membrane Fuel Cells – A New Era in Fuel Cells
13:00-14:30	Lunch and Poster Viewing	
14:00-14:30	General Assembly	
14:30-15:10	ICS-BioAnalytics Prize for an Excellent Ph.D. Student	Nadim Eghbarieh, HUJI
	ICS Prize for Excellent Graduate Students	Karina Abramov Harpaz, BGU Natanel Jarach, HUJI Martins Otikovs, WIS Renana Schwartz, BIU Radhey Shyam Yadav, AU
15:10-15:30	ICS Excellent Young Scientist Prize	Barak Hirshberg, TAU Have You Tried Turning It Off and On Again? Stochastic Resetting for Enhanced Sampling
15:30-15:50	ICS Excellent Young Scientist Prize	Graham de Ruiter, Technion A Flavor of Iron Chemistry: From Catalytic Novelties to Applicable Catalysis
15:50-16:10	ICS award for green chemical industry	Hen Dotan, H2Pro Ltd. Decoupled Water Electrolysis for a Renewable Energy Era: H2Pro's Solution
16:10-16:40	Coffee Break	
16:40-17:00	ICS Gold Medal	Joseph Klafter, TAU How Anomalous is Anomalous Diffusion?
17:00-17:20	ICS Gold Medal	Addy Pross, BGU The nature of stability: Bridging between chemistry and biology
17:20-17:40	Plenary	Renana Gershoni-Poranne, Technion Inverse Design of Polycyclic Aromatic Systems
17:40-18:10	Honorary Member of the ICS	Jonathan L. Sessler, UT Austin Texas-inspired Drug Discovery Efforts
18:10-18:20	Introducing the ACS Israel chapter	Mindy Levine, AU
18:20-20:30	Poster session - Sci-Mix	
19:00	ICS Awards Ceremony	

DAY 1 FEBRUARY 10, 2026

12:00-17:30	Chemical Education	
12:00-12:10	Chair: Debora Marchak, TAU	Opening remarks
12:10-12:35	Gilead Shafir, Israel police	Forensic chemistry in the DIFS, Israel Police
12:35-13:00	Ron Blonder, WIS	Binding school science and real science through contemporary content knowledge
13:00-14:00	Lunch and Poster Viewing	
14:00-14:30	Yehudit (Judy) Dori, Technion	Promoting 21st-Century Skills and STEM Career Pathways: Addressing Gender and Representation Gaps
14:30-14:55	Shelley Rap, WIS	Critical Thinking in Chemistry Education: Conceptualization, Challenges, and Research Findings
14:55-15:20	Yael Feldman-Maggor, BGU	A Conceptual Synthesis of SOLO Taxonomy and Generative AI in Nanotechnology
15:20-15:45	Tamar Traube, BIU	The Innovation in the Chemical Industry Course: Bridging Chemistry Studies and Industry
15:45-16:10	Shirly Avargil, Technion	Integrating Facilitation, Collaborative Regulation, and Formative Assessment in a Chemistry-based Educational Escape Room
16:10-16:40	Coffee Break	
16:40-17:05	Omry Morag, TAU	The Pedagogical Vision of Tel Aviv University Youth Programs for Chemistry Education: Cultivating Israel's Next Generation of Chemists
17:05-17:30	Ayelet Shvalb, Afeka College	"COFFEE TIME": a Virtual Chemical Escape Room

DAY 2 FEBRUARY 11, 2026

8:30-9:30	Gathering and light breakfast			
	Parallel sessions			
	Main Hall (1)	Balcony (2)	South Hall (3)	North Hall (4)
	Methodology and Catalysis in Organic Chemistry	Magnetic Resonance	Classic and Quantum Thermodynamics	Nanoscience and Nanotechnology
	Chair: Doron Pappo, BGU	Chair: Michal Leskes, WIS	Chair: David Gelbwaser-Klimovsky, Technion	Chair: Fernando Patolsky, TAU
	Michael M Meijler, BGU <i>Synthetic Probes to Unravel Mechanisms Behind Coexistence within Microbial Ecosystems</i>	Ilia Kaminker, TAU <i>From Investigation of Polarization Transfer to Materials Insight: DNP Mechanisms Probe Diamond Defects Distribution</i>	David Gelbwaser-Klimovsky, Technion <i>Necessary conditions for the Markovian Mpemba effect</i>	Uri Banin, HUJI <i>Excitons & multiexcitons in quantum dot molecules</i>
	Roman Dobrovetsky, TAU <i>Mimicking Transition Metals with Structurally Constrained P III and Sb III Cations</i>	Sharon Ruthstein, BIU <i>Exploring oligomerization states of proteins in solution using EPR spectroscopy</i>	Oren Raz, WIS <i>Thermodynamic Geometry Near Phase Transitions</i>	Adi Salomon, BIU <i>Seeing Depth in Color: Optical Encoding of Nanometric Axial Distances</i>
9:30-11:00	Anthony Cohen, ADAMA Ltd. <i>The development of an innovative route toward Prothioconazole at ADAMA</i>	Noam Shemesh, WIS <i>Correlation Tensor Magnetic Resonance as a probe of microstructure</i>	Haim Diamant, TAU <i>Relation between entropy and kinetics far from equilibrium</i>	Ernesto Joselevich, WIS <i>Enantioselective Guided Growth of Chiral Nanowires</i>
	Flash talks Anjali Soniwal, AU Batya Blank, WIS Keren Iudanov, BGU Michael Montag, WIS Omer Shaashua, BGU	Flash talks Ilia Moroz, WIS	Flash talks Tomer David Keidar, TAU Alon Krause, BIU Arad Lang, Technion Ido Avitan, Technion	Flash talks Achiad Goldreich, AU Elad Gaver, WIS Hagay Shpaisman, BIU Shai Kiriati, WIS Shir Abrahami Ben Harush, WIS
	Samer Gnaim, WIS <i>One-Electron Approach for Trans-Selective Alkyne Semi-Reduction via Cobalt Catalysis</i>	Amir Goldbourt, TAU <i>¹³³Cs NMR as a tool to study and guide waste immobilization in geopolymers</i>	Yonathan Dubi, BGU <i>Magnetic Moments at the Molecule-Metal Interface: A Seeming Violation of the Onsager Relations?</i>	Ronit Satchi-Fainaro, TAU <i>Rewriting the Rules of 3D Tumor-Host Interactions with Precision Nanomedicine</i>
	Ori Gidron, HUJI <i>A Twisted Synthron for Inducing Helicity and Handedness in Nanographenes</i>	Amnon Bar Shir, WIS <i>Introducing Fluorine Metabolic Imaging (FMI) for "Multicolor" MRI Mapping of Redox Biomarkers in Health and Disease</i>		Raz Jelinek, BGU <i>Capacitance-based carbon dot photodetector</i>
11:00-11:30	Coffee break			

	Polymer and Supramolecular Chemistry	Light-Matter Interactions	From Lab to Market: The Chemistry of Tech-Transfer	Bioinorganic Chemistry
	Chair: Charles Eliezer Diesendruck, Technion	Chair: Igal Levine, HUJI	Chair: Ronen Kreizman, RAMOT	Chair: Graham De-rutter, Technion
	Roy Shenhar, HUJI <i>Toward bimetallic nanowires: Insights from the co-impregnation of block copolymer films</i>	Daniel Grave, BGU <i>The Role of Optical Transitions in Determining Carrier Yields of Metal-Oxide Photoabsorbers</i>	Ronit Goldberg, LipoSphere Ltd. <i>Redefining the Treatment Paradigm for Knee Osteoarthritis</i>	Sotiris Hadjikakou, UoI <i>Hybrid Metallodrugs Targeting Breast Tumor Cancer Proliferation</i>
	Yossi Weizmann, BGU <i>Photoswitchable latent monomers as a new paradigm for latency in metathesis polymerization</i>	Tal Schwartz, TAU <i>Nothing can do something: Manipulating Molecules by Tailoring the Electromagnetic Vacuum</i>	Rotem Brakin, TomGrow Ltd. <i>TomGrow: reinventing soil</i>	Ori Green, Technion <i>Aza-Wittig based Sensors for Imaging Cellular CO₂ Production</i>
11:30 - 13:00	Shira Haber, BIU <i>Polymer Upcycling and Recycling: Insights from NMR Methodology</i>	Ron Tenne, Technion <i>Ultrafast spectroscopy at the single nanoparticle level</i>		Mindy Levine, AU <i>From Coordination to Color: Mechanistic Insights into Fluorophore- and Nanoparticle-Based Metal Ion Detection in Aqueous Media</i>
	Flash talks Alexander Laskavy, Volcani Arti Joshi, BGU Hadar Nasi, WIS Nir Lemcoff, BGU Ofer Burg, HUJI	Flash talks Michal Hartstein, WIS Anchal Vashishtha, BGU Paz Toledano, BIU Livin Paul, TAU Maya Levy Greenberg, WIS	Panel discussion Ronit Goldberg, LipoSphere Ltd. Ziv Kohav, ICL Ltd. Shoshi Mizrahi, RAMOT	Yuri Tulchinsky, HUJI <i>Formation and Reactivity of High-Valent Metal-Oxo Species Inside a Cavitand Pore</i>
	Ofer Reany, Open U <i>semiaza -Bambusurils as Versatile Macrocycles for Anion Transport and Sensing</i>	Sharly Fleischer, TAU <i>Ultrafast Triggering of Strong Coupling in a Semiconductor Terahertz Fabry-Pérot Cavity</i>	Itsik Bar-Nahum, ADAMA Ltd. Doron Shabat, TAU	Daniella Goldfarb, WIS <i>Unlocking Gd(III) Anisotropy: Determining the Zero-Field Splitting Axes to Enhance Spin-Label Structural Analysis</i>
	Tamar Segal-Peretz, Technion <i>Synthesizing water filtration polymer membranes, one monolayer at a time</i>	Igal Levine, HUJI <i>Mapping the Energetic Defect Landscape of Pb-free HaPs Using Surface PhotoVoltage</i>		

13:00-14:30	Lunch and poster			
14:20-14:30	Introducing Reaxys - Marta Da Pian, Elsevier GmbH (Main Hall)			
	Parallel sessions			
	Main Hall (1)	Balcony (2)	South Hall (3)	North Hall (4)
	Medicinal and Biological Chemistry	Translational Colloid Science: Bridging Materials, Medicine, and Agriculture	AI in Chemistry	Energy
	Chair: Muhammad Jbara, TAU	Chair: Guy Mechrez	Chair: Barak Hirshberg, TAU	Chair: Hannah-Noa Barad, BIU
	Ashraf Brik, Technion <i>Synthetic Proteins Behind the Plasma Barrier: Molecular Spies</i>	Avi Domb, HUJI <i>Solid lipid nanoparticles for the delivery of lipophilic drugs</i>	Ekaterina V. Skorb, ITMO University <i>AI-Driven Design of Biomimetic Interfaces: From Patterned Materials to Cellular Communication</i>	Michal Leskes, WIS <i>Tracking Lithium Dendrites and Solid Electrolyte Interphase Formation using Solid State NMR Spectroscopy</i>
	Moran Frenkel-Pinter, HUJI <i>Primordial Peptide Backbone Affects Assembly in Aqueous Solutions</i>	Dganit Danino, Technion <i>Engineered Alternative Casein Proteins for Drug Delivery</i>	Daniel Freedman, Genesis Molecular AI <i>A Theoretical Framework for an Efficient Normalizing Flow-Based Solution to the Electronic Schrödinger Equation</i>	Menny Shalom, BGU <i>Photocatalytic panels development for catalytic oxidation and reduction reactions</i>
	Micha Fridman, TAU <i>Chemical Probes for Antifungal Research: Illuminating Mechanisms of Action and Guiding Drug Design</i>	Sivan Antler, TEVA Ltd <i>Pharmaceutical Formulations: From API to Therapeutic Impact</i>	Yohai Bar Sinai, TAU <i>Machine Learning the Entropy to Estimate Free Energy Differences without Sampling Transitions</i>	Ido Hadar, HUJI <i>Organic Spacer Control of Charge Transport and Luminescence in Mn-Doped 2D Perovskites</i>
14:30 - 16:30	Gonen Ashkenasy, BGU <i>Mimicking Cyanobacteria Circadian Clock with Peptide Oscillators</i>	Ronit Bitton, BGU <i>Hierarchical structure of self-assembled peptide-polymer hybrids</i>	Ofir Lindenbaum, BIU <i>Interpretable deep learning for scientific discovery in chemistry</i>	Malachi Noked, BIU <i>On the Importance of Careful Electrochemical Analysis in Battery Performance Reporting</i>
	Flash talks Boaz Nutkovich, Technion Gal Raviv-Franco, WIS Miriam Gulman, BIU Shani Dvir, TAU Yuval Farchy, HUJI	Flash talks Men Guo, AU Yehonatan Levy, HUJI	Flash talks Yamin Ben-Shimon, TAU Evgenii Ziaikin, HUJI Netanela cohen, TAU Sofia Blyufer, Technion	Flash talks Anat Itzhak, DTU Mydhili Varma, AU Or Ben Zion, WIS Roy Marrache, TAU Yuval Mualem, BIU
	Sigal Saphier, IIBR <i>From basic physicochemical studies to a unique in-vitro ADME array: toward the development of improved opioid antagonists</i>	David Mocatta, ADAMA Ltd <i>Polymorphism in agrochemical formulations: A case study</i>	Barak Akabayov, BGU <i>Combining NMR-fragment screening with AI-based cheminformatics to design small molecules targeting RNA for antibiotic development</i>	Charlotte Vogt, Technion <i>Emergent Interfacial Dynamics: Rethinking Catalysis for a Sustainable Energy Future</i>
	Ariel Afek, WIS <i>Chemical Decoding of Protein-DNA Recognition in Health and Disease</i>	Levi Gottlieb – RAFAEL Ltd <i>Burn Rate Enhancement by In-Situ Catalytic Metathesis Reaction</i>	Mark Sierka, FSU Jena <i>Simulations of real-time electron dynamics in complex chemical environments</i>	Ahiud Morag, BGU <i>Reorganization of Mg Species Enables Cathode Electrochemistry</i>
	Doron Shabat, TAU <i>Unlocking the Barrier of Chemiluminescence in Water</i>	Lihi Adler Abramovich, TAU <i>Engineered Supramolecular Nanostructures for Tissue Regeneration</i>	Ilya Kuprov, WIS <i>Neural nets in Magnetic Resonance: how do they actually work?</i>	Lena Yadgraov, AU <i>Highly selective photocatalytic degradation of organic pollutants by core-shell nanoparticles via superoxide radical pathway</i>
16:30-17:00	Plenary talk - Kira Radinsky, Diagnostic Robotics <i>Chemistry in the Age of AI: Designing, Predicting, and Discovering</i>			
17:00-17:30	Poster awards and closing remarks			

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THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



Day 1: PLENARY AWARD SESSION

Chaired by: Roey J. Amir and Yuval Ebenstein

Invited lecture

Plenary session

Peptide Antibiotics that Matter: Linking Structure to Biological Effect

Roderich D. Süssmuth

¹Institut für Chemie, Technische Universität Berlin, 10623 Berlin, Germany

Natural peptides remain a prolific source of bioactive molecules with potent antimicrobial, anticancer, and immunomodulatory properties. Our research focuses on the discovery and characterization of peptide structures derived from cryptic bacterial and fungal biosynthetic pathways in the context of their mode-of-action and structure-activity-relations [1-3].

In recent years, major advances in antibacterial drug discovery came not only from natural peptides but also from their synthetic counterparts, including the exploration of novel antibacterial targets [4]. An example for an unusual natural product is Albicidin, a peptide produced by the plant-pathogenic bacterium *Xanthomonas albilineans* [5]. Albicidin exhibits remarkable potency against both Gram-positive and Gram-negative pathogens of the ESCAPE group. Recent studies have elucidated its mechanism of topoisomerase inhibition [6] and uncovered various natural resistance mechanisms [7,8,9]. In this context, chemical synthesis has enabled the generation of structural analogs with optimized pharmacological properties, facilitating proof-of-concept studies in animal models and further preclinical evaluation. The lecture will place Albicidin and other peptides within the broader framework of contemporary antibacterial and natural product research.

1. Sigurdsson A *et al.* (2023). *Angew Chem Int Ed*, 62, e202302490
2. Zhong L *et al.* (2025). *J Am Chem Soc*, 147, 20725-20734
3. Yao *et al.* (2021). *J Am Chem Soc*, 143, 14322-14331
4. Süssmuth RD *et al.* (2025). *Angew Chem Int Ed*, 64, e202414325
5. Cociancich *et al.* (2015). *Nat Chem Biol*, 11, 195-197
6. Michalzyk *et al.* (2023). *Nat Catal*, 6, 52-67
7. Rostock *et al.* (2018). *Nat Comm*, 9, 3095
8. Kosol *et al.* (2023). *Chem Sci*, 14, 5069-5078
9. Saathoff *et al.* (2023). *PLoS Biol*, 21, e3002186

Invited Lecture

Plenary session

Single-Molecule Fluorescence Deciphers the Translocation Mechanism of a Nanomachine

Gilad Haran, Weizmann Institute of Science

Multiple proteins function as nanomachines; how they utilize the energy of ATP to perform their work remains a fascination in Biological Physics. Single-molecule fluorescence resonance energy transfer (smFRET) spectroscopy is a powerful tool to study the internal motions of proteins during activity. We have used this capability to probe the ATP-dependent dynamics of ClpB, a machine that rescues proteins from aggregation. We find that protein translocation takes just milliseconds, two orders of magnitude faster than the rate of ATP hydrolysis by the machine. Using smFRET with three colors, we surprisingly observe both forward and retrograde substrate translocation. Supported by measurements of the pore loops, ClpB's elements that interact with substrates and pull them in, these findings suggest a stochastic, Brownian-ratchet-like mechanism of action.

Invited Lecture

Plenary session

Complex Shapes of Chiral and Colorful Crystals

Prof Milko van der Boom¹

Faculty of Chemistry, Weizmann Institute of Science, Israel

Single crystals with a multidomain morphology are a counterintuitive phenomenon. Growing such crystals in the lab is highly challenging, especially from organic molecules. Our pyridine-based ligands yield morphologies of remarkable complexity. We achieved the formation of uniform metal–organic crystals that exhibit single crystallinity with distinct domains and chirality. The crystals contain two types of continuous helical channels. This structural feature is atypical and has great potential for post-functionalization via selective inclusion of other components. Precise positioning and alignment of arrays of two different guest molecules within the crystalline host matrix produced new optically active materials. The color of individual micro-sized crystals depends on their orientation under polarized light. This angle-dependent behavior results from the geometrically constrained orientation of the dyes imposed by the crystallographic packing. Energy transport occurs between arrays of different dyes included in parallel nanochannels via Förster resonance energy transfer (FRET). Combining anisotropic optical properties with FRET may enable applications in optical switches and in bulk materials for light harvesting and conversion.

Plenary session

MOF-based tandem schemes for electrochemical small molecule activations

Prof. Idan Hod¹, Dr. Ran Shimoni¹, Dr. G. Shiva Shanker¹
Chemistry, Ben-gurion University Of The Negev (bgu), Israel

Metal-Organic Frameworks (MOFs) have emerged as promising electrocatalytic and solar energy conversion platforms. Initially, the key motivation behind the implementation of MOF-based porous platforms in electrocatalytic systems focused mainly on their capability to immobilize large quantity (high surface density) of electrolyte-accessible molecular catalysts which contains mass-transport conduits for diffusion of ions and catalytic-substrates towards the active sites (which constitutes a key advantage over conventional heterogeneous solids). Indeed, the initial examples of MOF-based electrocatalysis have laid the foundations for using MOFs as highly active and selective heterogeneous catalytic platforms for simple, small molecule activation reactions (i.e. 2-4 electrons/protons). Yet, as the field shifts toward more intricate catalytic proton-coupled electron transfer (PCET) reactions, such as: CO₂ conversion into multi-electron/multi-carbon products, reaching a further leap in our understanding of electrocatalytic MOF-based systems, one also must consider the well-defined structure and chemical modularity of MOFs as important virtue for efficient electrocatalysis. One can envision that MOFs-based electrocatalytic systems could draw inspiration from natural enzymes, which have evolved chemical and structural mechanisms that control and regulate the activity and selectivity of a desired catalytic reaction. For instance, MOFs offer unique, unparalleled tandem design opportunities due to their exceptional structural modularity, which allows precise spatial arrangement of multiple catalytic sites with controlled inter-site distances (at a nanometer length scale).

Here, we will present recent examples of: (a) MOF-based tandem schemes and investigation of their electrocatalytic CO₂ reduction performance, (b) molecular-level modulating of MOF-tethered active site's chemical environment and study its effect on the overall catalytic reaction.

Invited Lecture

Plenary session

Self-assembled Nanomaterials

Prof. Boris Rybtchinski¹

Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

We will present our work on self-assembled materials that employ organic nanocrystals, carbon nanotubes, and polymers. Our research focuses on the design and characterization of sustainable materials that can be recycled, advanced energy materials used in batteries and supercapacitors, and biodegradable plastics. Through these examples, we highlight how precise control over material structure enables improved performance and functionality. We will specifically address the importance of a fundamental understanding of crystallization mechanisms and molecular interactions as a guiding principle for rational materials design and the development of next-generation functional materials.

Invited Lecture

Plenary session

Anion-Exchange Membrane Fuel Cells – A New Era in Fuel Cells

Professor Dario Dekel¹

Technion, Israel

Since the first Anion-Exchange Membrane (AEM) Fuel Cell (AEMFC) with practical performance was announced about a decade ago [1], significant advances have been achieved in this field of research. This also opened the doors for the development of new technologies such as High-Temperature AEMFCs (HT-AEMFCs) [2], AEM Water Electrolyzers (AEMWEs) [3], and the very recent development of the novel AEM Oxygen Separation (AEMOS) [4].

We, at Technion, have recently presented the first results of AEMFCs tested at cell temperatures above 100 °C [5]. At these high temperatures, we could achieve not only high hydroxide ion conductivities close to 300 mS/cm [6] but also improved cell stability (yes, a very counterintuitive result). We have also demonstrated a novel approach to achieve high AEMFC performance while using PGM-free catalysts in both electrodes [7]. Altogether, these breakthroughs enable us to propose a novel strategy for CO₂ management [8] and to operate AEMFCs with ambient air, achieving record-high performance [9]. This represents a significant landmark for this technology.

In this talk, if time allows, all these breakthroughs will be shortly presented and discussed.

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1. ECS Transactions, 50 (2) 2051-2052 (2013).
2. J. Power Sources Adv. 5, 100023 (2020).
3. Chemical Soc. Reviews 51, 4583-4762 (2022).
4. ACS Org. Inorg. Au 4, 498-503 (2024).
5. Chemical Engineering J. Adv. 8, 100153 (2021).
6. J. Membrane Sci. 612, 118461 (2020).
7. Nature Catalysis, 2026.
8. Nature Energy, just accepted (2026).
9. ACS Energy Letters, just accepted, DOI: 10.1021/acsenorgylett.5c03124 (2026).

Invited Lecture

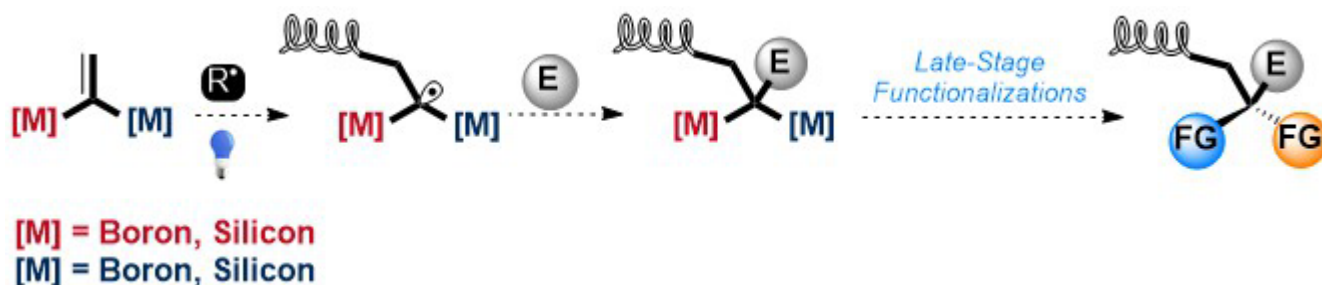
Plenary session

(Poly)borylated Species: Modern Tools for Advanced Synthetic Transformations

Nadim Eghbarieh¹

Chemistry, The Hebrew University of Jerusalem, Israel

Polyborylated molecules, which contain multiple carbon-boron bonds, have recently emerged as powerful compounds in modern organic chemistry. These systems, which are equivalent to polymetallated compounds, enable the generation and control of highly reactive α -metallated carbon-centered intermediates with unique electronic properties, allowing new and selective chemical transformations. In this talk, I will highlight our studies on the generation, stabilization, and functionalization of α -metallated carbon-centered radicals as versatile reactive intermediates that enable new and selective bond-forming processes. Their role in constructing structurally diverse organoboron architectures, ranging from sustainable and simple building blocks and natural materials to complex and biologically relevant scaffolds, will be discussed, alongside examples demonstrating their utility in synthetic late-stage transformations.



References:

- 1- N. Eghbarieh, N. Hanania, A. Zamir, M. Nassir, T. Stein, A. Masarwa, *J. Am. Chem. Soc.* **2021**, *143*, 6211–6220.
- 2- N. Kumar, N. Eghbarieh, T. Stein, A. I. Shames, A. Masarwa, *Chem. Eur. J.* **2020**, *26*, 5360–5364.
- 3- N. Hanania, N. Eghbarieh, A. Masarwa, *Angew. Chem. Int. Ed.* **2024**, *63*, e202405898.
- 4- N. Eghbarieh, N. Hanania, A. Masarwa, *Nat. Commun.* **2023**, *14*, 2022.
- 5- N. K. Vaishnav, N. Eghbarieh, R. A. Jagtap, A. E. Gose, B. E. Haines, A. Masarwa, *Angew. Chem. Int. Ed.* **2024**, *63*, e202412167.
- 6- N. Eghbarieh, A. Masarwa, *ChemistryEurope*, **2025**, *3*, e202500207.
- 7- N. Eghbarieh, N. Hanania, P. Nad, T. Alam, T. Kish, A. Masarwa, *Angew. Chem. Int. Ed.* **2024**, Accepted.

Invited Lecture

Plenary session

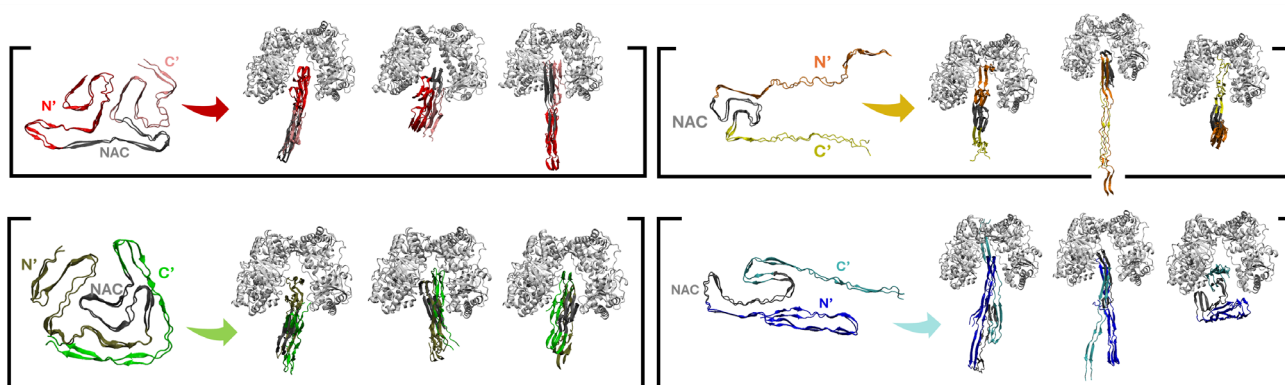
Non-proteolytic mechanisms of Insulin-Degrading Enzyme for inhibition of primary nucleation of amyloids

Karina Abramov Harpaz¹, Prof. Yifat Miller¹
Chemistry, Ben-Gurion University of the Negev, Israel

The primary nucleation of amyloids, e.g. amyloid- β (A β) and α -synuclein (AS) is a critical trigger in the pathology of Alzheimer's disease (AD) and Parkinson's disease, respectively. Isolating the earliest aggregation-prone species is experimentally challenging. The insulin-degrading enzyme (IDE) is known to degrade amyloidogenic peptides, e.g. A β . Our previous studies revealed the conformational plasticity of IDE (Inorg. Chem. Front., 2021, 8, 3205) and demonstrated its chaperone-like ability to entrap A β dimers (Biomolecules, 2022, 12, 1886). Although IDE has been experimentally shown to inhibit AS fibrillation in a non-proteolytic manner (Sci. Rep., 2015, 5, 12531), the molecular basis of this effect remains unclear.

Polymorphic AS dimers were systematically embedded into the IDE chamber in different orientations, generating a diverse set of starting conditions and molecular dynamics (MD) simulations were performed to investigate the effect of IDE on the conformational landscape of AS dimers and the inhibition of the primary nucleation of AS.

The inter-protein hydrophobic and electrostatic interactions, IDE conformational rearrangements and structural stability analyses provided an atomistic framework for understanding the structural determinants of the IDE non-proteolytic activity as well as the "dead-end" chaperone role in suppressing AS fibrillation. This work demonstrates the importance of MD simulations to uncover processes inaccessible to experiments and to bridge critical gaps between structural biology and mechanisms of diseases.



Atomistic framework of polymorphic α -synuclein dimers embedded in IDE in distinct orientations

Invited Lecture

Plenary session

Reversible Bonds in 3D Printing and Adhesives

Natanel Jarach^{1,2}, Michal Cohen¹, Rivka Gitt¹, Prof. Shmuel Kenig², Prof. Hanna Dodiuk², Prof. Shlomo Magdassi¹

¹*Institute of Chemistry, The Hebrew University of Jerusalem, Israel*

²*The Department of Polymer Materials Engineering, Shenkar – Engineering. Design. Art., Israel*

Thermoset polymers are integral to modern manufacturing but pose significant environmental challenges due to their irreversible cross-linked networks, which render them unrecyclable. Our work focuses on a sustainable approach to addressing these challenges by utilizing Covalent Adaptable Networks (CANs) in two distinct radiation-curing applications: Additive Manufacturing (AM) (i.e., 3D printing) and adhesives.

First, we introduce a fully recyclable photopolymer for Direct Ink Writing (DIW) based on cinnamaldehyde derivatives. Utilizing a novel tin-based catalyst, we achieved photopolymerization via [2 + 2] and [4 + 4] cycloaddition reactions. This system enables printing at 70°C, significantly lower than previously reported reversible systems, and enables complete depolymerization and multiple reprinting cycles without degrading material properties or requiring material replenishment.

Second, we present a solvent-free, reversible thermoset adhesive that incorporates disulfide bonds derived from α -lipoic acid. This adhesive demonstrates rapid photocuring (within 30 seconds) across a wide visible spectrum (400-650 nm) and maintains high adhesion strength on diverse substrates, including in underwater environments.

A key feature of both systems is the utilization of microwave irradiation as a trigger for reversibility. We demonstrate that microwave treatment efficiently induces depolymerization in the 3D-printed objects and controlled debonding in the adhesive, enabling a closed-loop life cycle. These findings highlight the potential of reversible chemistry to transform radiation-cured polymers into sustainable materials suitable for the circular economy.

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Invited Lecture

Plenary session

Development and applications of advanced MRI methods for imaging challenging regions

Martins Otikovs¹

Weizmann Institute of Science, Israel

MRI acquisitions incorporating diffusion weighting (DW) are gaining increasing importance in an array of clinical and research applications. However, they are often challenged by various factors that deteriorate the quality of acquired images. Among these, motion and sharp magnetic susceptibility variations play one of the most prominent roles. In this talk developments of image acquisition and data processing strategies to address aforementioned shortcomings using spatiotemporally encoded (SPEN) MRI will be presented and clinical applications enabled by these developments will be highlighted.

Invited Lecture

Plenary session

Mechanistic and Inhibitor Docking to Enzymes Catalysing complex Reactions Using EnzyDock.

Renana Schwartz¹, Dr. Shani Zev¹, Amit Hadar-Volk¹, Dr. Donghyuk Suh², Dr. Prashant Kumar Gupta^{1,3}, Prof. Wonpil Im², Prof. Kwangho Nam⁴, Prof. Dan T. Major¹

¹*Department of Chemistry, Israel National Institute of Energy Storage (INIES) and Institute for Nanotechnology & Advanced Materials, Bar-Ilan University, Israel*

²*Department of Biological Sciences, Lehigh University, United States*

³*Department of Chemistry, Central University of Kashmir, India*

⁴*Department of Chemistry and Biochemistry, University of Texas at Arlington, United States*

Enzymes perform essential biochemical functions. Docking uses computational methods to predict how small molecules bind to a target protein. Despite the broad availability of docking programs and modern AI-driven structure prediction tools, docking to enzymes that catalyse complex, multistep reactions remains challenging. This includes many enzymes involved in the biosynthesis of natural products with pharmaceutical and industrial value.

EnzyDock is a docking program that enables consensus docking of reactive intermediates - such as carbocations - to enzymes that mediate complex reaction pathways, while allowing users to incorporate chemical intuition or bias the docking toward experimental poses of ligand mimics. [1-3] Combined with other bioinformatic and simulation approaches, it revealed a key structural difference between terpene synthases from various organisms and those from plants. [4] In a separate study, it also suggested an explanation for how a single mutation alters the experimentally observed product profile of the diterpene synthase CotB2. [5] A webserver has been launched to make EnzyDock readily accessible to the broader academic community. [6]

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Invited Lecture

Plenary session

Pb-Induced Electronic Structure Modification Enhances Formic Acid Electrooxidation on Pd₃Pb

Dr Radhey Shyam Yadav^{1,2}, Prof. Haya Kornweitz²

¹*Space, Earth and Environment, Chalmers University of Technology, Sweden*

²*Department of Chemical Sciences, Ariel University, Israel*

The efficiency of formic acid electrooxidation (FAEO) is often hindered by CO poisoning via the indirect pathway, underscoring the need for catalysts that promote the direct, CO-free oxidation route. Pd-based catalysts are promising, but a limited understanding of their surface interactions and catalytic behavior restricts further development. The traditional d-band center model provides useful trends but does not capture the site-specific atomic environments and orbital interactions that govern adsorption and reaction steps. To overcome this limitation, we combined density functional theory (DFT) with Crystal Orbital Hamilton Population (COHP) analysis to gain deeper insight into the bonding of key intermediates during FAEO on Pd₃Pb(111) compared with Pd(111).

Our results reveal that incorporation of Pb into the Pd lattice enhances catalytic performance by modifying the electronic structure and introducing new active sites. Our analysis highlights the role of subsurface Pb, which strengthens HCOO binding at Pd–Pd bridge sites and reduces CO and H adsorption at the strongly binding fcc hollow sites. FAEO proceeds more efficiently on Pd₃Pb via O–H bond cleavage, forming an HCOO intermediate with a lower activation energy (0.29 eV) than on Pd (0.35 eV). Pd₃Pb favors the HCOO-mediated pathway, while Pd prefers the COOH-mediated route. Furthermore, COHP analysis shows that weaker Pb–O and Pb–C interactions reduce the HCOO rotation barrier from 0.84 to 0.51 eV, facilitating this key step and enabling the CO-free mechanism to proceed more efficiently. These insights reveal the mechanistic origin of superior FAEO activity on Pd₃Pb and provide guiding principles for designing next-generation CO-tolerant electrocatalysts.

Invited Lecture

Plenary session

Have You Tried Turning It Off and On Again? Stochastic Resetting for Enhanced Sampling

Prof. Barak Hirshberg¹

School of Chemistry, Tel Aviv University, Israel

Despite their widespread use in chemistry and biology, molecular dynamics simulations often suffer from a severe speed limit. They struggle to capture events that happen slower than a few microseconds, such as protein conformational changes or crystal polymorphism. While traditional methods, such as Metadynamics, attempt to force the system over energy barriers, they require prior knowledge of the reaction coordinate and bias the true dynamics of the system. I will present a new framework that overcomes these limitations by utilizing stochastic resetting. This approach accelerates rare events by periodically interrupting and restarting the simulation, effectively "teleporting" the system out of kinetic traps. I will show that it requires no prior knowledge of the reaction coordinate and minimally perturbs the natural dynamics of the system, allowing the inference of unbiased kinetic parameters. I will demonstrate how combining resetting with Metadynamics yields higher accelerations than either approach alone. Finally, I will present a machine-learning framework for designing resetting strategies that dynamically adapt to the state of the system. Adaptive resetting further accelerates sampling and can be used to shape the resulting nonequilibrium steady state.

Invited Lecture

Plenary session

A Flavor of Iron Chemistry: From Catalytic Novelties to Applicable Catalysis

Graham de Ruiter

Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Technion City, 3200008
Haifa, Israel

Email: graham@technion.ac.il

Ongoing efforts to advance sustainable chemistry have sparked renewed interest in using earth-abundant metals for homogeneous catalysis. Their natural abundance, low toxicity, and wide availability make them attractive alternatives to less sustainable noble metals. In this seminar, we will showcase how the unique properties of earth-abundant metals such as iron, cobalt and manganese can be unlocked through rational ligand design. Specifically, we will highlight how subtle modifications in ligand architecture can shift the focus from developing catalytic novelties to applicable catalysis. Building on our previously reported PC_{NHC}P iron complexes, [(PC_{NHC}P)FeCl₂] (**1**) and [(PC_{NHC}P)Fe(N₂)₂] (**2**), we will first demonstrate their catalytic activity in the stereoselective isomerization of alkenes, and their efficiency in H/D exchange. We will then show how the reactivity of these iron complexes can be redirected from alkene isomerization to iron catalyzed cross-coupling and alkene metathesis. Moreover, we will illustrate how transitioning from a PC_{NHC}P to an Cyclic Alkyl Amino Carbene (CAAC) based ligand framework can significantly alter the physicochemical properties of the resulting iron complexes resulting in unprecedented activity. Finally, we will demonstrate that through ligand design, we can understand the formation and decomposition pathways of an unprecedented iron metallacyclobutane that bears direct relevance for iron catalyzed alkene metathesis. Altogether, this work presents a new design paradigm, showing for the first time that two-electron chemistry with earth-abundant metals can be accessed through bespoke ligand design.

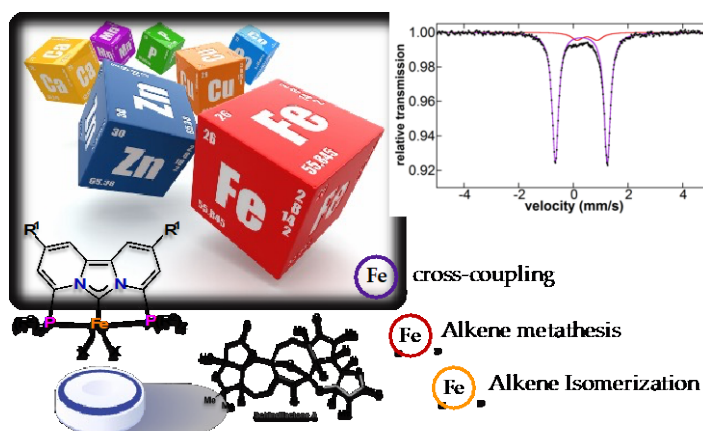


Figure 1 | Iron in Organic Synthesis. Iron PC NHC P pincer complexes for alkene metathesis, aryl-aryl cross-coupling, and alkene isomerization.

Invited Lecture

Plenary session

How Anomalous is Anomalous Diffusion?

Prof Joseph Klafter¹
Tel Aviv University, Israel

Anomalous diffusion describes a broad class of transport processes in which the mean-squared displacement deviates from the linear time dependence characteristic of classical Brownian motion. Here we examine the extent and origins of such deviations, focusing on subdiffusion and superdiffusion. In subdiffusion, the mean squared displacement increases slower than linearly with time which often reflects obstacles, trapping, or crowding that repeatedly interrupt motion. Examples include the movement of proteins in the dense interior of a living cell, contaminants spreading through water aquifer, or charge carriers in disordered semiconductors. In superdiffusion, the mean squared displacement increases faster than linearly with time. This behavior emerges when motion is persistent, strongly correlated, or dominated by long-range steps. Lévy walks represent a particularly striking form of superdiffusion. In these processes, many short steps are interrupted by rare but extremely long ones. These long flights dominate the spreading and cause the mean squared displacement to grow more rapidly than in normal diffusion. Lévy walk dynamics have been used to describe the foraging paths of animals, the dispersal of seeds carried by gusty winds, the propagation of light in strongly scattering materials, particles in turbulent flow, and even patterns of human mobility. Here we discuss the Lévy walk foraging hypothesis and how it led to new theories of the foraging brain and memory retrieval. We conclude that “anomalous” does not mean rare or exotic. Instead, it captures a wide spectrum of behaviors in nature.

Invited Lecture

Plenary session

The nature of stability: Bridging between chemistry and biology

Addy Pross

Ben Gurion University, Israel

The seeming incompatibility between central life attributes – agency, mind, consciousness – and the objective laws of physics and chemistry, continues to weigh on modern science. In this talk, I'll briefly outline a largely unrecognized dimension within chemistry, dynamic kinetic chemistry, and its underlying stability kind, dynamic kinetic stability (DKS), and show how these concepts might assist in the physical characterization of the living state.

Invited Lecture

Plenary session

Inverse Design of Polycyclic Aromatic Systems

Assoc. Prof. Renana Poranne¹

Schulich Faculty of Chemistry, Technion, Israel

Polycyclic aromatic systems (PASs) present a vast and intricate chemical space, where subtle structural changes can induce profound variations in electronic properties. This complexity, coupled with the high structural similarities among the molecules, pose a fundamental challenge for inverse molecular design: how can one reliably generate new PASs with predefined target properties?

I will present a data-driven framework that enables the inverse design of PASs by combining large-scale quantum-chemical data with modern deep-learning architectures. Central to this effort is the COMPAS Project (COMputational database of Polycyclic Aromatic Systems), which currently comprises nearly one million PASs across four curated datasets. To effectively learn from this data, we developed two complementary molecular representations—a text-based formalism and a graph-based encoding—tailored to the unique topology and aromaticity of PASs.

Building on these foundations, we introduce GaUDI, the first guided diffusion-based generative model specifically designed for PASs. GaUDI enables goal-directed molecular generation with flexible target functions, high structural validity, and—crucially—the ability to design molecules with properties extending beyond the training distribution. This allows systematic exploration of PAS chemical space toward regions inaccessible to conventional trial-and-error or forward-prediction approaches.

Through representative examples ranging from small benzenoid molecules to extended graphene-like systems, I will demonstrate how inverse design models can uncover new structure–property relationships and accelerate the discovery of functional PASs. Together, these results highlight how generative AI can transform PAS design from a descriptive endeavor into a predictive and creative scientific discipline.

Invited Lecture

Plenary session

Texas-inspired Drug Discovery Efforts

Prof. Jonathan Sessler¹

Chemistry, The University of Texas at Austin, USA

This lecture will present the development of expanded porphyrins--larger analogues of heme pigments--as a class of compounds and as potential drug leads. The presentation will center around my personal story of a 4x cancer survivor and how with the assistance of great coworkers and collaborators an effort has been made to fight back against this disease by studying the chemistry and anti-cancer biology of lanthanide(III) texaphyrins. Texaphyrins were the first of the so-called expanded porphyrins to stabilize a 1:1 complex with a metal cation. Subsequently, effort was made in our laboratories and those of many others to create additional expanded porphyrins. Hundreds are now known. They have helped probe the frontiers of aromaticity and antiaromaticity. Recently, efforts have been made to create so-called immunogenic cell death promoters designed to prevent cancer recurrence based on redox-active gold(I) carbenes. This new line of research will be reviewed as time permits.

Collaborations with a number of groups, including those of Profs. Dongho Kim, Jong Sung Kim, Shunichi Fukuzumi, Zahid Siddik, Rick Finch, Zhengrong Cui, Jingqin Chen, Aaron Tondreau, Chuanhu Lei, Hongyu Wang, Jun-long Zhang, and Tomas Torres, are gratefully acknowledged. Special thanks also go to former coworkers, including Jonathan F. Arambula, Gregory Thiabaud, Sajal Sen, Qing He, Zhan Zhang, Xian-sheng Ke, Xiaofan Ji, Xiaodong Chi, Atanu Jana, and Adam Sedgwick. Support for this work is being provided by the US NSF, US NIH, and the Robert A. Welch Foundation.

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THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



AI in CHEMISTRY

Chair: Barak Hirshberg

Invited Lecture

AI in CHEMISTRY

Neural nets in Magnetic Resonance: how do they actually work?

Prof Ilya Kuprov¹, Jake L. Amey², Jake Keeley², Tajwar Choudhury²

¹*Weizmann, Israel*

²*School of Chemistry and Chemical Engineering, University of, Southampton*

The arrival of teraflop-scale computing has set off a renaissance in Machine Learning methods in chemistry. Many methods proposed and abandoned in 1990-es (because ML models of sufficient size could not be handled at the time) are now viable. In particular, deep neural networks are successful in chemical shift prediction, chemical structure determination, and distance distribution extraction from double electron-electron resonance data.

Deep neural networks are trivially easy to train. However, a neural network is often an uninterpretable – and therefore untrusted – black box. In fully connected nets, the signalling between inner layers is scrambled because backpropagation training does not require perceptrons to be arranged in any particular order. This problem is particularly severe in scientific computing and digital signal processing, where neural nets perform abstract mathematical transformations that do not reduce to features or concepts.

We recently designed a group-theoretical procedure that attempts to bring inner layer signalling into a human-readable form, the assumption being that this form exists and has identifiable and quantifiable features – for example, smoothness or locality. We applied the procedure to DEERNet (a network used to process EPR data) and managed to descramble it. We found considerable internal sophistication: the network spontaneously invents a bandpass filter, a notch filter, a frequency axis rescaling transformation, frequency division multiplexing, group embedding, spectral filtering regularisation, and a map from harmonic functions into Chebyshev polynomials – in ten minutes of unattended training from a random initial guess.

[10.1073/pnas.2016917118]

Jake L. Amey, Jake Keeley, Tajwar Choudhury, Ilya Kuprov

Invited Lecture

AI in CHEMISTRY

Artificial intelligence driven glass discovery: from semantic data to autonomous synthesis

Prof. Dr. Marek Sierka¹, Mr. Ya-Fan Chen¹, Mr. Felix Arendt¹
*Otto Schott Institute of Materials Research, Friedrich Schiller University Jena,
Germany*

Artificial intelligence driven workflows are transforming how materials are discovered and optimized. Glasses are particularly attractive for such approaches because their compositions can be varied almost continuously, yet their properties respond in highly nonlinear ways. Mapping this design space by conventional experiments is not realistic.

We present an artificial intelligence based framework that combines a semantic data infrastructure, molecular dynamics (MD) simulations, machine learning (ML) models and robotic synthesis to navigate this landscape. A domain specific ontology integrates experimental data, simulation results and literature into knowledge graphs and connects to the SciGlass Next web platform for glass data and predictive models [1,3]. This enables consistent, queryable descriptions of compositions, processing histories and properties that follow the findable, accessible, interoperable and reusable (FAIR) principles.

Physics informed ML models trained on MD data and historical measurements predict thermophysical and mechanical properties across glass composition spaces [1,2]. Active learning strategies identify regions with high model uncertainty and trigger targeted experiments on the robotic melting platform, closing the loop between data, prediction and synthesis [2]. The approach, developed for glasses, provides a template for artificial intelligence driven discovery in wider materials and chemistry domains where continuous variables, complex processing and nonlinear responses are the rule.

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Invited Lecture

AI in CHEMISTRY

Machine Learning the Entropy to Estimate Free Energy Differences without Sampling Transitions

Prof Yohai Bar-Sinai^{1,2}

School of Physics, Tel Aviv University, Israel

Racah Institute of Physics, and Rachel & Selim School of Computer Science & Engineering, Hebrew University, Israel

Thermodynamic phase transitions, a central concept in physics and chemistry, are typically controlled by an interplay of enthalpic and entropic contributions. In most cases, the estimation of the enthalpy in simulations is straightforward but evaluating the entropy is notoriously hard. As a result, it is common to induce transitions between the metastable states and estimate their relative occupancies, from which the free energy difference can be inferred. However, for systems with large free energy barriers, sampling these transitions is a significant computational challenge. Dedicated enhanced sampling algorithms require significant prior knowledge of the slow modes governing the transition, which is typically unavailable.

We present an alternative approach, which only uses short simulations of each phase separately. We achieve this by employing a recently developed deep learning model for estimating the entropy and hence the free energy of each metastable state. We benchmark our approach by calculating the free energies of crystalline and liquid metals. Our method features state-of-the-art precision in estimating the melting transition temperature in Na and Al without requiring any prior information or simulation of the transition pathway itself.

Invited Lecture

AI in CHEMISTRY

A Theoretical Framework for an Efficient Normalizing Flow-Based Solution to the Electronic Schrödinger Equation

Professor Daniel Freedman¹

Applied Mathematics, Tel Aviv University, Israel

A central problem in quantum mechanics involves solving the Electronic Schrödinger Equation for a molecule or material. The Variational Monte Carlo approach to this problem approximates a particular variational objective via sampling, and then optimizes this approximated objective over a chosen parameterized family of wavefunctions, known as the ansatz. Recently neural networks have been used as the ansatz, with accompanying success. However, sampling from such wavefunctions has required the use of a Markov Chain Monte Carlo approach, which is inherently inefficient. In this work, we propose a solution to this problem via an ansatz which is cheap to sample from, yet satisfies the requisite quantum mechanical properties. We prove that a normalizing flow using the following two essential ingredients satisfies our requirements: (a) a base distribution which is constructed from Determinantal Point Processes; (b) flow layers which are equivariant to a particular subgroup of the permutation group. We then show how to construct both continuous and discrete normalizing flows which satisfy the requisite equivariance. We further demonstrate the manner in which the non-smooth nature (“cusps”) of the wavefunction may be captured, and how the framework may be generalized to provide induction across multiple molecules. The resulting theoretical framework entails an efficient approach to solving the Electronic Schrödinger Equation.

Invited Lecture

AI in CHEMISTRY

Combining NMR-fragment screening with AI-based cheminformatics to design small molecules targeting RNA for antibiotic development

Barak Akabayov¹

Ben-Gurion University of the Negev, Israel

I will present our strategy for developing novel antibacterial small molecules that specifically target an RNA hairpin located within the ribosomal peptidyl transferase center (PTC). Our approach combines an experimental platform of fragment screening with computational chemistry to identify a subset of molecules with a common molecular scaffold that bind our RNA target. By utilizing small molecules and their binding free energies to target the RNA hairpin, along with **AI-driven cheminformatics**, we established design principles that guide the optimization of molecular structures for improved bioactivity. The newly designed molecules were synthesized and tested using ribosome inhibition assays, with some exhibiting improved IC₅₀ values compared to standard antibiotic drugs. Importantly, biochemical and biophysical studies were conducted to clarify the binding mechanism of specific inhibitors to the RNA hairpin.

Invited Lecture

AI in CHEMISTRY

AI-Driven Design of Biomimetic Interfaces: From Patterned Materials to Cellular Communication

Ekaterina Skorb¹

Infochemistry Scientific Center, ITMO University, Russia

Recent advances in biomaterials and artificial intelligence (AI) are converging to create a new paradigm for designing biointerfaces with controlled cellular responses. Biomimetic material platforms, such as piezoelectric hydroxyapatite (HA) patterns formed via self-assembly, offer sophisticated scaffolds that mimic natural bone structure [Zyrianova et al. *Materials & Design*, <https://doi.org/10.1016/j.matdes.2024.112718>]. These platforms enable the non-invasive, extracellular study of intercellular communication by guiding cell localization and facilitating the detection of ionic signaling waves (Ca^{2+} , K^+ , Na^+) using integrated fiber-based biosensors. Concurrently, the complexity of designing such functional nanostructured materials necessitates advanced computational tools. Retrieval-Augmented Generation (RAG) systems, powered by large language models (LLMs), now automate the extraction and synthesis of knowledge from vast scientific literature [Krotkov et al. *J. Chem. Inf. Model.* <https://doi.org/10.1021/acs.jcim.5c01897>]. These AI systems can recommend material compositions, fabrication parameters, and nanostructure geometries linked to specific cellular behaviors like adhesion, proliferation, and differentiation. By bridging data-driven material design with experimental biological validation, this integrated approach accelerates the development of intelligent biointerfaces for neuroengineering, regenerative medicine, and fundamental studies of cell-cell communication, moving towards autonomous laboratories for advanced biomaterial discovery.

Invited Lecture

AI in CHEMISTRY

Interpretable deep learning for scientific discovery in chemistry

Ofir Lindenbaum¹

Engineering, Bar Ilan University, Israel

Chemical datasets are often high-dimensional, noisy, and heterogeneous, yet limited in sample size. These characteristics pose significant challenges for standard deep learning approaches and frequently limit interpretability. In this talk, I will present recent advances in interpretable-by-design deep learning that address these challenges by recovering chemically meaningful structure while improving generalization. I will highlight modeling strategies that identify key predictive variables either globally or within specific chemical subpopulations, enabling robust performance with substantially fewer features. The central message is that reliable feature selection can simultaneously enhance predictive accuracy and chemical insight, making interpretable deep learning a practical and trustworthy tool for scientific discovery when using tabular data in chemistry.

AI in CHEMISTRY

Principled Uncertainty Quantification via Diffusion Models for Analytical Continuation of Imaginary-Time

Sagi Meir¹, Prof. Daniel Freedman¹, Prof. Barak Hirshberg¹
Tel Aviv University, Israel

Inverse problems are ubiquitous in physics, chemistry, and engineering, arising when reconstructing hidden quantities from indirect measurements. In computational quantum chemistry, a key example is the analytical continuation of imaginary-time correlation functions (iTCFs) to real-time domains. This process requires an inverse Laplace transform which is an inherently ill-posed problem, highly sensitive to small input variations. Recent neural network (NN)-based methods have shown promising results by learning mappings from imaginary-time to real-time domains while outperforming traditional techniques such as maximum entropy. However, these regression-based approaches tend to approximate the mean of the solution space, failing to capture the full distribution of plausible power spectra. Building on advances in generative modeling, we introduce the first diffusion-based framework for analytical continuation of iTCF. Unlike regression-based NN approaches, diffusion models allow us to learn the density distribution of solutions, enabling rigorous estimation of both the intrinsic difficulty of the problem and the uncertainty associated with the inversion. In contrast to previous attempts at uncertainty quantification, our approach is derived from fundamental principles, providing a more theoretically grounded measure of confidence in the reconstructed power spectra.

AI in CHEMISTRY

Boltzmann subspaces in molecular junctions under a thermal bias

Yotam Gomeh¹, Prof. Uri Peskin¹
Chemistry, Technion, Israel

Single molecule junctions enable us to study molecules in new states far from equilibrium. In this work, we focus on molecules under a thermal bias imposed by coupling to two electrodes at different temperatures. We demonstrate that within the realm of weak electrode–molecule coupling (Pauli master equations), even far from equilibrium, the molecule can be assigned (at least approximately) an effective temperature at steady state. This is manifested in clustering of the molecular Hamiltonian eigenstates into groups with Boltzmann distributions of occupation probabilities. We demonstrate the emergence of such Boltzmann subspaces under thermal bias and identify the corresponding effective temperature in a variety of molecular junction models, including account for electron–electron interaction, molecular disorder, asymmetric coupling to the electrodes, and the orbital energy density. The results are promising from a practical perspective as we draw guidelines for controlling the temperature of single-molecule electronic devices. The existence of Boltzmann subspaces simplifies our understanding of transport in open quantum systems under thermal bias and holds promise for reducing the numerical effort in simulations of thermally driven molecular junctions.

AI in CHEMISTRY

Automated Discovery of Positive Energy Transport in 2D Layers via GVAE and Uncertainty-Driven Active Learning

Sofia Blyufer¹, Prof. Uri Peskin¹, Dr. Amir Kleiner²

¹*Technion, Israel*

²*Weizmann Institute, Israel*

Artificial intelligence is a transformative tool for exploring vast physical parameter spaces that are otherwise computationally inaccessible. In this study, we demonstrate an AI-driven framework for designing a nano-scale refrigerator. This device consists of a thin 2D layer coupled to heat baths and driven out of equilibrium by electrodes. Under optimal configurations, energy is absorbed from bosonic reservoirs at a steady state. While design principles are known for two-level models, scaling to larger systems presents an exponential computational challenge due to the complex interplay of quantum localization, orbital asymmetry, and energy level spacing.

To address this, we leverage a Graph Variational Autoencoder (GVAE) to learn a compressed, physically meaningful latent representation of the molecular junction. The GVAE distills site-level features and coupling matrices into a smooth, graph-level latent space. We employ multi-objective decoding for node feature reconstruction, edge weight preservation, and energy flux prediction to ensure the latent manifold reflects the underlying transport physics.

To enable efficient exploration, we coupled the GVAE with an Active Learning pipeline. Utilizing Monte Carlo dropout for uncertainty estimation, the framework autonomously identifies candidate configurations where predictive confidence is lowest, specifically targeting the boundaries of the desired flux regime. Results show that this uncertainty-driven strategy identifies highly informative configurations that random sampling overlooks. This work highlights the potential of combining graph-based generative models with active learning to automate the discovery of materials for optimized transport in complex quantum systems.

AI in CHEMISTRY

predictive modeling of quaternary ammonium degradation: machine learning-guided design for improved anion exchange membranes

Amit Manor Armon¹, Prof. Charles E. Diesendruck¹
Chemistry, Technion, Israel

Anion exchange membranes (AEMs) are essential components in multiple next-generation electrochemical devices, including fuel cells.¹ Quaternary ammonium (QA) functional groups embedded in the polymeric membrane backbone are responsible for facilitating hydroxide transport while blocking neutral and cationic species.^{1,2} To this day, no AEMFC presents suitable lifetime, as the QA groups decompose through reaction with the hydroxide ions.^{1,2}

Despite decades of research exploring diverse QA architectures, rational design principles for achieving kinetic stability remain elusive. This work addresses this challenge by developing a comprehensive computational framework combining systematic DFT calculations with Random Forest machine learning to establish quantitative structure-reactivity relationships across approximately 330 SN2 transition states. We sample diverse chemical space including aliphatic and benzylic CH₂ and CH₃ positions, extracting electronic parameters (NPA charges, LUMO energies), geometric features (bond distances, vibrational frequencies), and steric measures (buried volume, Sterimol parameters).^{3,4}

Although working with a relatively small but carefully designed dataset spanning a broad chemical landscape, our models achieve strong predictive accuracy, revealing that both electronic and steric parameters govern reactivity with position-specific importance. We demonstrate that three readily accessible descriptors can guide rational molecular design. This framework transforms QA development from trial-and-error exploration into systematic, predictive molecular engineering, providing practical design rules to accelerate the development of next-generation AEM.

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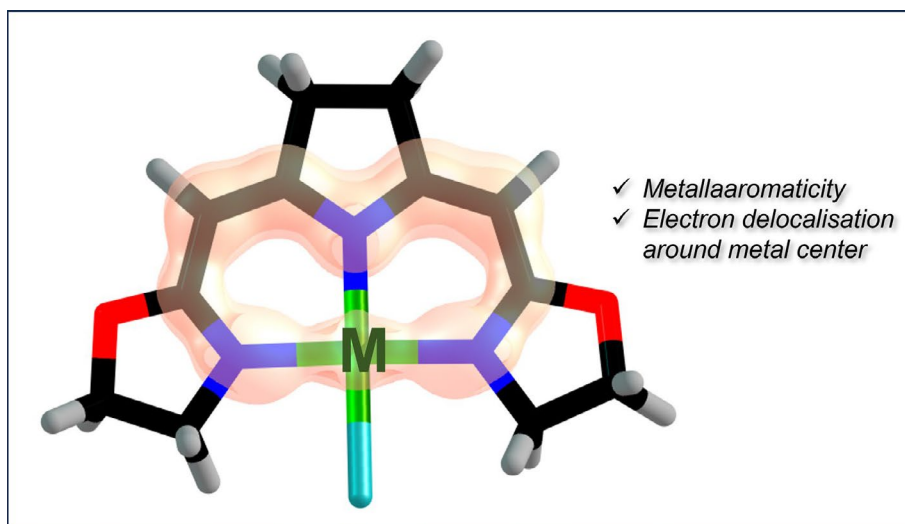
AI in CHEMISTRY

Computational Insights into Metallaaromaticity in Transition Metal Complexes

Ajeet Kumar Singh¹, Prof. Renana Gershoni-Poranne¹, Prof. Graham de-Ruiter¹
Schulich Faculty of Chemistry, Technion Israel Institute of Technology, Israel

Aromaticity, the phenomenon of cyclic electron delocalization that imparts molecular stability, has expanded from classical organic systems to include organometallic and inorganic frameworks. In metallaaromatic species, delocalization arises from a distinctive interplay between metal d-orbitals and ligand π -orbitals, resulting in tunable and complex electronic behavior. However, the role of metal identity, oxidation state, and ligand architecture in governing metallaaromaticity remains inadequately understood.

In this work, we present a systematic computational study of metallaaromatic transition metal complexes using density functional theory (DFT) combined with key aromaticity indices- nucleus-independent chemical shift (NICS), anisotropy of the induced current density (AICD), and electron density of delocalized bonds (EDDB). These complementary analyses provide qualitative and quantitative insights into electron delocalization and aromatic stabilization. Our results reveal that the electronic configuration and oxidation state of the metal center strongly influence aromatic character, while the ligand's donor-acceptor and conjugation properties modulate π -d orbital interactions. Visual analyses from AICD and EDDB distinctly capture ring current pathways, distinguishing aromatic from non-aromatic species. Correlations between theoretical aromaticity indices and available experimental data further validate the reliability of our computations.



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AI in CHEMISTRY

COMPAS-5: Data-Driven Investigation of Mono-substituted Cata-Condensed Polybenzenoid Hydrocarbons

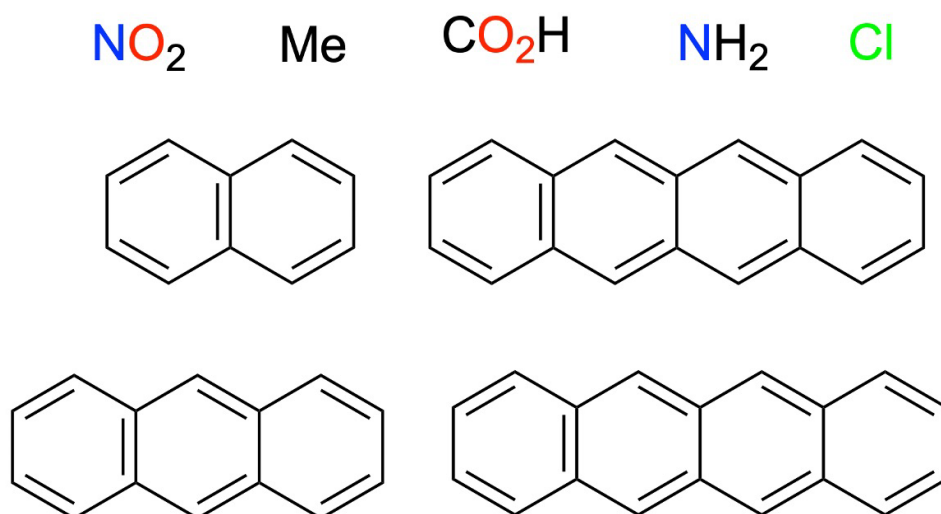
Pallavi Sarkar¹, Dr Sabyasachi Chakraborty¹, Prof Renana Gershoni-Poranne¹
Chemistry, Technion-Israel Institute of Technology, Israel

Cata-condensed polybenzenoid hydrocarbons (cc-PBHs) are aromatic molecules composed of fused benzene rings sharing only two carbon atoms between consecutive rings. Their exceptional stability, tunable optoelectronic properties, and solution processability make them valuable building blocks for organic electronics, including photovoltaics, light-emitting diodes, and field-effect transistors. The electronic properties of cc-PBHs can be systematically modulated through strategic incorporation of electron-donating or electron-withdrawing substituents at specific positions on the aromatic scaffold, enabling access to materials with tailored functionalities. However, the vast chemical space of substituted cc-PBHs presents both opportunities and challenges for molecular design.

In this work, we present the latest installment in the COMPAS Project (Computational Database of Polycyclic Aromatic Systems) series: COMPAS-5, a comprehensive dataset containing ground-state properties of mono-substituted cc-PBHs, built of ~8000 PBH scaffolds and 7 electronically diverse substituents. By analyzing substitution effects across different molecular positions and substituent types, we identify key chemical trends governing property modulation in cc-PBHs. These structure-property relationships provide fundamental insights into how substituents influence electronic structure and reveal design principles for constructing cc-PBHs with desired characteristics. This work establishes a systematic framework for understanding substituent effects in polycyclic aromatic systems, facilitating rational design of organic electronic materials.

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AI in CHEMISTRY

Data-Driven Design of Selective Ruthenium Metathesis Catalysts

Keren Iudanov¹, Prof. Matthew Sigman², Prof. N. Gabriel Lemcoff¹

¹Chemistry, Ben-Gurion University of the Negev, Israel

²Chemistry, University of Utah, United States

Traditionally, catalyst design has relied on chemical intuition and trial-and-error often leading to time-consuming and unpredictable outcomes. A powerful alternative is the application of data-driven methods. Olefin metathesis, catalyzed by transition metal carbene complexes, is an essential reaction in organic synthesis for forming new carbon-carbon double bonds.

Our group pioneered sulfur-chelated metathesis catalysts, modifying a known catalyst with a single-atom change. This structural modification enforced a cis-configuration of the anionic ligands and allowed for external regulation of activity. Subsequent research has generated a diverse library of these sulfur-chelated catalysts.

A key discovery was the unique ability of iodide ligands in these ruthenium benzylidenes to inhibit the coordination of non-terminal olefins. This unprecedented selectivity enabled ring-closing metathesis (RCM) of highly strained molecules, facilitating the synthesis of macrocycles and other valuable compounds.

We synthesized and evaluated a library of these catalysts in various metathesis reactions. Using Density Functional Theory, we computed the steric and electronic descriptors of the complexes. We then employed multivariate linear analysis to correlate these features with catalytic activity. The resulting model suggests that chemical hardness and the electronic environment around the sulfur significantly influence catalytic activity.

We are now extending data science methods to polymerization reactions to identify activity thresholds. This will guide the discovery of catalysts optimally suited for specific transformations such

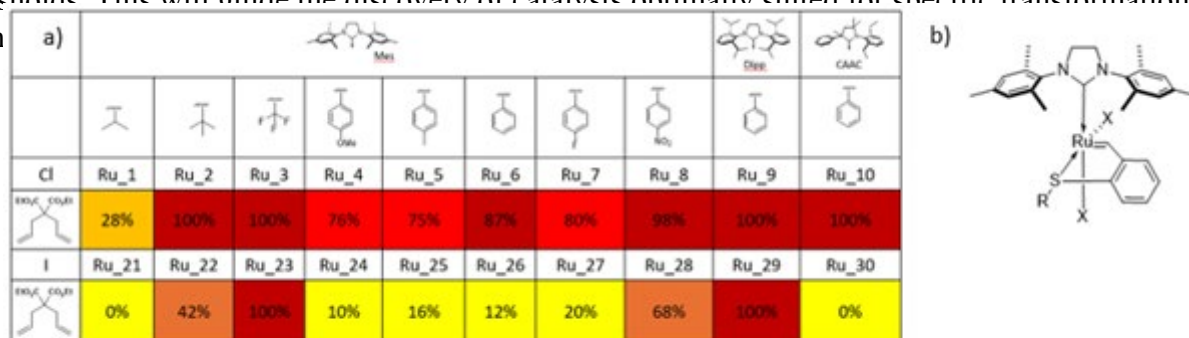


Figure 1. (a) Structures of the catalysts and their measured activity in the ring-closing metathesis of diethyl diallyl malonate. (b) General catalyst structure; X = Cl/I, R = benzylidene chelating substituent.

Y. Vidavsky, A. Anaby and N. G. Lemcoff, Dalton Trans., 2012, 41, 3

AI in CHEMISTRY

Defying Antiaromaticity- The Curious Case of Dipentalenes

Amrita Gogoi¹, Prof. Renana Gershoni-Poranne¹
Schulich Faculty of Chemistry, Technion, Israel

Antiaromaticity is one of the features in determining key candidates for organic electronic devices. Of the many antiaromatic molecules, Pentalene (C_8H_6) is an unstable, conjugated and non-alternant bicyclic hydrocarbon that consists of two fused cyclopentadiene rings that has 8π -electrons following Hückel's antiaromaticity rule ($4n$). Extending pentalene by a cyclopentadiene ring at either end affords two isomeric dipentalenes ($C_{14}H_8$), which are both formally Hückel aromatic polycyclic hydrocarbons containing 14 π -electrons. Dipentalene has two isomers based on the pattern of annelation: 1 and 2 which accounts to having cis-/trans- apical carbons in the pentalene core.

In this work, we explore the effect of further annelation with either benzene or cycloheptatriene, respectively (Figure 1). We investigate the individual effects of the type of core dipentalene structure, the annelation geometry, and the identity of the annelation ring on the (anti)aromatic character of the system. We find that, depending on the molecular geometry, the dipentalene core can either retain its aromatic behaviour, or revert to the antiaromatic nature of the parent pentalene. In some cases, we even observe enhanced antiaromaticity. These results can be rationalized with simple concepts, such as Clar sextets, providing a predictive conceptual framework, which paves the way towards designing stable antiaromatic functional molecules.

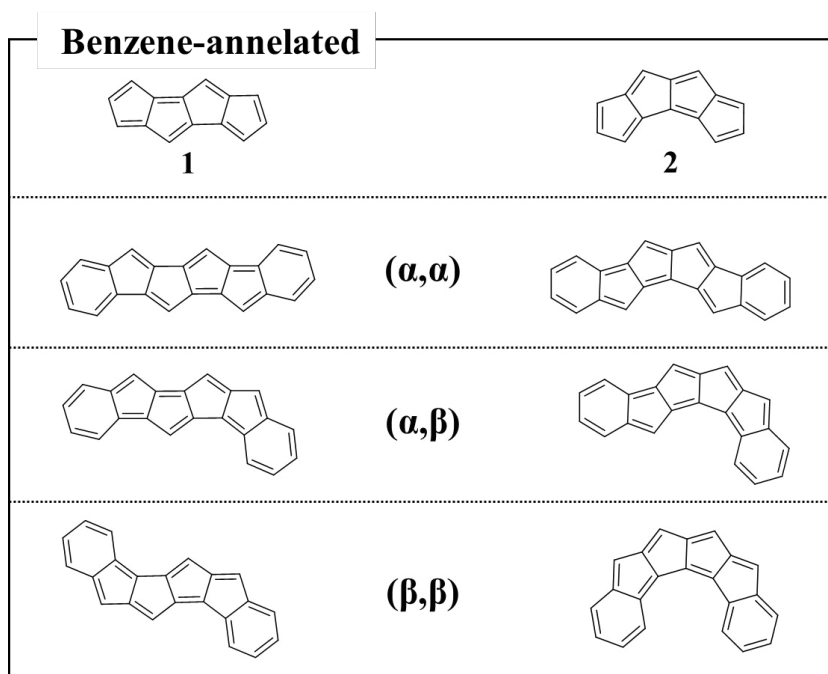


Figure 1. Representative examples of benzene-annelated dipentalenes

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AI in CHEMISTRY

Fusing functionality: A computational exploration of heterocycle-heptalene hybrids

Sabyasachi Chakraborty¹

Schulich Faculty of Chemistry, Technion, Israel Institute of Technology, Israel

Non-alternant polycyclic aromatic molecules, such as pentalenes and indenofluorenes, have captured the fascination of chemists for many years.¹ In contrast, heptalene—the bicyclic molecule comprising two fused 7-member conjugated rings—has remained relatively mysterious. The antiaromaticity of this 12π -electron system makes it highly reactive, e.g., towards polymerization, which may explain the lack of crystallographic data for unsubstituted heptalene. However, as with comparable antiaromatic cores, adding electron-withdrawing substitutions or further annulation may be promising strategies for stabilizing the system.²

Here, we computationally investigate the consequences of extended annulation on the heptalene core on its ground- and first excited states. We select a series of 4-, 5-, and 6-membered aromatic and hetero-aromatic moieties with varying degrees of aromaticity and explore the entire chemical space generated via annulation. We identify transferable chemical trends between optoelectronic properties and structural features; for example, a relationship between specific substitution patterns and stability. The observed effects can be rationalized by the varying aromatic character of the heptalene derivatives, thereby providing a strategy for tuning the extended systems' molecular properties and establishing design principles for generating functional molecules.

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AI in CHEMISTRY

NequIP Potentials for Energetic Crystals: Successes and Limits

Grigorii Livshits¹, Prof. Dan Major¹

Department of Chemistry, Bar-Ilan University, Israel

We present machine-learning interatomic potentials based on the NequIP architecture trained on a dataset of 20 energetic molecular crystals. The reference data were generated at the wB97M-V/def2-TZVPP DFT level and include monomers, dimers, and normal-mode distortions. The compound-specific models achieve high accuracy in reproducing polymorph energy ordering and equilibrium crystal densities, demonstrating that equivariant neural network potentials can reliably capture both structural and energetic trends across chemically diverse energetic materials.

Predictions of melting temperatures show a consistent overestimation relative to experimental values, suggesting that further refinement of simulation protocols or reference data may be required to fully capture high-temperature behavior. This discrepancy may stem from the finite timescales accessible to molecular dynamics or from subtle systematic differences in the underlying DFT energetics near melting. Fully ab-initio melting simulations at the wB97M-V level remain computationally prohibitive, leaving this distinction for future study.

Finally, we train a universal NequIP potential that spans all 20 materials simultaneously. This single transferable model retains nearly the same accuracy as the compound-specific versions for equilibrium densities and polymorph energetics, providing a practical route to large-scale simulations of diverse energetic crystals at a fraction of the cost of DFT.

AI in CHEMISTRY

Machine Learning the Entropy to Estimate Free Energy Differences without Sampling Transitions

Yamin Ben-Shimon¹, Prof Barak Hirshberg², Prof Yohai Bar-Sinai³

¹*School of Physics, Tel Aviv University, Israel*

²*School of Chemistry, Tel Aviv University, Israel*

³*School of Physics, Tel Aviv University, Israel*

Thermodynamic phase transitions, a central concept in physics and chemistry, are typically controlled by an interplay of enthalpic and entropic contributions. In most cases, the estimation of the enthalpy in simulations is straightforward but evaluating the entropy is notoriously hard.

As a result, it is common to induce transitions between the metastable states and estimate their relative occupancies, from which the free energy difference can be inferred. However, for systems with large free energy barriers, sampling these transitions is a significant computational challenge. Dedicated enhanced sampling algorithms require significant prior knowledge of the slow modes governing the transition, which is typically unavailable.

We present an alternative approach, which only uses short simulations of each phase separately. We achieve this by employing a recently developed deep learning model for estimating the entropy and hence the free energy of each metastable state.

We benchmark our approach by calculating the free energies of crystalline and liquid metals. Our method features state-of-the-art precision in estimating the melting transition temperature in Na and Al without requiring any prior information or simulation of the transition pathway itself.

AI in CHEMISTRY

AI in taste chemistry: from bitterness prediction to biotarget identification

Evgenii Ziaikin¹, Prof. Masha Niv¹

The Robert H. Smith Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem, Israel

Bitterness is a key taste modality that drives aversive responses to potentially harmful substances. This function is mediated by TAS2Rs, a family of G protein-coupled receptors (GPCRs) comprising 25 human subtypes. Beyond the oral cavity, TAS2Rs display diverse expression patterns across tissues and are activated by distinct sets of bitter molecules, with subtype TAS2R14 recognizing the majority of known bitterants, as summarized in the BitterDB.

BitterDB was recently expanded to provide the most comprehensive resource on bitter compounds, holding over 2200 molecules and in some cases information on associated receptors, encompassing human and non-human TAS2Rs.

Yet the structure (and the taste) of most natural products remains unidentified and information exists only as mass spectra of the so called “dark metabolome.” To address this gap, we developed BitterMasS, a machine-learning framework that predicts bitterness directly from mass spectra of natural molecules.

In parallel, Cryo-EM structure of TAS2R14 revealed that, unlike other TAS2Rs with experimental 3D structures, it possesses an intracellular binding pocket in addition to the canonical extracellular site. We evaluated the state-of-the-art generative co-folding model Boltz-2 on 22 experimental Cryo-EM complexes of TAS2Rs, and systematically analyzed TAS2Rs to identify structural features enabling intracellular pocket formation. Furthermore, by incorporating selected true-positive and true-negative ligand-receptor pairs into the Boltz-2 affinity module fine-tuning procedure, we optimized model estimates and improved the ability to recognize bitter ligands.

Our results indicate the effectiveness of ML and AI method to explain, predict and modify the taste of molecules.

AI in CHEMISTRY

On-the-Fly Machine Learning Force Fields for Surface Tension Prediction in Liquid Metals

Netanela Cohen¹, Prof. Oswaldo Diéguez¹

Department of Materials Science and Engineering, Faculty of Engineering, Tel Aviv University, Israel

Machine learning force fields (MLFFs) offer an efficient way to extend the accuracy of *ab initio* molecular dynamics (AIMD) to larger systems and longer timescales, enabling predictive simulations of dynamic systems such as liquids. Here, we develop and evaluate on-the-fly trained MLFFs for predicting the surface tension of liquid metals, using Li as a model system. AIMD simulations of the 128-atom bulk liquid provide reliable training data, as they successfully reproduce key thermodynamic and structural properties. To assess the role of interfacial environments, we compare force fields trained exclusively on bulk configurations with those that also include slab configurations. Surface tension is calculated using both a mechanical route, based on the pressure tensor, and a thermodynamic route from surface energy. This comparison enables a direct assessment of how training data selection influences force-field transferability to interfacial systems. Ongoing work extends this methodology to additional liquid metals to evaluate cross-element generalization and to determine minimal training requirements for accurate and scalable simulations of liquid metal surfaces.

AI in CHEMISTRY

A deep learning model for electronic structure prediction in crystalline materials

Ayala Cohen¹, Elizaveta Starykh², Klea Ziu², Aidar Alimbayev², Prof. Martin Takáč²,
Prof. Leeor Kronik¹

¹*Molecular chemistry and materials science, Weizmann Institute of Science, Israel*

²*Machine Learning Department, Mohamed bin Zayed University of Artificial Intelligence (MBZUAI), United Arab Emirates*

Density functional theory (DFT) calculations of electronic structure remain computationally expensive for high-throughput materials screening. Deep learning offers a promising alternative, but existing models struggle to accurately predict density of states (DOS) and partial DOS (pDOS) spectra, often over-smoothing critical fine features and sharp peaks. We present a graph neural network approach based on a modified polarizable atom interaction neural network (PaiNN) architecture, trained on approximately 30,000 publicly available DFT calculations from the Materials Project dataset. Our model takes atomic positions and atomic numbers as input and predicts element-resolved pDOS spectra. To improve prediction quality, we implement a specialized loss function that emphasizes band gaps and critical spectral features, combined with rigorous data filtering based on physical constraints. Our approach achieves state-of-the-art performance in pDOS prediction, greatly improving retention of fine spectral features across diverse crystal structures. However, challenges remain, especially for lighter elements such as H, N, and O, due to their strong environmental sensitivity and insufficient training data coverage. Reproducing sharp isolated peaks remains an issue as well. These results demonstrate significant progress toward fast, accurate electronic structure prediction for materials design applications while highlighting remaining opportunities for improvement.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



BIOINORGANIC CHEMISTRY

Chair: Graham de Ruiter

Invited Lecture

Bioinorganic Chemistry

From Coordination to Color: Mechanistic Insights into Fluorophore- and Nanoparticle-Based Metal Ion Detection in Aqueous Media

Mindy Levine¹, Jiawei Liu¹, Sharanya M. Karyadath¹, Jenisha John Peter¹, Ayala Dredzen¹, Nathaniel C. Roy¹, Prof. Flavio Grynszpan¹
Department of Chemical Sciences, Ariel University, Israel

The sensitive and selective detection of environmentally and industrially relevant metal ions in water remains a central challenge at the interface of supramolecular, analytical, and bioinorganic chemistry, owing to the competing influences of coordination equilibria, solvation, and surface-mediated processes. Our research groups have a long-standing track record of addressing this challenge through a mechanism-driven approach to optical sensor design, in which well-defined metal–ligand or metal–surface interactions are deliberately translated into colorimetric or fluorometric signal outputs.

In this presentation, three representative sensing platforms are discussed to illustrate how coordination chemistry governs both selectivity and response modality in aqueous systems:

- (1) The fluorometric detection of indium(III) cations via its coordination to a functionalized bimeane fluorophore and the resulting heavy-atom-induced fluorescence quenching, which was fully and selectively reversed upon addition of EDTA;
- (2) The colorimetric detection of arsenic(III) via aggregation of cystamine-functionalized gold nanoparticles, producing a visible red-to-purple shift (~80 nm) within 60 s and a detection limit of approximately 1 ppm; and
- (3) The colorimetric detection of mercury(II) via selective coordination to omeprazole-functionalized silver nanoparticles, yielding a visible yellow-to-brown color change within one minute and a solution-phase detection limit of approximately 200 pM.

Taken together, these systems reveal a unifying mechanistic framework in which the identity, geometry, and strength of analyte–sensor interactions dictate both signal transduction and selectivity. This perspective highlights how classical bioinorganic coordination principles can be leveraged to guide the rational design of next-generation optical sensors for complex aqueous environments.

Invited Lecture

Bioinorganic Chemistry

Hybrid Metallodrugs Targeting Breast Tumor Cancer Proliferation

Sotiris K. Hadjikakou* and Christina N. Banti

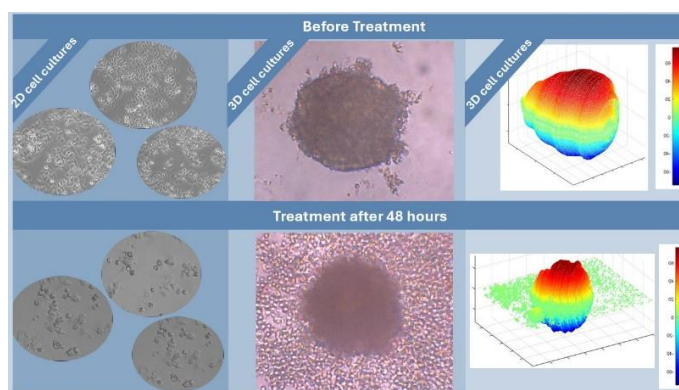
Biological Inorganic Chemistry laboratory, Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece

Email: shadjika@uoi.gr

Breast cancer is a highly heterogeneous disease comprising distinct molecular subtypes, including hormone receptor-positive (ER/PR+), HER2-enriched, and triple-negative breast cancer (TNBC), each characterized by different biological behaviors and therapeutic responses. Despite advancements in targeted therapies and chemotherapeutic regimens, a major clinical challenge remains the development of drug resistance, which allows cancer cells to evade treatment through mechanisms such as altered drug uptake, enhanced DNA repair, metabolic reprogramming, and activation of survival pathways. This acquired or intrinsic resistance significantly limits therapeutic effectiveness, leading to tumor relapses, disease progression, and reduced patient survival, thereby underscoring the urgent need for novel therapeutic strategies capable of overcoming these barriers.

Our research focuses on the development of next-generation metal-based chemotherapeutics, aiming to overcome drug resistance in cancer cells. This approach integrates multiple biologically active components into a single therapeutic entity, either by employing metal ions as structural linkers or by exploiting their intrinsic cytotoxic properties. These metal centers are conjugated to carefully selected carrier moieties that target specific intracellular biomolecules, enabling multi-targeted action within key subcellular compartments. Through this strategy, we aspire to create innovative chemotherapeutic agents capable of bypassing resistance mechanisms and achieving enhanced anticancer efficacy.

Thus, a wide range of bioactive molecules—including anti-inflammatory drugs, antibiotics, natural-product components, metabolites, antimetabolites, and amino acids—are conjugated to potent cytotoxic agents (e.g., mitochondriotropic groups or toxic metal ions), enabling simultaneous targeting and inactivation of multiple intracellular biomolecules.



Acknowledgements

The program "Supporting the Research Activities of the Laboratory of Biological Chemistry (MaRePBIC)" (University of Ioannina Research Committee program No 83718) is acknowledged.

Invited Lecture

Bioinorganic Chemistry

Unlocking Gd(III) Anisotropy: Determining the Zero-Field Splitting Axes to Enhance Spin-Label Structural Analysis

Alexey Bogdanov¹, Veronica Frydman², Xun-Cheng Su³, Manas Seal¹, Wenkai Zhu⁴, Angela M. Gronenborn⁴, Alexander Schnegg⁵, and Daniella Goldfarb¹

¹ Department of Chemical and Biological Physics, The Weizmann Institute of Science, P. O. Box 26, Rehovot, 7610001, Israel

² Department of Chemical Research Support, The Weizmann Institute of Science, P. O. Box 26, Rehovot, 7610001, Israel

³ State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071 P. R. China

⁴ Department of Structural Biology, University of Pittsburgh, 4200 Fifth Ave, Pittsburgh, PA 15260, United States

⁵ Max Planck Institute for Chemical Energy Conversion, 34-36 Stiftstraße, Mülheim an der Ruhr, 45470, Germany

The zero-field splitting (ZFS) of Gd(III) complexes is central to magnetic resonance applications, influencing nuclear relaxation in MRI and NMR, spin relaxation in EPR, and the performance of Gd-based spin labels for structural biology. Yet, despite its importance, determining the molecular-frame orientation of the ZFS tensor is experimentally and computationally demanding for Gd(III) chelate complexes in solution, where structural and dynamic heterogeneity complicates orientation determination. Here, we introduce a general experimental strategy that enables direct determination of the ZFS tensor orientation in Gd(III) complexes using ¹⁹F and ¹H orientation-selective (OS) electron-nuclear double resonance (ENDOR). Applied to the spin labels Gd-DO3A and Gd-PyMTA, this approach enabled the determination of the molecular-frame orientation of the ZFS, necessary for quantitative analysis of Gd(III) anisotropy. This allows for a dual-mode analysis of Gd–F ENDOR spectra, where electron-nuclear distances can be accurately extracted from measurements at the Gd(III) central transition, while the Gd–F vector orientation is determined using OS-ENDOR on high- $|m_S|$ transitions. Using this framework, we determined the placement of Gd-DO3A labels in two ¹⁹F-containing proteins and showed that utilizing existing rotamer libraries substantially overestimates conformational distributions. The experimentally determined ZFS orientations are further corroborated by simple molecular modeling based on the electric-field-gradient tensor. Our results provide a platform for improved structure determination with Gd-based labels and offer valuable benchmarks for improving quantum-chemical predictions of ZFS tensors.

Invited Lecture

Bioinorganic Chemistry

Aza-Wittig based Sensors for Imaging Cellular CO₂ Production

Dr Ori Green¹
Technion, Israel

Carbon dioxide (CO₂) is a fundamental molecule in biology, tightly linked to metabolism and organismal homeostasis. While the biological roles of CO₂ have been extensively studied in blood and respiration, where CO₂ is an established physiological biomarker, our understanding of CO₂ biology at the cellular and subcellular levels remains remarkably limited. Most existing studies study CO₂ function by manipulating exogenous CO₂ levels and examining the resulting biological responses. Although this approach has revealed important physiological effects, it does not address how CO₂ is endogenously produced, spatially organized, and regulated within living cells. This gap arises largely from the lack of selective chemical tools capable of imaging CO₂ in complex cellular environments.

In this talk, we discuss our efforts to address this challenge by leveraging the Aza-Wittig reaction as a general chemical platform for cellular CO₂ imaging. By exploiting the unique reactivity of phosphazenes with CO₂, we generate isocyanate intermediates that are rapidly trapped to form stable urea products with a distinct chemical fingerprint. Mechanistic studies reveal that this reaction is selective for CO₂, even over more electrophilic carbonyl species. Combined experimental and computational analyses show that this unexpected selectivity is governed primarily by steric effects and transition-state organization rather than electrophilicity alone. Finally, I will discuss how these CO₂-responsive sensors enable activity-based imaging of endogenous CO₂ in living cells, uncovering links to mitochondrial function and cellular metabolic state.

Invited Lecture

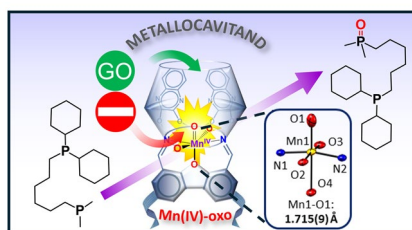
Bioinorganic Chemistry

Formation and Reactivity of High-Valent Metal-Oxo Species Inside a Cavitand Pore

Yuri Tulchinsky¹

Institute of Chemistry, Hebrew University of Jerusalem, Israel

Metal-functionalized cavitands are promising platforms for mimicking the chemical environments of hydrophobic pockets in natural metalloenzymes. However, successfully combining the unique supramolecular capabilities of cavitand scaffolds, with the high reactivity of transition metal complexes, still remains a major challenge. In my talk I will present a conceptually novel cavitand architecture featuring coordinatively-unsaturated M(II) centers (M = Mn, Fe) embedded deep within its pore. These metallocavitands were employed to generate highly reactive metal-oxo species inside their molecular cavity. The Mn(IV)-oxo congener was fully characterized spectroscopically (UV-vis, EPR, and HRMS) and – for the first time for a pseudo-octahedral Mn(IV)-oxo species – also by XRD. Reactivity and mechanistic studies, including monitoring the decay of this complex in various chlorinated solvents and its reactions with representative substrates, revealed that despite the steric protection provided by the cavitand scaffold, its Mn(IV)-oxo core remains highly reactive in both H atom abstraction (HAA) and O atom transfer (OAT) reactions. Moreover, this reactivity is subject to a high degree of steric control imposed by the cavitand framework capable of discriminating between potential substrate molecules based on their size and shape. This was further demonstrated by the regioselective oxidation of an asymmetric bisphosphine substrate – emulating the regioselectivity of natural metalloenzymes.¹ I will also present our recent reactivity studies of the Fe-based congener, indicating the possibility of a chemoselective hydroxylation of cyclic hydrocarbons.



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Bioinorganic Chemistry

Peptide-Based Strategies for Enhanced Drug Delivery of Titanium (IV) Complexes to Cancer Cells

Hadar Kowalski¹, Prof. Edit Tshuva¹

Institute of Chemistry, Israel

Titanium(IV) complexes have emerged as promising alternatives to platinum-based chemotherapy agents such as cisplatin, which are limited by severe side effects and resistance. PhenolaTi, a phenolato-based Ti(IV) compound developed by our group, exhibits strong cytotoxicity across multiple cancer cell lines, including cisplatin-resistant ones, while showing minimal in vivo toxicity. Unlike platinum drugs that target DNA, phenolaTi induces endoplasmic reticulum (ER) stress that triggers apoptosis and cell-cycle arrest. Genomic and cellular studies indicate activation of ER stress pathways, hypoxia-like responses, and altered mitochondrial function. This defines a distinct mechanism that supports its potential as a targeted anticancer agent.

Building on these findings, our research focuses on improving the delivery and bioavailability of Ti(IV) complexes through peptide conjugation. We designed a series of linear peptides inspired by signal recognition particles (SRPs) to facilitate intracellular transport and target the ER. These peptides were engineered to adopt α -helical structures with positively charged termini and hydrophobic cores. The C-terminus incorporates L-Dopa, whose catechol side chain coordinates with Salan Ti(IV) complexes by replacing isopropoxide ligands. Peptides were synthesized via solid-phase peptide synthesis, purified by reverse-phase HPLC, and conjugated to Ti(IV) complexes under anaerobic pyridine conditions. The resulting metal-peptide complexes were characterized using 2D NMR, revealing key structural features.

These results lay the groundwork for ER-targeted delivery of Ti(IV) complexes and indicate their potential as selective anticancer agents.

Bioinorganic Chemistry

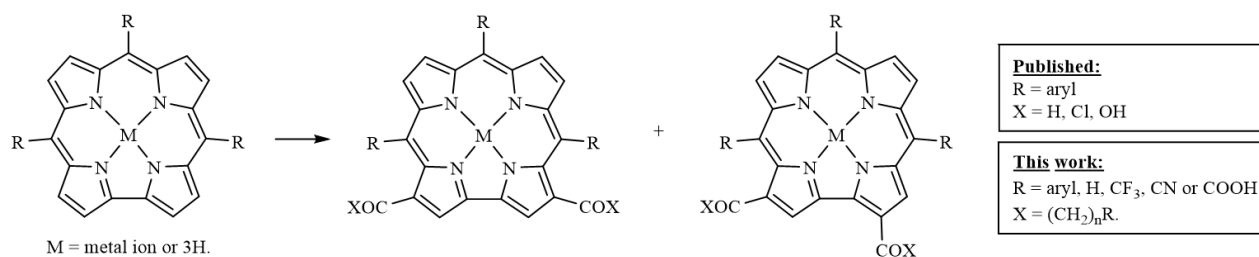
Synthesis of New β -Substituted Corroles

Shahar Tsur¹, Zeev Gross¹

Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Israel

The corrole macrocycle, with its trianionic and compact central cavity, is of high π electron density, and is highly relevant for electrophilic aromatic substitution at the β -pyrrolic positions.

Previous studies have shown that substitution of corroles by acyl moieties (CO-X, where X=H, Cl, OH; see Scheme 1) induces a redshift of both the Soret and Q bands in the UV-Vis spectrum [1]. This highlights the significant effect of β -substituents on the photophysical properties of corroles; and the redox potentials are strongly affected as well. Building on this concept, the current study introduces efficient and selective synthetic approaches to obtain corroles with β -pyrrole CO-X substituents, where X stands for moieties that may promote binding to proteins and surfaces, thereby expanding their applicability. The current studies are not limited to triarylcorroles but include also examples relating to derivatives with much smaller meso-C substituents, such as H, CF₃, CN and COOH.



Scheme 1: Published (upper box) and new (lower box) methods for post-functionalization of corroles.

References

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Bioinorganic Chemistry

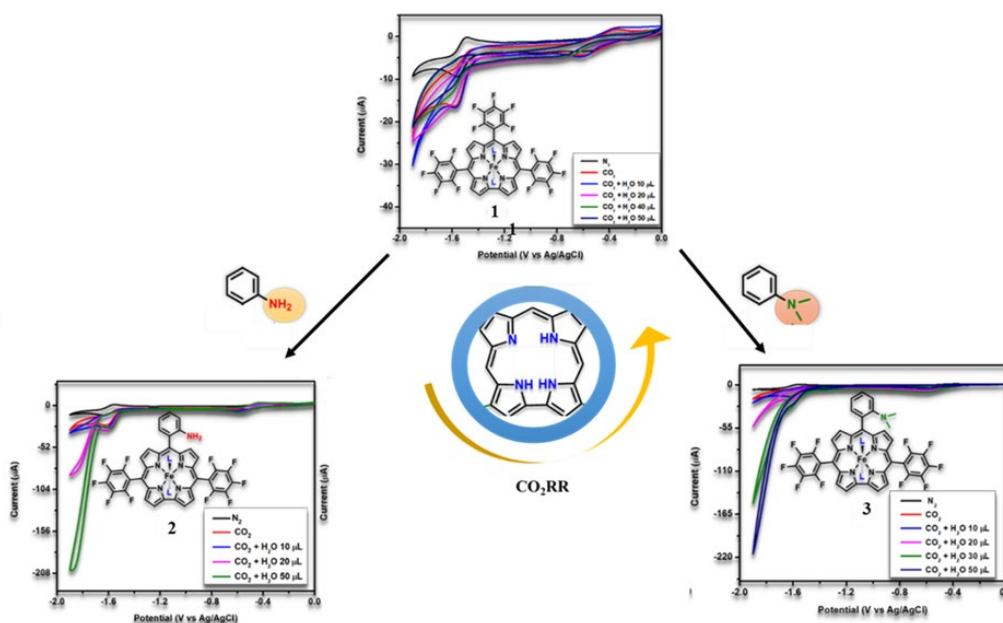
Effect of Secondary Sphere in Electrochemical CO₂ Reduction using Iron Corroles

Anubhi Rawat¹, Prof. Zeev Gross¹

Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa, Israel

Corroles, as contracted and trianionic tetrapyrrolic macrocycles, have emerged as promising analogues to porphyrins for CO₂ electroreduction. Despite several reports on corrole-based catalysts,^{1,2} the influence of second-sphere effects remains unexplored. Here, we examine the effect of amino-phenyl and dimethylamino-phenyl substituents on the electrochemical CO₂ reduction using iron corroles.

Two new iron corroles bearing nitrogenous substituents were synthesized and characterized by high resolution mass spectrometry, UV-vis and ¹H-NMR. The aminophenyl-group in corrole 2 enhances the catalysis via second-sphere hydrogen bonding interaction to intermediate species, leading to the enhanced CO₂ reduction activity, whereas 1 shows limited performance. Complex 3 exhibits a similar current increase but with distinct voltammetric features. The control experiments indicate that its response arises from a combination of CO₂ reduction and hydrogen evolution. These findings highlight the importance of tailored second-sphere design in tuning corrole-mediated CO₂ reduction pathways. The Current focus is the product determination.



Bioinorganic Chemistry

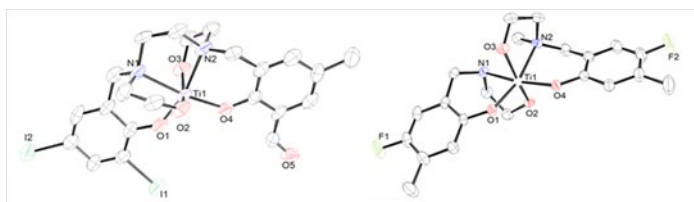
Ti(IV) Phenolato hexacoordinate complexes as anticancer chemotherapy: enhancement of solubility, hydrolytic stability, and cytotoxicity; and targeting aspects

Mohammad Taha¹

The Hebrew University of Jerusalem, Israel

Cisplatin is the first metal-based anticancer drug. It is effective, but suffers from two limitations: (a) it is toxic, which is a common feature of many chemotherapies; and (b) it is not widely active because some cancer cells can develop resistance to the treatment, limiting the potential use. Titanium is a good alternative to platinum because, although titanium is not considered an essential metal for the human body, it has biocompatible features. Nevertheless, the low stability in water of titanium complexes reported previously limited their potential use in anticancer therapy. In our group we aim to develop titanium-based complexes of enhanced stability and potency in anticancer therapy. To this aim, we employed a single hexadentate diaminobis-phenolato-bis-alkoxo ligand to give singly ligated complexes. Complexes of this type are highly stable and highly cytotoxic, but lack sufficient water solubility. PhenolaTi, a leading complex of this family, demonstrated significant activity toward all cell lines tested in the NCI-60 panel of the NIH, as well as in vivo efficacy. Mechanistic studies suggested that its cytotoxic activity involves ER stress; Nevertheless, knowledge of the exact mechanism of activity is still lacking.

Herein we present the synthesis of derivatives of phenolaTi complexes, aiming to improve their features and learn more on their mode of activity. We will discuss a new set of complexes demonstrating enhanced solubility, in addition to high cytotoxicity and hydrolytic stability. Additionally, aiming to shed additional light on mechanistic aspects, studies toward cellular, as well as sub-cellular, targeting of these complexes will be discussed.



Bioinorganic Chemistry

ZIPTAC-Mediated Relocalization to Correct Mislocalized Oncogenic RNA Binding Protein HuR

Liann Kassabri¹, Dr Raphael I. Benhamo¹
the hebrew university, israel

The RNA-binding protein HuR (ELAVL1) plays a central role in post-transcriptional gene regulation, and its aberrant cytoplasmic accumulation is a hallmark of many cancers. When mislocalized from the nucleus to the cytoplasm, HuR stabilizes and promotes the translation of oncogenic transcripts, thereby enhancing proliferation, preventing apoptosis, and driving tumor progression. We previously developed HuR-directed PROTACs that efficiently degrade the protein; however, complete elimination of HuR may be undesirable, as HuR retains essential physiological roles in stress response, RNA metabolism, and cellular homeostasis. To overcome these limitations, we introduce ZIPTAC, a relocalization-based therapeutic modality designed to correct the pathological cytoplasmic mislocalization of HuR rather than destroy it. ZIPTACs are hybrid small molecules that couple a HuR-binding ligand to a nuclear-directing element, enabling the active re-import of HuR into the nucleus and restoring its native subcellular distribution. We designed and synthesized a focused series of ZIPTAC derivatives with varying HuR ligands and linker architectures, identifying molecules capable of completely eliminating cytoplasmic HuR accumulation through efficient nuclear relocalization. Correcting HuR mislocalization markedly attenuates oncogenic downstream signaling, reflecting the loss of HuR's pathogenic activity in the cytoplasm. This subcellular-correction strategy represents a mechanistically distinct and potentially safer alternative to catalytic degradation, offering a new framework for therapeutically modulating RNA-binding proteins whose disease-driving functions arise from mislocalization rather than overabundance.

Bioinorganic Chemistry

Steroid-Functionalized Ti(IV)-Phenolato Complexes as Potential Anticancer Drugs

Karin Pichhadze¹, Prof. Edit Tshuva¹
The Hebrew University of Jerusalem, Israel

The disruption of normal cell growth lies at the core of cancer development, which encompasses nearly 100 different types and remains a prominent cause of mortality. Although cisplatin remains a key chemotherapeutic agent, its severe toxicity and propensity to induce resistance necessitate the pursuit of alternative metal-based therapeutics. Consequently, titanium(IV) has emerged as an attractive candidate owing to its bio-compatibility and activity against cisplatin-resistant cancer cells. Titanium(IV) complexes, including titanocene dichloride and budotitane, showcased potent anticancer activity across various cell lines with reduced side effects, entering clinical trials as pioneering non-platinum metal complexes. However, their clinical progress was curtailed mainly due to hydrolysis susceptibility. To overcome this, our group developed titanium(IV) complexes incorporating bis(phenolato)-ligands. The first generation featured diaminobis(phenolato)-salan ligands with labile isopropoxo groups, leveraging the chelate effect to enhance stability. The second generation eliminated labile groups by employing diaminobis(phenolato)-bis(alkoxo)-ligands, achieving further stabilization.

Elaborating further, we explored dipicolinic-acid derivatives as bridging ligands for attaching biomolecules to titanium(IV) complexes. These modifications aim to enhance tumor targeting and delivery capabilities while also elaborating on the therapeutic effects of titanium compounds alone. Using chelidamic acid, we synthesized Ti complexes that were further functionalized with steroidal groups. The dipicolinic-acid-Ti complexes were characterized by NMR spectroscopy and single-crystal X-ray diffraction, which confirmed a heptadentate coordination environment around the titanium center, even with a Cs-symmetric precursor bearing a flexible N-arm ligand. The steroid-modified complexes were characterized by NMR and are being evaluated for tumor-targeting and delivery properties. Various structural and activity studies will be discussed.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



CHEMICAL EDUCATION

Chair: Debora Marchak

Invited Lecture

Chemical Education

Critical Thinking in Chemistry Education: Conceptualization, Challenges, and Research Findings

Shelley Rap¹, Hanan Gbarin¹, Yael Schleifer¹, Prof. Ron Blonder¹
Department of Science Teaching, Weizmann Institute of Science, Israel

Critical thinking is widely regarded as a central competence in science education, essential for enabling learners to evaluate evidence, justify claims, and make reasoned decisions in a world saturated with information¹. In chemistry, developing such skills is particularly important for helping students connect abstract scientific knowledge to real-world contexts and to act as informed citizens in addressing global challenges like climate change. However, fostering critical thinking in chemistry classrooms remains a complex task. Teaching practices often emphasize the acquisition of factual knowledge and mastery of established procedures, leaving little space for reflection, argumentation, or discussion. Teachers may also hesitate to address controversial or uncertain issues, such as sustainability or energy use, because they fear losing control of discourse or exposing gaps in their own knowledge.

To explore how critical thinking can be fostered, a study was conducted among 238 high-school chemistry students from different sectors, using pre-post assessments based on the CRITIC model². It examined changes in students' critical reading and evaluation of scientific articles after an intervention with explicit instruction. Students' low performance improved, emphasizing the need for explicit guidance and teacher support. The lecture will review critical-thinking concepts, classroom challenges, key research contributions, and their implications.

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2. W. R. Bartz, in *The Skeptical Inquirer*, The Committee for the Scientific Investigation of Claims of the Paranormal (SCICOP), Buffalo, 2002, vol. 26, pp. 42-44.

Invited Lecture

Chemical Education

"COFFEE TIME": a Virtual Chemical Escape Room

Ayelet Shvalb¹, Dr Shelley Rap²

¹*Mechanical Engineering, AFEKA-The Academic College of Engineering in Tel Aviv, Israel*

²*Science Teaching, Weizmann Institute of Science, Israel*

Physical or digital escape games are a contemporary educational method adaptable to various age groups and academic disciplines, used for practice, reinforcement, or introducing new content. This method leverages the competitive group nature of escape rooms to enhance classroom learning.¹ Game-based learning is an innovative pedagogical approach that facilitates knowledge acquisition and skill development, contributing significantly to cognitive development and enhancing essential 21st-century competencies such as teamwork, critical thinking, problem-solving, and creativity. It also bridges the gap between formal and informal education, enabling experiential learning.²

The digital escape game "Coffee Time" was developed at Afeka College of Engineering for mechanical and biomedical engineering students taking an introductory chemistry course. The game aims to: 1) provide opportunities for applying 21st-century skills, 2) offer an alternative assessment to traditional quizzes, and 3) support first-year students' social adaptation through group-based activities. The development process focused on aligning chemistry principles, designing puzzles, and fostering peer interaction through immediate feedback.

Feedback from 251 participants revealed increased teamwork, creative thinking, and application of course content, suggesting the escape-room model is an effective tool for reinforcing scientific and engineering subjects in higher education.

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1. Veldkamp, A., van de Grint, L., Knippels, M.-C., & van Joolingen, W. (2020). Escape Education: A Systematic Review on Escape Rooms in Education. <https://www.preprints.org/manuscript/202003.0182/v1>
2. Yayon, M., Rap, S., & Blonder, R. (2023). Chemical escape rooms: Bridging the gap between formal and informal science learning. *Amplifying Informal Science Education*, 21(3), 400–415. <https://doi.org/10.1080/10509585.2023.2217994>

Invited Lecture

Chemical Education

Binding school science and real science through contemporary content knowledge

Ron Blonder¹, Dr. Ella Yonai²

¹*Department of Science Teaching, Weizmann Institute of Science, Israel*

²*Department of curriculum and teaching, College of education, Auburn University, Alabama, USA*

Science teachers are expected to help students make sense of a world shaped by rapidly advancing scientific knowledge. Yet most professional learning focuses on strengthening teachers' introductory content knowledge (ICK), while opportunities to engage with contemporary scientific knowledge (CCK) remain limited. In this presentation, we argue that treating teacher content knowledge (CK) as a single, static domain obscures the inherently tentative, creative, and socially embedded nature of science. We propose distinguishing between ICK, the foundational concepts found in introductory courses, and CCK, the emerging ideas, methods, and practices generated within the scientific community. This distinction better reflects the nature of science and highlights the need to support teachers in continually extending their knowledge.

We present a conceptual model describing the epistemic relationship between ICK and CCK and illustrate its implications through an authentic professional learning design centered on teachers' hands-on work with a scanning electron microscope (SEM) in a research institute. This authentic science environment fostered interactions with scientists, engagement with contemporary research, and opportunities to use scientific practices to extend and contextualize teachers' knowledge. Outcomes from this design show how teachers developed CCK and translated it into meaningful classroom resources.

We argue that cultivating teachers' CCK through authentic, socially situated experiences is essential for bridging "school science" and "real science," enriching instruction, and preparing students to use science as a framework for reasoning, decision making, and future career exploration.

Invited Lecture

Chemical Education

A Conceptual Synthesis of SOLO Taxonomy and Generative AI in Nanotechnology

Yael Feldman-Maggor¹

School of Education, Ben Gurion University of the Negev, Israel

As learners increasingly rely on generative AI (GenAI) tools to complete educational tasks, there is a growing need for frameworks that can evaluate the capabilities of these tools within chemistry education. This study contributes to addressing this need by applying the Structure of the Observed Learning Outcome (SOLO) taxonomy, a framework that categorizes learning outcomes based on their complexity. The SOLO taxonomy delineates five hierarchical levels: pre-structural, uni-structural, multi-structural, relational, and extended abstract. In this study, we used ChatGPT-4o to apply the SOLO taxonomy in order to solve and analyze 30 open-ended assignments on nanotechnology. The findings indicate that GenAI consistently performs at the relational level, but does not reach the highest learning level of extended abstract. Furthermore, some responses categorized as relational lacked precision in scientific content, highlighting the critical role that scientific knowledge and critical thinking continue to play when interpreting GenAI-generated outputs. Additionally, a comparison with a previous study about a professional development course on nanotechnology revealed greater variation in human responses. While current findings suggest that GenAI tools like ChatGPT-4o may help learners reach the relational level more consistently, they may also reduce the variability of responses. This potential reduction in answer variability poses a pedagogical concern, as such variation is essential for diagnosing different levels of student understanding. These results stressed the need to reassess the design of evaluation frameworks in chemistry education settings to ensure that the use of GenAI supports, rather than masks, students' individual learning processes and conceptual development.

Invited Lecture

Chemical Education

The Innovation in the Chemical Industry Course: Bridging Chemistry Studies and Industry

Tamar Traube¹, Dr Rachel Mamlok-Naaman²

¹*Bar-Ilan University, Israel*

²*Weizmann Institute of Science, Israel*

University chemistry courses often focus on theoretical content, while providing limited exposure to how chemistry is applied in professional industrial setting. Integrating industrial perspectives into university chemistry studies plays an important role in developing students' critical thinking and problem-solving abilities by engaging them with real-world industrial challenges. It also contributes to increased student engagement, strengthens the relevance of academic learning, and supports students' preparation for careers in chemistry-related fields.^{1,2} To address these goals, the Innovation in the Chemical Industry course was designed to connect academic chemistry studies with the professional world of the chemical industry. The course exposed students to contemporary industrial research and development through guest lectures delivered by experts from diverse industry sectors. The course included a project-based learning component in which students worked in teams to investigate the development of an industrial product or technology. The final project was presented in a poster conference format designed to simulate a professional scientific meeting and to encourage the development of key employability skills. Course evaluation results indicated that students improved their knowledge and understanding of industrial topics and increased their awareness of potential career opportunities.

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Invited Lecture

Chemical Education

FORENSIC CHEMISTRY IN THE DIFS, ISRAEL POLICE

Gilead Shafir¹

DIFS, Israel police, Israel

The Division of Identification and Forensic Science (DIFS) labs of the Israel police, are involved in nearly every criminal and terror investigations. The DIFS played critical role includ in the identification of the victims of October 7 and in the efforts to locate the hostages in the Gaza strip. The division integrates a broad spectrum of scientific disciplines, with particular emphasis on the chemical and biological sciences. In this lecture, I will outline the forensic chemistry aspect and the application of chemical analytical techniques and methods for purpose of investigating and the conviction of criminals and terrorists.

Invited Lecture

Chemical Education

Promoting 21st-Century Skills and STEM Career Pathways: Addressing Gender and Representation Gaps

Yehudit Judy Dori^{1,2}

Faculty of Education in Science and Technology, Technion, Israel
The Samuel Neaman Institute for National Policy, Israel

Career readiness in the 21st century requires both domain-general and STEM-specific interpersonal and thinking skills. A large-scale study of approximately 1,500 STEM students and alumni at the Technion examined the development of 21st-century skills during their academic studies. The findings indicated gaps in skill development across domains. STEM-specific and interpersonal skills showed lower growth compared to general skills, while active teaching methods demonstrated a moderate positive effect.

A series of complementary studies explored STEM career choices across diverse groups, integrating a gender perspective and focusing on underrepresented populations such as women, ultra-Orthodox (Haredi) students, and residents of geographic and socioeconomic peripheries (Edri et al., 2025; Tal et al., 2024). These studies identified unique challenges faced by these groups, including cultural and structural barriers, limited exposure to role models, and reduced opportunities to develop both interpersonal and STEM-specific skills.

Recognizing these barriers underscores the importance of equitable and tailored pedagogical interventions. Fostering both interpersonal and STEM-specific skills within inclusive learning environments has the potential to strengthen students' motivation to pursue STEM pathways, particularly among populations that have historically been underrepresented in the field.

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Invited Lecture

Chemical Education

The Pedagogical Vision of Tel Aviv University Youth Programs for Chemistry Education: Cultivating Israel's Next Generation of Chemists

Omry Morag¹, Ms. Roni Heliczer¹
Tel Aviv Youth University, Israel

Israel faces a critical strategic challenge: chemistry lies at the foundation of nearly every essential system—defence technologies, pharmaceuticals, advanced materials, energy, climate, water, and food security—yet the number of students studying chemistry at an advanced level in high school and university has reached a historic low. Addressing the national need to identify and promote the next generation of scientific leaders requires a bold and thoughtful reshaping of chemistry education.

The Tel Aviv University Youth Unit has developed a comprehensive pedagogical vision aimed at restoring chemistry to its central place in science and education. This vision is grounded in integrative, historical, and holistic teaching that is not confined to a rigid syllabus, but instead presents chemistry as it truly evolved: a journey of major questions, decisive experiments, scientific dilemmas, conceptual revolutions, and discoveries that shaped modern science. Close integration with physics enables students to view the laws of nature and the laws of matter as a single coherent system—an essential scientific toolbox for any young learner.

Chemistry instruction in the unit's academic programs combines high-level theoretical learning with authentic experimental work, demonstrations, data analysis, and applied reasoning. Students experience how scientists actually work—from curiosity, through challenges, to insight—supported by educational frameworks that encourage critical thinking, personal responsibility, and genuine passion for inquiry.

We will demonstrate how this pedagogical vision along with other activities for schools nationwide seeks to revive chemistry education.

Invited Lecture

Chemical Education

Integrating Facilitation, Collaborative Regulation, and Formative Assessment in a Chemistry-based Educational Escape Room

Shirly Avargil¹

Education in Science and Technology, Technion - Israel Institute of Technology, Israel

Educational escape rooms (ERs) are increasingly used in chemistry education as dynamic, collaborative learning environments that combine disciplinary problem-solving with authentic teamwork. This study integrates findings from three complementary investigations that examined ER-based learning from the perspectives of students, teachers, and facilitators, aiming to characterize instructional practices, collaborative regulation of learning, and teachers' formative assessment (FA) knowledge within a chemistry-based ER.

First, an analysis of verbal facilitation moves used by eight ER facilitators, both teachers and onsite instructors, identified twelve types of guidance strategies. Questioning emerged as the most dominant tool, and chemistry-related guidance was the most frequent content focus. These findings highlight the unique instructional demands placed on ER facilitators, who must balance autonomy with productive progression.

Second, high-school students' collaborative regulation during ER problem solving was examined through video observations and stimulated-recall discussions. Monitoring was the most prevalent regulatory phase, and socially shared regulation appeared primarily during orienting and monitoring. Students demonstrated chemical thinking across eight dimensions, with material identification and experimental skills most common, underscoring the role of ER tasks in promoting core chemistry practices.

Third, a professional development program involving 64 chemistry teachers explored teachers' FA knowledge when interpreting students' ER performance. Teachers emphasized 21st-century skills, chemical thinking, and affective aspects, identifying three characteristics of assessment knowledge.

Together, these integrated findings advance understanding of learning and assessment processes in chemistry-based ERs and offer practical implications for designing and facilitating collaborative, problem solving environments in chemical education.

Chemical Education

From Campus Blooms to Burettes: A 4-Hour Jacaranda Flowers-Based Acid–Base Titration Protocol in General Chemistry

Ariela Kaspi-Kaneti¹, Dr. Danny Zeng¹, Ms. Hannah Aranki¹, Ms. Brianna Morris¹,
Ms. Michelle Cornejo¹, Dr. Andrew Rice¹, Dr. Hou Ung¹, Dr. Nixon Mwebi¹
Chemistry, University of La Verne, CA USA

This study presents a four-hour, flower collection -to-finish laboratory protocol in which Jacaranda (*Jacaranda mimosifolia*) flower extract—prepared using only water as the solvent—is applied as a natural acid–base indicator in undergraduate General Chemistry. Designed to span a single lab session, the protocol leads students from flower collection to extraction and titration using core general-chemistry techniques. The initiative aimed to increase student engagement, strengthen conceptual understanding of titration, and connect laboratory learning to the campus environment. The project also actively involved undergraduate researchers in protocol development, optimization, and implementation. More than 200 students performed titrations using the Jacaranda extract and compared its performance to standard indicators for determining the molar concentration of hydrochloric acid solutions.

Chemical Education

Chemical Teachers' Knowledge across Career Stages

Boaz Hadas¹, Dr. Orit Herscovitz¹, Prof. Yehudit Judy Dori^{1,2}

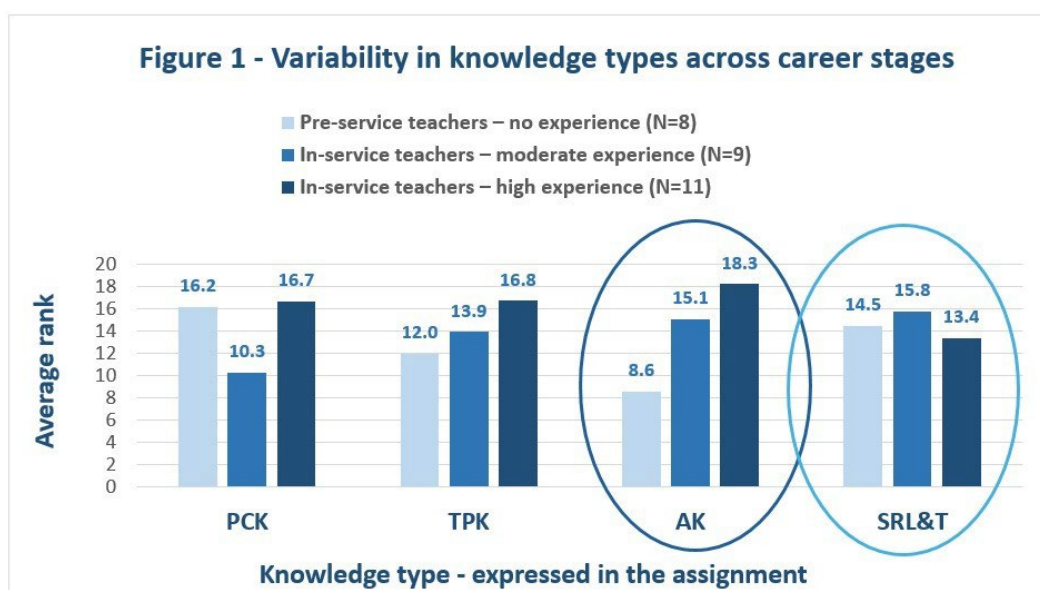
¹Faculty of Education in Science and Technology, Technion, Israel

²The Samuel Neaman Institute for National Policy, Technion, Israel

Chemistry teachers' professional growth unfolds across career stages, shaping how they manage instructional demands. In technology-enhanced environments, Self-Regulated Learning (SRL) becomes essential for navigating abstract and multimodal information. Beyond guiding SRL, teachers also regulate instruction, a dual responsibility conceptualized as SRL&T. This study examines how Pedagogical Content Knowledge (PCK), Technological Pedagogical Knowledge (TPK), Assessment Knowledge (AK), and SRL&T, manifest in SRL-oriented digital assignments developed by chemistry teachers across career stages.

This study used content analysis and quantitative comparisons of 28 assignments of 34 chemistry teachers. Teachers spanned three stages: pre-service, in-service (≤ 10 years), and in-service (10 years). A validated rubric (0–10) assessed PCK, TPK, AK, and SRL&T, enabling knowledge profiling and cross-career comparison.

The analysis showed high PCK and lower AK levels across all groups. Figure 1 illustrates that AK rises with experience and differentiates groups, aligning with the theoretical view that AK develops with teaching experience, whereas SRL&T levels remain stable, supporting SRL&T as a distinct knowledge domain. Findings highlight the need to strengthen AK and SRL&T through targeted professional development. The study also provides a rubric-based diagnostic tool for identifying chemistry teachers' knowledge.



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Chemical Education

Exploring Regulation of Collaborative Learning and Chemical Thinking in a Collaborative Dynamic Learning Environment

Noa Amir¹, Assoc. Prof. Shirly Avargil¹

Faculty of Education in Science and Technology, Technion, Israel

In recent decades, individuals' ability to collaborate and communicate when solving problems was acknowledged in educational and professional contexts. Addressing complex challenges requires combination of disciplinary expertise with the ability to engage in effective communication, collaboration, and regulation of social and cognitive processes within learning groups. However, there is still limited understanding of how regulation of learning unfolds in collaborative and dynamic learning environments. Educational escape rooms are innovative learning environments that engage students in active, face-to-face, team-based problem-solving grounded in real-world contexts. Through the social shared regulation of learning (SSRL) framework we examined how high school students jointly plan, monitor, and adapt their collaborative learning and employ chemical thinking within an educational chemistry escape-room environment.

The study employed video observations during the activity and structured group discussions following it, to characterize chemistry high school students' regulation of learning and expression of chemical thinking. Various regulation skills and types were identified and demonstrated throughout the activity. Monitoring emerged as the predominant regulatory skill, shared forms of regulation (co-regulation and SSRL) frequently co-occurred during complex tasks. Students' chemical thinking was mainly expressed through references to material identification and experimental procedures.

The findings demonstrate the collaborative nature and characterize the expression of chemical thinking within this authentic learning environment. The research offers tools for analysing students' chemical thinking and regulation of learning in a collaborative environment. Moreover, the results provide insights for educators on designing and facilitating collaborative, inquiry-based science learning environments that foster cognitive and metacognitive development.

Chemical Education

Critical thinking assessment tool for chemistry teachers using generative AI

Yael Schleifer¹, Dr Shelley Rap¹, Prof. Ron Blonder¹

Department of science teaching, Weizmann institute of science, Israel

The field of science education carries a great responsibility in preparing students for the new and challenging world. Critical thinking (CT) is essential when chemistry students, as chemists, make analysis of information, apply knowledge to real-world problems, identify reasoning and determine credibility, reliability and validity (Danczak et al., 2017). Chemistry is also an experimental subject that seeks to explain phenomena and expend the knowledge barriers through experiments and reasoning. CT is a transversal competence that can be developed within the context of chemistry. When teachers change their teaching and add a component to it (CT skill teaching), students' assessment of this component is an essential part. To ensure that the teaching process is productive and effective, assessment methods should be designed so that the marking and feedback-giving processes are not time consuming (Le & Tam, 2007). The current study, aims to develop GenAI tool to assess open-ended answers to critical thinking provoking questions in the context of chemistry-related issues. This tool will be provided for the use of chemistry teachers. Their considerations and decisions regarding the implementation, use and design of the assessment tool will be investigated.

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Chemical Education

Innovative chemistry outreach activities: Design features that enhance high-school students' understanding of the Nature of Science

Iris Shinar¹, Prof. Ron Blonder¹

Department of Science Teaching, Weizmann Institute of Science, Israel

Although developing students' understanding of the Nature of Science (NOS) is widely recognized as a key goal of science education, research consistently shows that secondary students often have limited opportunities to engage explicitly with NOS in their formal studies. Barriers include restricted curriculum time, the absence of appropriate teaching materials, and insufficient teacher preparation. To address these challenges, we designed innovative outreach activities for high-school chemistry students that combine explicit NOS instruction with contemporary chemical research practices through the use of Scanning Electron Microscopy (SEM) - a tool rarely accessible in school settings.

The activities were grounded in established design principles (*explicit and reflective NOS instruction, contextualized learning, authentic scientific practice and historical narratives*). By embedding SEM-based analysis within chemical inquiry, we created learning environments that reflect how modern chemists generate and interpret evidence.

To understand which aspects of these innovative chemistry-learning environments supported NOS understanding, we conducted an inductive qualitative analysis of students' written reflections. Beyond the planned design principles, students highlighted several emergent design features:

The visual power of SEM, which enabled students to connect chemical structure to scientific interpretation in an authentic way;

Collaborative group discussions, which facilitated comparison of observations and negotiation of explanations, mirroring real chemical research;

Cognitive conflict when experimental outcomes contradicted expectations, emphasizing the tentative and creative nature of chemical knowledge-building.

Our findings suggest that applying these design principles - both the established and the emergent ones - can effectively guide the development of other chemistry education activities that deepen students' NOS understanding.

Chemical Education

Teaching Students Nanomedicine Fundamentals and Synthesis through a Remote-Controlled Robotic Laboratory

Egor Egorov¹, Hagai Zeira², Yuval Ramrazker¹, Tiba Hamza¹, Zoe Nov¹, Prof. Avi Schroeder¹

¹*The Louis Family Laboratory for Targeted Drug Delivery & Personalized Medicine Technologies, Department of Chemical Engineering, Technion - Israel Institute of Technology, Israel*

²*Faculty of Education in Science and Technology, Technion - Israel Institute of Technology, Israel*

Direct engagement with experimental research is vital for scientific education, yet access to advanced infrastructure remains globally limited. To address this, we developed Robiochemistry, a hybrid initiative enabling remote participation in nanomedicine research. The program allows students with minimal laboratory access to conduct authentic lipid nanoparticle (LNP) synthesis using an automated liquid-handling platform. Supported by Technion International, the initiative attracted approximately 200 applications. Two cohorts of undergraduate and postgraduate students from Vietnam and China were selected for August and September 2025. Over four weeks, students navigated the complete research pipeline—from molecular assembly and in vitro analysis to data interpretation and presentation. Using a web-based interface, students progressed from theory to autonomous research, writing custom scripts to control a robotic workstation in real time. The majority of students successfully passed, completing all rigorous assignments and a final research project. The initiative received high praise, with students rating the engaging format and the utility of the material highly. By replacing passive simulation with active workflows identical to those used in nanomedicine, the program bridged the gap between manual understanding and automated execution. To scale this impact and provide a simulated user interface, we developed a prototype application that translates bench-top methods into robotic commands using AI. This foundation facilitates new collaborations and educational upgrades to expand outreach, demonstrating that automation can effectively extend laboratory experiences beyond physical boundaries.

Chemical Education

From teaching practices to student agency: Understanding how teachers' actions developing students' agency in the context of SDGs

Ayshi Sindiani- Bsoul¹, Prof. Ron Blonder¹, Dr Shelley Rap¹
Science teaching department, Weizmann Institute of Science, Israel

Agency is the ability to set goals, reflect, and act responsibly; student agency is applying these capacities to create change, supported by teacher-designed learning activities (OECD, 2019). This study focused on 9th grade students' agency, developed in the context of a program about SDGs (Rap et al., 2022). Studying 15 science teachers and their 9th and 10th grade students, we aimed to identify the role teacher play in developing the students' agency. We applied semi-structured interviews with the 8 teachers and 70 students (in groups), and classroom observations via a bottom-up qualitative research approach. In each of the classes, we looked for the connection between different actions teacher do and different component of students' agency. Our data analysis indicates a clear relationship between students' agency, as defined by Guerra et al. (2022) through its three components -personal values, actions, and the context of actions- and the practices teachers employ in the classroom. When teachers develop sustainability knowledge and encourage initiatives, students strengthen personal values, and meaningfully making plans for engagements that together foster their agency. We will present more details, discuss the results and the implications for teachers' professional development in the poster.

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Chemical Education

Developing an Educational Escape Room on Solar Panels: Expanding Exposure Beyond School Walls

Simona Shulman Tawily¹, Dr. Shelley Rap¹, Dr. Malka Yayon¹, Mrs. Gili Swary²,
Prof. Ron Blonder¹

¹*Science Teaching, the Weizmann Institute, Israel*

²*SolarEdge, Israel*

Studies show that students often perceive science as irrelevant or uninteresting (Osborne & Dillon, 2007; Stuckey et al, 2013), despite clear connections between personal interest, participation in science activities, and future study or career choices. Educational chemistry escape rooms were found to enhance students' engagement and motivation (Peleg et al 2019). However, a key pedagogical challenge in designing educational escape rooms (ERs) lies in balancing the informal nature of games that associated with enjoyment, curiosity, and challenge, with formal learning goals tied to scientific content, skills, and competencies.

In this study, we established an interdisciplinary team of engineers (from SolarEdge) and science educators (from the Weizmann Institute) to co-develop an innovative ER focused on renewable energy. Drawing on our experience in designing ERs, the activity was developed by integrating context-based learning theories with authentic industry challenges, emphasizing practical problem-solving.

At the conference, I will present puzzles from this innovative ER and discuss the development process that was based on collaboration between the engineering team and the science education research group.

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Chemical Education

Integrating citizen science into chemistry education: Fostering STEM literacy, critical thinking, and environmental agency through tree growth monitoring

Daniel Sorek^{1,2}, Dr. Shelley Rap¹, Prof. Tamir Klein¹, Prof. Ron Blonder¹

¹*Department of Science Teaching, Weizmann Institute of Science, Israel*

²*Hakfar Hayarok Youth Village, Israel*

Preparing learners for future challenges necessitates effective education addressing complex global issues, such as climate change, where immediate action is required. Chemistry is fundamental for understanding and responding to climate change, specifically regarding the global carbon cycle, photosynthesis, and ocean acidification. Citizen Science (CS) offers a unique and authentic arena for deep scientific learning¹

In a unique CS project, teachers and students were guided to participate in authentic research, specifically, monitoring the growth (or shrinkage) of mature urban trees in response to environmental factors, using band dendrometers. Previous research has shown that tree circumference can be directly linked to CO₂ uptake². This network of CO₂-photosynthesis-glucose-cellulose-tree growth, presents opportunities for interdisciplinary STEM connections, embedding CS principles into formal high school Chemistry curricula.

The project emphasized hands-on data collection and analysis. It coincided with an extreme drought year (2025), revealing significant scientific findings: pervasive stem shrinkage in 50–100% of monitored trees across school sites. Engaging with these real, sometimes non-intuitive, data promotes mathematical and scientific literacy. The requirement for teachers and students to analyze these findings and draw conclusions enhances critical thinking and data-based argumentation skills, connecting school chemistry to authentic science related to an urgent global issue of climate change.

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Chemical Education

Enhancing Student Preparation and Engagement in Chemistry Laboratories through LabBuddy: The First Implementation in Israel

Noach Treitel¹, Yaniv Geier¹, Dr. Ruthy Sfez¹
Azrieli College of Engineering Jerusalem, Israel

Laboratory courses are a central component of STEM education, enabling students to bridge theoretical concepts with practical experimentation. However, many students arrive at the laboratory insufficiently prepared due to cognitive overload, lack of structured guidance, and the absence of immediate feedback during the preparation phase. To address these challenges, we implemented LabBuddy, an interactive, web-based learning environment that supports students before, during, and after laboratory sessions.

LabBuddy was introduced for the first time in Israel at Azrieli College of Engineering, Jerusalem, within undergraduate chemistry laboratory courses for first- and second-year engineering students. The platform integrates theoretical background materials with clearly defined preparatory tasks, including conceptual questions, procedural guidance, and safety considerations. Students receive automated feedback that promotes active learning and reduces pre-lab anxiety.

Over the past two years, student engagement and performance have improved significantly. Learners reported higher confidence and satisfaction levels, while instructors observed enhanced readiness and deeper conceptual understanding during laboratory work. The seamless integration of LabBuddy into the Moodle learning management system further streamlined communication and assessment processes.

This study highlights the pedagogical benefits of combining interactive digital tools with traditional laboratory teaching. LabBuddy not only fosters self-regulated learning but also enables instructors to focus on inquiry-based discussions and higher-order skills. Our experience demonstrates that such blended learning approaches can substantially improve the quality and efficiency of chemical laboratory education in engineering curricula.

Chemical Education

How Teachers Guide Students in a Chemistry-Based Educational Escape Room: Types of Guidance Across Chemistry Learning Content

Hagai Zeira¹, Prof. Shirly Avargil¹

Faculty of Education in Science and Technology, Technion - Israel Institute of Technology, Israel

Educational escape rooms have recently emerged as immersive learning environments for teaching and practicing disciplinary content through collaborative problem-solving. In chemistry-based escape rooms, students engage with core concepts such as chemical reactions, stoichiometry, molecular structure, macroscopic and microscopic representations, and material properties while solving challenging puzzles in order to “escape” the room. During this process, the chemistry teacher assumes the role of a remote guide, providing pedagogical guidance aligned with students’ chemical reasoning and problem-solving processes.

Despite the increasing implementation of escape rooms in education, research on how teachers guide students’ disciplinary thinking during such dynamic learning experiences remains scarce. In particular, little is known about the nature of teacher guidance that supports students’ chemical understanding as they collaborate under time pressure.

This study investigates the characteristics of teacher guidance in a high school chemistry educational escape room. Eight experienced chemistry teachers participated, and all verbal guidance was segmented into discrete “comments” and analyzed using qualitative content analysis. Two complementary analytical dimensions were examined: (1) the enacted guidance type, based on established instructional guidance frameworks, and (2) the guidance content aspects, with a specific focus on the chemistry learning content, taking into account the chemical subtopic addressed, the level of chemical understanding and thinking, and the skills required.

Theoretically, the findings extend existing guidance models to a novel and underexplored learning environment. Practically, they offer actionable insights into instructional strategies that foster collaboration, engagement, and deep chemical learning in a unique learning environment.

Chemical Education

Integrating Chemical Engineering Aspects into High School Chemistry Teaching – Teachers' Knowledge and Perceptions

Mrs. Esraa Foqara¹, Mrs. Michal Bronstein-Tojen^{2,3}, Prof. Simon Brandon³, Shirley Avargil¹

¹*Faculty of Education in Science and Technology, Technion Israel Institute of Technology, Israel*

²*Centre for the Promotion of Learning and Teaching, Technion Israel Institute of Technology, Israel*

³*The Wolfson Department of Chemical Engineering, Technion Israel Institute of Technology, Israel*

Background:

There is a growing global gap between the number of science, technology, engineering, and mathematics (STEM) graduates and the demand for STEM professionals, emphasizing the need to understand factors influencing students' interest in STEM careers. International science education frameworks call for integrating engineering principles into science teaching, yet many teachers remain insufficiently prepared for this task, including in Israel.

Purpose:

The purpose of the study is to examine how exposure to chemical engineering concepts influences chemistry teachers' perceptions, knowledge, and readiness to integrate engineering practices into their teaching, and to adapt chemical engineering principles for high school chemistry instruction.

Methods:

The study employs a three-stage mixed-methods design:

1. A pre-professional development (PD) survey assessing chemistry teachers' (N=40) baseline conceptions, familiarity with chemical engineering, and perceived readiness to incorporate engineering practices.
3. A professional development day in the Faculty of Chemical Engineering during which chemistry teachers attend expert lectures, participate in laboratory tours, and engage in a collaborative instructional design workshop. Data collection tools include guided reflection sheets and structured observation protocols.
3. A post-PD survey and follow-up interviews exploring shifts in teachers' understanding, confidence, and instructional intentions.

Expected contribution:

Findings from this study are expected to provide insights into factors that support or hinder the integration of engineering practices in chemistry education. These insights may inform future teacher-training programs and contribute to long-term curriculum development efforts aimed at embedding chemical engineering concepts into the high school chemistry curriculum in Israel.

Chemical Education

Virtual Labs, Real Learning: A Comparative Analysis of Learning Outcomes and Skill Development in VR and F2F Thermodynamics Lab

Ilana Ram¹, Dr Lisa Bosman², Dr Shoval Gilboa³, Yulia Pavlov³, Michal Bronstein-Tojen⁴, Dr Alon Grinberg Dana³

¹*Faculty of Science and Technology Education, Technion Israel Institute of Technology, Israel*

²*Purdue Polytechnic Institute, Purdue University, USA*

³*The Wolfson Department of Chemical Engineering, Technion Israel Institute of Technology, Israel*

⁴*Centre for the Promotion of Learning and Teaching, Technion Israel Institute of Technology, Israel*

Virtual Reality (VR) is emerging as a powerful tool in STEM education, offering immersive environments that can enhance understanding of complex concepts. This study examined the effectiveness of VR in an undergraduate thermodynamics laboratory by comparing VR and face-to-face (F2F) formats across two cohorts (F2F: Spring 2024, n=34; VR: Spring 2025, n=36). We assessed perceived learning gains, skill development, and actual knowledge gains using a retrospective Post-Pre survey and identical knowledge-based questions.

Repeated measures analysis revealed significant improvements from Pre to Post in both cohorts for defining fugacity [$F(1,68)=17.56$, $p=0.001$], equipment usage [$F(1,67)=24.31$, $p=0.001$], and data collection [$F(1,68)=22.49$, $p=0.001$]. Knowledge assessments showed comparable performance overall, with VR students outperforming F2F peers on two items: dominant forces when fugacity coefficient exceeds one (47% vs. 15%, $p=0.005$) and residual volume at zero pressure (55% vs. 30%, $p=0.032$). VR students also scored higher in problem-solving ($t(64)=2.08$, $p=0.04$), while F2F students excelled in teamwork ($t(64)=5.64$, $p=0.001$). Other skills - knowledge application, posing questions, systems thinking, and design thinking - showed no significant differences.

Our findings indicate VR delivers learning outcomes comparable to traditional labs, successfully replicating critical skills such as equipment handling and data collection. VR offers a practical solution when physical labs are inaccessible, as during COVID-19, and opens opportunities for teaching topics constrained by safety or technical limitations. However, teamwork challenges in VR highlight the need for intentional design to support collaboration. Future research should explore strategies to enhance collaboration and extend VR applications to other domains where hands-on labs are impractical.

Chemical Education

From Grading to Learning: A Digital Reflective Assessment Framework for Chemistry Laboratories

Ruthy Sfez¹

Materials engineering, Azrieli, college of engineering, Israel

Laboratory courses are a central component of STEM education, offering a unique setting for active learning, development of critical thinking, and acquisition of professional laboratory skills. Yet, assessment of laboratory work is often intuitive, opaque, and largely summative, limiting its effectiveness as a learning tool during the course.

To address this gap, we developed MIRROR (Method for Instructor–Student Reflective Rubric-Based Observation & Review), an eight-parameter assessment framework designed to align instructor evaluation with guided student self-assessment. In each laboratory session, students and instructors independently evaluate performance using the same rubric. Comparison of these parallel evaluations highlights discrepancies between perceived and observed performance, creating structured opportunities for reflection, dialogue, and formative feedback.

This work presents the digital transformation of MIRROR from a paper-based tool into a mobile, rubric-based interface developed at Azrieli College of Engineering. The digital platform enables immediate data entry following laboratory sessions, automated comparison of instructor and student evaluations, and real-time alerts when discrepancies exceed predefined thresholds. This approach shifts assessment from retrospective grading to a continuous, formative learning process throughout the semester.

The system was piloted recently in first-year Analytical Chemistry Laboratory courses in the Departments of Materials Engineering and Pharmaceutical Engineering. Preliminary findings demonstrate high usability, strong student engagement with self-evaluation, and increased motivation to reflect on performance when students' self-assessments differ from instructor's evaluations. These results suggest that the digital implementation of MIRROR enhances transparency, engagement, and reflective learning in chemistry laboratories, with potential for broader adoption across STEM laboratory education.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
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CLASSIC AND QUANTUM THERMODYNAMICS

Chair: David Gelbwaser- Klimovsky

Invited Lecture

Classic and Quantum Thermodynamics

Thermodynamic Geometry Near Phase Transitions

Oren Raz¹, Omer Basri²

¹*Weizmann Institute of Science, Israel*

²*Weizmann, Israel*

Thermodynamic geometry provides a geometric framework, rooted in linear-response theory, for quantifying dissipation in driven systems, and is widely used in the analysis of heat engines, distillation processes, and chemical reactions. In this approach, the excess work defines a Riemannian metric on the space of control parameters, a metric that typically diverges at phase transitions. We show, however, that despite this divergence the thermodynamic length across a transition can remain finite. Consequently, optimal driving protocols may exist even though they do not satisfy the geodesic equation. In addition, we identify situations in which the globally optimal protocol crosses a phase-transition line twice, even when a path avoiding the transition entirely is available. These results clarify how geometric optimal-control methods behave near criticality and when they fail to reduce to geodesic minimization.

Invited Lecture

Classic and Quantum Thermodynamics

Necessary conditions for the Markovian Mpemba effect

David Gelbwaser-Klimovsky¹

Technion, Israel

The Markovian Mpemba effect is a counterintuitive thermodynamic behavior where the thermalization time does not depend monotonically on the difference between the bath and the initial temperatures (i.e., a hot system can cool down faster than a cold one (Direct Mpemba) or a cold system can heat up faster than a hot one (Inverse Mpemba). Here, we find simple conditions on the transition rates for a three-level system to exhibit the Mpemba effect. We prove analytically that these conditions can be used to obtain information about the Mpemba effect for an N-level system if the bath is at zero temperature. Moreover, we numerically demonstrate that this extends to any bath temperature. Finally, we study the implications of our results for different models of transition rates.

Invited Lecture

Classic and Quantum Thermodynamics

Relation between entropy and kinetics far from equilibrium

Prof. Haim Diamant¹

School of Chemistry, Tel Aviv University, Israel

The entropy of a material at steady state is a static property arising from the statistical distribution of its particles' configurations. Kinetic coefficients are dynamic properties related to how the particles move and transport momentum and energy. Despite this distinction, upon a change in thermodynamic variables such as temperature or density, the resulting changes in static and dynamic properties may be inter-dependent. For example, at equilibrium, the particles' self-diffusion coefficient and mobility (kinetics) are tied to the temperature (statics) via the Einstein relation. Using a variational principle, we derive general inequalities, which tie changes in the entropy to changes in kinetic coefficients for steady states arbitrarily far from equilibrium. We demonstrate the validity and usefulness of these relations in several examples.

Invited Lecture

Classic and Quantum Thermodynamics

Magnetic Moments at the Molecule-Metal Interface: A Seeming Violation of the Onsager Relations?

Prof. Yonatan Dubi¹

Chemistry, Ben Gurion University of the Negev, Israel

When organic molecules are adsorbed onto a metal surface, a constant, permanent magnetic moment can emerge. In the case of chiral molecules, this magnetic moment aligns with the molecular chiral axis, a phenomenon known as the Chiral-Induced Spin-Selectivity (CISS) effect. This effect has been evidenced both directly, through local magnetic detection, and indirectly, via the magnetoresistance of metal-molecule-metal junctions. However, the emergence of a magnetic moment from non-magnetic components and the observation of linear-response CISS magnetoresistance appear to challenge Onsager's theorem. According to the theorem, permanent magnetization cannot exist in a system where time-reversal symmetry is preserved. Is the presence of a molecule on a metal surface and the ensuing emergent magnetic moment truly a violation of the Onsager relations, or perhaps there is a simple explanation to this mystery?

Classic and Quantum Thermodynamics

Combining Harmonic Sampling with the Worm Algorithm to Improve the Efficiency of Path Integral Monte Carlo

Sourav Karmakar¹, Sutirtha Paul², Dr Adrian Del Maestro^{2,3}, Dr Barak Hirshberg^{1,4}

¹*School of Chemistry, Tel Aviv University, Israel*

²*Department of Physics and Astronomy, University of Tennessee, Knoxville, USA*

³*Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, USA*

⁴*Center for Computational Molecular and Materials Science, Tel Aviv University, Israel*

We propose an improved Path Integral Monte Carlo (PIMC) algorithm called Harmonic PIMC (H-PIMC) and its generalization, Mixed PIMC (M-PIMC). PIMC is a powerful tool for studying quantum condensed phases. However, it often suffers from a low acceptance ratio for solids and dense confined liquids. We develop two sampling schemes especially suited for such problems by dividing the potential into its harmonic and anharmonic contributions. In H-PIMC, we generate the imaginary time paths for the harmonic part of the potential exactly and accept or reject it based on the anharmonic part. In M-PIMC, we restrict the harmonic sampling to the vicinity of local minimum and use standard PIMC otherwise, to optimize efficiency. We benchmark H-PIMC on systems with increasing anharmonicity, improving the acceptance ratio and lowering the autocorrelation time. For weakly to moderately anharmonic systems, at $\beta\hbar\omega = 16$, H-PIMC improves the acceptance ratio by a factor of 6-16 and reduces the autocorrelation time by a factor of 7-30. We also find that the method requires a smaller number of imaginary time slices for convergence, which leads to another two- to four-fold acceleration. For strongly anharmonic systems, M-PIMC converges with a similar number of imaginary time slices as standard PIMC, but allows the optimization of the autocorrelation time. We extend M-PIMC to periodic systems and apply it to a sinusoidal potential. Finally, we combine H- and M-PIMC with the worm algorithm, allowing us to obtain similar efficiency gains for systems of indistinguishable particles.

Classic and Quantum Thermodynamics

Density Asymmetry Diagnostic for Coupled-Cluster Methods

Miss Kaila Weflen¹, Dr Megan Bentley², Dr James Thorpe³, Dr Peter Franke², Dr Gregory Jones², Dr Devin Matthews⁴, Dr Jan Martin¹, Dr John Stanton²

¹*Weizmann Institute of Science, Israel*

²*University of Florida, United States*

³*Argonne National Laboratory, United States*

⁴*Southern Methodist University, United States*

Diagnostic tools have long been used by theorists and experimentalists alike to assist in understanding different aspects of a molecular system – e.g., the *T1* diagnostic by Lee and Taylor,¹ which is used to provide insight into nondynamical correlation effects. Typically, existing wavefunction based diagnostics are evaluated at the CCSD level, which presents a limitation when moving to higher order coupled-cluster (CC) methods. Shortly before passing away, Prof. John Stanton and coworkers developed the density asymmetry diagnostic (DAD)² as a novel approach to judge the reliability of various CC methods. The DAD evaluates the degree of non-Hermiticity exhibited by an approximate CC method as contrasted to the fully Hermitian nature of the full configuration interaction limit. The initial implementation (presented at Sanibel 2023) first considered the asymmetry of the occupied-virtual/virtual-occupied blocks of the one-particle reduced density matrix (1PRDM), and has since evolved to evaluating the asymmetry of the entire 1PRDM (normalized based on the number of correlated electrons for size-intensivity). This diagnostic has been applied to various test cases of molecules ranging from the initial test suite of molecules,² the W4-17 dataset³ including open-shell systems, and presently to 3d and 4d transition metal-containing diatomics. We will discuss the DAD in its entirety from its inception to current applications, highlighting the contributions of Prof. Stanton to the field.

Classic and Quantum Thermodynamics

Thermally Stable Binary Hybrid Organic-Inorganic Perovskite Glasses

Arad Lang^{1,2}, Ms. Chumei Ye², Ms. Celia Chen², Ms. Emily V. Shaw², Dr. Lauren N. McHugh³, Prof. Sian E. Dutton⁴, Prof. Thomas D. Bennett²

¹*Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Israel*

²*Materials Science and Metallurgy, University of Cambridge, United Kingdom*

³*Chemistry, University of Liverpool, United Kingdom*

⁴*Physics, University of Cambridge, United Kingdom*

Two-dimensional hybrid organic-inorganic perovskites (2D-HOIPs) have recently garnered significant attention for their potential integration into next-generation optoelectronic applications. Their chemical diversity and straightforward synthesis, together with band gap tunability and enhanced stability, make them promising candidates to replace their three-dimensional counterparts as active materials in photovoltaics, light emitters, and photodetectors. Recent studies have revealed that 2D-HOIPs with the chemical formula $(RNH_3)_2MX_4$ (where R is a bulky organic moiety, M is a divalent metal cation, and X is a halide) can undergo melting — a reversible solid-liquid transition — upon heating. Furthermore, by carefully engineering the organic cation, the cooling-induced crystallisation can be suppressed, resulting in a glassy (amorphous) state. However, these so-called "HOIP glasses" exhibit thermal instability, reverting to their thermodynamically stable crystalline form upon mild heating or even at room temperature over a time span of hours to days.

In this work, we address the thermal instability of HOIP glasses through melt alloying, a technique we recently demonstrated to apply to meltable 2D-HOIP systems. Binary HOIP glasses were synthesized by blending powders of two glass-forming 2D-HOIPs: $(S-NEA)_2PbBr_4$ (where S-NEA = (S)-(-)-1-(1-naphthyl)ethylamine) and $(MIPA)_2PbI_4$ (where MIPA = methyl-iodopropylamine). Melt-quenching these blends resulted in the formation of glassy phases. The glass transition temperatures, optical band gap, and mechanical hardness of these glasses were found to depend on the blend composition. Most notably, the binary glasses exhibited complete thermal stability, with no recrystallisation observed even after one month of storage at room temperature.

Classic and Quantum Thermodynamics

Another angle on noncovalent interactions

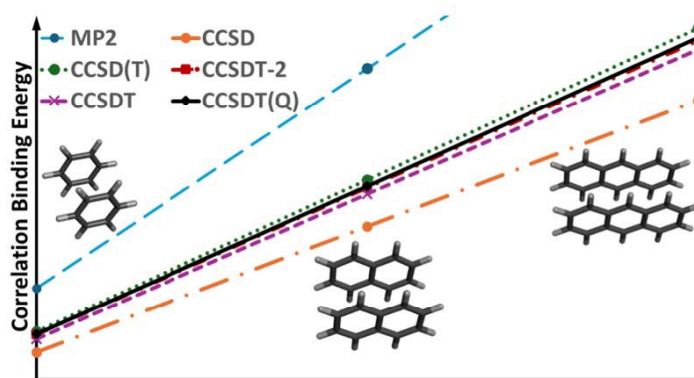
Vladimir Fishman¹, Prof. Michał Lesiuk², Prof. A. Daniel Boese³, Prof. Jan M. L. Martin¹

¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Faculty of Chemistry, University of Warsaw, Poland*

³*Department of Chemistry, University of Graz, Austria*

For noncovalent interactions, the CCSD(T) method is considered to be the "gold standard". However, recent FN-DMC (fixed-node diffusion [quantum] Monte Carlo) benchmarks have cast doubt on this, showing a discrepancy that grows progressively with system size, especially for pi-stacked complexes. One possible culprit is the neglect of higher-order correlation effects in CCSD(T). Unfortunately, CCSDT(Q) calculations scale as $O(N^9)$ with system size, making them impractical. We show, for pi-stacked sequences of polyacene and alkapolyene dimers, that the correlation energy scales almost linearly with the number of subunits in the monomers. We then compared the slopes of the lines for various approximate correlation methods to that obtained at the CCSDT(Q) level from benzene and naphthalene dimers. We thus find that, while CCSD(T) does overbind pi-stacks somewhat, it does not do so to the degree suggested by the FN-DMC simulations. The repulsive higher-order T3 terms are compensated to a large degree by the attractive contribution of connected quadruples (Q).

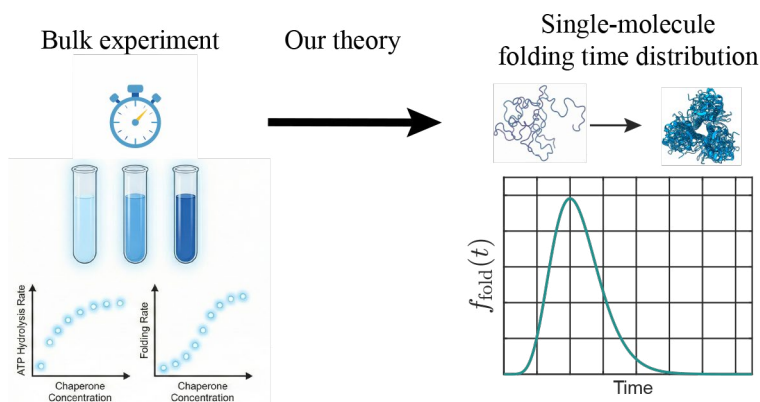


Classic and Quantum Thermodynamics

Inferring Complete Protein Folding-Time Distributions from Bulk Measurements of Chaperone-Assisted Folding

Tommer David Keidar¹, Prof. Shlomi Reuveni¹
School of Chemistry, Tel Aviv University, Israel

To function properly, many proteins need to fold into a well-defined 3D structure. To reduce folding time, living creatures evolved a system of chaperones – proteins that help fold other proteins. One of the mechanisms that chaperones use is to unfold misfolded proteins and give them a second chance to fold properly. In recent years, stochastic resetting, i.e., halting a process midway and bringing it back to its initial condition, emerged as a topic of growing interest in non-equilibrium thermodynamics. It was shown that stochastic resetting can accelerate processes with a broad completion time distribution. We treat chaperones as resetting agents; basically, we frame the “second chance to fold” mechanism as stochastic resetting. We derive the folding rate and ATP consumption rate as a function of chaperone concentration. Importantly, we show that based on our theory, it is possible to measure the entire folding time distribution, using bulk measurements only of the folding rate and ATP hydrolysis rate as a function of chaperone concentration. Currently, measuring the folding time distribution requires single-molecule experiments. Finding the entire folding time distribution without the need for single-molecule experiments will democratize production of this data, making it far more available. This could shed new light on protein folding pathways, en route to new and better cures to misfolding-related pathologies.



Classic and Quantum Thermodynamics

Morphology-Activated Second-Harmonic Generation in Metastable Para-Red Plate Crystals

Alon Krause¹, Prof. Adi Salomon¹
Bar Ilan University, Israel

Organic molecular crystals offer high optical nonlinearity, yet their application is frequently hindered by the thermodynamic drive toward energetically stable but non-functional forms. In this work, we utilize Para-Red as a model system to demonstrate how growth conditions can override these thermodynamic preferences. While Para-Red is historically considered optically inert due to its thermodynamically favored needle-like growth habit which masks the polar axis, we successfully stabilized a distinct 2D plate-like morphology using vapor deposition at 180-230°C.

Single-crystal X-ray diffraction confirmed that both the stable needles and our vapor-deposited plates belong to the same non-centrosymmetric space group. This reveals that the material's inactivity is not a fundamental structural limitation, but a morphological one defined by facet stability. By kinetically stabilizing the plate morphology, we exposed the active plane parallel to the molecular layers, granting direct optical access to the hyperpolarizability axis. Consequently, these plates exhibit strong Second Harmonic Generation (SHG), effectively "switching on" latent nonlinearity that is forbidden in the equilibrium needle form.

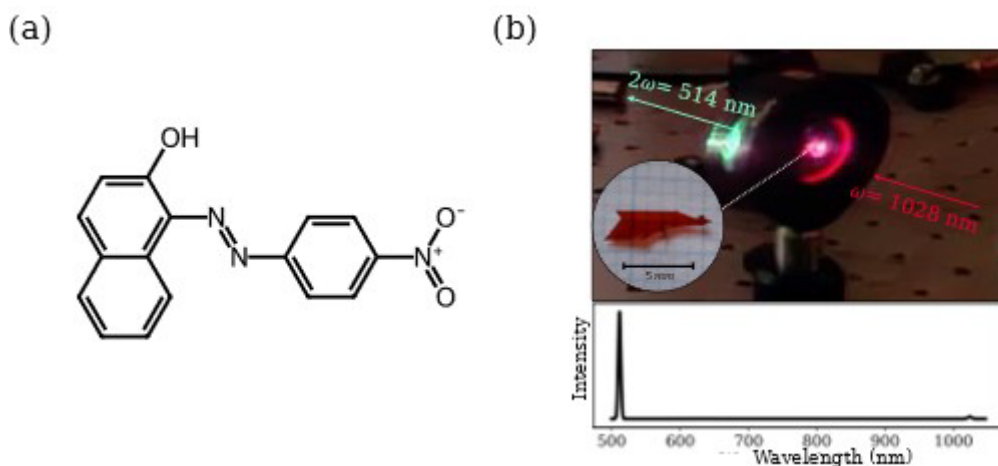


Figure: Para-Red as an optically active material (a) Para-Red molecule, possessing electron donor (OH) and acceptor (NO₂) groups inducing high polarizability. (b) A plate crystal in a laser setup; an incoming 1028 nm IR beam produces green 514 nm SHG. The optical spectrum shows a sharp SHG peak at 514 nm and a small remnant of the 1028 nm signal.

Classic and Quantum Thermodynamics

the markovian mpemba effect in 4 level systems

Mr Ido Avitan¹

Physics, Technion, Israel

The Mpemba effect is a counterintuitive phenomenon that has been observed, most famously in water, where hot water freezes faster than cold water. We study the Mpemba effect in a quantum mechanical setup, focusing on a Markovian N level system. Previous work analytically derived the necessary conditions for the effect to occur in a 3-level system. In this talk, we investigate how these conditions can be extended to systems with more levels. We identify emerging patterns in $N=3$ level systems, with several particularly curious phenomena appearing in the $N=4$ case.

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Energy

Chair: Hannah-Noa Barad

Invited Lecture

Energy

On the Importance of Careful Electrochemical Analysis in Battery Performance Reporting

Malachi Noked

Chemistry Department, Bar-Ilan University

Accurate and transparent reporting of battery performance are essential for meaningful comparison, reproducibility, and technological progress. However, several commonly used electrochemical characterization techniques are frequently over-interpreted or insufficiently contextualized in performance-oriented manuscripts. In my talk I will briefly review current practices in battery performance reporting, with particular emphasis on the limitations of half-cell measurements, differential capacity (dQ/dV) analysis, voltage window selection in anode studies, and the reporting(/ignoring) of coulombic efficiency. While half-cell data are valuable for mechanistic insight, they often fail to capture realistic operating conditions and can lead to inflated expectations when extrapolated to full-cell performance. Similarly, dQ/dV plots are powerful diagnostic tools, yet are highly sensitive to testing protocols, smoothing procedures, and cell history, which are not always adequately disclosed. The choice of voltage window, especially for anode materials, can strongly bias apparent capacity, stability, and degradation trends, complicating comparisons across studies. Finally, coulombic efficiency is frequently measured under irrelevant electrochemical conditions, limiting its relevance for assessing long-term stability. By highlighting these issues, my talk advocates for more careful, standardized, and context-aware use of performance metrics, aiming to improve the reliability and interpretability of battery research reported in the literature.

Invited Lecture

Energy

Reorganization of Mg Species Enables Cathode Electrochemistry

Ahiud Morag¹

Department of Chemical Engineering, Ben Gurion University, Israel

Mg-metal batteries (MMBs) offer a promising solution to the growing demand for advanced energy storage systems. However, challenges related to electrolyte compatibility with the Mg anode significantly impede their practical application. In this context, Cl-containing electrolytes are particularly attractive due to their superior anode performance. Nonetheless, a critical challenge in the utilization of these electrolytes is the high Mg-Cl dissociation energy, primarily caused by the presence of thermodynamically stable, large $\text{Mg}_x\text{Cl}_y^{2x-y}$ clusters. While previous studies have demonstrated the potential catalysis of Mg-Cl dissociation on the Chevrel phase (Mo_6S_8) surface, the phenomenon has not been replicated in other cathode systems. Here, we address the suboptimal cathode electrochemistry associated with Cl-containing electrolytes by manipulating the electrolyte species. The incorporation of ionic liquid additives into conventional MMB electrolytes results in the appearance of new voltage plateaus, indicating novel redox pathways. We employed electrochemical, structural, and chemical characterization techniques to elucidate the role of the ionic liquid additives. By combining spectroscopic methods with molecular dynamics simulations, we visualize the specific reorganization of Mg species. Our findings challenge the conventional paradigm that material engineering is the sole driver of MMB electrochemistry, revealing instead a complex multistep reaction mechanism enabled by the favorable reorganization of the electrolyte solvation structure.

References:

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- [2] A. Morag et al., *Energy Storage Mater.* 2022, 53, 435–443.
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Invited Lecture

Energy

Photocatalytic panels development for catalytic oxidation and reduction reactions

Menny Shalom

Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva, Israel

mennysh@bgu.ac.il

Heterogeneous photocatalysis is an attractive enabler of the efficient execution of various important environmental (e.g., hydrogen production and C-based fuel production) and organic reactions utilizing solar energy. In a typical batch reactor, a heterogeneous photocatalyst is dispersed in a given solution together with reactants, and upon illumination, a chemical reaction occurs. Despite its simplicity, the overall process faces some challenges related to the intrinsic nature of the reaction conditions: light penetration significantly decreases with distance, the photocatalyst should be continuously stirred to avoid sedimentation, separating the products from the photocatalyst is not trivial, the catalyst is hard to recycle, the reaction is dependent on the concentration of starting reactants, and scalability is questionable.

An alternative approach is to use a panel based on a photocatalytic material. This configuration enhances light management and facilitates easy recycling and scalability, similar to that of solar cells. Furthermore, the photocatalyst panel can be easily incorporated into a continuous-flow reactor, facilitating constant reactant feed and product separation. In recent years, polymeric carbon nitride (CN) materials have emerged as a class of photocatalysts for many reactions, from solar fuel production to biomass conversion and complex organic transformations. Nevertheless, most studies have focused on using CN powders as heterogeneous photocatalysts. Some pioneering works have shown the utilization of CN panels, primarily for H₂ production. However, all these panels were prepared by drop-casting or screen-printing a synthesized catalyst with a polymer containing perfluoro groups (i.e., Nafion) or a SiO₂ binder onto frosted glass or steel plates. The use of a binder can lead to photocatalyst detaching from the substrate due to the formation of radicals during the reaction, such as reactive organic species (ROS). This phenomenon primarily occurs in organic chemical reactions, where ROS intermediates can react with the binder to produce unwanted byproducts.

This talk will introduce facile and scalable approaches for growing polymeric carbon nitride (CN) layers on conductive substrates with tunable structural and photophysical properties for photocatalytic applications. We demonstrate CN-based photocatalytic panels as highly stable, efficient platforms for converting organic molecules into value-added chemicals while simultaneously producing hydrogen and hydrogen peroxide. Additionally, I will demonstrate the use of CN-films as highly stable photocatalytic panels for various catalytic and cascade reactions.

Invited Lecture

Energy

Tracking Lithium Dendrites and Solid Electrolyte Interphase Formation using Solid State NMR Spectroscopy

Prof. Michal Leskes¹

Weizmann Institute of Science, Israel

Polymer-ceramic composite electrolytes enable safe implementation of Li metal batteries with potentially transformative energy density. Nevertheless, the formation of Li-dendrites and its complex interplay with the Li-metal solid electrolyte interphase (SEI) remain a substantial obstacle which is poorly understood.

In this talk I will present our approach to tackle this issue by a combination of solid-state NMR spectroscopy and Overhauser dynamic nuclear polarization (DNP) which boosts NMR interfacial sensitivity through polarization transfer from the metal conduction electrons. We achieve unprecedented molecular-level insight into dendrites formation and propagation within the composites and determine the composition and properties of their SEI. We find that the dendrite's quantity and growth path depend on the ceramic content and correlated with battery's lifetime. We show that the enhancement of Li resonances in the SEI occurs through Li/Li⁺ charge transfer in Overhauser DNP, allowing us to correlate NMR signal enhancements with Li transport and thus directly determine the SEI lithium permeability. These findings have promising implications for SEI design and dendrites management which are essential for the realization of Li metal batteries.

Invited Lecture

Energy

Emergent Interfacial Dynamics: Rethinking Catalysis for a Sustainable Energy Future

Charlotte Vogt¹

Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Israel

Advancing the global transition to sustainable energy requires catalytic systems capable of operating efficiently under inherently dynamic, electro-driven conditions. Yet many of the processes governing activity and selectivity unfold on timescales and in interfacial regions that remain inaccessible to conventional operando methodologies. In this talk, I will discuss our recent efforts to uncover these hidden dynamic regimes by integrating time-structured perturbations, broadband operando spectroscopy, and data-driven analysis to resolve the nonlinear, multi-timescale behavior of catalytic interfaces. Applied to CO₂ electroreduction, these approaches reveal that key steps, ranging from electric-double-layer reorganization to adsorbate interconversion, proceed not through smooth relaxation but through discrete, emergent dynamical events that strongly depend on cation identity and solvation structure. By distinguishing the temporal signatures of interfacial, diffuse-layer, and concentration-gradient processes, we expose how fluctuating water networks and charge redistribution events govern catalytic pathways far beyond the active site itself. These insights recast catalytic function as a product of dynamically coupled fields, structures, and reaction intermediates, and provide a foundation for rationally designing catalysts that leverage, rather than fight against, interfacial complexity. This dynamic viewpoint opens new avenues for controlling electrochemical transformations central to the future energy landscape.

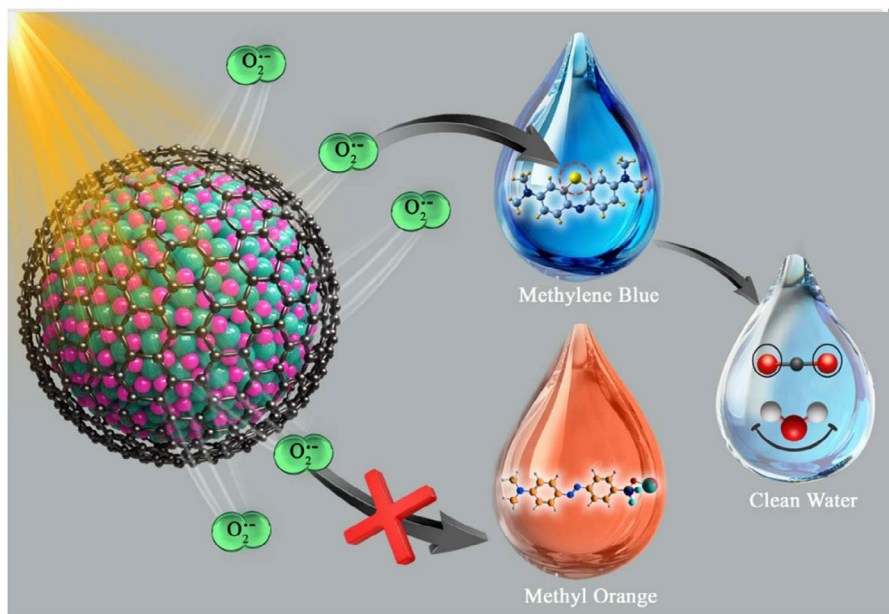
Invited Lecture

Energy

Highly selective photocatalytic degradation of organic pollutants by coreshell nanoparticles via superoxide radical pathway

Lena Yadgarov

Rapid industrialization and extensive human activities have led to severe environmental challenges, particularly water contamination by persistent organic pollutants, which pose serious risks to ecosystems and human health. Photocatalytic technology provides a sustainable approach to pollutant degradation using solar energy. In this study¹, we employ ultrathin carbon-encapsulated ZnO nanoparticles, ZnO@C, as an efficient photocatalyst, using methylene blue and methyl orange as model pollutants. The carbon has a favourable band alignment with ZnO for efficient charge transfer. In fact, optical absorption studies and finite-difference time-domain simulations establish enhanced absorption and light–matter interaction upon thin, uniform carbon encapsulation. Photoluminescence quenching (~80%) indicates reduced electron–hole recombination, facilitated by defect-induced charge transfer from ZnO to carbon. Electron paramagnetic resonance measurements reveal that superoxide radicals ($\text{O}_2^{\bullet-}$) are the dominant reactive species, driving a selective radical-mediated degradation pathway. Compared to pristine ZnO, the ZnO@C system exhibits over 60% higher degradation efficiency. Liquid chromatography–mass spectrometry analyses elucidate the sequential degradation pathway driven by $\text{O}_2^{\bullet-}$. The ZnO@C exhibits excellent photostability and reusability across multiple cycles, with a sixfold increase in kinetic rate constants compared to pristine ZnO. These improvements highlight the potential of ZnO@C core@shell nanostructures for sustainable environmental remediation.



¹ Prasad, N., et al. "Highly selective photocatalytic degradation of organic pollutants by ZnO@C core–shell nanoparticles via superoxide radical pathway." *Small* (2025): e08852.

Invited Lecture

Energy

Organic Spacer Control of Charge Transport and Luminescence in Mn-Doped 2D Perovskites

Dr. Ido Hadar¹

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

Two-dimensional (2D) halide perovskites have emerged as a versatile platform for tunable optoelectronic materials, owing to their layered crystal structure and chemical flexibility. In these materials, organic spacer ligands separate the inorganic perovskite layers and play a central role in governing structural rigidity, charge transport, and light emission. Understanding how spacer chemistry influences excited-state processes is therefore essential for rational materials design.

In this talk, I will present a comparative study of manganese (Mn)-doped 2D perovskites incorporating either aromatic phenethylammonium (PEA) or aliphatic butylammonium (BA) spacer ligands. Mn doping provides a robust route to introduce strong, broadband luminescence, yet the interplay between dopant emission, exciton transport, and spacer identity remains poorly understood. By systematically varying Mn concentration and sample morphology, from nanoplatelets to bulk crystals, we uncover distinct doping regimes, including edge-localized Mn incorporation at high doping levels and uniform dopant distribution at lower concentrations.

Despite similar Mn incorporation behavior, the two spacers lead to markedly different optical responses. PEA-based perovskites exhibit significantly stronger Mn-related emission than their BA-based counterparts. Using transient reflection microscopy, we directly probe exciton transport and find nearly a twofold enhancement in exciton diffusivity for PEA systems. These differences are correlated with crystal rigidity and exciton–phonon coupling.

Overall, this work highlights how organic spacer ligands control both charge mobility and luminescence in 2D perovskites, offering design principles for next-generation light-emitting materials.

Energy

Unveiling Solid Electrolyte Interphase Doping

Roy Marrache¹, Dr. Tzach Mukra¹, Mr. David Stark¹, Dr. Evelina Faktorovich-Simon¹,
 Prof. Emanuel Peled¹

School of Physical Chemistry, Tel-Aviv University, Israel

Energy storage systems (ESSs) are essential for large-scale renewable energy utilization and electrification across technologies. Improving cycle life, safety, and energy density remains a central priority. Among the critical components influencing ESSs performance, the solid electrolyte interphase (SEI), controls safety and energy parameters in rechargeable lithium systems¹.

Multiple strategies tune SEI composition and structure²: electrolyte additives³, salt composition⁴, incorporation of inert inorganic nanoparticles into the electrolyte (suspension electrolytes, SE)⁴⁻⁷. These could be referred to as doping, which alter the SEI's chemistry and microstructure, hypothesized to increase grain boundaries (GBs), introducing ionically conductive paths, reducing inactive metal accumulation and thus improving safety and power density.

This concept was first suggested in 1979: "...the ionic resistivity of the SEI should be decreased by doping. This way both the electric field, which be developed on the SEI, and the electrical heating of the SEI will be reduced¹." It was found that this approach increases ionic conductivity, reduces electrolyte consumption and reduces "dead-Li" accumulation during cycling³⁻⁷. SEI doping is an attractive, inherently scalable approach for next generation ESSs.

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6. R. Marrache et al, *J. Solid State Electrochem.*, 26, (2022).
7. T. Mukra et al, *J. Electrochem. Soc.*, 168, (2021).

Energy

Pressure Driven Interplay of Rashba, Rashba-Dresselhaus and Persistent Spin Texture in Lead-free Quasi-2D Hybrid Perovskites

Jagjit Kaur^{1,2}, Prof. Sudip Chakraborty¹

¹*Physics, Harish-Chandra Research Institute, India*

²*Chemistry, Bar Ilan University, Israel*

The quasi-2D hybrid halide perovskites have emerged as promising nano-structures in the field of optoelectronics. However, the toxicity related to the presence of lead (Pb) in such lower dimensional systems remain as a challenge, which leads to the discovery of lead-free analogues. In this work, we have envisaged two such quasi-2D hybrid halide perovskites with orthorhombic crystal structure (space group Pca21), based on germanium (Ge) and tin (Sn) in the form of (A-Pyr)₂GeI₄ and (A-Pyr)₂SnI₄, where A-Pyr is the organic counterpart C₆H₁₀N₂. Based on the systematic electronic structure calculations and spin texture analysis, we have witnessed structural, electronic, optical and most interestingly spin texture evolution in both the perovskites under the evolution of pressure. We have considered the pressure limit of 10.4, and 7.5 GPa respectively for Ge and Sn based systems, till the thermodynamic stability prevails with negative formation energy. The unique transition between Rashba (R), Rashba-Dresselhaus (RD) and persistent spin texture (PST) has been observed through the tuning of pressure on the systems. For (A-Pyr)₂GeI₄, PST emerges above 4.3 GPa in the valence band and throughout all the pressure point in the conduction band, with Rashba splitting strength reaching 0.73 eVÅ. Interestingly, (A-Pyr)₂SnI₄ exhibits dynamic transitions between Rashba, Rashba-Dresselhaus splitting and PST, influenced by Sn-5p orbital contributions.

Energy

Interaction of lithium dendrites in composite ceramic-polymer solid-state electrolyte in lithium-metal batteries

Guy Saller¹, Nadav Maimon¹, Dr. Ayan Maity¹, Prof. Michal Leskes¹
*Department of Molecular Chemistry and Materials Science, Faculty of Chemistry,
 Weizmann Institute of Science, Israel*

The increasing global energy demand requires the development of novel technologies of energy storage. Lithium-metal batteries yield much higher theoretical specific capacity compared to lithium-ion batteries. Solid electrolytes offer a safe route for utilizing metal anodes, with polymer-based electrolytes being advantageous due to their mechanical flexibility. However, polymer electrolytes suffer from relatively low ionic conductivity and are susceptible to growth of lithium dendrites which can cause short-circuits. Introducing ceramic particles to the polymer matrix increases its ionic conductivity. Nevertheless, the intricate interaction between dendrites and the ceramic particles, resulting in the formation of the solid electrolyte interphase (SEI) and controlling the dendrites propagation path, remains unclear.

High sensitivity solid-state NMR spectroscopy enables a detailed examination of dendritic growth and of the composition of the SEI layer. The enhanced sensitivity, gained by transfer of spin polarization from the lithium conduction electrons, allows identifying distinct blockage mechanisms of dendrites. Lithium-based ceramics, namely $\text{Li}_{1.5}\text{Al}_{0.5}\text{Ge}_{1.5}(\text{PO}_4)_3$, have been shown to hinder the growth of dendrites via a chemical interaction. The resulting SEI layer incorporates unique chemical environments, originating from the lithium ceramics. However, passive additives are known to physically block the progression of dendrites across the cell. We have demonstrated that ZrO_2 -based electrolyte forms a new unrecognized environment near the dendrites, which may be either an intercalation of lithium or a new intermetallic phase. These findings may indicate about a previously unknown interaction mechanism. It may contribute to the mitigation of dendrites in lithium metal batteries and to the development of high-capacity energy storage technologies.

Energy

High-capacity polydiacetylene cathode for high-performance zinc ion batteries

Anita Samage¹, Dr. Nitzan Shauloff¹, Prof. Raz Jelinek¹

Department of chemistry, Ben Gurion University of the Negev, Israel

Organic cathodes are perceived as promising alternatives to metal-based electrodes in energy storage devices, considering their structural and electrochemical tunability and benign environmental impact. Most organic cathodes in zinc ion batteries, however, operate at relatively low voltages (1.0 V vs. Zn^{2+}/Zn), thereby limiting their practical applicability. We constructed an organic cathode exhibiting excellent electrochemical properties, utilizing, for the first time, polydiacetylene—a unique conjugated polymer exhibiting remarkable structural and electronic properties. Specifically, a zinc ion battery comprising anthraquinone-functionalized polydiacetylene cathode, further doped with polyaniline (PANI) for conductivity enhancement, and $\text{Zn}(\text{ClO}_4)_2/\text{acetonitrile}$ as electrolyte, exhibited excellent electrochemical features, including high specific capacity (330 mAh g⁻¹ at 0.1 A g⁻¹) and energy density (277 Wh kg⁻¹ at 0.1 A g⁻¹), excellent rate capability and long-term cycling stability. The polydiacetylene-based cathode is inexpensive, readily synthesized, and environmentally friendly, offering a pathway toward the introduction of high-performance organic zinc-ion batteries.

Energy

Long-Range Electrostatics and Configuration Ensembles Are Key to Predicting Electrolyte Redox Potential Trends: Insights from MD and QM/MM Simulations

Khorsed Alam¹, Dr. Shubham Patel^{1,2}, Dr. Amreen Bano^{1,3}, Dr. Langyuan Wu⁴, Prof. Netanel Shpigel⁴, Prof. Dan Thomas Major¹

¹*Bar-Ilan University, Israel*

²*IIT Kharagpur, India*

³*TCG-CREST, India*

⁴*Ariel University, Israel*

The stability and performance of electrolytes are central to advancing energy storage technologies. In particular, their redox potentials define the electrochemical window accessible during battery cycling. Although redox trends can be inferred from computed frontier orbital energies or ionization potentials (IP) and electron affinities (EA), accurately capturing long-range electrostatics remains challenging. Established solution-phase embedding methods (e.g., continuum solvation, cluster–continuum, polarizable embedding, and QM/MM) have seen limited application and validation in complex electrolytes. In this study, we adopt an integrated approach combining classical molecular dynamics (MD) simulations and quantum mechanics–molecular mechanics (QM/MM) calculations to estimate electrochemical stability. MD simulations generate representative solution configuration ensembles, which are then subjected to QM/MM calculations to determine the HOMO, LUMO, and vertical IP and EA. To capture long-range electrostatics and configurational effects, we include increasingly larger solvation shells and perform ensemble averaging. Using this framework, we study two widely used electrolytes for lithium- and sodium-ion batteries and investigate the effect of anion additives. We conclude that it is important to include several solvation shells and to average over configuration ensembles to accurately compute the frontier orbitals of electrolyte molecules. This approach, for the first time, computes oxidative and reductive stability trends of electrolyte species while capturing long-range and configurational effects. We also observe that, while vertical IP and EA values correlate with HOMO–LUMO energies, structural relaxation of oxidized and reduced species—particularly for organic carbonates upon reduction—weakens this correlation, underscoring the need to account for geometry relaxation in realistic redox modeling.

Energy

Improving the Properties of the Interface between Lithium/Sodium Anode and Solid Electrolyte

Lina Faktorovich¹, Prof. Emanuel Peled¹

Faculty of Exact Sciences, School of Chemistry, Tel Aviv University, Israel

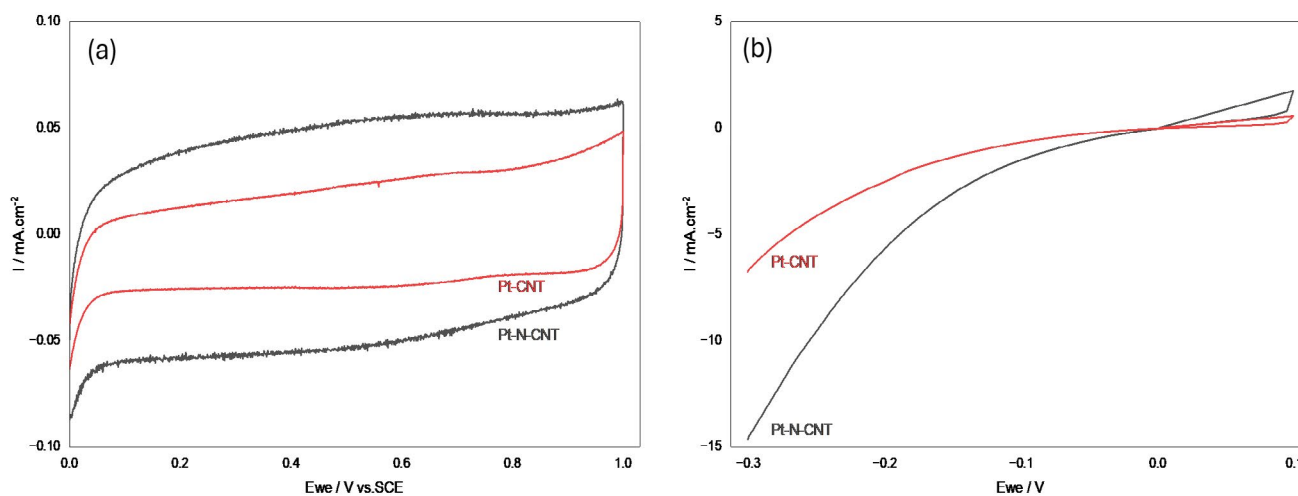
The development of solid-state lithium and sodium metal batteries necessitates improved the interfacial stability between the solid electrolytes (SEs) and the metallic anodes to enhance their efficiency, safety, and cycle life. This study introduces a simple and cost-effective approach using a porous polyethylene micro-layer (PEML) preloaded with a liquid electrolyte containing metal oxide nanoparticles (MONPs) to enhance the interfacial contact in all-solid-state batteries. LLZO-Ta and Na- β'' -alumina were employed as SEs for the lithium and sodium metal cells, respectively. The results indicated that most MONPs reduced the interfacial resistance between the SE and metallic anode, as well as the apparent SEI thickness, leading to improved interfacial properties. Additionally, MONP additives improved the coulombic efficiency (CE) in both cell types; 2% SnO₂ yielded the highest CE (96.3%) in the LLZO-Ta cells and 1% Al₂O₃ enhanced the CE from 82.1% to 91.9% in the Na- β'' -alumina cells. These findings highlight the potential of MONP-modified PEMLs for mitigating the interfacial challenges in all-solid-state batteries, thus offering a promising pathway for next-generation energy storage solutions.

Energy

Enhancing Stability and Activity in Hydrogen Evolution: Nitrogen Doping & Catalyst Coordination within Carbon Nanotubes

Samuel Itziksohn¹, Dr. Manoj Shanmugasundaram¹, Prof. David Zitoun¹
Chemistry, Bar Ilan University, Israel

Platinum encapsulation within carbon nanotubes (CNTs) is a promising route for improving long-term catalyst stability (Shanmugasundaram et al., 2024). Building on recent achievements in spatial confinement of metal catalysts within single-walled CNTs, we investigate how heteroatom doping, specifically nitrogen, modifies the coordination environment and catalytic performance of Platinum (Li et al., 2023; Pan et al., 2024). Our ongoing work explores the synthesis of N-doped CNTs and the incorporation of single atom Pt catalysts in such nanotube. Nitrogen dopant introduces active sites with new coordination and can influence the electronic structure and charge localization within CNTs. Preliminary findings suggest (Fig. 1a) significantly higher capacitive and non-faradaic current response for Nitrogen doped samples compared to undoped ones and significant increase in HER current and decrease in onset potential (Fig. 1b). These results demonstrate a clear impact of nitrogen doping on Platinum catalytical performance. This would indicate potential real-world application for similar catalyst synthesis.



Energy

Plasma-catalytic NO_x production: CaO as plasma moderator

Thierry Slot¹, Max Bernard¹, Yair Shahaf¹, Prof. Joe Lefkowitz¹, Prof. David Eisenberg¹

Technion - Israel Institute of Technology, Israel

The Haber–Bosch process made industrial ammonia possible, but its 1–2% share of global energy use and fossil dependence makes it a prime target for reinvention. We explore a zero-emission pathway that converts air to ammonia by combining plasma-catalytic nitrogen oxidation with electrochemical reduction (Figure 1a).

Plasma-based nitrogen fixation typically suffers from poor energy efficiency, as much of the input power is lost to gas heating or non-reactive excited states. By introducing catalysts into the discharge (Figure 1a,b), we aim to drive plasma energy into bond formation and away from filamentary arcs and unstable discharges.

Initially we explored a series of transition metals (Co, Cu, Ni, Mo, V, W) impregnated on Al₂O₃ as catalysts, but many catalysts behaved frustratingly similar to the blank: the same yields. This pushed us to ask a different question: how does the plasma couple to the catalyst? and can we change the support to one *actively shaping the discharge*?

This quest led us to CaO, a basic, thermally robust oxide. CaO improves plasma–catalyst contact, suppresses filamentary arcs (allowing higher O₂ fractions), and provides a strongly basic surface that stabilizes NO_x intermediates.

As a bonus, within the CaO-based transition-metal screening, Co/CaO emerged as our most active formulation, combining a characteristic “firefly” microdischarge pattern with high NO_x productivity and well-defined NO/NO₂ selectivity (Figure 1c).

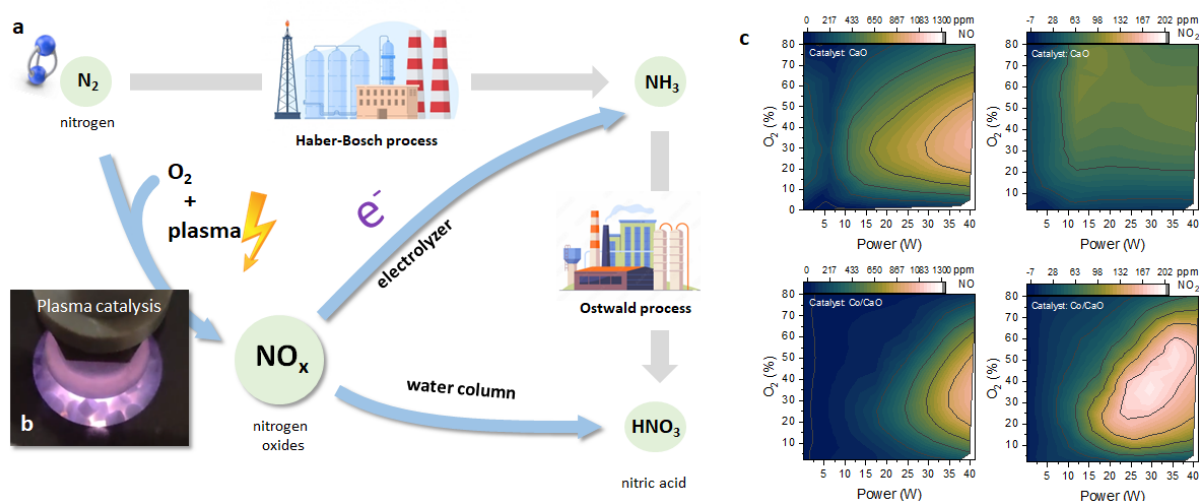


Figure 1: (a) schematic drawing of our oxidative nitrogen fixation approach (b) image of catalyst in custom-designed plasma chamber, (c) results of plasma-catalytic NO/NO₂ production for catalysts CaO and Co/CaO.

Energy

Two Electrons in a Li-S Cage: A Novel Lithium Cubic Electride—[(tBu₂MeSiS)₆Li₈]²⁺•2e[−]

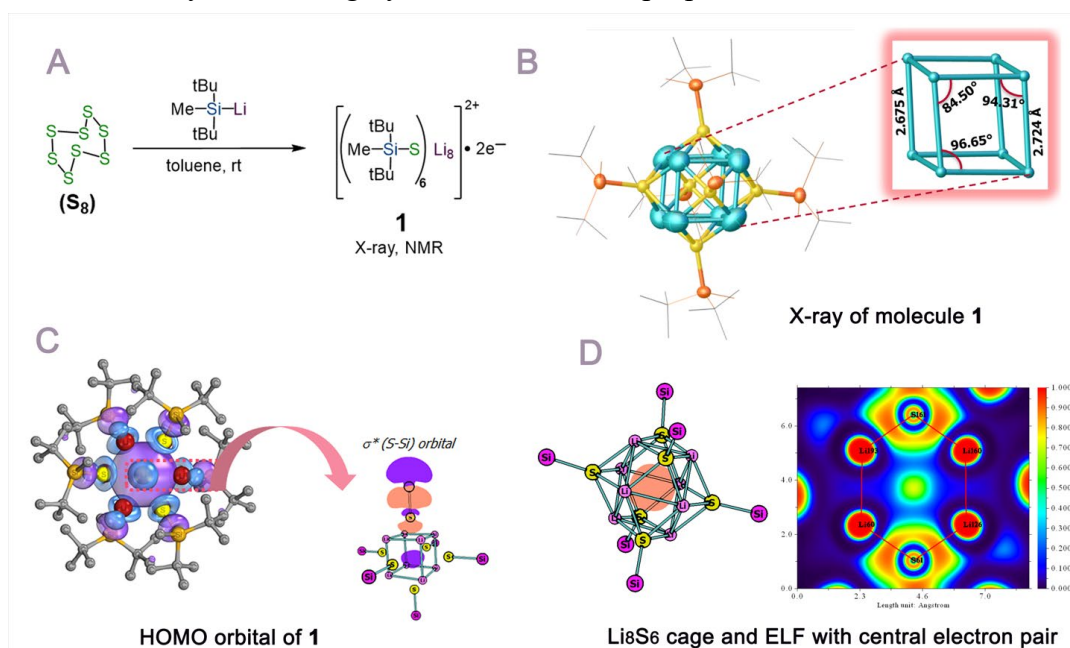
Devendra Yadav^{1,2}, Dr Alexander Kaushansky¹, Yuri Glagovsky¹, Dr Dmitry Bravo-Zhivotovskii^{1,2}, Prof Malachi Noked², Prof Yitzhak Apeloig¹

¹Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Israel

²Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel

Electrides—materials in which electrons serve as anions—show exceptional catalysis, energy storage, and quantum material properties.^{1–2} However, thermally stable, single-molecule electrides with centrally stored electrons remained a major synthetic challenge. In 2003, Matsuishi *et al.* reported the first thermally stable electride [Ca₂₄Al₂₄O₆₄]⁴⁺•4e[−].³ While such solid-state electrides are well studied, singly isolated electrides with high thermal stability and truly central electron(s) are mostly unknown.

Here we report an unprecedented lithium–sulfur–silyl cluster, [(tBu₂MeSiS)₆Li₈]²⁺•2e[−], (1)—**the first thermally stable and structurally characterized molecular electride featuring confined interstitial electrons** (Scheme 1, A–B). X-ray and ELF analyses confirm the confinement of an interstitial electron pair within the S₆Li₈ cluster (Scheme 1, D) and the cubic Li₈ cavity of 15.23 Å³. NBO data reveal dominant contributions from Li(s) and σ*(S–Si) orbitals (Figure 1C). The electride-like HOMO is high-lying (−1.66 eV), and its HOMO–LUMO gap is small (1.17 eV), indicating strong central electron localization. **No electrides with high electron density inside a single-isolated molecule cage have been previously reported.** Our findings establish a unique class of electride with centered electron density to show highly elevated electride properties.



Scheme 1: (A) Synthesis of 1; (B) X-ray structure of 1, showing a Li₈ cubic arrangement; (C) HOMO orbital of 1, showing s* (S–Si) orbital contribution; (D) ELF graph of the Li₈S₆ cage showing the central electron pair density.

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Energy

Synthesis and study of novel $[(R_3Si-AlR_3) Li]$ compounds as precursors for atomic layer deposition (ALD)

YOGENDRA KUMAR¹

chemistry, Bar-Ilan University, Israel

Recently, we discovered that $(R_3SiLi)_n$ ($R = Me, Me_2N, Me_3Si$, etc.) compounds serve as highly useful precursors for ALD (Atomic Layer Deposition) for coating NMC (lithium nickel manganese cobalt oxide) cathode material in lithium-ion batteries.¹ Protecting coating formed by ALD of unsolvated $tBuMe_2SiLi$ and following oxidation by O_3 improved the cathode capacity by 35% compared to the uncoated electrode. The obtained coating was studied by solid-state NMR and it was found that the protecting layer consists of three phases: SiO_2 , Li_2O , and alkyl-substituted siloxane polymers $-(RSi-O-SiR)_n$.²

Herein, we report a synthesis of the first volatile silyl aluminum precursors for ALD with the general formula $(R_2R'SiAlR_3Li)_n$. These compounds were characterized using NMR, X-ray, XRD, MS, and DFT calculations. We plan to further investigate their volatility in the conditions of the ALD and to study the thermal stability of these novel reagents with the aim of optimizing solid-electrolyte interphase (SEI)/cathode-electrolyte interphase (CEI) formation, thus improving overall battery performance. We hope to obtain better SEI (with the better conductivity, made of siloxane-aluminoxane polymers with a more regular structure as shown in Figure 1.

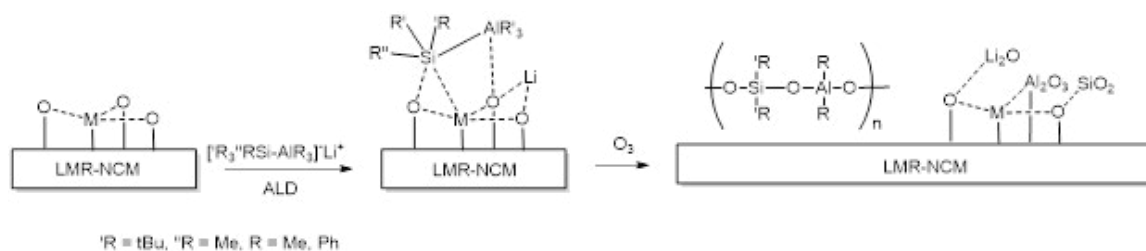


Figure 1: Proposed mechanism for the interaction of $(R_2R'SiAlR_3Li)_n$ with the metal-oxide surface.

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Energy

Synthesis and study of novel silyl aluminum lithium salts $[(R_3R''Si-ALR_3)Li]_n$ as a promising electrolyte additive for LMB

ROBIN KUMAR¹

Chemistry, Bar-Ilan University, Israel

The development of advanced electrolyte additives for lithium metal batteries (LMBs) requires a deep understanding of how molecular structure influences interphase chemistry and long-term electrochemical performance.¹ We previously demonstrated that silyl ketones function as effective LMB additives, forming xOSiFy-rich cathode–electrolyte interphases (CEIs) that markedly enhance cycle life.² However, silyl–aluminum–based lithium salts have not yet been explored in LMB systems.

In this work, we report for the first time novel silyl–aluminum lithium salts, formulated as $(R_2R''SiAlR_3Li)_n$, as electrolyte additives for LMBs (Figure 1). Incorporation of these silyl–aluminum salts leads to a substantial improvement in battery lifespan, highlighting their potential as multifunctional additives for next-generation high-energy LMBs.

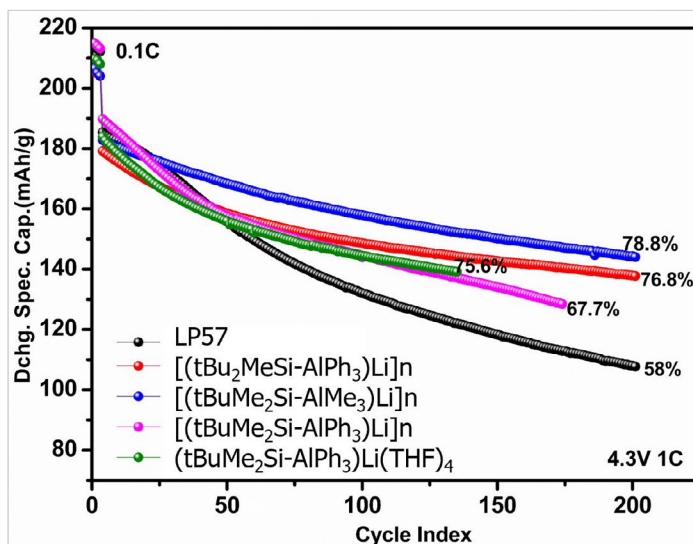
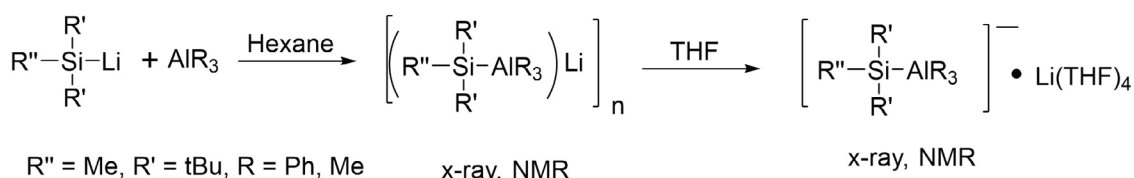


Figure 1: General synthesis scheme for $[(R_2R''SiAlR_3)Li]_n$ and preliminary electrochemical data.

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Energy

Investigating the Effect of Nickel Hydroxide Phases on the Oxidation of Small Molecules for Energy Conversion

Ana Elisa Lejtman¹, Prof. David Eisenberg¹
Chemistry, Technion, Israel

Nickel hydroxide is a promising electrocatalyst for energy applications due to its strong performance, low cost, and material abundance. It primarily exists in two polymorphs, α -Ni(OH)₂ and β -Ni(OH)₂, which differ in structure and associated stability. The α -phase contains layered sheets separated by intercalated water molecules and anions, resulting in a more expanded and less ordered structure, whereas the β -phase has compact, well-ordered layers without interlayer species, giving it a greater structural stability.[1] These distinctions influence their electrocatalytic activity in the oxidation of small molecules[2], including urea, methanol, glycerol and other alcohols.

In this study, both α and β phases were synthesized, characterized using HRSEM, XRD, and Raman spectroscopy, and the oxidation reaction were evaluated using cyclic voltammetry. By examining how each phase affects activity, onset potentials, and reaction pathways, we aim to identify clear performance trends that could be linked to their structural differences. These comparisons could support a deeper understanding of structure–activity relationships in Ni(OH)₂-based catalysts and highlight considerations relevant to alcohol oxidation in energy-conversion systems.

Overall, the work underscores the importance of tuning phase composition to design efficient, stable, and cost-effective nickel hydroxide electrocatalysts for future electrochemical technologies.

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Energy

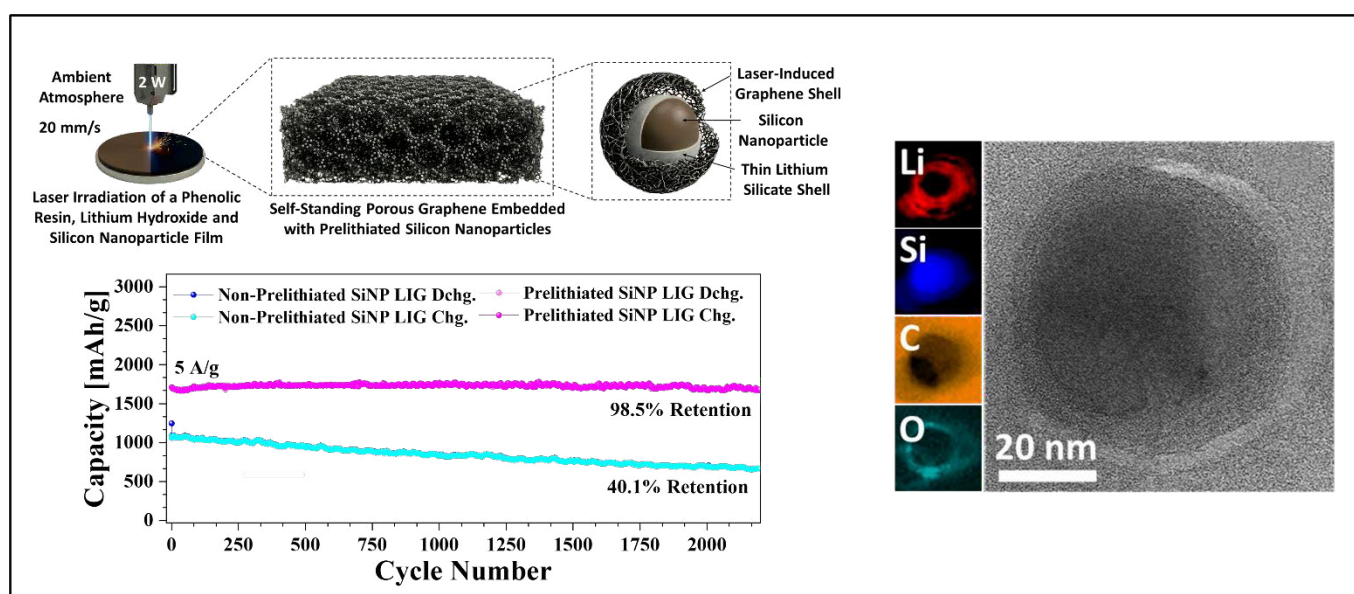
Single-Step Laser-Driven Synthesis and Prelithiation of Monolithic Silicon-Graphene Anodes for High-Performance Zero-Decay Lithium-ion Batteries

Gil Daffan¹, Avinash Kothuru², Fernando Patolsky^{1,2}

1. Department of Materials Science & Engineering, Faculty of Engineering, Tel Aviv University, Israel

2. School of Chemistry, Faculty of Exact Sciences, Tel Aviv University, Israel

Silicon is one of the most promising anode materials for next-generation lithium-ion batteries (LIBs) due to its theoretical capacity nearly ten times higher than graphite. However, its practical use is limited by large volume changes during cycling, causing particle fracture, unstable contact, and repeated rupture of the solid-electrolyte interphase (SEI), leading to capacity fading and low initial coulombic efficiency (ICE). While nanostructuring and carbon embedding improve stability and conductivity, they do not fully prevent lithium loss or long-term degradation. Prelithiation can offset lithium loss and stabilize the SEI, but conventional methods are ex-situ and rely on reactive lithium metal or complex reagents, making them multistep, air-sensitive, and unsuitable for scalable or ambient fabrication. This work introduces a laser-driven, solid-state, in-situ prelithiation approach that occurs simultaneously with electrode formation, combining the advantages of prelithiation and silicon-carbon composite synthesis in one step. A ternary mixture of phenolic resin, silicon nanoparticles (SiNPs), and common lithium salts were exposed to localized laser irradiation, inducing carbothermal conversion of the resin into a porous graphene matrix while driving solid-state lithiation of Si. The process proceeds under ambient conditions, forming Li-Si and Si-C bonds and a stable artificial SEI without post-treatment. The resulting prelithiated SiNP/LIG anodes deliver over 1700 mAh g⁻¹ with less than 2% capacity decay after 2000 cycles at 5 A g⁻¹ and ICE above 97%. Non-prelithiated electrodes retain only ~40% capacity and 83% ICE. This single-step laser process offers a scalable, low-cost route to high-performance silicon-graphene anodes for next-generation LIBs.



Energy

Towards "Lung-Inspired" Porosity

Nicola Seraphim^{1,2,3}, Kerem Har-Zahav Reshef^{1,2,3}, Noa Soffer-Lugassy^{1,2,3}, Prof.
David Eiseneberg^{1,2,3}

¹*Schulich Faculty of Chemistry, Technion, Israel*

²*Nancy and Stephen Grand Technion Energy Program, Technion, Israel*

³*Resnick Sustainability Center for Catalysis, Technion, Israel*

Fuel cells and electrolyzers represent promising sustainable energy storage technologies that harness redox reactions at electrodes. However, their efficiency is compromised by challenges including low power density and expensive catalysts.

Porous electrode architectures offer a potential solution to overcome mass transfer limitations, with hierarchical structures being on the spotlight for many researchers. However, the variety in design and complexity of these structures poses a challenge, as it leads to trial and error strategy in the implementation. In our approach, we decided to enhance the hierarchical structure by using bio-mimic inspired "lung design" in the catalyst layer. N-doped carbon electrodes are synthesized via a hard-template method with acrylonitrile precursor and ZnO "Lung-Inspired" templates.

By synthesizing ZnO templates through two-step hydrothermal methods, we were able to achieve a structure imitating lungs in its hierarchy. Materials were characterized using scanning electron microscopy, nitrogen adsorption isotherms, and Raman spectroscopy. We compare between carbons with different porosities, through electrochemical activity in oxygen reduction reaction, using cyclic voltammetry and ring-rotating disk electrode (RRDE) analysis.

Our results reveal the enhancement of mass transfer limit through porosity, adding fundamental insights into the rational design of hierarchy in carbons. These findings contribute to addressing a critical limitation in fuel cell and electrolyzer technologies, advancing their practical implementation for sustainable energy conversion and storage.

Energy

Scalable Route to High-Quality BaZrS₃ Absorbers for Next-Generation Solar Cells

Anat Itzhak¹, Prof Andrea Crovetto¹

National Centre for Nano Fabrication and Characterization (Nanolab, Technical University of Denmark (DTU, Denmark)

BaZrS₃ is an emerging chalcogenide perovskite offering a stable, non-toxic, and earth-abundant alternative to lead-halide perovskites. However, unlike halides, BaZrS₃ is not defect-tolerant; grain boundaries and intragap states severely limit carrier transport, typically necessitating synthesis temperatures >900 °C to achieve device-compatible quality.

We report a robust synthesis route for BaZrS₃ films at device-compatible temperatures (600 °C) using a glovebox-integrated reactive sputtering system, followed by post-annealing. By using amorphous sulfide precursor films, we control precursor oxidation and degradation, yielding crystalline films of comparable quality to those synthesized at 900 °C.

We observed that the films exhibit a distinct absorption onset and a photoluminescence (PL) peak blue-shifted to ~2 eV, compared with 1.9 eV for single crystals.^{1,2} We attribute the shift to the incorporation of some oxygen in the lattice, which widens the band gap. This hypothesis is supported by Terahertz spectroscopy, which reveals a sum of carrier mobilities of ~70 cm²V⁻¹s⁻¹, in line with TRPL measurements of single crystals.³

The carrier diffusion length of ~26 nm closely matches the crystallite size of ~35 nm, suggesting that grain boundaries might be the primary bottleneck for macroscopic transport. These results demonstrate that reactive sputtering can produce high-quality films at low temperatures, offering a scalable path to high-efficiency and environmentally friendly tandem devices.

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Energy

Development of analytical methods for quantification of N-cycle species.

Gennadiy Itov¹, Thierry Slot¹, Yair Shahaf¹, Prof. David Eisenberg¹
Technion - Israel Institute of Technology, Israel

The chemistry of Nitrogen-containing compounds is extremely diverse as the title element can exist in all possible oxidation states from +5 to -3. These species are important players both in biological and industrial cycles. Monitoring transformations of N-compounds is crucial for understanding and manipulating their behavior. This work is aimed at developing practical analytical tools for complex mixtures that are formed during electrochemical oxidation or reduction of these materials. Ion Chromatography (IC), Voltammetry (VA), Nuclear Magnetic Resonance (NMR), and Wet Chemistry (Indophenol Blue and Griess) procedures were developed for analysis of solutions of nitrate, nitrite, hydroxylamine and ammonium. Differential Electrochemical Mass Spectrometry (DEMS) was used for detection and quantification of gas phase components such as N₂, N₂O, NO and NO₂.

Energy

Using bond characteristics to predict self-healing properties in materials for sustainable energy conversion

Mr. Yuval Mualem^{1,2,3}, Prof. David Cahen⁴, Dr. Yevgeny Rakita⁵, Dr. Hannah Noa Barad^{1,2,3}

¹*Department of Chemistry, Bar-Ilan University, Israel*

²*Institute of Nanotechnology & Advanced Materials (BINA), Israel*

³*Israel National Institute of Energy Storage (INIES), Israel*

⁴*Department of Molecular Chemistry & Material Science, Weizmann Institute of Science, Israel*

⁵*Department of Materials Engineering, Ben Gurion University of the Negev, Israel*

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 materials occurs through a mass transfer inside the lattice that drives the healing process through two main mechanisms: through kinetically-stabilized defects in a ‘static lattice’ (‘class 1’), or through thermodynamically-stabilized defects in a ‘dynamic lattice’ (‘class 2’) where the bonds are portrayed as being ‘metavalent’. Although self-healing is very important in many applications, there are no clear physical or chemical guidelines for self-healing in semiconductors that can be used to predict their self-healing mechanism.

This work takes a data-driven approach to find bond character parameters that may affect the mechanism in known self-healing semiconductors, by data mining of four parameters: optical deformation potential (ODP), relative structural polarization (RSP), Pauling’s ionicity and microhardness. Statistical analysis of the data and matching the trends with known theory result in a clear definition of the two mechanism classes based on ODP and RSP, and an elevated understanding of the difference between the bond metavalency in class 2 materials and the defect-informed nature of class 1 materials based on ionicity and microhardness. The results shown in this work present preliminary steps in the understanding of the self-healing process, which can direct the search for sustainable self-healing materials for energy uses.

Energy

Effect of hydration on electrical properties of lanthanum-cerium oxides

Or Ben Zion¹, Dr David Ehre¹, Prof Isaac Abrahams², Prof Igor Lubomirsky¹

¹*Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Chemistry, Queen Mary University of London, United Kingdom*

The search for efficient and environmentally friendly energy sources has driven major interest in fuel cells, which convert the chemical energy of fuels directly into electricity. Solid oxide fuel cells (SOFCs), employing ion-conducting ceramics as electrolytes, are among the most promising technologies. However, their operation at high temperatures (300-900°C) limits long-term stability due to thermal stress.

SOFCs and solid oxide electrolyzers (SOEs) operating above 300 °C exhibit rapid electrode kinetics, especially in proton-conducting systems, yet suffer from thermal degradation. Ceramic devices functioning between 150–250°C could maintain fast kinetics without Pt-based catalysts and avoid thermal stress, but suitable proton conductors for this range remain unidentified.

Hydrated rare earth oxides, known for their chemical and thermal stability, have emerged as potential low-temperature proton conductors. Our study of La(OH)₃, a material insoluble in water and stable in CO₂, shows dominant protonic conductivity below 200°C, though still too low for applications. The non-blocking grain boundaries suggest promise for further development.

To enhance conductivity, partial substitution of La³⁺ with Ce⁴⁺ was explored in La_xCe_{1-x}O_{2-x/2} (LCO) ceramics. Compositions with $x \leq 0.5$ decompose to La(OH)₃ and CeO₂ upon hydration, restricting stability to $x \leq 0.5$. A tailored hydration protocol for LCO45 achieved ~38.5% hydration of the theoretical limit, causing a 0.413% lattice expansion and a marked increase in conductivity. Excess hydration, however, led to mechanical disintegration, while LCO40 showed negligible water uptake.

These findings highlight hydrated LCO ceramics as promising candidates toward developing stable, low-temperature proton-conducting ceramics for fuel cell and electrolyzer applications.

Energy

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

Philip Immanuel¹, Dr Lena Yadgarov¹

Department of Chemical Engineering, Ariel University, Israel

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 Cs₄PbBr₆ and 3D CsPbBr₃ 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 CsPbBr₃ NCs starts after 3 min of light exposure, while Cs₄PbBr₆ 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 CsPbBr₃ NCs performed as superior photocatalysts compared to their 0D Cs₄PbBr₆ NCs counterparts. Yet, linking the results of EPR measurements with the photocatalytic efficacy suggests that the CsPbBr₃ 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 contributing to advancements beyond the HP family.

Energy

Computational electronic structure analysis of Ru-based vacancy ordered halide perovskites

Shachar Gold¹, Prof. Leeor Kronik¹

Department of Molecular Chemistry and Material Science, Weizmann Institute of Science, Israel

Halide perovskites have been examined for their potential attractive electronic properties for photovoltaic applications. However, many promising candidates are known for issues with their stability, limiting their usefulness. In order to expand the available chemical space, a perovskite-derived structure of the form $A_2B(IV)X_6$, with Pt-group metals (such as Ru), being common candidates for the B-site. Due to the vacancies in the structure, the octahedra are relatively isolated, and have been experimentally shown to have 0D like properties, such as having magnetic properties. However, some systems, such as the Ru-based ones, lack an appropriate supportive computational backing. In this study, we present a computational analysis of selected Ru-based perovskites, focused on the electronic structure and magnetic properties, using a purely predictive method for structure determination and proper level of theory for the electric structure.

Energy

Does non-planarity affect electro-oxidation on Fe-N₄-C?

Noa Soffer-Lugassy¹, Prof. David Eisenberg¹

Chemistry, Technion-Israel Institute of Technology, Israel

Electrochemistry plays a central role in clean energy conversion technologies. One of its major challenges is efficient energy storage. Fuel cells, batteries, and supercapacitors all require high-performance electrode materials. Developing sustainable and affordable fuel-cell electrodes is especially important because many current catalysts, such as Pt, are costly. Single-atom catalysts (SACs) offer a promising alternative, providing nearly 100% atomic utilization, high stability, and easy separation from reaction media.

Heme-cofactors in enzymes are almost always non-planar; a feature so conserved it must be linked to function. For example, the hydrazine dehydrogenase (HDH) enzyme, which oxidizes N₂H₄ to N₂, contains a ruffled heme core. Inspired by biological systems, we aim to mimic a non-planar FeN₄ site in an inorganic electrocatalyst to optimize Fe³⁺ stabilization and improve binding properties. Our approach involves synthesizing Fe–N–C materials through a "ligand-mediated" method on differently structured carbon supports, creating catalysts with a variety of both planar and non-planar sites.

Direct hydrazine alkaline fuel cells are promising due to hydrazine's high energy density and flexible catalyst requirements, making the hydrazine oxidation reaction (HzOR) an excellent model. Using electrochemical and microscopy techniques (CV, RRDE, fuel-cell testing, HRTEM, Raman), we aim to clarify how active-site geometry controls activity and guide the design of improved DHFC catalysts.

Energy

Intercalation of urea oxidation intermediates in alpha-nickel hydroxide: first experimental step for supporting the dynamic intercalation model

Aviv Bryger¹, Jeremie Zaffran², David Eisenberg¹

¹*Schulich Faculty of Chemistry, Technion–Israel Institute of Technology, Israel*

²*Eco-Efficient Products & Process Lab (E2P2L), China*

The alpha phase of nickel hydroxide (α -Ni(OH)₂) has emerged as a promising catalyst for both the urea oxidation reaction (UOR) and the oxygen evolution reaction (OER). While OER studies suggest that part of the reaction occurs within the interlayer region of α -Ni(OH)₂—effectively increasing catalytic surface area—the situation for UOR is less straightforward. Because urea molecules and their oxidation intermediates are significantly bulkier than typical OER intermediates, the standard α -Ni(OH)₂ interlayer spacing (7–8 Å) is unlikely to accommodate them, seemingly ruling out interlayer UOR activity.

Building on our previous findings linking structural disorder in α -Ni(OH)₂ to enhanced UOR performance, we now propose that such disorder enables temporary interlayer expansion during operation. Defects may disrupt rigid stacking in the alpha phase, imparting structural flexibility that allows larger species—urea and its intermediates—to infiltrate the interlayer galleries. This “dynamic intercalation” effectively expands basal spacing under reaction conditions, increases accessible active sites, and enhances in-layer diffusion, thereby improving catalytic efficiency.

In this study, direct experimental evidence from X-ray diffraction (XRD) confirms that UOR-related anions intercalate into α -Ni(OH)₂ and expand its interlamellar spacing. Systematic testing of multiple anions with two alkali cations (Na⁺ and K⁺) supports our central hypothesis: UOR intermediates require greater spacing than that offered by pristine α -Ni(OH)₂, and such expansion occurs only when structural disorder permits it.

In parallel, ongoing density functional theory (DFT) calculations aim to map the arrangement and interactions of these intercalated species, providing mechanistic insights that complement and validate our experimental observations.

Energy

MOF Encapsulated Activated Carbon for Electrochemical CO₂ Reduction

SANTANU JANA¹, Prof Arie Borenstein¹

Department of Chemistry, Ariel University, Israel

Electrochemical CO₂ reduction (CO₂RR) provides a sustainable route to mitigate atmospheric CO₂ while producing value-added chemicals. Although noble metals are highly efficient CO₂RR catalysts, their cost limits large-scale application, motivating the development of cheaper alternatives. Transition-metal sites in metal–organic frameworks (MOFs) show strong catalytic promise, but their poor conductivity is a major limitation. Activated carbon (AC), with high surface area and excellent conductivity, enhances charge transport and CO₂ adsorption, while encapsulated MOFs supply tunable, selective active sites. Their synergy increases exposed active sites, improves charge-transfer kinetics, and suppresses hydrogen evolution. Here, Cu-Zeolitic Imidazolate Framework (Cu-ZIF) nanoparticles were grown inside a hierarchically porous AC matrix rather than physically blended with additives. This encapsulation maintained MOF crystallinity, improved conductivity, and strengthened interfacial electronic coupling. In CO₂RR, the Cu-ZIF@AC composite achieved 10 mA/cm² at only –0.56 V (vs. RHE) and selectively produced hydrogenated products such as acetic acid, methanol, and formic acid, demonstrating strong potential for scalable CO₂ electroreduction.

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Energy

First-Principles Investigation of Cu₃XN (X= Ni, Pd, Pt) Antiperovskite Electrocatalysts for CO₂ Reduction

Gaurav Mukherjee¹, Dr Itay Pitussi¹, Dr. Arie Borenstein¹
Department of Chemical Science, Ariel University, Israel

Antiperovskite-type Cu₃XN (X = Ni, Pd, Pt) materials have recently emerged as promising candidates for catalytic CO₂ electroreduction due to their metallic conductivity, tunable surface chemistry, and structural flexibility. In this work, we employ first-principles density functional theory (DFT) calculations to investigate the electronic and catalytic properties of Cu₃XN systems with a focus on identifying active surface terminations and understanding their role in CO₂ activation. Surface energies were calculated to determine the thermodynamically preferred facets, followed by detailed electronic structure analysis through band structure, density of states (DOS), and projected DOS (PDOS) evaluations. The results reveal strong hybridization between Cu-d and X-d orbitals near the Fermi level, facilitating enhanced electron transfer essential for catalytic activity. We further evaluated key reaction intermediates and adsorption energetics along the CO₂ reduction pathway, including *COOH and *OCHO species, to assess reaction feasibility and selectivity. Overall, our findings highlight the potential of Cu₃XN antiperovskites as efficient electrocatalysts for CO₂ conversion and provide valuable insights for the rational design of next-generation catalytic surfaces.

Energy

Zirconium-doped ceria as electromechanical energy converter

Nimrod Barak¹, Sergei Khodorov¹, Dr David Ehre¹, Prof Igor Lubomirsky¹
Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

Small-Scale energy harvesters are in growing demand as efficient and sustainable energy sources. These devices convert ambient mechanical vibrations into useful electricity. Current devices rely primarily on piezoelectric materials which have good energy conversion but are typically lead-based and have subpar long-term performance. Electrostrictive materials, though less developed commercially, offer a promising alternative. Among them, Zirconium-Doped Ceria (ZCO) has emerged as a promising candidate. ZCO demonstrates an electrostriction coefficient comparable to Lead Magnesium Niobite (PMN-PT), while being non-toxic, low-cost, easy to produce, and silicon microfabrication compatible. Additionally, the electrostrictive response of ZCO can be adjusted through Zr concentration and ZCO bulk oxidation.

My work aims to assess the feasibility of using ZCO as an electrostrictive energy-harvesting material. I designed a machine that applies alternating stress on a ZCO sample which causes the material's capacitance to alternate. Connecting this alternating plate capacitor to a DC circuit should produce useful AC current. Additionally, I am optimizing the Zr concentration and level of oxidation to find a balance of high electrostriction with low conductivity for optimal energy harvesting.

Energy

Pressure-induced modulation of band characteristics in 2D hybrid perovskites

Eti Mahal^{1,2}, Prof. Biswarup Pathak¹

¹*Chemistry, Indian Institute of Technology Indore, India*

²*Chemistry, Bar-Ilan University, Israel*

Since the advent of 2D hybrid perovskites for optoelectronic devices, achieving significant out-of-plane charge transport and strong organic-inorganic orbital coupling has been a major challenge. Recent research has focused on incorporating polycyclic amine-based spacer cations to address this issue. In this study, we used density functional theory to explore the pressure tunability of perovskite electronic structures. Applying external pressure to naphthalene-based spacer cation containing 2D perovskites, specifically (NaphDA)PbI₄, resulted in significantly enhanced out-of-plane carrier transport, with a hole effective mass approaching 0.15 m_0 . Additionally, for another perovskite we noticed significant inorganic-organic orbital overlap at the band edges. We discovered that the direction of applied pressure alters the intramolecular band alignment: a material with a type I_a alignment can shift to a type II_a alignment under pressure.

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Energy

Development of FA_{0.9}Cs_{0.1}PbI₃ perovskite based flexible solar cells

Ayush Tara¹, Naba Kumar Rana¹, Sidharth Reghunathan¹, Areen Shawahni¹, Dr.
Hannah-Noa Barad¹

*Department of Chemistry, Institute of Nanotechnology and Advanced Materials, and
Israel National Institute for Energy Storage (INIES), Bar-Ilan University, Israel*

Flexible perovskite solar cells (f-PSCs) have attracted significant attention for next-generation wearable and portable energy applications due to their lightweight nature, mechanical flexibility, and low-temperature processability. However, their efficiency remains limited by polymer substrates that cannot withstand high processing temperatures, leading to poor perovskite crystallization and high defect densities. Low-temperature fabrication on flexible substrates often compromises phase stability, interfacial quality, and mechanical durability of FACsPbI₃ devices. Among various substrates, polyethylene naphthalate (PEN) offers superior thermal stability, optical transparency, and mechanical robustness compared to conventional polymer substrates, making it highly suitable for flexible photovoltaic devices. In this work, we report the fabrication and performance of PEN substrate based flexible FA_{0.9}Cs_{0.1}PbI₃ PSCs, processed entirely under low-temperature conditions compatible with plastic substrates.

High-quality perovskite films were deposited via a controlled solution-processing route, enabling uniform grain morphology, reduced defect density, and enhanced crystallinity, despite the constraints imposed by flexible substrates. Optimized electron transport layers and interface engineering suppressed non-radiative recombination and improved charge extraction. The resulting flexible devices exhibit power conversion efficiencies comparable to their rigid counterparts, along with excellent mechanical durability. Devices retain over 85% of their initial efficiency after repeated bending cycles at small bending radii, demonstrating outstanding mechanical resilience. These results indicate the strong potential of f-PSCs for scalable, high-performance flexible energy-harvesting applications.

Energy

Dynamic Heterogeneity and Dielectric Breakdown in Polycarbonate-Polysulfone Multilayer Films using Broadband Dielectric Spectroscopy

Mydhili Varma¹, Mindy Levine² & Paul Ben Ishai¹

¹Dielectric & THz Science Laboratory, Department of Physics, Ariel University of Samaria, Ariel, Israel.

²Laboratory of Supramolecular Chemistry, Department of Chemical Sciences, Ariel University of Samaria, Ariel, Israel.

High-K dielectrics find useful applications in energy storage devices operating under high frequencies. Polymer-polymer composites, embedded polymers containing inorganic and organic conducting and semiconducting nanofillers are in high demand. However, these nanofillers contribute to high conductivity losses, inducing thermal dissipation. Additionally, the huge disparity in the dielectric properties of individual entities in these composites can cause local electric field distortions, accelerate the electrical breakdown and thereby reducing the dielectric breakdown strength. This restricts practical applications for prolonged use [1]. A strategically designed multilayer dielectric with different materials, fillers and configuration would allow polarization manipulation and avoid the problems mentioned beforehand [1,2].

In this work, we choose two high performance thermoplastic polymers, polycarbonate (PC) and polysulfone (PSF), with similar dielectric characteristics to design an all-polymer, flexible, freestanding multilayer dielectric film. An optimized concentration of 10 w/v% of PC and 5 w/v% of PSF in chloroform were spin coated to form a PC/PSF/PC multilayer structure for various post-fabrication heating times of 0-30 min at 65 °C. The XRD pattern was recorded to analyze the change in crystallinity of the samples with heating duration while FT-IR spectroscopy and SEM imaging was used to confirm the bonding between PC and PSF and morphological changes due to the amorphous to crystalline transition of PC/PSF/PC multilayers. Polarization and relaxation mechanisms due to confinement of dipoles in the interfaces, dielectric breakdown in PC/PSF/PC were studied using broadband dielectric spectroscopy (BDS) as functions of the morphology and post-fabrication heating times.

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Energy

Direct Graphene Growth Enhances the Photo-electro Properties of WS₂ Nanotubes

Asmita Dutta¹

Ariel University, Israel

We report the first-ever direct growth of few-layer graphene on WS₂ nanotubes (NTs), achieving a hybrid architecture with unprecedented electronic, optical, and electro-optical characteristics. Encapsulation of WS₂ NTs by graphene forms a core-shell structure that integrates the semiconducting behavior of WS₂ with the exceptional electronic conductivity of graphene. Photo-absorption spectroscopy reveals distinct excitonic transitions characteristic of WS₂ NTs, along with an additional $\pi \rightarrow \pi^*$ transition in the hybrid system, evidencing strong interfacial interactions. Finite-difference time-domain (FDTD) simulations further demonstrate enhanced light-matter coupling, showing an 18% increase in electric field intensity and cavity mode confinement relative to pristine WS₂ NTs. The improved photoresponse arises from modulation of the dielectric environment and Fermi-level alignment within the hybrid nanotubes. Density functional theory (DFT) calculations indicate pronounced bandgap reduction upon graphene coating—an 87.5% decrease for tubular WS₂ NTs versus 38.5% for the planar analogue—attributed to electronic hybridization and curvature-induced strain at the WS₂/graphene interface. Although graphene itself is non-photoactive, its incorporation significantly enhances charge transport and photon harvesting capabilities. This synergistic effect was exploited in photo-electrocatalytic hydrogen evolution reaction (HER) studies, where WS₂/graphene NTs exhibited a 49.1% increase in reduction current under illumination, compared to only an 8.9% enhancement for uncoated WS₂. Overall, the WS₂/graphene hybrid nanotubes offer tunable optoelectronic properties, improved charge carrier dynamics, and superior photocatalytic activity, presenting a promising platform for next-generation PEC systems and broader energy conversion technologies.

Energy

Proton conduction at middle range temperatures, from room temperature to 473K, in $\text{La}_2\text{Ce}_2\text{O}_7$ thin films for renewable energy applications

Hadar Dessau¹, Dr David Ehre¹, Prof Isaac Abrahams², Prof Igor Lubomirsky¹
¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Department of Chemistry, Queen Mary University of London, Mile End Road
London E1 4NS, United Kingdom*

Solid state inorganic proton conductors have raised a lot of interest in the last few years. One of these proton conductors is $\text{La}_2\text{Ce}_2\text{O}_7$ (LCO50). This material competes with the existing proton conductors such as polymers (e.g. Nafion), which have problems of compatibility with other materials and with conductivity under dry conditions.

In this presentation, I will discuss the fabrication and impedance measurements of LCO50 thin films. I will show the effect of hydration on the film that deposited at 733K. I will also discuss the improved properties of the nanocrystalline LCO50, which is deposited at room temperature. The latter spontaneously hydrated at ambient conditions and shows relatively high proton conductivity even at room temperature. In addition to the LCO films, I will present composite films of nanocrystalline LCO50 and WO_x . I will discuss the fabrication of these films and show their advantages as solid state electrolytes.

Energy

Determination of local structural and dynamic descriptors using EXAFS in Zr-doped Ceria, a non-classical electrostrictor

Tali Savich¹, Kaifeng Zheng², Dr. Ryuichi Shimogawa^{2,3}, Dr. Prahlad Routh², Dr. Maxim Varenik¹, Dr. David Ehre¹, Prof. Igor Lubomirsky¹, Prof. Anatoly I. Frenkel^{2,4}

¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, 761001, Israel*

²*Department of Materials Science and Chemical Engineering, Stony Brook University, NY 11794, USA*

³*Science & Innovation Center 1000, Mitsubishi Chemical Corporation, Japan*

⁴*Division of Chemistry, Brookhaven National Laboratory, NY 11973, USA*

Ceria oxides have rising interest in many energy applications, such as fuel cells and thermochemical cycles. Our group studies electrostriction (ES) in dense, ceria-based ceramics with fluorite symmetry. Electrostriction is a second-order electromechanical response, where $u_3 = M_{33} \times E_3^2$; E_3 - applied electric field; M_{33} is the longitudinal ES coefficient. We recently observed non-classical electrostriction (NCES) in 10mol% Zr-doped Ce (10ZDC), with strain performance comparable to commercial materials^[1]. Unlike classical electrostriction, which depends on oxygen vacancies, 10ZDC- with isovalent dopants, exhibits strong strain response ($|M_{33}| = 10\text{--}16 \text{ m}^2/\text{V}^2$, $|u_3| \geq 220 \text{ ppm}$) up to 3 kHz, rivaling commercial piezoelectrics like PMN-PT while maintaining a lower dielectric constant and higher elastic modulus. However, aliovalent co-doping ($\geq 0.5 \text{ mol}\%$) suppresses NCES, highlighting oxygen vacancies as the key suppressors^[2]. X-ray absorption spectroscopy (XAS) reveals that even low vacancy concentrations introduce structural disorder.

To probe the mechanism of NCES in ZDC, temperature-dependent XAS was used to identify structural and dynamic descriptors^[3]. These descriptors (static bond length disorder, anharmonicity of the effective pair potential, and effective force constants for the probed atomic pairs) derive from quasi-harmonic approximation for the nearest-neighbor Zr (/Ce) bonds. The emerging structural model emphasizes significant free volume around Zr in the oxygen cube, explaining both the mechanical anomaly (Young's modulus decreases with Zr%) and correlating at least one descriptor (static disorder) to the measured M_{33} . This descriptor-based approach can be extended to further applications in ceria-based ceramics.

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Energy

Enhancing Sodium Plating Efficiency in a Carbonate-Based Electrolyte - A Mechanistic Study

Tamir Assa¹, Mr. Hadar Shlomo¹, Mr. Itamar Charit¹, Mr. David Stark¹, Prof.

Emanuel Peled¹

Tel Aviv University, Israel

The instability of the Solid Electrolyte Interphase (SEI) in carbonate-based electrolytes hinders the development of high-energy-density sodium batteries. This study elucidates the stabilization mechanism provided by a C65-coated aluminum electrode, representing the nucleation host in an anode-less sodium battery architecture, within a half-cell configuration against a sodium-metal counter electrode, using a carbonate-based electrolyte (1 M NaPF₆ in EC:DMC with 5% FEC). We demonstrate that the high-surface-area C65-coating homogenizes the local effective current density, thereby facilitating the selective reduction of FEC prior to bulk solvent decomposition, fostering the formation of a flexible, NaF-rich SEI. Conversely, the high local current density on bare aluminum electrode drives nonselective electrolyte decomposition, resulting in a brittle, inorganic-rich SEI and severe accumulation of "dead sodium". Consequently, the C65-coated electrode enhances the average Coulombic Efficiency to 85%, representing a significant relative improvement over the bare substrate. Furthermore, X-ray photoelectron spectroscopy reveals that the SEI composition on the bare aluminum electrode eventually evolves to resemble the stable interface on the coated electrode, yet electrochemical performance remains inferior. This underscores the long-term impact of the early-stage SEI composition on cell cyclability.

Energy

Understanding Sodium Storage Mechanisms in Soft and Porous Carbon Materials for Sodium-Ion Battery Anodes

Elizaveta Lukovskaya¹, Prof. David Zitoun¹
Chemistry, Bar Ilan University, Israel

The growing demand for sustainable and cost-effective energy storage technologies has intensified interest in sodium-ion batteries (SIBs) as an alternative to lithium-ion systems¹. Despite significant progress, the fundamental mechanism of sodium storage in carbon anodes remains insufficiently understood, limiting the rational design of high-performance materials. This research aims to elucidate the sodiation mechanism in engineered carbon structures by systematically studying the roles of surface adsorption, intercalation, pore filling, and sodium electroplating. Carbon materials synthesized via hydrothermal carbonization of glucose, followed by controlled pore modification, are investigated alongside commercial activated carbon and hard carbon to determine how variations in porosity, defect density, and surface chemistry influence sodium uptake^{2,3}. Structural characterization (BET, Raman spectroscopy, HR-SEM) is combined with electrochemical analysis in half-cell configurations to correlate carbon morphology with storage behavior. Preliminary results show that hydrothermal treatment effectively reduces surface area and alters pore accessibility, leading to measurable changes in charge–discharge profiles and sodiation dynamics. By resolving the order of storage events and identifying conditions that promote or suppress sodium electroplating, this work seeks to construct a unified model for sodium storage in disordered carbons. The insights gained will guide the development of tailored carbon anodes with improved efficiency, stability, and safety for next-generation sodium-ion batteries.

Energy

Mechanistic Study of Humidity-Driven Energy Generation in Thin Protein Films

Prashant Kumar¹, Prof. Nadav Amdursky¹
Technion, Israel

This study explores the mechanism of power generation from atmospheric humidity using spin-coated protein films composed of the Bovine Serum Albumin (BSA) protein. BSA's hygroscopic properties and functional groups facilitate proton conduction, enabling efficient energy harvesting through moisture gradients. Experimental results demonstrate that BSA generates maximum average open-circuit voltage (avg V_{oc}) of 0.56 volts at around 60% relative humidity (RH), with a maximum average short-circuit current (avg I_{sc}) of 7.07×10^{-8} ampere at 80% RH and the values increase as RH rises from low to high. The work highlights advancements and research gaps in biomaterial-based energy-harvesting systems.

Energy

Development of Bismuth-Matrimid based Electrocatalyst for Efficient CO₂ Reduction

Sonal Rajput¹, Prof. Eran Edri¹

*Department of Chemical Engineering, Ben Gurion University of the Negev, Beersheba,
Israel, Israel*

The importance of CO₂ separation and conversion has been growing as it a significant greenhouse gas that aggravates global warming. Therefore, the distinct properties of functionalized inorganic fillers in polymer matrices have enabled the development of mixed-matrix membranes (MMMs) for selective CO₂ separation and conversion. Traditional methods for CO₂ conversion such as biochemical and thermal are time-consuming, relatively expensive and produce less yields; hence cannot preferred in the field. Therefore, due to its excellent selectivity and cost-effectiveness, the electrochemical reduction of CO₂ can thus assist store renewable energy and reduce the impact of CO₂ emissions on the environment. Among CO₂RR products, formic acid requires low energy consumption and holds great importance in pharmaceutical industry, thus producing formic acid is generally considered as a profitable line for CO₂RR. Mainly, bismuth-containing electrocatalysts show high selectivity to formic acid during the process of CO₂ reduction. This work focuses on how to develop bismuth matrimid based mixed membrane as electrocatalyst with a scalable approach with high selectivity. Hence, mixed matrix was synthesized by casting membrane using doctor's blade method. Their physicochemical properties were subsequently investigated by characterization techniques such SEM/EDX, XRD, XPS etc. Then, the fabricated membrane was induced to laser to develop a potential electrode for CO₂ reduction. Hence the developed electrode will be used as electrocatalyst for efficient CO₂ reduction.

Energy

Incorporation of transition metal substituents into LaNiO₃ improves electrocatalytic activity and stability of acidic oxygen evolution

Nophar Tubul¹, Dr. Johannes D. Bartl², Dr. Adi Kama¹, Uriel Vaknin¹, Kohav Lifshitz Shimoni¹, Dr. Hannah-Noa Barad¹

¹*Chemistry, Bar Ilan University, Israel*

²*Materials, Ruhr University, Germany*

A hydrogen-based energy economy is one of the ways to mitigate climate change. Thus, water electrolyzers for H₂ are crucial. Acid-based electrolyzers use expensive and non-abundant Ir as the catalyst for the anodic oxygen evolution reaction (OER), thus, new precious metal free materials need to be studied.

This work presents one of the first studies of LaNiO₃ (LNO) electrocatalysts operating in acidic conditions, an area largely unexplored until now. We investigate how incorporating acid-stable transition metals, Mo, W, and Mn into LNO stabilize and improve OER performance in a pH 4 electrolyte. Using high-throughput materials libraries (20–55 at% substitution), material characterizations (XRD, XPS, EDS, SEM) and electrochemical screening (CV, LSV, CA), we map the activity across a wide compositional space.

Two exceptional compositions—LNO-Mo (35 at%) and LNO-W (20 at%)—achieve overpotentials 100 mV lower than pristine LNO and show up to 240% higher stability, even outperforming Ir-based benchmarks.

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THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



LIGHT-MATTER INTERACTIONS

Chair: Igal Levine

Invited Lecture

Light-matter Interactions

Nothing can do something: Manipulating Molecules by Tailoring the Electromagnetic Vacuum

Tal Schwartz¹

Physical Chemistry Department, Tel Aviv University, Israel

Light-matter interactions are at the core of many physical and chemical processes, but when these interactions are confined to the nanoscale, entirely new phenomena can emerge. In this talk, I will present our recent explorations of how strong coupling between photons and excitons gives rise to hybrid light-matter states with novel optical and electronic properties. I will discuss how such effects can modify molecular emission, energy flow, and even chemical reactivity, pointing toward new horizons in material sciences.

Invited Lecture

Light-matter Interactions

Ultrafast Triggering of Strong Coupling in a Semiconductor Terahertz Fabry-Pérot Cavity

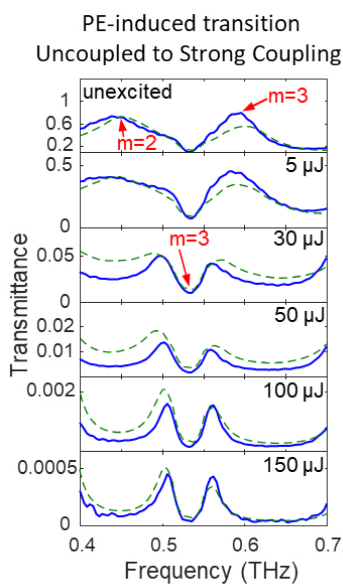
Prof. Sharly Fleischer^{1,2}, Dr. Soumitra Hazra^{1,2}, Hanna Turchinsky^{1,2}, Prof. Tal Schwartz^{1,2}

¹Physical Chemistry, Tel Aviv University, Israel

²Tel Aviv University center for Light-Matter Interaction, Israel

Strong light-matter coupling, the hybridization of material excitations with the electromagnetic modes of a photonic resonator, has led to striking modifications in the physical and chemical properties of materials, including their chemical reactivity [1,2]. A key capability however, remains elusive: the ability to switch strong coupling 'on demand' and noninvasively - that is, without perturbing the molecular system itself. Such control is crucial for isolating the causal role of strong coupling in chemical dynamics and for accessing the microscopic temporal domain of polaritonic chemistry under strong coupling conditions.

I will introduce an ultrafast, optically switchable Fabry-Pérot cavity that enables 'on-demand' triggering of strong coupling with a switch-on time of just a few picoseconds, shorter than the cavity photon lifetime (~ 45 ps) and even shorter than the characteristic time for coherent energy exchange between the photonic and molecular systems (Rabi period, $1/\Omega \sim 17$ ps).



By photoexciting silicon-based cavity mirrors, we induced an *abrupt spectral shift* and *linewidth narrowing* of the photonic cavity mode - leading to a substantial increase in the Q-factor and tuning the cavity mode into resonance with the vibrational transition of the α -lactose powder pellet embedded within the cavity [3]. This, in turn, triggers ultrafast light-matter hybridization celebrated by the formation of vibrational polaritons.

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- [2] W. Ahn et. al., Science 380, 1165 (2023).
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Invited Lecture

Light-matter Interactions

The Role of Optical Transitions in Determining Carrier Yields of Metal-Oxide Photoabsorbers

Daniel Grave¹

Department of Materials Engineering, Ben Gurion University, Israel

Transition metal oxide semiconductors are promising photoabsorbers for solar-fuel generation. Oxides with d^0 and d^{10} cation configurations can exhibit high internal quantum efficiencies, but their wide band gaps limit solar utilization. In contrast, oxides with open d-shells often possess ideal band gaps but show markedly lower photoconversion efficiencies. To identify the origins of these losses, we combine epitaxial thin-film growth with optical spectroscopy, photoelectrochemistry, and time-resolved microwave conductivity. We find that open d-shell oxides exhibit intrinsically low mobile charge-carrier yields, with a substantial fraction of absorbed photons failing to generate carriers capable of driving redox chemistry. Across Fe-based oxides, including α -Fe₂O₃, β -Fe₂O₃, and ZnFe₂O₄, we find that despite substantial differences in structure and transport behavior, the carrier-generation yield and its spectral dependence remain remarkably similar. This invariance points to Fe-centered ligand-field excitations as dominant nonproductive relaxation pathways that do not produce mobile carriers on nanosecond timescales. To further probe the electronic origins of these losses, we examine ilmenite-type MTiO₃ (M = Mn, Co, Ni), where the balance between ligand-field and charge-transfer excitations can be systematically tuned by the d-electron configuration. In these Ti-containing oxides, mobile carriers arise primarily from O²⁻ to Ti⁴⁺ charge-transfer transitions, whereas ligand-field excitations fail to generate mobile carriers on nanosecond timescales. Overall, these results demonstrate that carrier-generation efficiency in open d-shell oxides is governed predominantly by electronic excitation pathways, providing guidance for the design of oxide photoabsorbers for solar-fuel applications.

Invited Lecture

Light-matter Interactions

Mapping the Energetic Defect Landscape of Pb-free HaPs Using Surface PhotoVoltage

Dr. Igal Levine¹

Chemistry, Hebrew University of Jerusalem, Israel

Non-radiative recombination of electronic charge carriers via defect states in the bulk and at semiconductor interfaces significantly limits the performance of optoelectronic devices, including solar cells, photoelectrochemical cells, and light-emitting diodes.

Detecting and characterizing deep bulk and interfacial defect states is, therefore, crucial for identifying performance-limiting factors in electronic devices. However, defect characterization poses both technical and scientific challenges due to the low density of defect states in high-quality semiconductors and their very low absorption cross section.

In this presentation, I will demonstrate how Surface PhotoVoltage (SPV) under light modulation or pulsed excitation can directly probe the energetic location of defects in various semiconductor families. The influence of several key parameters such as halide composition/organic cation/Pb contents, on the defect distribution will be addressed and discussed in detail.

Invited Lecture

Light-matter Interactions

Ultrafast spectroscopy at the single nanoparticle level

Dr. Ron Tenne¹

Schulich Faculty of Chemistry, Technion - Israeli Institute of Technology, Israel

Nanoparticles serve as inherent sources for quantum states of light such as single photons and entangled photon pairs. Ideally, under cryogenic conditions, their radiation is fully coherent – maintaining a constant phase relation throughout the emission process. Often, however, the interaction of excited electrons with the lattice limits the coherence lifetime to the picosecond timescale. Experimentally, such a timescale necessitates the use of pump-probe measurements with ultrashort laser pulses. While the generation of short pulses is hardly a novelty, applying them to the sensitive spectroscopy of single nano objects is a highly challenging task. Here, we present the first transient-transmission experiments directly measuring the coherent dynamics of excitons in an individual epitaxial CdSe QD.

Using a highly stable femtosecond Er: fiber laser source, we generate the pump and probe beams that are focused through a high-numerical-aperture objective lens within an optical cryostat (T=1.6 K). In this setup, we readily observe the signature of coherence in the periodic oscillations of phase between two spectral features. Moreover, directly exciting the p-shell electrons we form a hot excitonic state that remains populated and coherent for hundreds of picoseconds. This last result is especially surprising considering the typical fast relaxation of states with excess energy. In fact, it is an indication of a robust phonon bottleneck.

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Light-matter Interactions

Unravelling quantum dot–molecule interactions for π -conjugated ligands: insights into binding and anchoring group effects

Yinon Deree¹

Chemistry, hebrew university, Isreal

To explore triplet energy transfer (TET) efficiency in quantum dots (QDs) coated with π -conjugated ligands, we investigated the effect of ligand binding and orientation on the quenching rate of QD photoluminescence. By comparing anthracene ligands with different anchoring groups (carboxylate, thiol, and dithiol), we found that replacing the carboxylate group with thiol or dithiol groups enhanced quenching rates by factors of 3 and 4.5, respectively.

To quantify these results, we developed a modified Stern–Volmer model that accounts for the Poisson distribution of ligand binding on QDs. We observed distinct spectral changes in the absorption spectra of bound ligands, including a ligand-dependent bathochromic shift and altered vibronic progression, attributed to deprotonation of the anchoring groups and the confined environment on the QD surface. These changes enable the distinction between bound and free ligands upon ligand addition, allowing for accurate determination of binding stoichiometry and reliable quenching rate extraction.

Consistent with DFT calculations, the improved quenching for thiolated anthracenes is attributed to the parallel orientation of the π -system relative to the QD surface, which allows for greater orbital overlap and faster TET rates via the Dexter mechanism.

This work contributes to design principles for efficient QD–organic hybrid systems for improved triplet energy transfer.

Light-matter Interactions

Optoelectronic Behavior of BaZrS₃: An Emerging Semiconductor with Perovskite Structure

Yraden Ben Arosh Arad¹, Dr. Matan Menahem¹, Prof. Igal Levine², Prof. Rafael Jaramillo³, Prof. Omer Yaffe¹

¹*Department of Chemical and Biological Physics, Weizmann Institute of Science, Israel*

²*Department of Nanoscience and Nanotechnology, Hebrew University of Jerusalem, Israel*

³*Department of Materials Science & Engineering, MIT, Cambridge, USA*

BaZrS₃ (BZS) is a chalcogenide perovskite that has gained much interest as an emerging semiconductor, exhibits a direct band gap of ~ 1.9 eV, an unusually large dielectric constant (50–100, compared to 11.7 in Si and 10.9–12.9 in GaAs), and offers enhanced stability. When processed as thin film form, it presents an attractive option for various optoelectronic devices.

I will presents preliminary results, studying the optoelectronic dynamics in BZS thin films, towards comparison between thin films and single crystals, with emphasis on differences in dynamics defect states and their role in recombination processes. A surprising finding that I will present is that some of the films show better quantum efficiency than a single crystal although surface-to-bulk ratio is lower.

To explore these effects, I employ two complementary approaches. Timeresolved photoluminescence (TRPL) measurements are used to probe carrier recombination dynamics and evaluate the influence of defects on radiative pathways. Concurrently, modulated surface photovoltage (mSPV) measurements provide direct insights into non-radiative processes not captured by PL. Together, these techniques enable a comprehensive mapping of the defects in BZS thin films and their impact on electronic behavior.

Light-matter Interactions

Exploring the Multiple Scattering of Organic Exciton-Polaritons Using Interferometric Imaging

Gal Sandik

Molecular exciton-polaritons, having a dual photonic and material nature, are not localized like excited molecular states - they are instead delocalized over length-scales comparable to the optical wavelength [1–3]. This delocalized nature of polaritons has major implications to the design of organic solar cells, which are largely limited in their efficiency by the mobility of the generated excitons. Additionally, this partially excitonic nature of polaritons indicates that they can interact with each other, enabling the design of photonic analogous of electronic components.

While the delocalized and coherent nature of polaritons was demonstrated more than a decade ago [1], recent experimental and theoretical works [3, 4] have revealed that polaritons have intricate propagation dynamics, undergoing a transition from ballistic propagation - movement at a constant velocity - to a diffusive type of movement, dominated by multiple scattering.

In this work, we further examine the delocalized nature of polaritons and their long-range coherence properties, in order to understand the importance of incoherent (phase-destructive) scattering vs. coherent (phase-preserving) scattering in the two transport regimes. In our studies, we employ wide-field interferometric imaging (Fig. 1) to measure the mutual coherence of polariton emission at distant points along the polariton propagation and for varying photonic weights. Interestingly, we find that not only does the fringe visibility depend on the separation between the measured points, but also on where along the propagation they are located. By providing information on the loss of coherence, such experiments can shed further light on the nature of the scattering processes involved in polaritonic transport and on the transition between ballistic motion and diffusion.

Light-matter Interactions

Towards modeling laser-induced homogeneous ice nucleation from first principles

Margarita Shepelenko¹, Prof. Leeor Kronik¹, Prof. Gershon (Jan M. L.) Martin¹,
Prof. Leslie Leiserowitz¹

Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

The phenomenon of ice nucleation from supercooled water, with ramifications for living and nonliving systems, occurs at a heterogeneous interface. Homogeneous ice nucleation, meaning nucleation far from pre-existing interfaces, is a challenge to induce and explore. Here we focus on laser-induced homogeneous ice nucleation reported by Nevo et al. in 2020, which we aim to understand from first principles. Our basic hypothesis is that ice nuclei are formed without the help of the laser beam, but these ice nuclei are metastable; interaction with the laser beam stabilizes their formation and promotes their growth. We started our computational study from ice XI, a proton-ordered orthorhombic polymorph of ice, which has a triple point with hexagonal ice and gaseous water at (72 K, 0 Pa) and is stable below this temperature. Ice XI is of interest owing to similarities between its crystal structure and that of hexagonal ice I_h . By virtue of an orthorhombic-to-hexagonal cell transformation applied to the ice XI crystal structure, we obtained a proton-ordered ice structure in a hexagonal-ice-like cell and were able to compare lattice energies and other parameters of interest of “proton-ordered” and disordered hexagonal ice. In order to simulate a hexagonal ice (I_h) nucleus lying in liquid water, we made use of a model composed of 96 water molecules to generate a pseudo proton-disordered crystal of ice surrounded by a water shell. This work is in progress, and next we intend to study the effect of linearly and circularly polarized light on the ice nucleation process.

Light-matter Interactions

Double-well spectroscopic signatures induced by hydrogen-bonds

Noam Pinsk¹, Dr Nimrod Benshalom¹, Michal Hartstein², Dr Yael Diskin-Posner³, Dr Matan Menahem¹, Dr Olle Hellman², Prof Leeor Kronik², Prof Omer Yaffe¹

¹*Chemical and Biological Physics, Weizmann Institute of Science, Israel*

²*Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

³*Chemical Research Support, Weizmann Institute of Science, Israel*

Vibrational modes in crystals are typically modeled by quasi-harmonic potentials, where temperature modifies only the mode frequency and curvature. In a molecular crystal α -glycine, we identify two Raman features whose temperature evolution cannot be captured within this framework. Using temperature- and polarization-dependent Raman spectroscopy together with density-functional theory, we exclude a quasi-harmonic origin and show that these features arise from a double-well potential whose asymmetry changes with temperature. Isotopic substitution ($H \rightarrow D$) confirms that this behavior is governed by α -glycine's hydrogen-bond network. Our results directly connect macroscopic Raman signatures to the underlying microscopic potential that shapes the vibrational dynamics.

Light-matter Interactions

Equilibrium and Nonequilibrium Raman Spectroscopy of Aqueous Systems

Noam Lusthaus¹, Prof. Omer Yaffe¹

Weizmann Institute, Israel

Low-frequency Raman scattering provides a sensitive probe of molecular dynamics in liquids, revealing how intermolecular interactions and molecular conformations govern energy transport. In this work, we employ equilibrium and time-resolved Raman spectroscopy to bridge the microscopic and macroscopic levels.

At equilibrium, we investigate distilled water and aqueous amino acid solutions over a range of temperatures, focusing on the evolution of the quasielastic band and the intermolecular bending and stretching modes near 60 cm⁻¹ and 170 cm⁻¹ of water molecules. Heating or the addition of amino acid solutes disrupts the hydrogen-bond network, which can be directly observed through the waning of the modes associated with the intermolecular vibrations of the hydrogen bonds.

To extend these insights beyond equilibrium, we implement a time-resolved Raman setup with sub-nanosecond temporal resolution. A near-infrared pump pulse induces a controlled temperature jump, and the subsequent relaxation of the low-frequency Raman spectrum is tracked in real time. These measurements enable us to follow molecular rearrangements through the evolution of the intermolecular bending and stretching modes of water.

In future work, we will exploit this time-resolved Raman setup to study more complex systems, namely aqueous amino acid solutions, providing temporal insight into the relaxation dynamics of solute–solvent arrangement.

Light-matter Interactions

**Many-Body Effects in Lattice Dynamics: A Case Study of the
Displacive Phase Transition in BiVO₄**

*Shlomo Rand,¹ Adi Lanton (Cohen),¹ Ian D. Sharp,^{2, 3} Omer Yaffe,¹ and Matan Menahem¹, **

¹Weizmann Institute of Science, Rehovot, Israel

²Walter Schottky Institute, Technical University of Munich, 85748 Garching, Germany

*³Department of Physics, TUM School of Natural Sciences,
Technical University of Munich, 85748 Garching, Germany*

Displacive phase transitions, characterized by structural instabilities driven by the soft-ening of a vibrational mode, are central to the behavior of many functional materials. These transitions are often described using simplified models that treat soft modes as independent vibrational excitations. However, such treatments neglect the critical role of mode coupling and many-body interactions, which become especially significant near structural instabilities. A more complete framework is needed to capture the rich and often anomalous features observed in vibrational spectra during these transitions.

This work introduces a coupling-based dynamical model that integrates explicit interaction terms into the lattice equations of motion. Using BiVO₄ as a representative system, we demonstrate that this framework captures key spectral anomalies, such as intensity redistribution, asymmetric lineshapes, and polarization-dependent snaking that elude conventional Lorentzian descriptions. These results highlight that mode coupling is a fundamental aspect of displacive phase transition dynamics. Our approach establishes a direct connection between many-body lattice interactions and experimentally observed spectral features, offering a powerful tool for investigating anharmonic behavior and phase transitions across a broad class of materials.

Light-matter Interactions

What can chemical bonding tell us about photoinduced self-healing reactions in inorganic semiconductors? Insight from Bismuth-Antimony Selenide

Anchal Vashishtha¹, Prof. Eran Edri¹

Chemical Engineering, Ben-Gurion University of the Negev, Israel

Photo-reactive self-healing semiconductors with suitable bandgaps for solar energy conversion offer an intriguing path to making resilient and low-cost photovoltaic devices through the introduction of a self-recovery path. However, only few inorganic photovoltaic materials have such quality, and the underlying chemical properties that enable it are unknown, which poses a significant limit to our ability to study and discover new self-healing semiconductors. Recently, we have found antimony trichalcogenide (Sb_2Se_3 , Sb_2S_3) and chalcogenides (e.g., SbSeI) can undergo a reversible photo-induced phase transition (PIPT) in which the structure is restored after photo-induced damage is incurred to the materials. This group of materials offer a unique opportunity for studying PIPT and its limits. In particular, this group of materials facilitates the study of functional permutation to specific crystalline sites, and to finding the limits of PIPT occurrence, which sheds light on the origin of the PIPT and self-recovery of this class of materials. We found that PIPT magnitude decays upon gradual $\text{Bi}_{\text{Sb}(1)}$ substitution in a $\text{Sb}_{2-x}\text{Bi}_x\text{Se}_3$ homologous series, until nearly one in five Sb ions is substituted with Bi. Then, PIPT diminishes completely. The homologous series occurs along a transition from a covalent to metavalent chemical bonding. By expanding our search, we find a correlation between bonding type and photoreactivity does exist but is an insufficient condition. Instead we suggest that sufficient bonding states at the bottom of the conduction band are also required. This study pushes the limits of designing self-healing inorganic semiconductors for various applications and provides tools to further expansion.

Light-matter Interactions

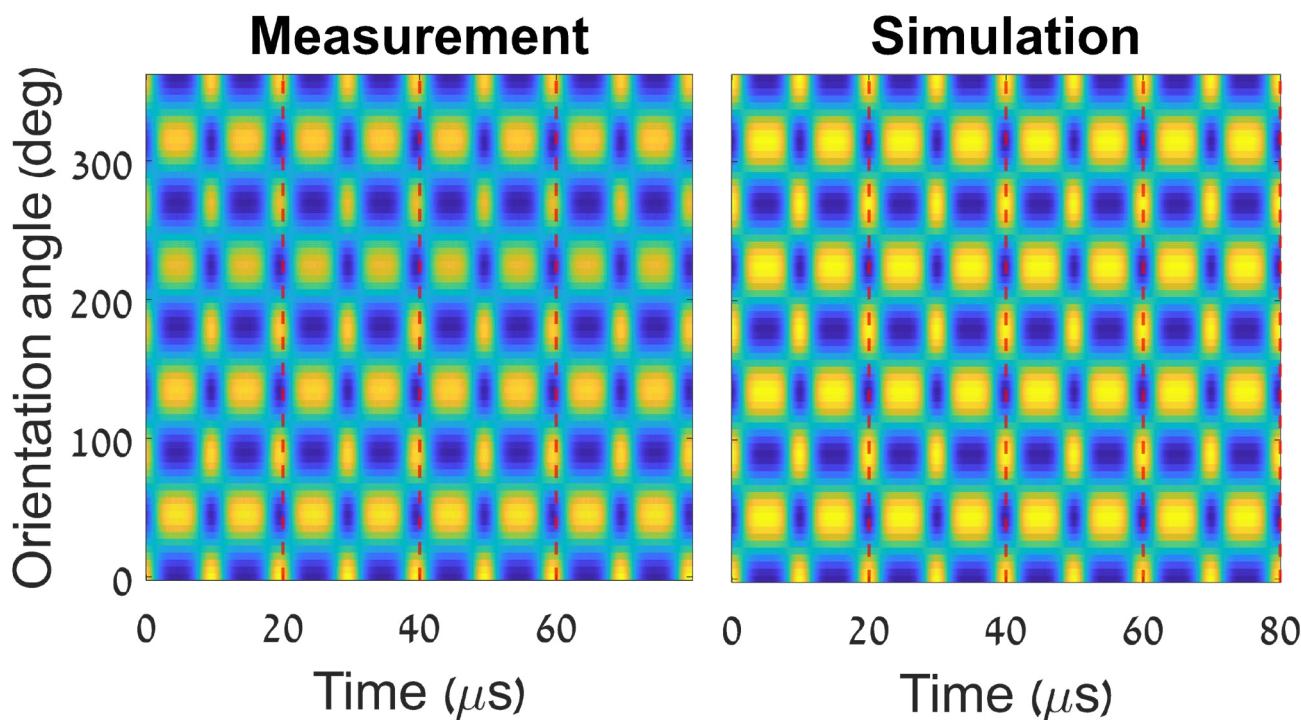
Linear and Circular Polarization Modulated Raman

Shaked Ezra Brandwein¹, Dr. Matan Menahem¹, Alina Shafir¹, Prof. Omer Yaffe¹
Chemical and Biological Physics Department, Weizmann Institute of Science, Israel

Linear polarization effects in Raman scattering have been systematically studied in our lab using Polarization Orientation (PO) measurements. PO Raman experiments reveal the symmetry of lattice vibrations, enabling the extraction of the corresponding Raman tensors and locating the material within the continuum between crystalline and amorphous order. However, such measurements require long acquisition times due to angular scanning, which demands high system stability and leaves the results susceptible to temperature fluctuations, illumination noise, and focus variations caused by mechanical drift.

To address this challenge, we developed a high sensitivity setup based on 50kHz modulation of the incident polarization using a photoelastic modulator (PEM). The measurement method is Time Correlated Single Photon Counting (TCSPC). In TCSPC, photon arrival times relative to a periodic trigger are recorded and accumulated into a histogram over many cycles. Here, the periodic trigger signal corresponds to the modulation frequency of the PEM.

We demonstrate the performance of the new setup on silicon, comparing measured polarization patterns with simulations based on the known Raman tensor (see the attached figure). After establishing the linear response capability, we are extending the system to circular polarization measurements, enabling access to chiral light-matter interactions and, ultimately, Raman optical activity in solid-state samples.

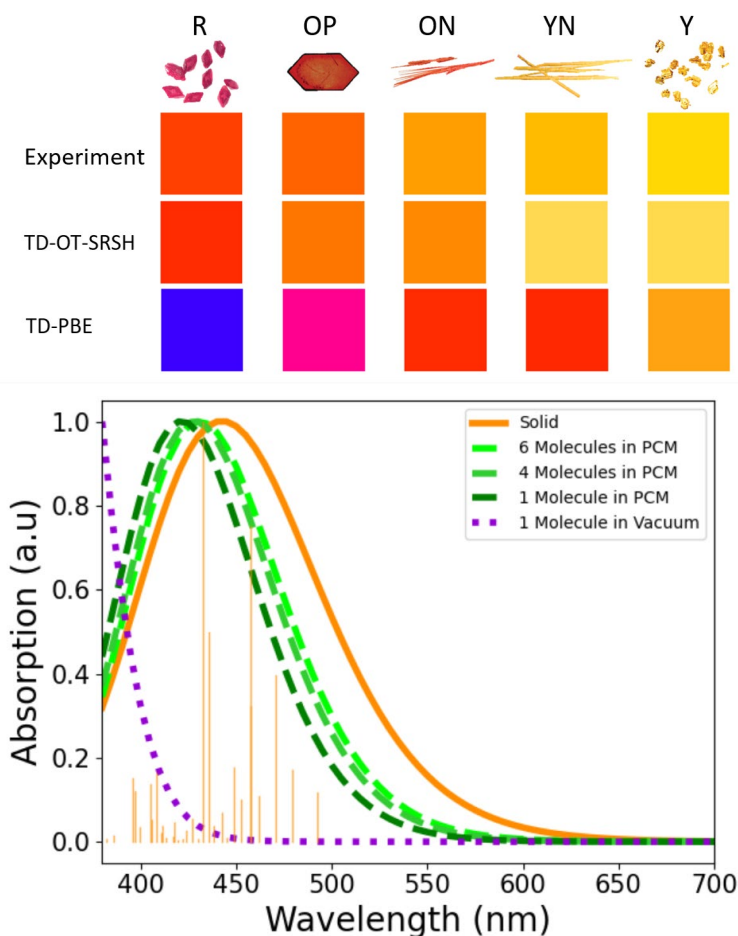


Light-matter Interactions

Accurate non-empirical predictions of color polymorphism in ROY: the role of solid-state effects

Michal Hartstein¹, Dr. Guy Ohad¹, Prof. Leeor Kronik¹
Weizmann Institute of Science, Israel

Predicting accurately the absorption spectra of molecular solids is a long-standing challenge for time-dependent density functional theory (TD-DFT). A particularly demanding test case is color polymorphism, where different polymorphs of the same molecular solid exhibit different perceived colors that arise from relatively modest spectral changes. A striking example is the molecular crystal ROY (5-methyl-2-((2-nitrophenyl)amino)thiophene-3-carbonitrile), known for its red, orange, and yellow polymorphs. Here, we show that non-empirical optimally-tuned screened range-separated hybrid (OT-SRSH) functionals can accurately predict the experimental optical spectra and colors of ROY polymorphs. Beyond accurate predictions, our analysis reveals that the origin of the observed color variation arises not only from conformational changes at the molecular level but also from solid-state effects, including dielectric screening and excitonic delocalization across the crystal. These findings challenge the prevailing assumption that color in such systems is predominantly molecular in nature, and highlight the importance of modeling the full solid-state environment to understand and predict color polymorphism in molecular crystals.



Light-matter Interactions

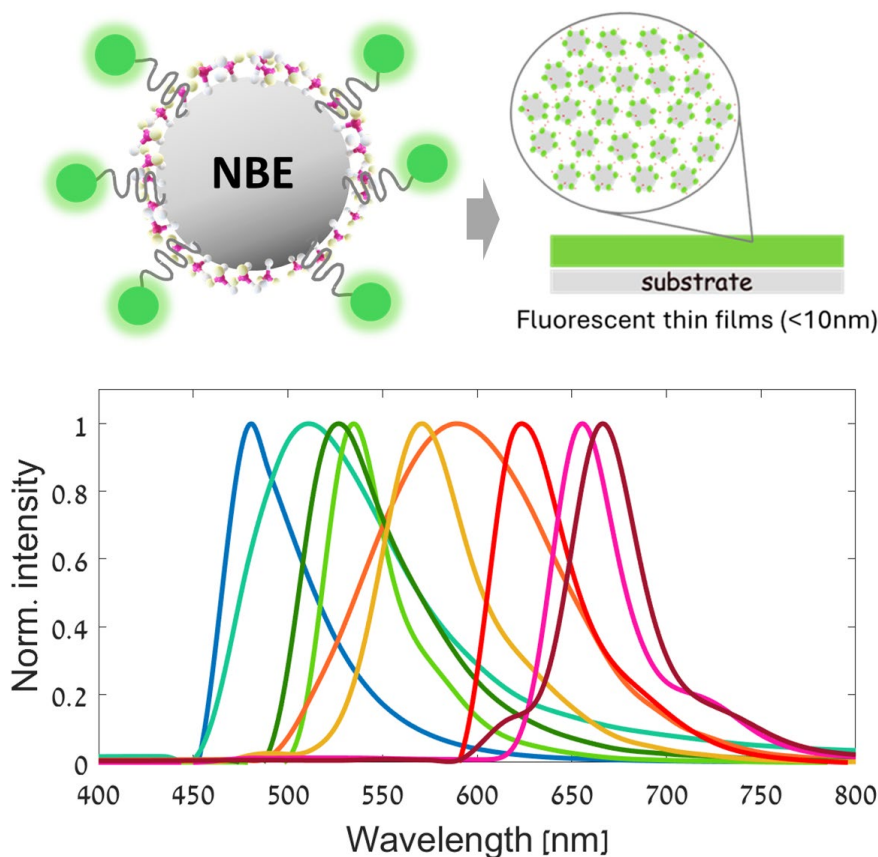
Nano Bead Emitters: A Versatile Toolkit for Advanced Optical Thin Films

Ilya Olevsko¹, Prof. Gerardo Byk¹, Prof. Adi Salomon¹

Department of Chemistry, Bar-Ilan University, Israel

The precise engineering of optical surfaces with controlled fluorescent properties is a critical challenge in biophotonics and super-resolution microscopy. Here, we introduce the Nano Bead Emitter (NBE) platform, a versatile, bottom-up toolkit for fabricating custom fluorescent thin films using size-controlled, dye-functionalized nanohydrogels. By leveraging the mono-dispersity and strong negative zeta potential of the precursor nanohydrogels, we achieve exceptionally bright, transparent, and uniform optical layers where the film morphology is strictly dictated by the nanobead size.

A key advantage of the NBE platform is its profound modularity; virtually any fluorescent dye can be incorporated and printed with high fidelity onto diverse substrates. We demonstrate this versatility by fabricating custom axial calibration standards matched to specific excitation lines (e.g., 405, 488, 561, 640 nm) for instruments like TIRF and confocal microscopes. Furthermore, the platform supports the creation of precise 3D multi-layer architectures, opening new possibilities for modeling optical effects such as Förster Resonance Energy Transfer (FRET). We also report on the platform's remarkable stability retaining high fluorescence with minimal degradation after 12 months and its robust biocompatibility, supporting direct cell culture. This work establishes NBEs as a powerful, adaptable solution for engineering advanced optical surfaces for both materials science and biological applications.



Modular Hydrogel-Based Nano-Bead Emitters for Bright, Homogeneous Fluorescent Thin Films

Light-matter Interactions

Simulations of real-time electron dynamics in complex chemical environments

Prof. Dr. Marek Sierka¹, Dr. Manas Sharma²

¹*Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Germany*

²*Department of Chemical Engineering, Indian Institute of Science, India*

Understanding light–matter interactions in complex chemical environments requires capturing ultrafast electron dynamics and environmental response. We present a real-time time-dependent density functional theory (RT-TDDFT) framework combined with density functional embedding theory (DFET) in TURBOMOLE [1–2]. The approach, implemented with Gaussian basis functions and density fitting, supports kinetic-energy density functional and projection-based embeddings, enabling subsystem simulations that retain environmental polarization at modest cost [2,4].

We highlight two applications. First, high-harmonic generation (HHG) from water: embedding a single H₂O in liquid water lowers the ionization potential by ≈ 2 eV and red-shifts the cutoff from the 18th harmonic (22.3 eV) to the 15th (18.6 eV), consistent with hydrogen-bond screening [2]. Second, resonance-enhanced Brunel harmonics in organic semiconductor films: tetraphenylporphyrin exhibits a five-photon S₀→S₂ pathway that amplifies the fifth harmonic and drives an early deviation from perturbative scaling, in agreement with RT-TDDFT simulations [3].

These results establish real-time density functional embedding (RT-TDDFET) as a practical tool for light-induced dynamics in realistic environments, bridging molecular and condensed-phase descriptions from solvated chromophores to organic thin films.

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Light-matter Interactions

2D Metal Halide Perovskites with Iodo-aromatic Ligands - Structural and Optoelectronic Properties

Rawan Hirzalla¹, Dr Ido Hadar¹

department of chemistry, Hebrew university of Jerusalem, israel

Two-dimensional (2D) metal halide perovskites are emerging as a promising class of semiconductors with the general formula A_2BX_4 , where A is an organic spacer, B a metal cation, and X a halide anion. Unlike their three-dimensional counterparts, 2D perovskites offer enhanced chemical and structural tunability by varying elemental composition—metals, halides, organic spacers, and inorganic layer thickness—allowing for tailored optical and electronic properties. This flexibility presents both opportunities and challenges associated with studying these compounds.

Here, I present the synthesis of single-layer 2D metal halide perovskite structures stabilized by aromatic-ring-based ligands, which are anticipated to induce lattice modifications influencing their optoelectronic behaviors. I specially prepared iodide-substituted ligands, including Iodoaniline, Iodolphenylmethyamine, and Iodophenylethylamine, with different positions of iodide substitution (ortho and para) and alkylamine tail lengths. The perovskites were synthesized in solution, and their structures were characterized via single-crystal and powder X-ray diffraction. Composition analysis involved NMR spectroscopy, while optical properties were examined using UV-Vis absorption and photoluminescence spectroscopy. Results indicated that minor structural distortions could significantly impact properties like band gap and emission energy.

Overall, this work introduces a series of novel 2D metal halide perovskites, most of which are reported here for the first time, highlighting the potential for further exploration of their optoelectronic applications.

Light-matter Interactions

Direct Observation of Carrier-Induced Phonon Asymmetry in Hematite via Time-Resolved Raman Spectroscopy

Maya Levy Greenberg¹, Prof. Omer Yaffe¹

Chemical and Biological Physics, Weizmann Institute of Science, Israel

The interaction of phonons with charge carriers governs transport, recombination, and functionality in materials with strong polaronic and carrier-localization effects. A key open issue is the long-lived, non-coherent lattice state that follows photoexcitation; it is rarely probed because its subtle anharmonic vibrational signatures require high spectral resolution and lie beyond the scope of harmonic models. To address this, I developed a time-resolved Raman system that combines pulsed photoexcitation with a continuous-wave probe, providing nanosecond-resolved vibrational measurements with high spectral precision and directly probing lattice distortions driven by photoinduced carriers. Applied to hematite (α -Fe₂O₃), a prototypical small-polaron oxide, our experiment reveals a mode-dependent asymmetry in the Raman lineshape that persists for more than 200 ns. Steady-state temperature-dependent spectra show no comparable evolution, ruling out transient heating and indicating that the long-lived distortions arise from carrier-induced modifications of the phonon self-energy.

These results demonstrate that time-resolved Raman spectroscopy can directly capture nonequilibrium carrier-lattice coupling, providing a new route to tracking polaronic relaxation pathways in materials dominated by localized carriers.

Light-matter Interactions

Highly Stable CsPbBr₃ Vertical Nanowire Arrays for Efficient Light-Matter Interaction and CO₂ photoreduction

Neena Prasad¹, Dr. Lena Yadgarov¹

Chemical Engineering, Ariel University, Israel

Halide perovskite nanowires (HP-NWs) exhibit fascinating optical properties, making them attractive for advanced technologies. However, instability and lack of an effective synthetic protocol limit their commercialization. To address this, nanoporous anodized aluminum oxide (AAO) metamaterial is used as templates for the growth of CsPbBr₃ NW arrays. These cutting-edge membranes will play a pivotal role in highly efficient carbon dioxide (CO₂) reduction via photocatalysis. AAO functions as a growth template and a stabilizing medium. The NW array exhibits strong light-trapping ability, and the pore geometric features (pore radius-*R* and distance between pores-*d*) can potentially enhance the light-matter interactions (LMI). The impact of *R* and *d* on LMI within the AAO/CsPbBr₃ system using theoretical finite difference time domain (FDTD) simulations is demonstrated for the first time. Optimal LMI is observed with *R* = *d* = 25 nm and 50 nm. Ligand-free synthesis of CsPbBr₃ NW arrays via spin-coating, drop-casting, and inverse temperature crystallization (ITC) is reported. The modified ITC method achieves 90% pore filling with significant NW lengths. This AAO/CsPbBr₃ system exhibited strong light-trapping abilities, further enhanced by the integration of electron and hole transport layers (ETL and HTL). MoS₂ as a promising ETL material due to its capability to enhance charge separation and reduce recombination losses. This design not only facilitates solar energy conversion but also promotes favorable electron-hole separation, which is beneficial for CO₂ reduction. Hence, this device structure forms a robust foundation for the stable HPs required in efficient CO₂ reduction, opening pathways for sustainable and ecofriendly energy solutions.

Light-matter Interactions

concentration and thickness dependent optical transparency in biological tissues via refractive index modulation

Paz Toledano¹, Prof Yaakov R. Tischler²

¹*Bar-Ilan University, Israel*

²*Chemistry, Bar-Ilan University, Israel*

Recent progress in tissue optical clearing has introduced a non-traditional mechanism for achieving optical transparency in biological samples. Conventional optical clearing agents (OCAs) reduce light scattering by matching the refractive indices of the aqueous and lipid components of tissue, typically through dehydration or chemical modification. In contrast, a resonance-based OCA approach exploits spectral engineering with highly absorbing dyes to modulate the real part of the refractive index and thereby lower scattering.

Notably, Ou et al. [Science 385, eadm6869 (2024)] demonstrated that tissue transparency can be achieved not by direct absorption at imaging wavelengths but through a Kramers–Kronig (KK) resonance effect. In this mechanism, intense and narrowband absorption near 428 nm increases the real refractive index in the red and near-infrared regions, reducing refractive-index contrast and suppressing optical scattering without inducing chemical or structural damage.

We systematically investigated KK-OCA efficacy as a function of tartrazine concentration and tissue thickness using ex-vivo chicken breast and a custom optical setup enabling precise thickness control. Transmission measurements at 785 nm revealed a strong dependence on both parameters: low concentrations (1–10 mM) reduced transmission, while above threshold levels (~100 mM for thin and ~400 mM for thick samples) transparency increased up to 26-fold at 200 mM.

These results quantitatively confirm the KK-dispersion mechanism and establish a practical “Transparency Scale” linking optimal dye concentration to tissue thickness for rational design of resonance-based optical clearing strategies.

Light-matter Interactions

Three-Photon Cascaded Emission from Triexcitons in Giant CsPbBr₃ Quantum Dots and in CdSe/CdS Nanoplatelets at Room Temperature

Dekel Nakar¹, Dr. Miri Kazes¹, Dr. Daniel Amgar¹, Nadav Frenkel¹, Dr. Ihor Cherniukh^{2,3}, Dr. Maryna I. Bodnarchuk^{2,3}, Leon G. Feld^{2,3,4}, Dr. Chenglian Zhu^{2,3}, Mariia Svyrydenko^{2,3}, Dr. Gabriele Rainò^{2,3,4}, Prof. Maxym V Kovalenko^{2,3,4}, Prof. Dan Oron¹

¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Laboratory for Thin Films and Photovoltaics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*

³*Institute of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland*

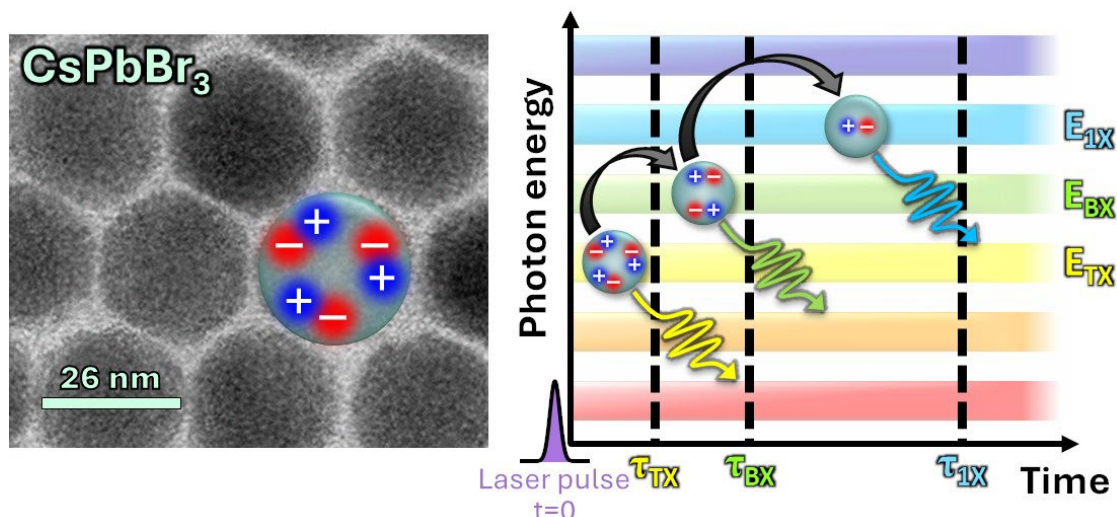
⁴*National Centre of Competence in Research (NCCR) Catalysis, ETH Zürich, Switzerland*

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, which limits their investigation and applications. Here, we present the heralded spectroscopy of three-photon cascades from triexcitons in giant CsPbBr₃ nanocrystals at room temperature.[1] We show that this system exhibits second- and third-order correlation function values, $g^{(2)}(0)$ and $g^{(3)}(0,0)$, close to unity, demonstrating efficient emission and very weak binding of both biexcitons and triexcitons. Combining fluorescence lifetime analysis, photon statistics, and spectroscopy, we can readily identify and characterize emission from higher multiexcitonic states. Finally, we compare the multiexciton properties of the giant CsPbBr₃ QDs with our recent findings on CdSe/CdS nanoplatelets, showing correlation between triexciton and exciton binding energies, and a transition from repulsion to attraction, via heterostructure engineering.[2] Our results suggest a potential pathway toward control of multiexcitonic emission cascades and high-order photon correlations, with potential applications in non-classical light emission.

[1] Kazes, M.,* Nakar, D.,* et al., Nano Lett. 24, 13185 (2024). * Equal Contribution.

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Triexciton Heralded Spectroscopy



Light-matter Interactions

Resolving the parameter dilemma in structural and electronic properties of CuBr via non-empirical density functional theory

Guy Ohad¹, Conan Weiland², Eric Cockayne², Eric L. Shirley², Leeor Kronik¹, Joseph C. Woicik²

¹*Weizmann Institute of Science, Israel*

²*National Institute of Standards and Technology, USA*

Simultaneous description of both structural and electronic properties of cuprous bromide (CuBr) within density functional theory (DFT) has proven to be challenging. Previous work showed that adding a Hubbard U term to semilocal DFT remedies structural deficiencies, but at the cost of an insufficiently accurate electronic structure. Here, we revisit this challenge by using non-empirical tuning of a range-separated hybrid functional. We find that this approach matches DFT+ U in the prediction of structural properties, while significantly outperforming it in reproducing the electronic structure, specifically the valence-band photoemission spectrum and the band gap. Finally, we explore temperature effects on spectral broadening, including the low temperature regime which is inaccessible experimentally.

Light-matter Interactions

Enhancing the Solid-State Emission of Carbonyl-Containing Compounds with a Bifuran-Core

Hadar Roizman Yakir¹, Prof Ori Gidron¹

Institute of Chemistry, Hebrew university of Jerusalem, Israel

Organic luminescent materials, particularly those used in optoelectronic devices such as organic light emitting diodes (OLEDs), have drawn significant interest due to their tunable emission properties. However, many aromatic compounds that luminesce strongly in solution possess little to no luminescence when aggregated (e.g., in the solid state), which limits their practical application. The discovery of the reverse phenomenon, whereby aggregation induces emission, has prompted research into luminescent aggregates and their potential to enhance solid-state emission properties. This study investigates a series of bifuran dialdehydes and diketones (F1–F3) and their bithiophene analogs (T1–T3), comparing their photophysical properties in solution and the solid state. The incorporation of carbonyl groups into bifuran cores significantly enhances their fluorescence, with solid-state quantum yields reaching 35% for F2, in contrast to low emissions from the thiophene-based analogs. Structural analysis via X-ray crystallography reveals that bifuran derivatives exhibit tighter packing and more rigid molecular backbones, which contributes to the observed aggregation-induced emission. The carbonyl group also stabilizes the furan core, resulting in stronger luminescence and better stability compared with unmodified bifurans. These findings suggest that bifuran-carbonyl materials have significant potential for high-performance luminescent applications, offering a promising alternative to traditional thiophene-based systems for optoelectronic devices.

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Light-matter Interactions

The Critical Role of π -Electron Count ($4n$ vs. $4n+2$) in Dictating the Singlet and Triplet Excited State Photophysics of π -Conjugated Macrocycles

Noam Levinsky¹, Prof Ori Gidron¹
Chemistry, Hebrew university, Israel

The quinoidal character of π -conjugated macrocycles incorporating small aromatic subunits enables the formation of planar π -conjugated systems at sizes exceeding the practical limit of annulenes. As a result, these materials hold a central position in the development of newest applications, including OPV devices, OFETs, and molecular switches. They also possess larger ring sizes while maintaining a higher degree of Hückel aromaticity in the ground state than corresponding annulene systems. In the last few years, research on this type of macrocycle has expanded from the ground state to the excited states to investigate the possibility of identifying Baird's Aromaticity. This theory argues that an aromaticity reversal occurs in the excited state: $4n$ π -electron systems become aromatic, and $4n+2$ π -electron systems become antiaromatic.

In the present study, we investigate the photophysical properties of furan-acetylene macrocycles (C5-C8), comprising five to eight monomers, utilizing ultrafast femtosecond and nanosecond transient absorption spectroscopy in conjunction with theoretical calculations. Our results demonstrate that the electronic excited states and molecular dynamics are dictated primarily by the aromaticity and π -electron count, rather than the size of the macrocycle.

Light-matter Interactions

When Cavity Fields Meet Localized Plasmon Resonances

Livin Paul¹, Prof. Tal Schwartz¹

Physical Chemistry Department, Raymond & Beverly Sackler Faculty of Exact Sciences and Center for Light–Matter Interaction, Tel Aviv University, Israel

The confinement of light within specially tailored optical structures gives rise to new quantum states, such as localized plasmons and excitons in metal nanoparticles and molecules, as well as confined electromagnetic modes within nanocavities.¹ The interaction between the quantized optical modes of nanocavities and molecular excitations leads to the formation of hybrid light–matter states known as polaritons.² Likewise, the coupling between localized plasmon resonances and excitons generates hybrid states referred to as plexcitons.³ Here, I will present the emergence of new hybrid modes arising from the strong coupling between localized surface plasmon resonances in metal nanoparticles and microcavity modes, and I will explain the properties of the resulting energy levels. Most importantly, I will demonstrate how the cavity field can mediate cooperative quantum-coherent interactions between otherwise uncoupled localized surface plasmons and molecular excitons, manifesting as cavity-mediated long-range dipole–dipole interactions. The optimized and unique configuration of the localized plasmon resonance–cavity field–exciton system results in the emergence of new hybrid states that incorporate contributions from plasmons, excitons, and cavity fields.

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Light-matter Interactions

Interfacial Engineering of Auto-Reversible Reactions: A 4DSTEM Study of Encapsulated SbSeI Phase Change Materials

Anchal Vashishtha¹, Dr. Alexander Upcher², Dr. Vladimir Ezersky², Prof. Yevgeni Rakita³, Prof. Eran Edri¹

¹*Chemical Engineering, Ben-Gurion University of the Negev, Israel*

²*Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of the Negev, Israel*

³*Materials Engineering, Ben-Gurion University of the Negev, Israel*

Auto-reversible reactions resemble self-healing processes, while irreversible reactions can be used to switch between bright and dark states, as well as conductive and non-conductive states. SbSeI, a wide bandgap semiconductor ($E_{\text{gap}} \sim 1.8$ eV), exhibits a 'volatile' photochemical reaction, during which Sb metal clusters form as intermediates. However, the structural properties of these clusters, such as size, shape, crystal structure, and their relationship with parent crystal orientation, remain unknown. To investigate the structure of SbSeI nanorods after reaction, we employed 4D scanning transmission electron microscopy (4DSTEM). To prevent oxidation of photoexcited nanorods, we coated them with thin layers (~ 60 nm) of alumina/zinc oxide using ALD. Surprisingly, alumina coating facilitated a non-volatile state, resulting in Sb clusters of varying sizes (100 nm), which were primarily located near alumina-nanorod interface. A thermal annealing process, monitored in-situ by Raman spectroscopy, enabled the reactivation of intermediates and nearly complete recovery of SbSeI. In contrast, microscopic analysis of the zinc oxide-coated rods, which showed spectroscopic signs of SbSeI auto-recovery without a thermal step, revealed voids formed at the center of the rods. This phenomenon is likely due to a Kirkendall effect, where halide diffuses faster than other components, leading to the formation of reduced species (Sb and SbSe_x). In summary, this study demonstrates that transition from volatile to non-volatile conditions can be controlled by selecting the appropriate coating. This finding has significant implications for enabling or disabling 'self-healing'-like reactions in semiconductors for photovoltaic applications or for advancing computing technologies.

Light-matter Interactions

Numerical simulations of Ni, Cu, and Al plasmonic nanoparticles for localized surface plasmon resonance biosensing

Iryna Hovor¹, Dr Lena Yadgarov¹

Chemical Engineering, Ariel University, Israel

Plasmonic nanoparticle-based biosensors are noninvasive, highly sensitive for the detection of disease biomarkers due to their ability to detect minimal changes in the refractive index (RI) of the surrounding medium without analyte labeling. The development of efficient biosensors based on localized surface plasmon resonance (LSPR) requires a detailed understanding of the optical properties of nanostructures. Numerical simulations of spherical Ni, Cu, and Al nanoparticles were performed as low-cost alternatives to Au and Ag using the finite-difference time-domain (FDTD) method.

Nanoparticles with diameters ranging from 10 to 90 nm were modeled in media with refractive indices from 1 to 4. The sensitivity (S) was defined as the slope of the resonance wavelength on RI. The simulation results revealed that the sensitivity of metals increases with particle diameter. The relative sensitivity enhancement ($S_{90\text{nm}}/S_{10\text{nm}}$) followed the trend: Ni (3.2) Al (2.2) Cu (1.9), demonstrating the strongest size dependence for Ni. Despite their high sensitivity, Ni NPs exhibited the lowest extinction efficiency ($Q_{\text{ext}} = 3.6$) across all RI values with shifting LSPR peak to the near-infrared region, outside the desired UV–Vis range. Cu NPs showed the highest Q_{ext} values (11.7 and 11.5 for RI = 3 and 4, respectively), but also in the near-infrared region. In contrast, Al NPs maintained high Q_{ext} (8.6–6.9, RI 1–4) values within the visible range across all RI values, demonstrating stable optical performance. Ultimately, 20 nm Al NPs exhibited optimal characteristics — visible resonance and high sensitivity, which makes them promising candidates for low-cost label-free LSPR biosensors.

Light-matter Interactions

Synthesis of Biocompatible Fluorescent Nano Beads for Advanced Optical Applications

Maria Shehadeh¹, Prof Adi Salomon¹
Chemistry, Bar Ilan University, Israel

A major challenge in the field of optical imaging is the fabrication of fluorescent thin films that are bright, and morphologically uniform, key attributes required for reliable calibration in advanced microscopy techniques, especially in two-photon (2P) excitation microscopy. Conventional fluorescent films frequently suffer from limitations such as aggregation-induced quenching, uncontrolled surface morphology, and rapid photobleaching, all of which compromise imaging quality and reproducibility. In this work, I address these issues by synthesizing hydrogel-based nanoparticles that are designed to conjugate efficiently with a wide range of fluorescent dyes bearing NHS-ester functional group. These resulting nano bead emitters (NBEs) can be processed into ultrathin films that maintain exceptional brightness, homogeneity, and photostability, making them highly promising candidates for use in 2P microscopy calibration and other demanding bioimaging applications. The particles were synthesized in aqueous conditions and further processed into nanometric thin films, either directly or following polymer coating.

The resulting fluorescent films exhibit strong two-photon absorption properties and high spatial uniformity, with thicknesses below 10 nm. Their emission characteristics were confirmed by spectroscopic analysis, and their morphology was evaluated by atomic force microscopy (AFM). The films demonstrated exceptional photostability and brightness under 2P excitation, making them suitable as axial calibration standards for nonlinear optical imaging.

In addition to optical calibration, these films also find application in biological imaging scenarios, including plant tissues, where deep penetration, low background, and spectral tunability are essential for tracking and imaging in plant science.

Light-matter Interactions

Weak-Field Coherent Control of Ultrafast Molecule Making

Zohar Amitay¹

Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Israel

We experimentally demonstrate for the first time coherent control of ultrafast molecule making in the weak-field regime [Phys. Rev. Lett. 133, 193201 (2024)]. It is achieved even under thermally hot conditions typical of chemical reactions, which are extremely challenging due to the initial incoherent population of a vast number of scattering eigenstates. The weak-field regime corresponds to a photo-excitation that is fully described perturbatively. We coherently control by weak linearly-chirped femtosecond pulses the making of KAr complexes from thermally-hot pairs of colliding K and Ar atoms via a resonance-mediated two-photon transition. Our ab initio studies are in excellent agreement with the experiments and explain them. The control mechanism is identified to combine Franck-Condon filtering and phase-dependent shaped excitation of the selected excitation channels. The former purifies the huge thermal ensemble of excitation channels and selects a sub-ensemble of channels that is susceptible to coherent control, while the latter realizes their control by manipulating intra-channel interferences. This mechanism is utilized to further enhance the coherent control degree by tuning the pulse spectrum [paper in preparation]. The demonstrated control of the KAr system serves as a basic model for controlling triatomic systems, with an atom and a diatomic molecule as the reactants, that are non-reactive in their ground electronic state and all their excited electronic states are weakly-bound or unbound. All this opens up new feasible routes for the realization of the yet-to-be-realized dream of coherent control of binary chemical photoreactions.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



MAGNETIC RESONANCE

Chair: Michal Leskes

Invited Lecture

Magnetic Resonance

Exploring oligomerization states of proteins in solution using EPR spectroscopy

Sharon Ruthstein¹

Chemistry, Bar-Ilan University, Israel

Protein oligomerization is a central regulatory mechanism in biology, influencing gene expression, enzyme activity, receptor signaling, and cell–cell interactions. Understanding how proteins change conformation and assembly state remains challenging, especially when oligomerization is dynamic and sensitive to factors such as concentration, metal ions, nucleic acids, or interacting partners. Recent advances in site-directed spin labeling have positioned electron paramagnetic resonance (EPR) spectroscopy as a powerful tool for probing these mechanisms in solution.

In this work, we used EPR spectroscopy to investigate the oligomeric state of CsoR, a copper-sensing transcriptional repressor in *Mycobacterium tuberculosis*. CsoR regulates the *cso* operon by dissociating from its promoter upon copper binding. Our measurements reveal that CsoR exists primarily as a tetramer in equilibrium with a smaller dimer population, and that this distribution is maintained regardless of DNA binding. Continuous-wave EPR, relaxation analyses, and DEER experiments collectively indicate that DNA does not shift the tetramer–dimer equilibrium but does alter the exchange dynamics between oligomeric species. These findings provide mechanistic insight into how CsoR oligomerization contributes to transcriptional regulation.

Invited Lecture

Magnetic Resonance

Introducing Fluorine Metabolic Imaging (FMI) for "Multicolor" MRI Mapping of Redox Biomarkers in Health and Disease

Dan Cohen¹, Libi Saad¹, Balamurugan Subramani¹, Hyla Allouche-Arnon¹, **Amnon Bar-Shir¹**

Weizmann Institute of Science, Israel

The ability to map glucose and other monosaccharides in living systems has revolutionized the field of molecular imaging, providing unprecedented insight into cellular metabolism and transforming diagnostic medicine. Radiolabeled and magnetic resonance detectable sugars have become indispensable imaging agents for assessing metabolic activity in health and disease using non-invasive imaging modalities. For example, positron emission tomography (PET) with [¹⁸F]2-fluoro-2-deoxy-glucose (2FDG) enables visualization of enhanced glucose uptake in tumors; ²H-labeled glucose used in deuterium metabolic imaging (DMI) allows non-radioactive detection of downstream glycolytic products; and ¹H chemical exchange saturation transfer (CEST) MRI with native monosaccharides facilitates imaging of glucose transport and accumulation. Despite their impact, all these approaches report on enhanced glycolytic fluxes and phosphorylation-dependent trapping, leaving non-glycolytic metabolic pathways largely unexplored.

To achieve a more comprehensive and informative report on additional metabolic processes, in both health and disease, we introduced Fluorine Metabolic Imaging (FMI), a new ¹⁹F-MRI-based platform designed to visualize cellular redox metabolism rather than glycolytic fluxes. FMI utilizes synthetic 3-fluorodeoxy sugars as MRI-detectable molecular probes, which, unlike conventional glucose and galactose analogs, bypass phosphorylation and undergo redox transformations mediated by Aldo Keto Reductase (AKR) and Aldehyde Dehydrogenase (ALDH) enzymes. These reactions yield distinct oxidized and reduced fluorinated metabolites with well-resolved ¹⁹F-NMR signatures, enabling multiplexed, "multicolor" imaging of redox fluxes in vivo.

Invited Lecture

Magnetic Resonance

Correlation Tensor Magnetic Resonance as a probe of microstructure

Noam Shemesh¹

Research, Champalimaud Foundation, Portugal

Porous media - from emulsions and rocks to cells and living tissue - contain complex networks of microscopic compartments and barriers whose noninvasive characterization is essential across physics, materials science, geoscience, and biology. Since the 1960s, diffusion NMR has been recognized as an effective intrinsic probe of such microstructure: molecular displacements become sensitive reporters of restriction, disorder, and compartmentation, enabling inference of properties such as density, organization, and permeability without exogenous labels. In modern MR, diffusion is often summarized by low-order descriptors such as the diffusion tensor and diffusional kurtosis, which quantify deviations from Gaussian transport. However, these metrics are notoriously non-specific: similar values can emerge from distinct microstructural mechanisms, including microscopic anisotropy, heterogeneity of diffusivities across environments, and intrinsically non-Gaussian motion within restricting domains.

In this talk, I will present Correlation Tensor NMR/MRI (CTI), a framework based on advanced double diffusion encoding pulse sequences that exploits correlated molecular displacements to disentangle these competing sources of diffusion non-Gaussianity. CTI decomposes conventional kurtosis into three interpretable contributions: anisotropic kurtosis (arising from locally anisotropic barriers), isotropic kurtosis (reflecting variance in diffusivity), and microscopic kurtosis (capturing intra-compartment restriction/disorder or exchange). We will explore CTI through examples spanning controlled validation, in vivo brain measurements, and clinical translation to human 3T MRI, and show how CTI reveals distinct microstructural signatures in acute ischemic stroke, providing mechanistic interpretability beyond conventional diffusion metrics. Finally, I will discuss emerging extensions toward directional, tensorial microscopic biomarkers, opening routes to quantify biophysical tissue properties in a more specific MR-based manner.

Invited Lecture

Magnetic Resonance

^{133}Cs NMR as a tool to study and guide waste immobilization in geopolymers

Noy Vaisleib¹, Dr. Nurit Manukovsky¹, Dr. Michal Arbel-Haddad², **Professor Amir Goldbourt¹**

¹*School of Chemistry, Tel Aviv University, Israel*

²*NRCN, Israel*

The immobilization of radioactive cesium remains a key challenge for the nuclear industry. Alkali-activated geopolymers, which provide a low-temperature route to durable wasteforms, were suggested as an immobilization matrix for Cs-bearing radioactive waste streams. Recent work shows that Cs ions induce the formation of specific zeolites within metakaoline-based geopolymer formulations. Silica-rich formulations yield pollucite, which is the only naturally known Cs mineral, while formulations with a lower silica content yield the Cs bearing form of zeolite F (EDI).

Consequently, site-resolved ^{133}Cs SSNMR was combined with leaching tests in order to identify Cs sites across coexisting phases in the geopolymer matrices (zeolites A/X/F and amorphous phase) and tracks its migration during leaching. ^{133}Cs spectra indicate preferential retention in zeolite F and evolving occupancy of A/X zeolite sites, providing direct evidence that crystalline Cs-binding phases enhance immobilization.

To improve structural assignments where sites overlap, we developed enhanced triple-quantum (TQ) ^{133}Cs SSNMR. New three- and four-pulse schemes roughly double excitation efficiency versus two-pulse methods for Cs experiencing weak quadrupolar couplings ($C_q \lesssim 20$ kHz), enabling more informative 2D spectra on hydrated Cs-containing zeolites.

Finally, DFT-GIPAW calculations benchmarked on Cs salts and simple solids are used to link measured chemical shifts and quadrupolar couplings to candidate binding sites, and to screen functionals suitable for Cs systems, leading eventually to more reliable assignments of Cs spectra to in more complex geopolymer immobilization matrices.

Overall, the talk will present an SSNMR-led framework that provides guidance for durable Cs immobilization.

Invited Lecture

Magnetic Resonance

From Investigation of Polarization Transfer to Materials Insight: DNP Mechanisms Probe Diamond Defects Distribution.

Prof. Ilia Kaminker¹

School of Chemistry, Tel-Aviv University, Israel

Magnetic resonance techniques provide a powerful, non-destructive probe of point defects and their interactions in solids. Beyond sensitivity enhancement, dynamic nuclear polarization (DNP) can serve as a mechanistic tool that reveals microscopic information about defect structure and spatial heterogeneity. Here, we show that a systematic investigation of DNP mechanisms yields new insights into the nature and distribution of paramagnetic defects in diamond.

Using a combination of high-field electron paramagnetic resonance (EPR), electron–electron double resonance (ELDOR), and ^{13}C DNP at 7 and 14 Tesla, we investigate nitrogen-related defects in diamond, focusing on substitutional nitrogen (P1) and nitrogen–vacancy (NV) centers. By comparing samples with different defect compositions, we demonstrate that distinct DNP mechanisms—such as the solid effect (SE) and cross-effect (CE) are selectively activated depending on defect proximity and the strength of the electron–electron coupling. The DNP efficiency, spectral signatures, and polarization buildup dynamics directly reflect the presence of isolated versus clustered P1 centers.

Extending this approach to NV centers, we show that NV- and P1-driven DNP hyperpolarize different subsets of ^{13}C nuclei. Nuclear relaxation measurements and sequential DNP experiments reveal that while both P1 and NV centers polarize nuclei in their immediate vicinity, the two polarize distinct ^{13}C populations. The additivity of NV- and P1-induced hyperpolarization provides direct experimental evidence for a heterogeneous spatial distribution of defects within the same diamond crystal.

These results demonstrate that the high-field EPR -based investigation of DNP mechanisms may reveal previously unknown features of the materials used in hyperpolarization experiments.

Magnetic Resonance

Synthesis of 3-fluoro-3-deoxy pentoses for multicolor fluorine metabolic imaging via redox-dependent ¹⁹F-NMR fingerprints

Balamurugan Subramani¹, Dr Dan Cohen¹, Dr. Hyla Allouche-Arnon¹, Prof. Amnon Bar-Shir¹

Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

Early studies showed that 3-fluoro-3-deoxy-glucose and 3-fluoro-3-deoxy-galactose undergo intracellular reduction to polyols or oxidation to acids,^{1,2} producing distinct fluorine nuclear magnetic resonance (¹⁹F-NMR) signatures suitable for multicolor fluorine metabolic imaging (FMI). FMI can differentiate tumors based on their ¹⁹F metabolic fingerprints and report on redox biomarkers AKR1B1 and ALDH1A1.³ Motivated by this, we developed the unified synthetic strategy to a panel of 3-fluoro-3-deoxy pentoses: 3-fluoro-3-deoxy-D-xylose, 3-fluoro-3-deoxy-D-lyxose, 3-fluoro-3-deoxy-D-arabinose, and 3-fluoro-3-deoxy-D-ribose, and focused on 3-fluoro-3-deoxy-D-xylose (3FDXyl) as a prototype FMI probe.

3FDXyl was prepared by selective fluorination of allofuranose to give 3-fluoro-D-glucofuranose, followed by isomerization and deprotection.⁴ Its redox metabolites, 3-fluoro-3-deoxy xylitol (FDXtol) and 3-fluoro-3-deoxy xylonic acid (3FDXylA), were obtained by sodium borohydride reduction and sodium bicarbonate/bromine oxidation, respectively. In solution at 9.4 T, ¹⁹F-NMR showed two anomeric peaks for 3FDXyl (-196, -201 ppm) and distinct resonances for FDXtol (-212 ppm) and 3FDXylA (-207 ppm).

After intravenous 3FDXyl administration in a mouse, in vivo ¹⁹F-NMR revealed new signals consistent with metabolic conversion to these redox products. Multiplex three-dimensional FMI maps showed strong accumulation of FDXtol in skeletal muscle, resembling uptake patterns of 2-[¹⁸F]FDG in non-fasted subjects and suggesting transport via insulin-dependent glucose pathways. These results support fluorinated pentoses as promising candidates for expanding FMI probe chemistry.

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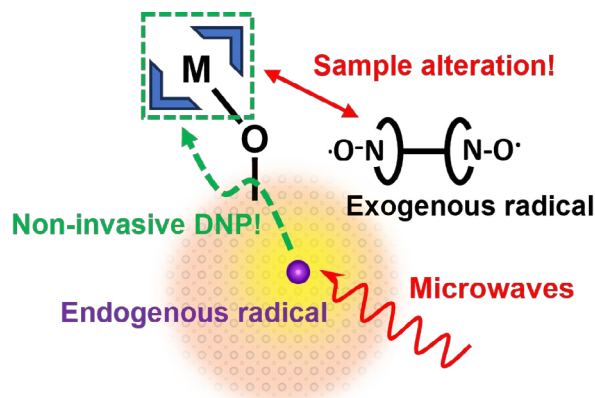
Magnetic Resonance

Development of metal-ion dynamic nuclear polarization NMR tool for non-invasive characterization of supported organometallic catalysts

Ilia Moroz¹

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

Surface organometallic chemistry (SOMC) is an approach that applies organometallic chemistry principles to solid surfaces to create well-defined supported catalysts, combining the advantages of both homogeneous and heterogeneous catalysis.¹ Although solid-state NMR spectroscopy is a powerful technique to study SOMC-made catalytic sites, their small quantity coupled with low inherent sensitivity of NMR make conventional NMR measurements impractical.



Dynamic Nuclear Polarization can significantly enhance NMR signals by transferring polarization of unpaired electrons to nuclear spins upon microwave irradiation.² Typically, the unpaired electrons are introduced by impregnating materials with a solution of organic radicals. Despite its effectiveness, this approach might not be suitable for catalytic surfaces: organic radicals can decompose and alter the material.

In our group we develop an alternative approach, metal-ion DNP (MIDNP), where materials are doped with a minute quantity of paramagnetic metal ions.³ This strategy avoids possible interactions between the PA and the investigated surface sites. Here we extend the application of MIDNP to SOMC-made systems and demonstrate that NMR signals of grafted molecules can be enhanced with minimal impact on samples integrity.

This work is supported by the Israeli Ministry of Absorption and Integration Postdoctoral Fellowship.

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MEDICINAL AND BIOLOGICAL CHEMISTRY

Chair: Muhammad Jbara

Invited Lecture

Medicinal and Biological Chemistry

Unlocking the Barrier of Chemiluminescence in Water

Doron Shabat¹

Tel Aviv University, Israel

Chemiluminescence probes are considered to be among the most sensitive diagnostic tools that provide a high signal-to-noise ratio for various biological applications. We have developed a new molecular methodology to design and foresee light-emission properties of chemiluminescence 1,2-dioxetane luminophores suitable for use under physiological conditions. The methodology is based on incorporating a substituent on the benzoate species obtained during the chemiexcitation pathway of a phenoxy-dioxetane probe. The substituent effect was initially evaluated on the fluorescence emission generated by the benzoate species and then on the chemiluminescence of the dioxetane luminophores. A striking substituent effect on the chemiluminescence efficiency of the probes was obtained when acrylate and acrylonitrile electron-withdrawing groups were installed. The chemiluminescence quantum yield of the best probe was more than three orders of magnitude higher than that of a standard, commercially available phenoxy-dioxetane probe. These are the most powerful chemiluminescence-dioxetane probes synthesized to date that are suitable for use under aqueous conditions. In addition, our probes are capable of providing high-quality chemiluminescence *in vitro* and *in vivo* images based on the endogenous activity of native enzymes or bio-analytes. We anticipate that the strategy presented here will lead to the development of efficient chemiluminescence probes for various applications in the field of sensing and imaging. This presentation outlines the conceptual insights that guided the development of these unprecedented luminophores and provides a historical perspective on the evolution of chemiluminescent phenoxy-dioxetane probes.

Invited Lecture

Medicinal and Biological Chemistry

Synthetic Proteins Behind the Plasma Barrier: Molecular Spies

Ashraf Brik¹

*Schulich Faculty of Chemistry, Technion-Israel Institute of Technology / Schulich
Faculty of Chemistry, Israel*

Understanding how posttranslational modifications (PTMs) shape protein function in living cells remains a central challenge in chemical biology. Genetic methods have transformed our ability to visualize and manipulate proteins. Yet, they provide limited control over events after translation and cannot fully access the vast chemical space of PTMs. Synthetic and semisynthetic proteins—prepared through solid-phase peptide synthesis and chemoselective ligation—offer atomic-level precision, enabling the incorporation of natural and unnatural PTMs, caging groups, reactive handles, and fluorophores. However, the inability of proteins to cross the plasma membrane has long restricted these powerful constructs to *in vitro* studies.

Recent advances in intracellular delivery now enable the introduction of synthetic proteins directly into living cells, although the full potential of this capability has yet to be realized. In this talk, I will highlight our strategies that enable such breakthroughs, including cell-penetrating peptides and physical delivery approaches such as multiplexed bead loading. Using case studies from our laboratory, I will describe improved live-cell delivery using DABCYL-modified cyclic deca-arginine; multiplexed delivery of ubiquitin and SUMO2 variants to probe conjugation-dependent localization in cells; and insights into the maturation process of SUMO2.

Together, these advances demonstrate the potential of combining synthetic proteins with intracellular delivery to expose dynamic PTM-encoded information and unlock mechanistic studies previously inaccessible using genetic tools alone. As delivery technologies continue to evolve, the integration of chemical synthesis with cell biology promises powerful new ways to analyze—and ultimately modulate—the molecular logic governing cellular function.

Invited Lecture

Medicinal and Biological Chemistry

Primordial Peptide Backbone Affects Assembly in Aqueous Solutions

Dr. Moran Frenkel Pinter¹

Chemistry, The Hebrew University of Jerusalem, Israel

One of the most fascinating mysteries in the field of origins of life concerns the driving force that led to the selection of today's 20 universal L-alpha amino acids in biology. An essential aspect of life's emergence involves the formation of compartments, which offer encapsulation for molecules and provide protection from hydrolysis in aqueous environments. Thus, polymers capable of assembly may have had a chemical evolutionary advantage over polymers that lacked this ability. We postulated that primordial peptide assembly could be one of the driving forces that led to the chemical selection of alpha amino acids in life today. To test this hypothesis, we generated depsipeptides, oligomers composed of ester bonds and peptide bonds that form readily under mild drying conditions, as model prebiotic peptides. However, it is unknown whether depsipeptides form assemblies in an aqueous environment similarly to peptides and proteins. To test the hypothesis that depsipeptides with alpha backbones will form assemblies more readily than beta backbones, we synthesized depsipeptides using a matrix of eight alpha- and beta- hydroxy acids and six alpha-, beta-, and gamma- amino acids. The reaction products were analyzed by microscopy and a physical stability analyzer to study assembly formation as well as various analytical techniques for chemical analysis. Our results demonstrate assembly formation in depsipeptide systems containing hydrophobic hydroxy acids and indicate that depsipeptide assemblies containing alpha hydroxy acid backbones are significantly more stable than beta analogs. Overall, our results offer an assembly-driven mode of selection for the alpha backbone in present-day biology.

Invited Lecture

Medicinal and Biological Chemistry

Chemical Decoding of Protein–DNA Recognition in Health and Disease

Ariel Afek¹, Irina Miodownik¹, Yumi Yao¹, Tamir Avioz¹, Noga Levy¹
Chemical and Structural Biology, Weizmann Institute of Science, Israel

Chemical and epigenetic DNA modifications can strongly reshape transcription factor binding, yet the underlying mechanisms are poorly understood. By systematically introducing natural and synthetic modifications—including 5mC, 5hmC, mismatches, and controlled nicks—we quantify energetic contributions of bases and backbone contacts and reveal alternative binding modes hidden in canonical DNA. Strikingly, several naturally occurring modifications dramatically alter the binding of disease-related TFs, including oncogenic regulators. These results expose a multilayered recognition code and highlight chemical perturbation as a powerful strategy to understand and modulate transcription factor activity in disease.

Invited Lecture

Medicinal and Biological Chemistry

Chemical Probes for Antifungal Research: Illuminating Mechanisms of Action and Guiding Drug Design

Micha Fridman¹

Chemistry, Tel Aviv University, Israel

The rising prevalence of fungal infections and drug resistance underscores the urgent need for a deeper understanding of how antifungal agents function within living cells. Our group has developed a suite of fluorescent chemical probes based on the three major classes of clinically used antifungal drugs: azoles, echinocandins, and polyenes. These probes enable direct visualization of drug behavior in live fungal cells, providing mechanistic insight into antifungal action and resistance. Using azole-based fluorescent probes, we showed that intracellular localization influences antifungal efficacy. Probes that accumulate in the endoplasmic reticulum, where the azole target resides, display markedly increased potency. These probes also enable rapid identification of resistance phenotypes such as enhanced efflux. Fluorescent echinocandin analogues revealed that accumulation at the fungal cell surface correlates with antifungal activity. An imaging-based assay employing a fluorescent echinocandin allows prediction of resistance by quantifying cellular uptake. Moreover, we demonstrated that subtle structural modifications to the echinocandin scaffold can restore activity against resistant strains, illuminating structure–activity relationships and target engagement. To investigate polyene drugs, we designed a unified set of fluorescent probes derived from amphotericin B, nystatin, and natamycin. Although these probes share a general mode of action, they exhibit distinct subcellular localization patterns across fungal species. In resistant strains, pronounced vacuolar accumulation suggests sequestration as a resistance mechanism and provides a potential marker identifiable by live-cell microscopy. Altogether, our work demonstrates how chemical biology and live-cell imaging uncover key principles of antifungal drug action and resistance, advancing the development of more effective antifungal therapies.

Invited Lecture

Medicinal and Biological Chemistry

Mimicking Cyanobacteria Circadian Clock with Peptide Oscillators

Gonen Ashkenasy¹

Ben-Gurion University of the Negev, Israel

Living organisms are replete with rhythmic and oscillatory behavior at all levels, to the extent that oscillations have been termed as a defining attribute of life. Recent studies of synthetic oscillators that mimic such functions have shown decayed cycles in batch-mode reactions or sustained oscillatory kinetics under flow conditions. Considering the hypothesized functionality of peptides in early chemical evolution and their central role in current bio-nanotechnology, we have recently developed a *peptide-based oscillator*. Oscillatory behavior was achieved by coupling coiled-coil-based replication processes as positive feedback to controlled initiation and inhibition pathways in a continuously stirred tank reactor (CSTR). Our results stress that assembly into the supramolecular structure and specific interactions with the replication substrates are crucial for oscillations. The replication-inhibition processes were first studied in batch mode, which produced a single damped oscillatory cycle. Thereafter, combined experimental and theoretical characterization of the replication process in a CSTR under different flow and environmental (inhibitor amount, temperature, pH, redox) conditions demonstrated sustained oscillations. We propose that studies in this direction might pave the way to the design of robust oscillation networks that mimic the autonomous behavior of proteins in cells (e.g., in the cyanobacterial circadian clock) and hence hint at feasible pathways that accelerated the transition from simple peptides to extant enzymes.

Invited Lecture

Medicinal and Biological Chemistry

From basic physicochemical studies to a unique in-vitro ADME array: toward the development of improved opioid antagonists

Sigal Saphier¹

Organic Chemistry, IIBR, Israel

In our campaign to discover the next generation of opioid antagonists with improved pharmacokinetics, mainly onset time, we adopted the properties-based drug design approach, which led us to the establishment of a unique in-vitro ADME array. This array was used for screening a series of new fluorinated/methylated opioid antagonists designed to modulate lipophilicity and other physicochemical properties that may show improved pharmacokinetics, over the FDA approved antidotes, naloxone and nalmefene. In order to study in-depth, the structure-activity/properties relationship of our new drug candidates, we developed new methods and approaches, focusing on aspects that may affect both pharmacokinetics and pharmacodynamics. The in-vitro ADME array includes the determination of logD using novel methods, H-bond acidity (A) and basicity (pK_{HB}), PAMPA-BBB permeability, metabolic stability, water-solubility, amine pK_a and assessment of intramolecular H-bonding. The drug candidates have been screened using different assays, and the multiparameter optimization through all tests indicated lead compounds that will be subjected to animal testing.

Medicinal and Biological Chemistry

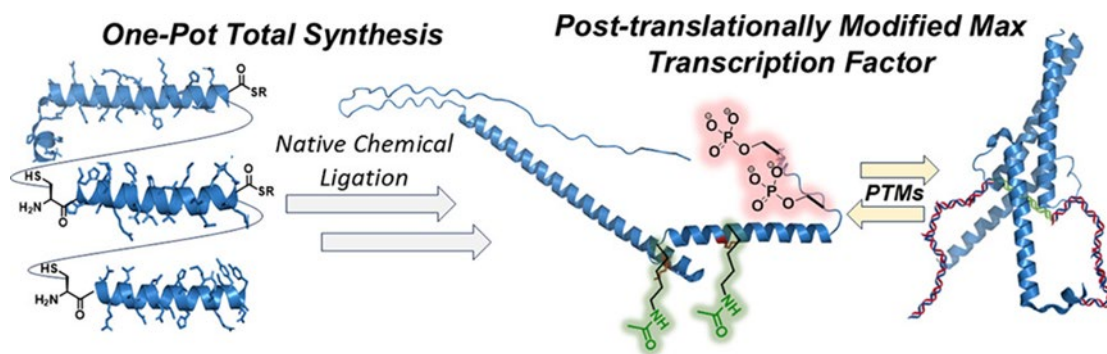
Deciphering the Role of Posttranslational Modifications on the DNA-Binding Activity of Max Transcription Factor Using Chemical Protein Synthesis

Nithun Raj Vakkayil¹, Yumi Minyi Yao², Omer Harel¹, Shada Khoury¹, Shaimaa Habiballah¹, Xiaoxi Lin¹, Ariel Afek², Muhammad Jbara¹

¹*School of Chemistry, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Israel*

²*Department of Chemical and Structural Biology, Weizmann Institute of Science, Israel*

Transcription factors (TFs) are proteins that regulate gene transcription by binding to specific DNA sequences. TF activity is tightly regulated by dynamic post-translational modifications (PTMs); covalent modifications that can modulate TF-DNA interactions and impact gene expression. Among these TFs, Max plays a pivotal role in controlling the expression of 15% of the human genome. The activity of Max is regulated by PTMs; Ser-phosphorylation and Lys-acetylation are considered key regulatory mechanisms. In this study, we developed a practical synthetic strategy to prepare homogeneous full-length Max for the first time, to explore the impact of Max PTMs on its DNA binding activity.^[1] We prepared a focused library of modified Max variants, with distinct modification patterns, including phosphorylated and acetylated analogues as well as fluorescently labeled variants through solid phase peptide synthesis coupled native chemical ligation approach. Through comprehensive DNA binding analyses, we discovered that phosphorylation and acetylation play a crucial role in the DNA-binding activity of Max.^[2,3] Furthermore, our results indicate that PTMs, e.g., Lys-acetylation can alter the binding specificities of Max towards certain sequences flanking its consensus binding sites. Our work provides insights into the hidden molecular code of PTM-TFs and DNA interactions, paving the way to interpret gene expression regulation programs.^[4,5]



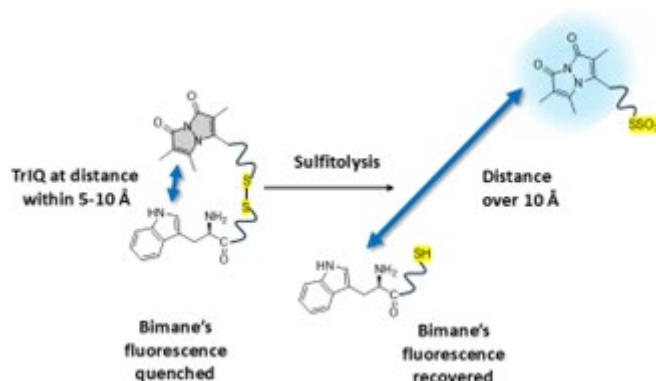
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Medicinal and Biological Chemistry

Tryptophan-Quenched Bimane Fluorophores for Sensor Development

Shira Glasberg¹, prof. Flavio Grynszpana¹, Dr Vincent Joseph¹, Prof. Mindy Levine¹
Chemical Sciences, Ariel University, israel

Leveraging short-range fluorescence quenching interactions provides an effective strategy for designing responsive molecular probes. Here, we present a bimane–tryptophan construct that exploits tryptophan-induced quenching (TrIQ) to create a reduction-activated sensor for sulfur dioxide (SO₂). SO₂ and its pH-dependent sulfite species are widely used in industry and food preservation, yet their associated health risks, including epithelial damage and inflammatory responses, highlight the need for sensitive detection and quantification methods. Our sensor consists of a syn-bimane fluorophore connected through a disulfide bond to a tryptophan-containing oligopeptide. In its intact form, the close Trp–chromophore proximity enables efficient quenching of bimane emission, while exposure to sulfite induces reductive cleavage of the disulfide bond, releasing the bimane unit and generating a strong fluorescence turn-on signal (Fig. 1)



Syn-bimane derivatives were selected due to their favorable photophysical properties, including high quantum yield, rigidity, and low molecular weight. Their versatility has enabled applications in biomolecular labelling and various sensing platforms. DFT geometry optimization suggests that the sensor can adopt a compact arrangement with an average bimane–tryptophan distance of approximately 5 Å, consistent with efficient TrIQ. Fluorescence measurements show a clear concentration-dependent increase in emission with an LOD of 0.129 ppm and an LOQ of 0.260 ppm, demonstrating high analytical sensitivity toward sulfite.

Ongoing studies aim to evaluate additional reductants capable of cleaving disulfide bonds, including biological systems such as glutaredoxin, as well as small-molecule reducing agents such as NaBH₄, to determine the selectivity profile of the sensor and guide the development of next-generation TrIQ-based probes.

Medicinal and Biological Chemistry

Analyte–Metabolite Interactions Govern Ion Suppression in Electrospray Ionization

Anna Morshina¹, Dr Katherine Margulis¹, Ori Shalev¹
The Hebrew University of Jerusalem, Israel

Electrospray-based ionization methods provide a direct link between solution-phase chemistry and gas-phase ion formation, yet the chemical origins of ion suppression remain poorly understood. Suppression is often attributed to co-present species or bulk matrix effects, but whether it reflects intrinsic suppressor strength or selective molecular interactions is unresolved.

Here, we investigate ion suppression using a combination of direct-infusion electrospray ionization (ESI) and desorption electrospray ionization mass spectrometry (DESI-MS). Using a panel of small molecules spanning basic amines, nucleobases, nucleosides, amino acids, and zwitterionic metabolites, we demonstrate that ion suppression is analyte-specific and non-symmetric. A representative example is shown in Figure 1, where increasing molar excess of deoxycytidine strongly suppresses hypoxanthine ionization while exerting only weak suppression on a basic amine analyte [Dimethyltryptamine] under identical conditions. Similar interaction-dependent behaviour is observed across additional analyte–co-solute combinations.

In DESI-MS, where no chromatographic separation is present, suppression effects arise directly from competitive ionization at the surface and display patterns that differ from LC-MS measurements. Together, these results show that ion suppression arises from specific analyte–co-solute interactions, while the observable matrix-effect behaviour depends on the ionization context. This interaction-based view reframes ion suppression as a chemically selective phenomenon across electrospray-based platforms.

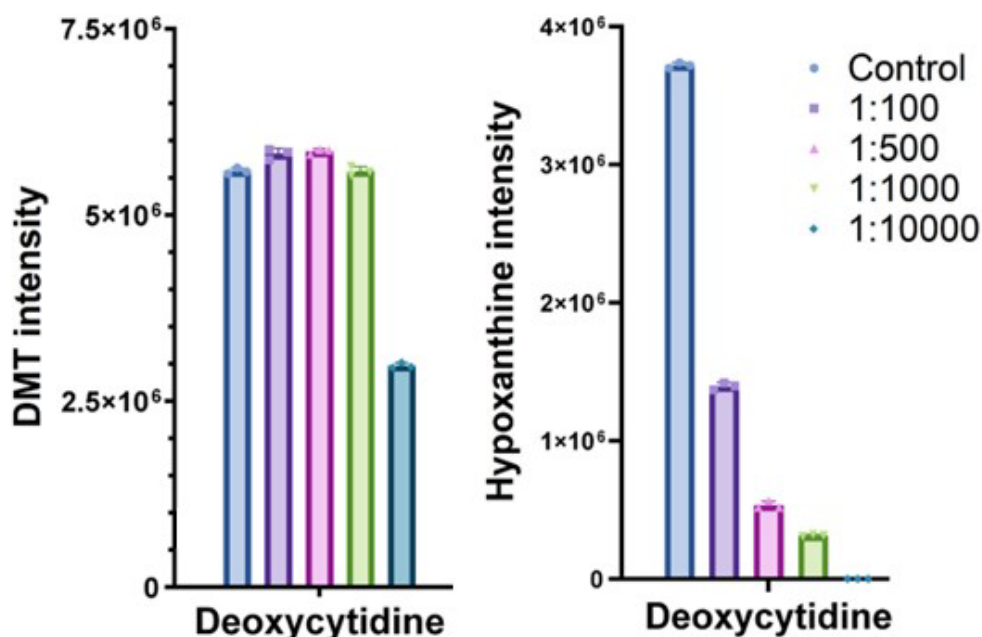


Figure 1. Same co-solute, different ion suppression

Medicinal and Biological Chemistry

Amyloid- β fibrils induce calcium phosphate crystallization via catalysis of ATP hydrolysis

SISIRA Mambram Kunnath^{1,2}, Dr. Elad Arad^{1,2,3}, Ms. Elinor Slavsky², Dr. Lonia Friedlander¹, Prof. Hanna Rapaport^{1,4}, Prof. Raz Jelinek^{1,2}

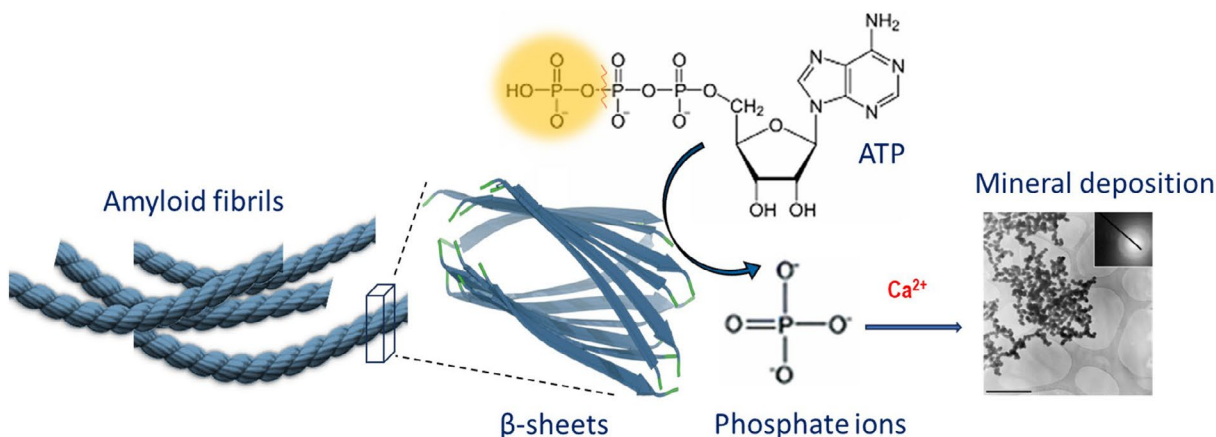
¹*Ilse Katz Institute (IKI) for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer Sheva, Israel*

²*Chemistry, Ben-Gurion University of the Negev, Beer Sheva, Israel*

³*Department of Chemical Engineering, Columbia University in the City of New York, USA*

⁴*Avram and Stella Goldstein-Goren Department of Biotechnology, Ben-Gurion University of the Negev, Beer Sheva, Israel*

Brain-localized deposits of crystalline calcium phosphate, mainly comprising of hydroxyapatite, are a pathological hallmark of Alzheimer's disease (AD). While calcium phosphate crystals are specifically identified in the neuronal amyloid plaques in AD, consisting mostly of beta amyloid ($A\beta$) fibrils, the mechanisms and factors affecting the biomineralization are unknown. Here, we present a novel mechanism for AD plaque-induced formation of crystalline calcium phosphate¹. Specifically, we show, for the first time, that $A\beta$ amyloid fibrils catalyse dephosphorylation of adenosine triphosphate (ATP)¹. Furthermore, incubating $A\beta$ fibrils, ATP, and calcium ions gave rise to pronounced deposition of hydroxyapatite crystals upon the $A\beta$ amyloid fibril matrix, originating through reaction between calcium ions and the monophosphate released through the catalytic dephosphorylation reaction (Experimental scheme). This pathway may explain amyloid plaque-associated calcification in AD, as elevated levels of both ATP and calcium are key features of the disease.



Experimental scheme: The experimental scheme depicting calcium phosphate crystallization induced through reaction between calcium and phosphate ions released by $A\beta$ -catalysed ATP dephosphorylation.

Reference

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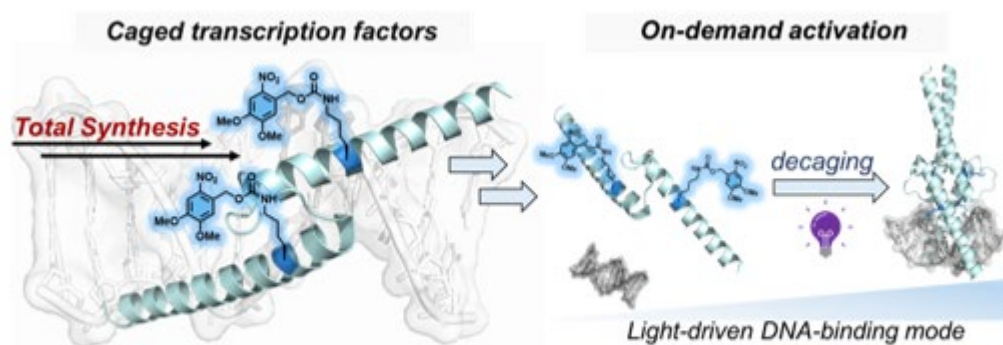
Medicinal and Biological Chemistry

engineering light-responsive transcription factor switches via strategic masking of post-translational modification residues

Shada Khoury¹, Nithun Raj V¹, Dr. Muhammad Jbara¹
School of Chemistry,

Faculty of Exact Sciences Raymond & Beverly Sackler, Tel Aviv University, Israel

The development of transcription factor switches that generate functional outputs in response to specific stimuli has significant potential for modulating key cellular processes for basic research and biomedical applications. In this study, we engineered light-responsive caged transcription factors derived from Max that can be unmasked and activated on demand by photolysis. By combining native chemical ligation and palladium-mediated C-S cross-coupling, we synthesized caged Max in which key Lys residues (e.g., Lys31 and Lys57) were masked with the o-nitroveratryloxycarbonyl group. Caged Max can be rapidly unmasked and activated within minutes using simple photolysis to modulate its DNA binding activity. Remarkably, whereas engineered Max showed a significant reduction in DNA-binding activity, potent binding to the enhancer box was rapidly restored upon site-selective unmasking of Lys31/57 residues. Our approach enables the effective production and activation of protein switches, paving the way for developing light-responsive analogs for on-demand control of transcription factors across various applications.



TOC

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Medicinal and Biological Chemistry

Tracing the path from photodynamic efficiency to sonodynamic capability in cyclohexene cyanine dyes

Amartya Sanyal¹, Dr. Arjun Veliyil Prakash², Prof. Gary Gellerman¹

¹*Department of Chemical Sciences, Ariel University, Israel*

²*Department of Chemistry, Bar-Ilan University, Israel*

While photodynamic therapy (PDT) has advanced significantly through the development of novel photosensitizers, the demand for organic dyes with strong near-infrared (NIR) absorption and high phototoxicity under biologically relevant light conditions remains high. Cyanine dyes, despite their advantageous NIR optical properties, have been comparatively underexplored relative to conventional porphyrin-based photosensitizers. Building upon our previous work on cyclohexene-based cyanine dyes containing indolenine, benzothiazole, and benzoselenazole terminal groups—shown to efficiently eradicate *S. aureus* and *E. coli* under low NIR light doses with minimal dark toxicity—we extend these investigations into the emerging field of sonodynamic therapy (SDT).

SDT offers a compelling alternative to PDT because ultrasound penetrates biological tissues more deeply and is less limited by optical scattering, enabling therapeutic activity in sites inaccessible to light. Despite its promise, sonodynamic studies of cyanine dyes have not been explored, and the sonodynamic antibacterial effect itself remains insufficiently investigated. Furthermore, minimal reports exist on the sonodynamic quantum yield of NIR-absorbing dyes, an essential parameter for understanding mechanistic efficiency and guiding rational dye design.

In this work, we evaluate the sonodynamic activity of our cyanine dye series against pathogenic bacteria and quantify reactive oxygen species (ROS) generation under ultrasound irradiation. Sonodynamic quantum yields were determined using H₂DCFDA as a ROS-sensitive fluorescent probe, enabling direct comparison with PDT performance. Our results highlight the potential of cyanine dyes as dual-modal photo- and sonosensitizers and underscore the broader importance of developing SDT-active NIR dyes for overcoming limitations inherent to light-based antimicrobial therapies.

Medicinal and Biological Chemistry

IPET: an excellent tool for diagnostic applications for human pathologies

Tasneem Rass¹

Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Age-related diseases and metabolic disorders, such as cancer, are closely associated with increased protein oxidation. As oxidative stress rises and in various metabolic conditions, proteins undergo damaging chemical modifications due to the interaction with reactive oxygen species (ROS) and other oxidative agents. This process can lead to significant functional impairments, as the accumulation of oxidized proteins contributes to cellular dysfunction, inflammation, and the progression of various diseases, highlighting the critical role of oxidative damage.

Currently, there are no efficient, sensitive, and affordable commercially available tools to perform extensive and quantitative redox proteomics analysis. In response to this gap, an innovative method has been developed for detecting, identifying, quantifying, and monitoring changes in redox-sensitive cysteines within complex proteomes. This approach involves the design, synthesis, and application of two differentially sized alkylating reagents, IPET, which specifically target reduced cysteine thiols. IPET refers to modified peptides that are chemically synthesized using solid-phase peptide synthesis (SPPS). These peptides feature an enrichment affinity tag and a cleavable tag, which can be removed in a single-step reaction. The cleavage of the tag does not alter the properties of the labeled peptides, resulting in a precise mass difference.

Since non-small cell lung cancer (NSCLC) is closely related to elevated oxidants and protein oxidation, the IPET approach presents a promising model for identifying, monitoring, and diagnosing cancer cases through redox proteomics in general, and specifically with IPET.

Medicinal and Biological Chemistry

Dual-color epigenetic profiling of myeloproliferative neoplasms

Sigal Avraham¹, Prof. Maya Koren-Michowitz², Dr. Miri Neaman¹, Ilana Sofronyuk²,
Dr. Jasline Deek¹, Shir Michowitz¹, Prof. Irit Avivi³, Prof. Yuval Ebenstein¹

¹*Department of Chemistry, Raymond and Beverly Sackler Faculty of Exact Sciences,
Tel Aviv University, Israel*

²*Department of Hematology, Shamir Medical Center, Israel*

³*Department of Hematology, Tel Aviv Sourasky Medical Center, Israel*

Myeloproliferative neoplasms (MPNs), including polycythemia vera (PV), essential thrombocythemia (ET), and myelofibrosis (MF), are clonal hematologic malignancies driven by shared genetic mutations yet characterized by distinct phenotypes, prognoses, and therapeutic responses. Growing evidence indicates that epigenetic regulation, particularly DNA methylation (5mC) and hydroxymethylation (5hmC), contributes to this biological heterogeneity.

Here, I developed a dual-color chemoenzymatic fluorescence labeling assay that enables simultaneous detection of 5mC and 5hmC on the same DNA sample. The platform employs two modification-specific chemoenzymatic reactions, each introducing an azide functionality at the target site. In a subsequent step, click chemistry is used to attach distinct fluorophores to each modification, enabling dual-color fluorescence readout that allows parallel analysis of 5mC and 5hmC patterns within a single experiment. The dual-labeling strategy was applied to custom-designed DNA microarrays targeting disease-relevant genomic loci, enabling high-resolution, locus-specific epigenetic profiling.

Using DNA from peripheral blood, I analyzed samples from PV, ET, and MF patients, as well as Hydroxyurea (Hydrea)-treated and untreated individuals. Each MPN subtype exhibited distinct and non-overlapping 5mC and 5hmC patterns, clearly separating disease groups from healthy controls. Although the direct epigenetic mechanisms of Hydrea are still incompletely understood, when patients were grouped by Hydrea treatment, both PV and ET cohorts showed robust, treatment-specific changes in 5mC and 5hmC that were independent of disease-driven differences.

Overall, this work establishes a dual-color microarray assay that detects both disease-specific and Hydrea-specific epigenetic markers with clear clinical relevance, enabling low-cost diagnosis and monitoring from minimally invasive blood samples (~60\$ per sample).

Medicinal and Biological Chemistry

Spatio-Temporal Protease Fluorescent Sensing (STEPFS)

Laura Levy¹, Dr Ori Green¹

Department of Chemistry, Technion, Israel

Fluorescent activity-based sensing (ABS) is a powerful strategy for visualizing protease activity in living systems, yet most protease-responsive sensors lack precise spatiotemporal control. Sensors can activate prematurely during uptake, producing off-target signals, high background, and poor spatial accuracy in complex biological environments. To address this gap, we introduce the Spatio-Temporal Protease Fluorescent Sensing (STEPFS) platform: a modular, dual-channel system that integrates photochemical gating with protease-responsive substrates. In STEPFS designs, a photolabile protecting group cages the protease-cleavable motif, keeping the sensor inert, while Channel 1 emission reports sensor localization in the OFF state. Upon localized irradiation, uncaging occurs only at the desired site and time, enabling protease-mediated cleavage that releases a bright reporter with a spectrally separated Channel 2 signal. This architecture encodes both delivery (Channel 1) and activity (Channel 2) within a single ratiometric design and minimizes off-target activation. We validate this strategy using a penicillin G acylase-responsive coumarin model and advance toward red/NIR ICT reporters. By extending the same photoprotected trigger strategy to diverse proteases (e.g., cathepsin B, caspase-3, and leucine aminopeptidase), STEPFS provides a general blueprint for spatiotemporally controlled protease imaging, enabling quantitative mapping of protease function and therapeutic response in live-cell and disease-relevant models.

Medicinal and Biological Chemistry

Energetic prepayment or complex stabilization?

Using DNA mismatches to reveal potential mechanisms governing the kinetics of DNA-protein recognition

Dr Michael O'HAGAN¹, Dr Ariel AFEK¹

Department of Chemical and Structural Biology, Weizmann Institute of Science, Israel

Transcription factors (TFs) bind DNA to orchestrate gene expression programs. To fulfil their function, TFs must efficiently search for the appropriate response element amidst a sea of genomic DNA and bind to their target sequences with high specificity. As the cell is a dynamic system operating out of equilibrium, TF specificity is not determined solely by thermodynamics but also the kinetics of the binding association and dissociation reactions. However, the molecular mechanisms by which TFs tune their binding kinetics are challenging to probe. Herein, we leverage single-base DNA mismatches as a tool to probe the complementary roles of conformational penalty and complex stability in dictating the kinetics of protein/DNA binding reactions. Our results reveal strikingly different kinetic behaviours between TFs, shedding further light on the mechanism of TF/DNA recognition and suggesting a means by which TFs exploit contrasting kinetic regimes to tune their biological functions.

Medicinal and Biological Chemistry

Molecular Design of Peptidic ligands for Cortactin-SH3

Miriam Gulman^{1,2}, Dr. Inbal Sher¹, Prof. Jordan Chill¹, Prof. Dan Major^{1,2}

¹*Chemistry, Bar-Ilan University, Israel*

²*Nanotechnology Advanced Materials, Bar-Ilan University, Israel*

Cortactin is a cytoplasmic protein that regulates actin polymerization and cytoskeletal rearrangement. Upon activation, it stabilizes nucleation sites for actin branching and is essential for lamellipodia, invadopodia, migration, and endocytosis. The cortactin SH3 domain (CortSH3) recognizes proline-rich peptides containing the “PXXP” motif, such as those from Proline-rich tyrosine kinase 2 (Pyk2) and hematopoietic cytoskeleton regulator WIP. Our objective is to identify peptides with improved affinity for CortSH3 and stability. These competitors block cortactin activation and thereby suppress lamellipodia and invadopodia assembly in cancer cells—key structures that drive motility, matrix degradation, and invasion. By inhibiting CortSH3 interactions, we aim to reduce metastatic potential while also probing how peptide sequence influences binding affinity.

This research combines experimental and computational approaches. Peptides are studied using Surface plasmon resonance and Nuclear Magnetic Resonance spectroscopy to measure binding affinities and derive distance restraints. These restraints are incorporated into docking with HADDOCK (High Ambiguity Driven DOCKing) to determine CortSH3–peptide structures and predict peptide orientation in the SH3 binding groove. To optimize this process, we developed a restraints scoring function that determines how many NOE restraints are needed to accurately solve docking, thereby making structure determination more efficient.

Complementing experiments, in silico screening of 4,608 peptides identified several promising CortSH3 ligands. One peptide bound ~50-fold stronger than the original 12-residue Pyk2 segment, and key interacting residues were mapped. Several variants were synthesized and tested, revealing sequence–affinity relationships. Overall, this work identifies a potent CortSH3-binding peptide and provides design principles for inhibitors that block cortactin-driven cancer cell invasion.

Medicinal and Biological Chemistry

Robust synthesis of prebiotic precursors in drying reactions of amino acids and keto acids

Eliav Marland¹, Gal Lipson¹, Dr. Rotem Edri¹, Or Cohen¹, Prof. Aikomari Guzman-Martinez², Dr. Ori Shalev³, Prof. César Menor Salvan⁴, Dr. Moran Frenkel-Pinter^{1,5,6}

¹*Institute of Chemistry, The Hebrew University of Jerusalem, Israel*

²*Department of Chemistry, University of Puerto Rico, Puerto Rico*

³*The Metabolic Profiling Unit, Core Research Facility, The Hebrew University of Jerusalem, Israel*

⁴*Departamento de Biología de Sistemas, Universidad de Alcalá, Spain*

⁵*The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel*

⁶*Casali Center of Applied Chemistry, The Hebrew University of Jerusalem, Israel*

There are several long-standing questions that we must answer to construct a coherent theory of the origin of life. In our research we explore two of those questions:

All extant biopolymers require dehydration-condensation reactions to polymerize from monomers. These reactions are thermodynamically suppressed in aqueous solutions. However, the most basic functions of life require a wide variety of polymers.

Furthermore, there is the question of the formation of metabolites and enrichment of the molecular inventory. For life to evolve, a diverse supply of organic material would need to be available. The earliest life would require metabolic cycles to exist, and therefore some form of prebiotically-plausible formation and transformation of metabolites would have to arise for first life to form.

In our recent work (accepted to ChemSystemsChem), we demonstrate for the first time the potential role of wet-dry cycling in the formation of metabolites and possible polymerization precursors. Dehydration of aqueous solution shifts equilibria to favour condensation-dehydration reactions, as well as exponentially increasing concentration of solutes, while adding water hydrolyses weak bonds and allows for further reactions. We have found that drying reactions between amino acids and keto acids, organic molecules central to polymerization and metabolism, form a multitude of heterogeneous products under mild conditions without added catalysts. These findings significantly broaden the expected chemical landscape in the prebiotic milieu on early Earth, and open new avenues for research on possible metabolic cycles and formation of building blocks in mild, plausible prebiotic conditions.

Medicinal and Biological Chemistry

Chemical Engineering of Transcription Factors Uncovered Cell-Permeable μ Max Modulators

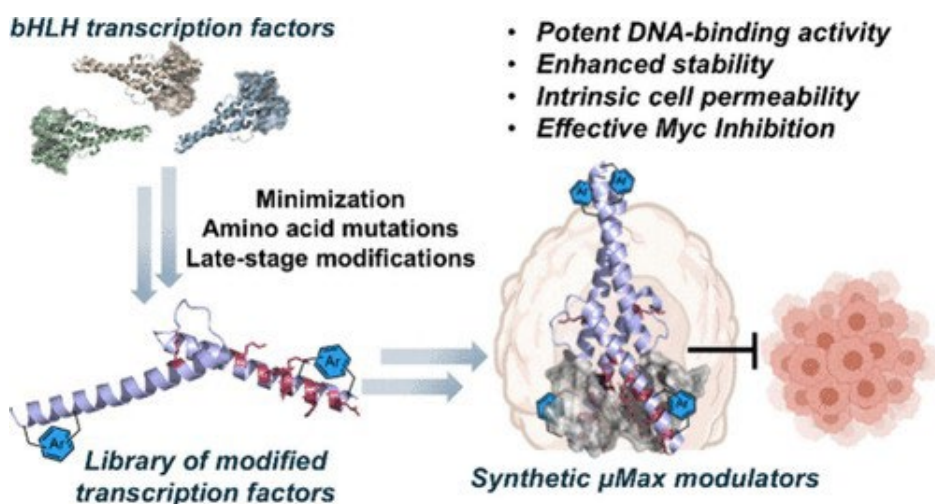
Omer Harel¹, Ferran Nadal-Bufi², Nithun Raj¹, Yumi Yao³, Ariel Afek³, Marc Vendrell², Muhammad Jbara¹

¹*School of Chemistry, Tel Aviv University, Israel*

²*Centre for Inflammation Research and IRR Chemistry Hub, The University of Edinburgh, Scotland*

³*Department of Chemical and Structural Biology, Weizmann Institute of Science, Israel*

Transcription factor engineering has emerged as a powerful strategy for generating novel proteins for fundamental research and biomedical applications.¹ Although various analogs have been developed, they remain largely constrained to native sequences and structures. The generation of advanced analogs bearing noncanonical modifications with enhanced functional properties remains limited. Here we combined rational design with total synthesis to engineer novel abiotic transcription factors with enhanced stability and cell permeability.^{2,3} Using solid-phase synthesis and native chemical ligation, we created a library of 30 Max-derived transcription factor analogs incorporating novel modifications, such as sequence mutations and aromatic staples at strategic sites. Through DNA-binding analysis and cellular uptake studies, we identified the μ Max20 analog, which contains two mutations (Lys31 and Lys57 to hArg) and exhibits potent DNA binding to the canonical enhancer box (E-box) as well as intrinsic cell permeability. Notably, further site-specific modifications of μ Max20 with aromatic staples yielded improved analogs with enhanced stability and remarkable cellular delivery at nanomolar concentrations.⁴ Our lead μ Max20 analog suppressed Myc-driven gene expression, as demonstrated by reporter gene assays and antiproliferative activity against Myc-dependent cancer cells. Altogether, these results highlight how combining chemical protein synthesis with late-stage modifications can be leveraged to enhance protein function and engineer novel bioactive modulators.



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Medicinal and Biological Chemistry

DNA Nuclease and ATPase Like Amyloid Fibrils: A Pathway Towards Amylin Pathology

Arunavo Chatterjee¹, Ms. Sisira Mambram Kunnath¹, Dr. Shubhra Kanti Bhaumik¹,
Prof. Raz Jelinek¹

Department of Chemistry, Ben Gurion University of the Negev, Beer-Sheva, Israel

Amylin aggregation is central to Type 2 Diabetes where amylin aggregates into toxic amyloid fibrils and contribute to β -cell death and disease progression. The mechanisms of this toxicity have not been fully elucidated. The high blood glucose and H_2O_2 level can result into DNA damage and cause systematic cell death, which can also intensify amylin aggregation and further growth of the already matured fibrils. The amylin fibrils also can cause ATP depletion due to higher energy accumulation in mitochondrial disruption involved in β -cell death. Although there are reports on modification and role of amylin aggregation in the context of T2DM, the catalytic activity of the amylin fibrils is yet to be explored. Here in, we have envisaged on the catalytic properties of the amylin fibrils for the DNA nuclease and ATPase like activities, mimicking various hyperglycemic conditions with different concentrations of glucose and H_2O_2 for delineating on the mechanism of the amylin pathology. The ability of high glucose and H_2O_2 concentrations to cause further growth and clustering of the already matured fibrils amplifies the catalytic activity of the amylin fibrils in hyperglycemic conditions. The exploration of the DNA nuclease and ATPase like activity of amylin fibrils may reveal new mechanisms of β -cell death and disease progression in T2DM.

Medicinal and Biological Chemistry

Near Infra-Red Fluorescent Sensor Based on Si-Rhodamine for CO₂ sensing

Boaz Nutkovich¹, Dr Ori Green¹

Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Israel

Carbon dioxide (CO₂) plays a key role in numerous biological processes, including cellular metabolism and signalling. To better understand its dynamics in living systems, real-time monitoring is essential.

Our group previously developed a CO₂-sensing platform based on a CO₂-reactive trigger coupled to a fluorophore reporter, enabling real-time monitoring of CO₂ at the cellular level. However, the current sensors emit at relatively short wavelengths, which limits their signal-to-noise ratio and hampers tissue imaging. To overcome these limitations, we integrated our CO₂-reactive trigger with a silicon-rhodamine (Si-rhodamine) scaffold, in which the bridging oxygen of rhodamine is replaced by a silyl group, resulting in red-shifted emission. Upon CO₂ activation, the sensor undergoes a structural transformation that shifts its fluorescence into the near-infrared (NIR) region.

The resulting sensor exhibits high hydrolytic stability, suitable kinetics under physiological conditions, and cell permeability with minimal cytotoxicity in THP-1 cells. This work introduces the first NIR CO₂ imaging platform, expanding the toolbox for CO₂ visualization from live-cell to tissue and potentially in vivo imaging.

Medicinal and Biological Chemistry

proto-peptide backbone affects assembly in aqueous solutions

Yishi Ezerzer¹, Sarah Fischer¹, Dr. Moran Frenkel-Pinter¹

Chemistry, Hebrew university of jerusalem, Israel

One of the most fascinating mysteries in the field of origins of life concerns the driving force that led to the selection of today's 20 universal L-alpha amino acids in biology. An essential aspect of life's emergence involves the formation of compartments, which offer encapsulation for target molecules and provide protection from hydrolysis in aqueous environments. Thus, polymers capable of assembly may have had a chemical evolutionary advantage over polymers that lacked this ability. We postulated that primordial peptide assembly could be one of the driving forces that led to the chemical selection of alpha amino acids in life today. To test this hypothesis, we generated depsipeptides, oligomers composed of ester bonds and peptide bonds that form readily under mild drying conditions, as model prebiotic peptides. However, it is unknown whether depsipeptides form assemblies in an aqueous environment similarly to peptides and proteins. To test the hypothesis that depsipeptides with alpha backbones will form assemblies more readily than beta backbones, we synthesized depsipeptides using a matrix of eight alpha- and beta- hydroxy acids and six alpha-, beta-, and gamma- amino acids. The reaction products were analyzed by microscopy and a physical stability analyzer to study assembly formation as well as various analytical techniques for chemical analysis. Our results demonstrate assembly formation in depsipeptide systems containing hydrophobic hydroxy acids and indicate that depsipeptide assemblies containing alpha hydroxy acid backbones are significantly more stable than beta analogs. our results offer an assembly-driven mode of selection for the alpha backbone in present-day biology.

Medicinal and Biological Chemistry

real-time probing intracellular CO₂ metabolism using aza-wittig-based sensors

Rawan Shahen¹, Dr Ori Green¹
Schulich, Technion, Israel

Carbon dioxide (CO₂) plays vital roles in cell proliferation, inflammation, immune regulation, and metabolism, yet its biology remains underexplored due to the lack of tools for real-time detection in living systems. To bridge this gap, we have developed an activity-based sensing strategy that enables fluorescence imaging of CO₂ in cells, using a molecular sensor that exhibits a fluorescence turn-on response upon reacting with CO₂. Previously, we demonstrated the capability of this approach to image exogenous CO₂ in living cells. Here, we extend the strategy to validate its ability to image endogenously produced CO₂, demonstrating responsiveness across physiological and pathophysiological concentration ranges. Using flow cytometry and live-cell fluorescence microscopy, we reveal mitochondrial-associated CO₂ microdomains indicative of localized metabolic activity. This work establishes activity-based CO₂ sensing as a versatile platform for probing CO₂ dynamics in living systems, which will potentially open new opportunities for exploring CO₂ regulations in metabolism and immune function.

Medicinal and Biological Chemistry

Encapsulation Efficiency of a Therapeutic Material Within Nanoparticles Produced from Epithelial Cells.

Hadar Nissan^{1,2}, Valeria Rahamim¹, Dr Roni Azaguri¹

¹*Department of Chemical Engineering, Ariel University, Israel*

²*Alpha program, Future Scientists Center, Israel*

This study focuses on the development of a novel carrier system for non-invasive drug delivery that combines the convenience of non-invasive administration with the efficacy typically associated with invasive methods. While non-invasive drug delivery is user-friendly and pain-free, its effectiveness is often limited because the drug undergoes metabolism in the liver, which reduces the bioavailability of the active compound. In contrast, invasive delivery routes offer high efficacy but are accompanied by pain, discomfort, and an increased risk of infection.

The aim of this research is to design a non-invasive drug delivery system that enables drug absorption through the mucous membrane of the oral cavity while maintaining the pharmacological advantages of invasive administration. The study explores the use of liposomes - microscopic vesicles composed of lipid bilayers - to effectively entrap a therapeutic agent. Liposomes derived from TR-146 epithelial cells were engineered to entrap both hydrophilic and hydrophobic substances, depending on the drug's properties. As a model system, the encapsulation of the fluorescent hydrophilic compound FITC-dextran was investigated to assess encapsulation efficiency under varying sonication conditions.

The results demonstrate that higher sonication intensities, longer exposure durations, and an additional sonication cycle following cooling in an ice bath significantly enhanced encapsulation efficiency. These findings suggest that optimizing sonication parameters can substantially improve the ability of liposomes to encapsulate therapeutic agents, thereby advancing the potential of non-invasive drug delivery systems that mimic the effectiveness of invasive approaches.

Medicinal and Biological Chemistry

On the Different Synthetic Routes of RNF4

Saed Bisher¹, Dr Rajesh Pallava¹, Prof Ashraf Brik¹
Chemistry, Technion, Israel

RNF4, a RING-type E3 ubiquitin ligase, targets polySUMOylated proteins for ubiquitination and subsequent proteasomal degradation. The ability to chemically synthesize RNF4 will open up future opportunities to study its structure and biological function, especially its role in degrading the oncoprotein PML-RAR α in acute promyelocytic leukemia (APL).

To achieve this, we performed a total chemical synthesis of RNF4 using sequential native chemical ligation (NCL). The presence of nine cysteine residues enables stepwise ligation through five peptide fragments to assemble the full-length protein. Two synthetic strategies were explored: the first employed a convergent ligation approach, while the second used a linear N-to-C ligation. In the convergent approach, all cysteine residues were protected with acetamidomethyl (Acm) groups to prevent side reactions during ligation, though this required multiple deprotection and purification steps. Conversely, the N-to-C synthesis method proceeded efficiently without cysteine protection, providing a simplified workflow with minimal purification needs.

This research provides a reliable and accessible method for the complete chemical synthesis of RNF4, addressing major challenges in synthesizing large proteins and enabling new opportunities for future biological research.

Medicinal and Biological Chemistry

Investigating the Aza-Wittig reaction: from mechanistic insight to carbon dioxide (CO₂) sensing

Anupama Yadav¹

Department of Chemistry, Technion-Israel Institute of Technology, Israel

The Aza-Wittig reaction, involving iminophosphoranes, was first introduced by Hermann Staudinger in 1919. Despite its long history and broad synthetic utility, a fundamental gap remains in our understanding of its structure–reactivity relationship. In this study, iminophosphoranes generated from different phosphines were reacted with carbon dioxide, selected as a model electrophile and role in CO₂ sensing. Reaction progress was systematically monitored using HPLC at various time intervals to gain kinetic insights and evaluate product formation. This approach not only provides a deeper understanding of the reaction course but also highlights the potential of these systems in CO₂ recognition and sensing. The ongoing work aims to establish a comprehensive structure–activity relationship by correlating reactivity trends with steric and electronic factors through Hammett analysis and buried volume/cone angle parameters. Overall, this study revisits a century-old reaction from a modern mechanistic perspective, bridging fundamental chemistry with emerging applications in molecular sensing.

Medicinal and Biological Chemistry

Synthesis of Deuterated Tetrahydrocannabinol and Cannabidiol for Improved Metabolic Stability

Sivan Bahar Ouzan¹

Chemistry, Bar Ilan university, Israel

Cannabis, also known as Marijuana, is a psychoactive drug, produced by the Cannabis sativa plant. Among its ~500 constituents, THC (trans- Δ^9 -tetrahydrocannabinol) is estimated to be the main ingredient that produces the psychoactive effect. It binds to specific cannabinoid receptors on brain nerve cells, such as CB1, and influences their activity. In oral administration (as medicines are taken), THC is rapidly oxidized in the liver to 11-hydroxy-THC (11-OH-THC) and further to the corresponding inactive carboxylate derivative (THC-COOH). 11-OH-THC penetrates the blood-brain barrier faster than THC itself, causing a faster and stronger psychoactive effect. This limits the use of THC as an orally administered drug, especially for patients with chronic medical conditions.

Cannabidiol (CBD) is the second most prevalent bioactive constituent of the Cannabis sativa plant. CBD is non-psychoactive but exerts several beneficial pharmacological effects.

Our research focuses on the development of THC and CBD analogs that differ from the parent compounds in the methyl group that undergoes oxidative metabolism. The new compounds are designed to have the same biological activity as THC and CBD but with much slower metabolism. The THC analog will convert much slower to the psychoactive substance 11-OH-THC, avoiding the latter undesired side effects. Thus, this modification will circumvent the original substances side effects and enable the use of lower dosage, providing an advantage for the use of these modified compounds as drugs.

Medicinal and Biological Chemistry

nitroreductase-activated switchable corrole for tumor imaging

Nitroreductase-Activated Switchable Corrole for Tu Yuval Guetta¹

chemistry, technion, israel

Phosphorus corroles are promising candidates for fluorescence imaging of cancer owing to their high fluorescence intensity and excellent photostability [1]. Among various bioimaging strategies, enzyme-responsive fluorescence activation has emerged as an effective approach for achieving selective tumor visualization with high signal-to-background contrast.

In this study, a novel nitro-substituted phosphorus corrole probe was designed and synthesized. This probe exhibits switchable fluorescence behavior, where emission is quenched by nitro-phenyl substituents and restored upon enzymatic reduction catalyzed by nitroreductase, which is frequently overexpressed in hypoxic tumor environments [2]. Possible organelle-specific targeting will be approached by incorporating morpholine moieties to facilitate lysosomal accumulation, thereby improving the selectivity of imaging.

Medicinal and Biological Chemistry

Development of Covalent Binders for E3 Ligases

Zohar Ben Arrosh¹, Prof. Nir London¹

Chemical and Structural Biology, Weizmann institute of science, Israel

Targeted protein degradation is an innovative therapeutic approach that eliminates disease-causing proteins, surpassing the limitations of traditional inhibition methods. By leveraging the ubiquitin-proteasome system (UPS), this strategy enhances the specificity and effectiveness of treatments. Proteolysis-targeting chimeras (PROTACs) and molecular glues are small molecules that facilitate targeted degradation by recruiting E3 ligases to mark these proteins for degradation, offering a promising new pathway in drug development. However, both approaches rely on a limited set of recruitable E3 ligases. There's a need to develop more ligands for new E3 ligases, which would broaden the scope and effectiveness of PROTACs and molecular glues. The E3 ligase plays a key role in the UPS by recognizing the substrate and leading to its degradation. FBXL17 and FEM1B are two structurally distinct E3 ligases with emerging roles in cellular regulation. FEM1B is a better-studied ligase compared to FBXL17 with known PROTACs and binders, so it's an attractive ligase for covalent binder development. Together, these ligases represent complementary models for expanding the toolbox of E3 candidates in targeted degradation strategies.

In this study, we discovered covalent binders for FBXL17 and FEM1B, designed to enable targeted degradation. Our approach involved high-throughput screening of electrophilic fragment libraries, structure-activity relationship studies, and iterative design-make-test cycles followed by biochemical and biological assays to evaluate their effectiveness in cells. These covalent binders serve as valuable tools to probe the biological functions of FBXL17 and FEM1B, laying the groundwork for the future development of novel PROTACs and molecular glues for therapeutic applications.

Medicinal and Biological Chemistry

Synthesis and Identification of a Novel Retinoid Metabolite as a Potential Endogenous RXR Ligand Derived from 9-cis β -Carotene

Meital Sklarz¹, Dr Svetlana Furman¹, Prof Amnon Albeck¹
Chemistry, Bar Ilan university, Israel

Vitamin A (retinol) and its natural derivatives play vital roles in numerous physiological processes, primarily through activation of the nuclear Retinoic Acid Receptor (RAR) and Retinoid X Receptor (RXR). These receptors regulate gene expression in inflammation, metabolism, and vascular function, making them especially relevant in diseases such as atherosclerosis. While 9-cis-retinoic acid (9c-RA) was initially proposed as an endogenous RXR ligand, its physiological presence remains uncertain. In contrast, 9-cis-13,14-dihydroretinoic acid (9CDHRA) was confirmed as the first endogenous RXR ligand, validated in mouse liver, serum, and brain. 9CDHRA was shown to activate RXR-mediated signaling at physiologically relevant concentrations and in cholesterol metabolism. To investigate the possible dietary origins of 9CDHRA, mice were given 9-cis β -carotene-enriched diets, including extracts from *Dunaliella salina* algae. Although 9CDHRA itself was not detected, a structurally similar substance was identified, particularly in the liver of mice supplemented with 9-cis β -carotene. This substance exhibited similar mass and retention time to 9CDHRA but showed distinct MS/MS fragmentation patterns and lacked the UV absorption typical of conjugated retinoids. These characteristics suggest the presence of a previously unidentified retinoid metabolite that may function as a novel endogenous RXR ligand.

This research focuses on synthesizing and characterizing this new class of substances that adhere to the spectroscopic data, as potential metabolite ligands for retinoid receptors, offering new insights into vitamin A metabolism and RXR signaling pathways. Shown below are the structures of compounds consistent with the experimental results obtained from our mouse model.

Medicinal and Biological Chemistry

Pharmacological Activation of Signaling by Homodimer Induction

Dana Shkolnik Ella¹, Prof. Nir London¹
Weizmann Institute of Science, Israel

Symmetry, and in particular homodimerization, plays a crucial role in numerous biological processes. Many proteins are only active when found in their homodimeric form, the formation of which is heavily regulated by mechanisms that ensure timely and condition-dependent activation.

We aimed to bypass the cell's regularity mechanisms by pharmacological induction of homodimerization of target proteins, thereby selectively activating signaling pathways. To achieve this goal, we rely on chemistry previously developed in our lab, Covalent Ligand-Directed Release (CoLDR). CoLDR enables covalent tagging of endogenous proteins while preserving their function. Efficient chemical approaches exist for inducing proximity between two distinct proteins using heterobifunctional molecules. Surprisingly, extending this concept to molecules capable of inducing homodimerization introduces several unexpected challenges.

This work focuses on identifying the key obstacles to inducing homodimerization of proteins by synthesizing a range of homodimer recruiters that vary in their linker and recruiting ligand. We designed several symmetric proximity inducers for Bruton's Tyrosine Kinase (BTK) and K-ras^{G12C} proteins, which control pivotal cellular signaling pathways. We identify two obstacles in the design of homodimeric ligands, and explore possible strategies to mitigate them. Thus far, we were able to demonstrate successful dimerization of both target proteins in live cells.

This proof-of-concept establishes a generalizable framework that we are currently extending to additional targets, where enforced homodimerization is expected to modulate signaling. Such activators should have a significant impact on our ability to dissect complex signaling biology and represent promising starting points for more nuanced therapeutics.

Medicinal and Biological Chemistry

Examining the Effect of the Ultrasonic and LiposoFast Systems on Size and Polydispersity of Nanoparticle Solutions Produced from 146TR Epithelial Cells

Talia Malek^{1,2}

Chemical Engineering, Ariel University, Israel

Future Scientists Center, Alpha program, Israel

The present study focuses on developing a system for non-invasive drug delivery using advanced technologies for highly efficient drug transport while maintaining patient comfort. Two basic types of medication administration procedures exist: invasive and non-invasive.

While invasive delivery systems include injections, non-invasive delivery offers various options such as administration through the oral cavity, the skin and more. The system developed in this study focuses on drug delivery through the buccal region, which is considered a highly vascularized area with large surface area, enabling more efficient absorption of the therapeutic compound.

The study is based on 146TR cancerous epithelial cells derived from the human neck region, which produce liposomes (vesicles) intended to transport therapeutic substances. The vesicles must be adjusted to different sizes in order to encapsulate drugs with varying molecular dimensions. For this purpose, the effects of the Ultrasonic and LiposoFast devices on the size and polydispersity index of the nanoparticles were examined.

During the study, Ultrasonic and LiposoFast devices were operated on the vesicles produced under different conditions of amplitude intensity and Duty Cycle, and their effects were examined. Results show that applying LiposoFast to nanoparticle suspensions after sonication slightly reduced the surface charge values. In addition, sonication intensity was shown to effect nanoparticle size in that working at higher amplitude percentages led to particles with smaller diameters.

Medicinal and Biological Chemistry

S. aureus biofilm formation in a 3D bioengineered in vitro microenvironment

Inbar Shmuely¹, Prof Liraz Chai¹

chemistry, The Hebrew University of Jerusalem, Jerusalem

Biofilms are clusters of bacteria embedded in a protective matrix that form on natural and synthetic surfaces. When biofilms develop on implants, they can delay tissue healing and potentially cause implant failure. Traditionally, biofilm-related implant infections are studied in vitro under simplified conditions that do not replicate the physiological environment in vivo.

This project aims to investigate biofilm formation in a physiologically relevant microenvironment, using biofilms embedded in gelatin methacryloyl (GelMA) as a tissue mimetic. GelMA is a tunable, biocompatible material commonly used to model tissues in biomedical applications. *S. aureus* bacteria were embedded in GelMA samples of varying stiffness and cultured for 21 days in two media: Tryptone Soya Broth (TSB), a standard bacterial growth medium, and Minimum Essential Medium (MEM) supplemented with fetal bovine serum, mimicking in vivo nutrient composition.

GelMA samples, were analysed for biofilm formation via optical microscopy, mechanical properties using compression tests and rheology, and water content through DSC.

We found that bacteria degraded GelMA in TSB, while in MEM, GelMA remained stable and biofilm clusters developed over time. The culture medium influenced GelMA's mechanical properties and water content: in TSB, storage and Young's moduli decreased over time and samples failed at higher strains. In MEM, these moduli remained stable and comparable to controls. Water content increased in TSB but remained unchanged in MEM.

These findings show that *S. aureus* biofilms affect GelMA's mechanical and water properties in a medium-dependent manner, emphasising the importance of using 3D tissue-mimetic models to study biofilm formation in vitro.

Medicinal and Biological Chemistry

QUMA-Based RIBOTACs for Selective Targeted Degradation of mRNA G-Quadruplexes

Elias Khaskhia¹, Dr. Dipak Dahatonde¹, Dr. Raphael Benhamou¹

*The Institute for Drug Research of the School of Pharmacy, Faculty of Medicine,
Hebrew University of Jerusalem, Israel*

RNA G-quadruplex (G4) structures are noncanonical four-stranded secondary structures formed by guanine-rich RNA sequences that are highly stable and regulate key cellular processes. Among them, G4-forming messenger RNAs (mRNA G4s), such as KRAS, NRAS, FGF2, or ADAM10, are enriched in key regulatory and disease-associated transcripts. G4 regulates translation, localization, and stability, influencing signaling and stress responses. They are implicated in oncogenic signaling, stress adaptation, and cell-cycle control. Dysregulation of mRNA G4 formation or resolution has been linked to aberrant gene expression and uncontrolled proliferation, potentially contributing to disease, including cancer. Despite their critical roles, strategies to specifically target mRNA G4 remain limited. Here, we report the development of novel small molecules utilizing RIBOTAC (Ribonuclease-Targeting Chimera) technology to selectively degrade G4-forming mRNAs by targeting their G4 structures. These RIBOTACs combine a G4 binder named QUMA, known for its high affinity for RNA G-quadruplexes, with an RNase L recruitment module, enabling site-selective cleavage of G4-containing mRNA. Quantitative binding assays reveal that these compounds bind mRNA G4 with high affinity while showing negligible interaction with non-G4 control sequences, confirming their strong preference for G4 structures. Furthermore, in cell-free RNase L cleavage assays, these degraders promote efficient degradation of G4-forming substrates, demonstrating that G4 recognition can be coupled to RNase L recruitment to achieve targeted RNA cleavage in vitro. Together, these results establish QUMA-based RIBOTACs as a modular platform for exploiting mRNA G4 as druggable regulatory elements and lay the foundation for future therapeutic strategies aimed at selectively modulating G4-containing disease-associated transcripts.

Medicinal and Biological Chemistry

Induced Lysosomal Targeted Degradation of the Oncogenic RNA-Binding Protein HuR Complex

Binyamin Insler¹, Liann Kassabri¹, Dr Raphael I. Benhamou¹

The Institute for Drug Research of the School of Pharmacy, Faculty of Medicine, The Hebrew University of Jerusalem, Israel

Human antigen R (HuR, also known as ELAVL1) is an RNA-binding protein that stabilizes and enhances the translation of numerous mRNAs involved in cell proliferation, survival, inflammation, and stress responses. In many cancers, HuR becomes aberrantly overexpressed and mislocalized to the cytoplasm, where it exerts potent oncogenic effects by protecting transcripts that encode oncogenes, anti-apoptotic factors, and metastatic drivers. Notably, HuR directly stabilizes key cancer-promoting mRNAs such as MYC, BCL2, CCND1, VEGFA, and MMP9, thereby amplifying proliferative signaling, preventing apoptosis, and promoting angiogenesis and invasion. Autophagy-Targeting Chimera (AUTOTAC) are bifunctional small molecules that simultaneously bind a target protein and a specific autophagy-activating ligand, thereby tagging the target for selective degradation through the autophagy-lysosome pathway. We have previously demonstrated that HuR can be successfully degraded using Proteolysis Targeting Chimera (PROTAC) technology; however, this approach eliminates only the protein and not the oncogenic transcripts it protects. With AUTOTAC, we aim to degrade not only HuR itself but also its associated pathogenic mRNAs through autophagy-mediated co-degradation, offering a more comprehensive suppression of HuR-driven oncogenic programs. We designed and synthesized multiple AUTOTAC derivatives incorporating different HuR-binding ligands and linker lengths, allowing us to systematically tune target engagement, autophagy recruitment, and degradation efficiency, thereby increasing the therapeutic potential for coordinated removal of HuR and its associated oncogenic RNAs. These findings establish a powerful induced-proximity strategy for lysosomal elimination of HuR and its oncogenic RNA cargo, paving the way toward a next-generation therapeutic platform for targeting previously undruggable RNA-protein oncogenic networks.

Medicinal and Biological Chemistry

Synthesis, development, and optimization of PLGA-PEG-based polymeric nanoparticles for targeted drug delivery, enabling the encapsulation and controlled release of small bioactive molecules

Ohad Hasin¹, Adi Yona¹, Dr. Marina Green Buzhor¹, America Garcia Alvarado¹, Dr. Shani Koshrovski-Michael¹, Daniel Rodriguez Ajami¹, Ron Kleiner¹, Dr. Shahar Tevet², Prof. Ronit Satchi-Fainaro^{1,3}

¹*Physiology and Pharmacology, Tel Aviv University, Israel*

²*Organic Chemistry, Tel Aviv University, Israel*

³*Sagol School of Neurosciences, Tel Aviv University, Israel*

Polymeric nanoparticles (NP) for drug delivery offer improved therapeutic efficacy with reduced systemic toxicity. We designed amphiphilic PLGA–PEG block-copolymer NP to achieve controlled release of small-molecule therapeutics. The hydrophobic PLGA segment facilitates efficient drug loading, while the hydrophilic PEG shell enhances colloidal stability and prolongs circulation time. Incorporation of terminal sulfate ($-\text{OSO}_3^-$) groups provided P-selectin–targeting capability, exploiting its overexpression in the tumor microenvironment. By systematically varying polymer composition, particle size, and surface chemistry, we optimized encapsulation efficiency, release profiles, and targeting performance, highlighting the versatility of PLGA–PEG NP for precision medicine. For polymer synthesis, a selective allylation of bifunctional PEG–OH was optimized to favor mono-substitution, generating HO–PEG–Allyl. This intermediate underwent ring-opening polymerization with lactide and glycolide using $\text{Sn}(\text{Oct})_2$ to yield PLGA–PEG–Allyl. The PLGA terminus was acetylated, and the PEG terminus was sulfated via a thiol–ene reaction, producing $\text{AcO-PLGA-PEG-(OSO}_3)_2$. Structural confirmation and batch consistency were validated by $^1\text{H-NMR}$, PDI, and MALDI-TOF MS. The PLGA–PEG synthesis was successfully scaled up with improved yields and greater control over PLGA chain length, enhancing polymer properties such as drug encapsulation capacity. Through targeted chemical washes and selective precipitation, we achieved precise polymer lengths, higher yields, and improved PDI relative to commercially available materials. The resulting NP effectively encapsulated either a single bioactive compound or a dual therapeutic combination of Dabrafenib (DBF) and Trametinib (TRM), demonstrating efficient co-loading and release for synergistic melanoma treatment.

Medicinal and Biological Chemistry

3D-Bioprinted Capsules for the Co-Delivery of Live Bacteria and Small Molecule Immunotherapies

Or Kandli¹, Dr. Marina Green Buzhor¹, Prof. Ronit Sachi-Fainaro¹

Department of Physiology and Pharmacology, Gray Faculty of Medical and Health Sciences, Tel Aviv University, Israel

Immunotherapy has revolutionized cancer treatment, however, many patients remain unresponsive. Co-delivering live bacteria with computer-assisted drug-design (CADD) small-molecule immunotherapeutics (SMi) offers a promising strategy to overcome therapeutic resistance. Certain gut bacteria positively correlate with improved immunotherapy outcomes, and their targeted delivery may enhance treatment efficacy.

We developed innovative 3D-bioprinted, enteric capsules that encapsulate live bacteria and SMi. The selected bacterial strains, both aerobic and anaerobic, include those reported to be positively correlated with the response to immunotherapy. Capsules were 3D-bioprinted using growth-promoting hydrogel bio-inks based on alginate and gelatine that support bacterial survival and improve printability. An additional enteric outer layer was 3D-printed to ensure gastric resistance and colon-targeted release. Capsules were evaluated for mechanical strength, release kinetics under simulated gastrointestinal conditions, and bacterial viability using fluorescent imaging and flow cytometry.

Our developed capsules successfully encapsulated live bacteria and PD-L1, withstanding gastric conditions and maintaining the viability of anaerobic bacteria for over 15 days. In contrast, aerobic strains survived for up to 3 days. Additionally, the encapsulated SMi demonstrated chemical stability for 21 days, with complete release achieved after 6 hours in simulated gastrointestinal conditions. These results support the feasibility of this platform for co-delivering viable bacteria and immunotherapeutics with controlled spatial and temporal release.

This 3D-bioprinted capsule represents a novel strategy to sensitize tumors to immunotherapy by combining live bacteria and SMi co-delivery. Incorporating bacteria associated with enhanced immunotherapy responses may improve therapeutic efficacy and provide a personalized approach for patients who do not benefit from current treatments.

Medicinal and Biological Chemistry

Reprogramming the Cationic Choline Ether Headgroup of the Second-Generation Echinocandin
Rezafungin Restores Activity Against Resistant *Candida* Pathogens

Moriah Jospe-Kaufman¹, Prof. Micha Fridman¹

*School of Chemistry, Raymond & Beverly Sackler Faculty of Exact Sciences, Tel Aviv
University, Israel*

Echinocandins are a clinically important class of antifungal agents that inhibit β -1,3-D-glucan synthase, yet their effectiveness is increasingly compromised by resistance arising from mutations in the *FKS* gene, which encodes the catalytic subunit of the glucan synthase complex. Rezafungin, a second-generation echinocandin distinguished by a choline ether modification at the C5 ornithine position, offers improved pharmacokinetics relative to earlier agents; however it remains vulnerable to *FKS*-mediated resistance. Given our prior finding that benzylic dehydroxylation of the homotyrosine residue of rezafungin significantly enhances activity against resistant *Candida* strains, we sought to investigate whether strategic C5 headgroup redesign could further improve antifungal activity. We synthesized rezafungin derivatives in which the choline ether was replaced with aromatic quaternary ammonium moieties, including pyridinium, pyrazinium and pyridazinium groups, alone or combined with benzylic dehydroxylation. These modifications introduce delocalized cationic character and expanded π -surface area, features hypothesized to strengthen interactions within the membrane-associated target environment. Fungal growth-inhibition assays revealed that several derivatives exhibit improved potency against echinocandin-resistant *Candida* strains. These findings demonstrate that rational headgroup redesign, particularly when paired with benzylic dehydroxylation, can restore activity against *FKS* mutant pathogens and offers a promising direction for next-generation echinocandin development.

Medicinal and Biological Chemistry

Discovery of Novel Small-Molecule Inhibitors to the P-selectin/PSGL-1 Pathway for Enhanced Cancer Immunotherapy

Rina Sevostianov¹

Tel-Aviv University, Israel

Inhibiting the PD-1/PD-L1 axis has demonstrated significant clinical efficacy in various cancers, but the limited response rates to current monoclonal antibody-based therapies underscore the urgent need for alternative strategies. In a previous study, we employed a transdisciplinary approach combining in silico drug discovery with in vitro, ex vivo, and in vivo experiments to identify novel small molecules capable of inhibiting the PD-1/PD-L1 interactions. By screening a custom-prepared library of compounds from readily available sources and the published crystal structure of PD-L1, a structure-based screening approach using docking was employed, followed by filtering the compounds for drug-like properties. The best-scoring compounds were further validated in vitro to identify those with the most inhibitory activity. The hits were found to stimulate human adaptive immune responses and uniquely facilitate extensive T-lymphocyte infiltration into three-dimensional solid tumor models. Additionally, they enhanced the recruitment of cytotoxic T cells to the tumor microenvironment in vivo. This new family of small-molecule candidates holds great potential to advance cancer immunotherapy by addressing the current limitations of antibody-based immune checkpoint inhibitors. Following this successful drug discovery campaign, we turn our attention to P-selectin/P-selectin ligand-1 axis, which we recently discovered as an immune checkpoint in several cancer types. Efforts are now focused on developing small-molecule inhibitors for this axis using the Schrödinger computational platform.

Medicinal and Biological Chemistry

comparative flocculation responses to antifungal drug classes reveal microenvironmental barriers to uptake in *Candida albicans*

Tal Kopp¹, Melissa Shbeta¹, Prof. Micha Fridman¹
School of Chemistry, Tel Aviv University, Israel

Candida albicans is the most common fungal pathogen worldwide, causing infections that affect millions of people and posing a major challenge in modern medicine. *C. albicans* is capable of switching between yeast and hyphal forms, with hyphae arising through a filamentation program that produces long filaments suited for tissue invasion and survival under diverse conditions. *C. albicans* can form compact yeast clusters, a phenomenon termed flocculation, which is mediated by adhesins through calcium-dependent cell-cell interactions under nutrient limitations and other stresses. The echinocandin antifungal caspofungin has been shown to trigger flocculation in yeast at subinhibitory concentrations. However, it remains unclear whether other antifungal drugs induce flocculation in yeast or hyphae, or if this behavior is specific to echinocandins. Here, we address this gap by testing drugs from the three major antifungal classes (echinocandins, polyenes, and azoles) for their ability to induce flocculation in yeast and hyphal forms of *C. albicans* under defined nutrient conditions, and by assessing how drug exposure reshapes population structure. We found that the entire echinocandin class induced flocculation, with stronger effect in hyphae than in yeast. In contrast, none of the tested azoles triggered flocculation, and among polyenes, only amphotericin B induced this response. These findings indicate that antifungal classes differentially reorganize *C. albicans* populations, potentially affecting drug penetration, treatment response, and therapeutic outcomes. Echinocandin induced flocculation may promote transient drug tolerance or resistance within aggregates, whereas the lack of flocculation with azoles and most polyenes may enable more uniform drug exposure and consistent antifungal activity.

Medicinal and Biological Chemistry

Fluorescent probes derived from the polyene class of antifungal drugs reveal distinct localization patterns and resistance-associated vacuolar sequestration in *candida* species.

Melissa Shbeta¹, Tal Kopp¹, Ivan Voronov¹, Adi Yona¹, Dr. Rania Hasib Afana¹,
Prof. Shmuel Carmeli¹, Prof. Micha Fridman¹
School of chemistry, Tel Aviv university, Israel

Amphotericin B, nystatin, and natamycin are the only polyene antifungals in clinical use and remain last-resort therapies for severe fungal infections. These agents disrupt fungal membranes through ergosterol binding, but how structural differences between the three polyenes influence subcellular distribution, and whether such distribution is linked to resistance, remains uncharacterized. To investigate these relationships, we developed fluorescent probes from each clinically used polyene by conjugating a common fluorophore to a conserved functional group, preserving the amphoteric nature and ergosterol-dependent antifungal activity of the parent drug while enabling live-cell imaging. This unified design allowed direct comparison of localization and trafficking across *Candida* species, including sterol biosynthesis mutants with a high level of polyene resistance. The probes revealed structure-specific distribution patterns, with resistant strains showing enhanced accumulation within the vacuole lumen for all three polyenes. These findings suggest that vacuolar sequestration contributes to polyene resistance and may represent an unrecognized aspect of the fungal stress response. More broadly, this work provides the first direct visual evidence that polyene structure dictates subcellular distribution patterns in fungal cells.

Medicinal and Biological Chemistry

the effects of single post-translational modifications on the aggregation of the R3 domain of Tau protein

Yuval Farchy¹, Shachar Guy Bressler¹, Prof. Mattan Hurevich¹, Prof. Assaf Friedler¹
Organic Chemistry, The Hebrew University of Jerusalem, Israel

Aggregation of the Tau protein is a hallmark of several neurodegenerative diseases, termed tauopathies. Tau aggregation is initiated by hyperphosphorylation of the protein and is also regulated by other post translational modifications (PTMs). To elucidate how specific PTMs and PTM patterns regulate Tau aggregation, it is crucial to obtain libraries of Tau derivatives with all the relevant PTM patterns. This is difficult to achieve at the protein level, and indeed most current studies rely on mutations that mimic certain aspects of native PTMs. Studies at the domain level using synthetic peptides is an excellent way to access such libraries. We have previously developed several methods for the rapid, efficient and automated synthesis of multi-PTM peptides and utilized it to synthesize libraries of the R4 domain of Tau, showing how distinct Ser and Thr phosphorylations can determine if it will undergo aggregation or condensation¹. Here we expanded this approach to also combine tyrosine phosphorylation and lysine acetylation and studied how single PTMs affect the aggregation of the R3 domain of Tau. Using a combination of biophysical methods such as DIC, SEM, ThT and Turbidity we have shown if and how each PTM affects the aggregation of Tau R3. Our results provide insight into the regulation of Tau aggregation by various PTMs and highlights that synthetic peptide libraries are essential for fully understanding which PTMs and combinations thereof affect biological processes.

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Medicinal and Biological Chemistry

Walking DNA: A Tunable Platform for Multivalent Binding and Intracellular Delivery

Gal Raviv-Franco¹, prof. David Margulies¹
Chemistry, Weizmann Institute of Science, Israel

We present a novel multivalent DNA nanostructure, the DNA tetrapod, as a highly tuneable platform to investigate the dynamic interactions between ligands and cell surface receptors. The tetrapod self-assembles from G-rich single-strand DNA and displays multiple small-molecule ligands, providing multivalency for enhanced binding affinity. The design is engineered to allow for the precise control of the spacing between the displayed ligands via variable linker lengths. We found that the linker length is a critical parameter for achieving strong multivalent binding, as excessively short or long linkers resulted in weak binding due to neighbouring receptors being out of reach or having too many degrees of freedom, respectively. Crucially, Molecular Dynamics simulations suggest that long linkers enable the tetrapod to engage in an "active search" or "walking" motion across the cell membrane surface. This dynamic motion, reminiscent of bacteriophages on bacterial surfaces ("Touch and search"), enhances the ability of the structure to effectively locate and engage clustered receptors even at low densities. Furthermore, the tetrapod walking behaviour is being investigated further using dSTORM super-resolution microscopy. Finally, we were able to show that binding an antisense molecule- a DNA-based drug to the tail of the tetrapod structure results in the inhibition of the targeted protein expression, enabling a platform for a new class for drug delivery. This work offers insights into how receptor density and clustering dictate the binding and internalization of nanoscale materials at the cell surface.

Medicinal and Biological Chemistry

A Fluorescent Probe Inspired by the Quorum-Sensing Molecule Farnesol
Suppresses *Candida albicans* Morphogenesis and Shows Pronounced
Mitochondrial Enrichment

Ivan Voronov¹, Student Melissa Shbeta¹, Prof. Micha Fridman¹
School of Chemistry, Tel Aviv University, Israel

Farnesol, a quorum-sensing sesquiterpene produced and released by *Candida albicans*, is known to inhibit filamentation, the transition from the unicellular yeast form to the filamentous hyphal form that underlies fungal invasion and virulence, a key determinant of pathogenicity. Yet it remains unclear if and how its intracellular distribution relates to this filamentation-inhibitory activity. To investigate this relationship, we synthesized two farnesyl-derived fluorescent probes, F-1 and F-2, together with dodecyl-chain controls. Both analogues retain the native farnesyl isoprenoid chain but differ in fluorophore identity: F-1 incorporates tetramethylrhodamine, whereas F-2 carries 7-diethylaminocoumarin. In live *C. albicans* cells, the TAMRA–farnesyl probe F-1 displayed pronounced mitochondrial localization and inhibited filamentation to the same extent as exogenous farnesol, while F-2 localized to several membranous compartments and was inactive. The dodecyl derivatives exhibited subcellular distributions identical to those of their farnesyl counterparts but lacked inhibitory activity, indicating that while the fluorophores modulate subcellular localization, they do not contribute to the biological function. F-1 also maintained mitochondrial association and filamentation-inhibitory activity in strains resistant to azoles, echinocandins, and polyenes, the three principal classes of clinically used antifungal agents. These findings demonstrate a direct association between farnesol's mitochondrial localization and its inhibition of filamentation, providing new insight into how subcellular targeting influences quorum-sensing control of fungal morphogenesis and virulence.

Medicinal and Biological Chemistry

Using Adenine Synthetic Modification as a Tool for Identifying Protein Footprint on DNA

Shani Dvir¹

Physical Chemistry, Tel Aviv University, Israel

We present a chemical strategy for mapping protein–DNA interactions based on localized adenine modification by the sequence-independent adenine methyltransferase Hia5. We successfully demonstrated that in the presence of the synthetic cofactor AdoYnAzide, Hia5 catalyzes the transfer of an azide group to adenines in double-stranded DNA, enabling subsequent bioorthogonal labeling. We intentionally employ azide-modified adenine because unmodified adenine and N6-methyladenine produce highly similar signals in nanopore sequencing, whereas azide modified adenine generates a distinct signal, making it a promising chemical handle for future singlemolecule sequencing readout.

To achieve protein-targeted DNA modification, Hia5 is fused to protein A/G (pAG-Hia5), enabling antibody-mediated recruitment of the enzyme to specific protein. Upon localization, pAG-Hia5 modifies nearby adenines, creating a spatially confined chemical footprint. Fluorescent detection was achieved via strain-promoted azide-alkyne cycloaddition with DBCO-ATTO647. As a controlled model system, site-specific single-strand nicks were introduced using the enzyme Nt.BspQII, followed by incorporation of biotinylated-nucleotides and recognition by anti-biotin antibodies. Experiments were performed on λ and T7 genomes, which differ in the number and distribution of nicking sites. Single-molecule fluorescence-imaging revealed labeling patterns that closely match theoretical predictions.

This work establishes antibody-guided, azide-based adenine labeling as a chemically precise approach for detecting protein–DNA interactions, with strong potential for future integration with nanopore sequencing as an orthogonal, label-free readout.

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Medicinal and Biological Chemistry

Rotaxanes as a Targeted Dual Modality Agents

Sapir Paryente¹, Dr. Arjun Prakash¹, Helal Metawi¹, Dr. Abed Saady¹
Chemistry, Bar-Ilan University, Israel

In recent years, mechanically interlocked molecules (MIMs) have gained increasing attention for biological applications and bioimaging,¹ driven by their unique topological bonding, stability, and modularity. Among these systems, rotaxanes² provides an attractive platform for constructing multifunctional molecular probes within a single, well-defined scaffold.³

Here, we present an efficient synthesis of targeted dual-modality imaging agents based on rotaxanes using a high-yielding active-template copper-catalyzed alkyne azide cycloaddition (AT-CuAAC) strategy. This approach enables the modular assembly of functional half-axles and macrocycles, facilitating the integration of targeting and imaging units within one mechanically interlocked structure.

The resulting rotaxanes are designed to selectively target cells expressing the genetically encoded SNAP-tag enzyme. Ongoing live-cell fluorescence microscopy studies aim to evaluate cellular labeling efficiency and cytotoxicity, while magnetic resonance imaging (MRI) measurements are being explored to assess contrast enhancement. Overall, this work highlights the growing potential of rotaxane-based MIMs, enabled by efficient active-template synthesis, as versatile platforms for targeted multimodal bioimaging.

Medicinal and Biological Chemistry

Photocatalytic Proximity Labeling for Mapping SUMO Interactors in Live Cells

Nasreen Nasser¹, Mahdi Hasan¹, Ashraf Brik¹

Chemistry, Technion – Israel Institute of Technology, Israel

Protein–protein interactions (PPIs) are fundamental to cellular regulation and represent important therapeutic targets. Proximity labeling proteomics (PLPs) enables mapping of protein interaction networks in native cellular environments; however, commonly used enzyme-based methods such as APEX and BioID are limited by relatively low spatial resolution. Photocatalytic approaches, including μ Map and Multiscale, overcome these limitations by generating short-lived reactive intermediates upon light activation of a photocatalyst tethered to a protein of interest, enabling nanometer-scale labeling with minimal cellular perturbation.

Here, we apply high-resolution photocatalytic proximity labeling to investigate the interactomes of Small Ubiquitin-like Modifier (SUMO) analogs in live cells. SUMO is a regulatory protein that modifies target proteins through reversible SUMOylation, thereby controlling protein localization, stability, and PPIs. Defining the SUMO interactome is essential for understanding its roles in cellular regulation and disease. We have previously demonstrated that SUMO2 undergoes efficient covalent conjugation to target proteins and localizes predominantly in the nucleus, particularly within PML nuclear bodies. In contrast, SUMO2 Δ G93, which lacks the essential C-terminal glycine required for activation and conjugation, remains unconjugated and is distributed mainly in the cytoplasm.

We hypothesize that the interactomes of SUMO2 and SUMO2 Δ G93 will differ significantly, potentially revealing distinct molecular interactions and cellular pathways. To capture these interactions at high spatial resolution, we propose a photocatalytic labeling strategy in which SUMO analogs are conjugated to a photocatalyst that activates a range of photoreactive probes upon LED illumination. Overall, this study aims to define SUMO interaction networks in live cells with high spatial resolution.

Medicinal and Biological Chemistry

Mirror-image proteins display distinct cellular uptake behaviours: L-Forms prevail

Eman Nassar¹, Dr. Ashok Donthoju¹, Mr. Mahdi Hasan¹
Chemistry, Technion, Israel

Mirror-image peptides and proteins are attracting interest as therapeutics, key building blocks for constructing mirror-image life, and as tools to probe the origin of life. To fully exploit their potential, it is essential to understand how their intracellular uptake compares to that of their natural L-counterparts. Here, we systematically investigate the impact of cargo chirality on cellular internalization while keeping the delivery vehicle constant. Three model cargos of increasing size and structural complexity were synthesized in both L- and D-configurations and conjugated to an identical cyclic deca-arginine (cR10) cell-penetrating peptide (CPP). Using this fixed CPP scaffold, we quantified uptake across multiple cell lines to directly isolate the contribution of cargo stoichiometry. Our results consistently show superior uptake of L-cargos relative to their mirror-image D-counterparts, demonstrating that cargo chirality is a key determinant of uptake efficiency across the chiral biological membrane.

Medicinal and Biological Chemistry

Access to 2,5-Disubstituted Thiazoles Via Cyclization of N-Substituted α -Amino Acids

Hajar Aledwan¹, Mr. Guy Zimmermann¹, Dr. Abed Saady¹
Chemistry, Bar Ilan University, Israel

Thiazoles are ubiquitous heterocyclic motifs found in natural products, pharmaceuticals, and functional materials, yet efficient and general methods for their direct construction remain limited.^{1,2} We report a simple, mild, and metal-free one-pot strategy for the synthesis of 2,5-disubstituted thiazoles from readily available N-substituted α -amino acids.³ The transformation proceeds via in situ carboxylic acid activation with thionyl chloride, followed by intramolecular cyclization and sulfoxide deoxygenation, delivering the target thiazoles in excellent yields under ambient conditions.

The protocol exhibits broad substrate scope and high functional-group tolerance, accommodating electron-rich and electron-poor aryl substituents, heteroaryl groups, alkynes, and extended π -systems. Importantly, the reaction is insensitive to air, avoids transition metals and complex reagents, and is readily scalable to gram quantities. Mechanistic investigations suggest a multirole function of thionyl chloride, serving as the activating agent, sulfur source, and deoxygenation reagent.

This operationally simple and robust methodology significantly streamlines access to structurally diverse 2,5-disubstituted thiazoles and provides a valuable platform for the rapid synthesis of biologically and materially relevant heterocycles.

Medicinal and Biological Chemistry

Direct Cellular Screening of Pd-Mediated Arylation of Cyclic Peptide Binders Targeting Ubiquitin Chains: Toward Modulating NEMO Liquid–Liquid Phase Separation

Mahdi Hasan¹, Nagaraju Vodnala¹, Yuri Glagovsky¹, Yakop Saed¹, Julia Kriegesmann¹, Prof. Hiroaki Suga², Prof. Ashraf Brik¹

¹*Schulich Faculty of Chemistry, Technion, Israel*

²*Department of Chemistry, Graduate School of Science, The University of Tokyo, Japan*

Ubiquitination is a critical post-translational modification that regulates key cellular processes such as protein degradation and DNA damage repair. Targeting a specific type of ubiquitin chain (e.g., Lys48 or Lys63-linked ubiquitin chain) via cyclic peptides presents a new strategy to modulate biological processes with therapeutic potential for various diseases. However, such a strategy remains challenging due to the obstacles of cell permeability and bioactivity. Here, we present a new method that directly assesses these parameters by integrating palladium-mediated Cys arylation with direct cellular screening. Using CP4, a previously identified cyclic peptide modulator of Lys63-linked ubiquitin chains, we generated a focused library of arylated analogues and optimized the Pd-mediated arylation for direct cellular screening. We discovered a new analog, CP-P12-Ar^H, that demonstrated enhanced binding affinity and robust bioactivity, as evidenced by increased γ -H2AX phosphorylation and apoptosis induction in cancer cells. Furthermore, CP-P12-Ar^H effectively inhibited the in vitro formation of NF- κ B essential modulator (NEMO) biomolecular condensates by disrupting the elongation of Lys63-linked ubiquitin chains, offering a novel way to modulate NF- κ B signaling. This work establishes a generalizable platform for the rapid optimization of cyclic peptide therapeutics targeting protein–protein interactions.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



METHODOLOGY AND CATALYSIS IN ORGANIC CHEMISTRY

Chair: Doron Pappo

Invited Lecture

Methodology and Catalysis in Organic Chemistry

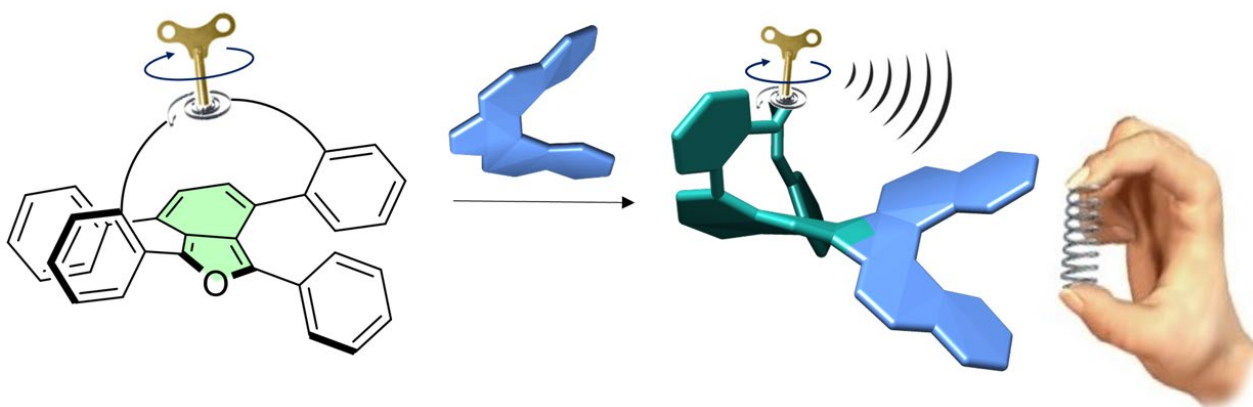
A Twisted Synthon for Inducing Helicity and Handedness in Nanographenes

Ori Gidron¹

Institute of Chemistry, The Hebrew University of Jerusalem, Israel

The helicity of nonplanar polyaromatic hydrocarbons dictates their electronic, optical, and chiroptical properties. However, controlling this helicity requires complex, target-specific synthesis.

In this talk, I will present a new approach for inducing curvature to nanographenes based on a versatile helical synthon, isobenzofuranophane. This synthon enables late-stage induction and remote control of helicity in polyaromatic frameworks. Reacting isobenzofuranophane with a [5]helicene aryne precursor, we show that the system's handedness and pitch can be controlled by varying the tether length. X-ray analysis reveals that this method induces significant curvature, with up to 35° torsion in a single benzene ring, thereby enabling tunable (chiro)optical properties. This work establishes isobenzofuranophane as a synthon for inducing a specific curvature to nanographenes.



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Invited Lecture

Methodology and Catalysis in Organic Chemistry

Mimicking Transition Metals with Structurally Constrained P^{III} and Sb^{III} Cations

Roman Dobrovetsky¹

School of Chemistry, Tel Aviv University, Israel

Structurally constrained main-group compounds and the unusual reactivity that emerges from geometric distortion have recently become a major focus in modern chemistry. In particular, constrained group 15 species have drawn significant attention due to their ambiphilic character, which enables transition-metal-like behavior. Our research centers on structurally constrained Pn(III) (Pn = pnictogen) cations that, as we have recently demonstrated for P(III) systems, exhibit ambiphilic small-molecule reactivity and can mimic transition metals in catalysis.

In this presentation, recent advances in the chemistry of structurally constrained P(III) and Sb(III) cations will be highlighted, including H₂ activation and metallomimetic catalytic hydrogenation with constrained P(III) cations, as well as metallomimetic catalytic silane redistribution mediated by structurally constrained Sb(III) cations.

Invited Lecture

Methodology and Catalysis in Organic Chemistry

The development of an innovative route toward Prothioconazole at ADAMA

Anthony Cohen¹, Dr Itsik Bar-Nahum¹, Dr Eran Fogler¹, Dr Liza Pen¹, Mr. Eli Gelman¹, Dr Avihai Yacovan¹
Chemical R&D, ADAMA, Israel

Prothioconazole is a triazole fungicide produced by ADAMA. It is produced on a multi-thousand-ton annual scale and is widely used for the protection of major cereal crops against fungal diseases. As part of ADAMA's ongoing commitment to chemical and process excellence, a new synthetic route toward M-243, a key intermediate in the manufacture of prothioconazole, has been developed.

The route incorporates several innovative process technologies. The first step is a copper-catalyzed photochemical transformation, which required extensive engineering efforts to optimize photon utilization while minimizing local overheating. This reaction was evaluated in batch and continuous-flow reactor configurations. The second step involves a phase-transfer-catalyzed cyclization, where careful catalyst selection enabled the use of mild sodium hydroxide instead of hazardous strong bases such as sodium hydride. Optimization of reagent stoichiometry, addition order, and dosing rates suppressed competing oligomerization and hydrolysis pathways.

The third step comprises an industrial-scale Grignard reaction, where precise control of reagent addition proved essential to avoid thermal runaway and Wurtz-type coupling. The final step required development of a selective epoxidation of ketone M-228, a substrate prone to side reactions due to an acidic benzylic α -proton. Competing methylation and Favorskii rearrangement pathways were mitigated through design-of-experiments optimization, resulting in a robust, scalable, and sustainable manufacturing route.

Beyond synthetic feasibility, the route was designed with strong emphasis on green chemistry principles and industrial viability, including maximization of atom economy, minimization of waste streams, reduction in step count, solvent recovery and recycling.

Invited Lecture

Methodology and Catalysis in Organic Chemistry

One-Electron Approach for Trans-Selective Alkyne Semi-Reduction via
Cobalt Catalysis

Prof. Samer Gnaim¹

Weizmann Institute, Israel

Selective partial reduction of alkynes to alkenes is a cornerstone of synthesis, yet broadly applicable catalytic routes to E-configured products remain scarce. We report a cobaltcatalyzed electrochemical platform that converts internal alkynes to trans-alkenes with high stereoselectivity via a radical pathway. The method accommodates diverse electronic and steric environments, delivers excellent chemoselectivity and functional-group tolerance, and enables straightforward access to trans-deuterated products. It also operates selectively in substrates bearing multiple alkyne motifs. Mechanistic studies-cyclic voltammetry, UV-vis spectroelectrochemistry, and DFT-support a dual catalytic cycle in which cathodic generation of a Co-H species engages an organometallic radical relay to forge E-alkenes. Guided by these insights, we developed a complementary, purely chemical oxidative variant that provides E-alkenes from substrates unreactive under electroreductive conditions. Together, these results establish a general cobalt-based strategy for accessing stereodefined trans-alkenes and open a new avenue for radical-mediated alkyne functionalization.

Invited Lecture

Methodology and Catalysis in Organic Chemistry

Synthetic Probes to Unravel Mechanisms Behind Coexistence within Microbial Ecosystems

Michael Meijler¹

Chemistry, Ben Gurion University of the Negev, Israel

Life on earth is heavily based on chemical communication between cells. Quorum sensing enables unicellular organisms to coordinate their behavior and function in such a way that they can adapt to changing environments and compete, as well as coexist, with multicellular organisms. Prime examples of this phenomenon are displayed by the opportunistic pathogens *Pseudomonas aeruginosa* and *Staphylococcus aureus*, which cause disease in humans – but most often do not. In recent years we embarked on a quest to unravel questions regarding coexistence, based on chemical signaling. The Meijler group is targeting and examining signaling within and between various microbes (e.g. pathogens in humans and beneficial soil microbes) with several chemical tools, such as a set of electrophilic and photoactivatable ‘tag-free’ probes that are designed to bind QS receptors covalently. These probes are used as molecular tools to obtain new insights into the mechanisms of activation, deactivation and recognition of bacterial quorum sensing. Diverse species, including eukaryotes, have been found to react strongly to the presence of these compounds, and the recognition of QSMs is mediated by mostly unknown receptors. Recently we identified and validated the role of a human receptor for HSLs, called the Major Vault Protein (MVP), as an important immunomodulator, and we also identified new receptors for QSMs in other species. We also recently identified an exciting new mode of coexistence between bacterial pathogens using untargeted metabolomics and synthetic confirmation, and we are developing new ABPP probes to identify the unknown receptors that mediate these events.

Methodology and Catalysis in Organic Chemistry

Free Oxoboranes: Formation, Structure, and Reactivity

Stav Deri¹, Dr Moran Feller¹, Dr Shibaram Panda¹, Batya Blank¹, Dr Mark A. Iron¹, Dr Yael Diskin-Posner¹, Dr Liat Avram¹, Dr Linda J. W. Shimon¹, Dr Rakesh Mondal¹, Dr Samer Gnaim¹

weizmann institute of science, Israel

We introduce a novel class of boranobornadiene derivatives, termed boranoanthracene, along with an in-depth study of their structures and reactivities. Using these versatile precursors, we propose a fundamentally novel mechanism for generating free oxoborane species. This pathway enables the formation of aminoxoborane species, which are rarely reported in the literature. The proposed mechanism unfolds via coordination of an oxygen-Lewis base (dimethyl sulfoxide) to the boron center, triggering a fragmentation cascade propelled by oxidative aromatization. Comprehensive experimental analysis, NMR measurements, and DFT calculations provide strong evidence supporting this mechanism.

We identify three distinct reactivity modes of the resulting oxoborane species. First, we show insertion of oxoboranes into B–C bonds, representing, to the best of our knowledge, the first example of this transformation. Second, we demonstrate a [3 + 2] cycloaddition between oxoboranes and nitrones, affording new boranoheterocycles. Third, we report the first [5 + 2] cycloaddition of oxoboranes with azomethine imines, delivering a seven-membered boracycle.

The diverse reactivities and facile generation of aminoxoboranes highlight their potential as versatile tools in organic chemistry and open new avenues for exploring the chemistry of highly reactive boron–oxygen species.

Methodology and Catalysis in Organic Chemistry

Unveiling the Fenton-Like Reactivity of Magnesium–Bicarbonate Complexes: Kinetic and Mechanistic Insights

Anushka Lucas¹

Chemical Sciences Department, the Schlesinger Family Center for Compact Accelerators,

Radiation Sources and Applications, and The Radical Research Center, Ariel University, Israel

In this work, we introduce a magnesium-based alternative to the conventional iron-driven Fenton system for oxidative catalysis. Instead of relying on redox-active transition metals, we show that a simple aqueous mixture of Mg^{2+} , bicarbonate, and hydrogen peroxide can activate peroxide and generate strong oxidizing species under mild conditions.

What makes this system fundamentally different from classical Fenton chemistry is the nature of the reactive intermediate. Through a combination of kinetic experiments and density functional theory (DFT) calculations, we demonstrate that the dominant oxidant is the carbonate radical ($\text{CO}_3^{\bullet-}$), rather than the hydroxyl radical. Our results indicate that this radical forms via the decomposition of a short-lived magnesium–carbonate–peroxo complex, highlighting a coordination-driven, rather than redox-driven, activation pathway.

We further show that this Mg(II) –bicarbonate– H_2O_2 system is capable of oxidizing a range of organic substrates and environmentally relevant pollutants in water. Using magnesium offers clear practical advantages: it is Earth-abundant, non-toxic, and avoids the sludge formation and metal contamination typically associated with iron-based processes.

Taken together, this work proposes a new way of thinking about peroxide activation using non-transition metals. Beyond its potential for water treatment, the chemistry opens up opportunities to design greener oxidation methodologies in both aqueous and organic reaction systems. We believe these findings contribute to the broader effort to develop sustainable catalytic strategies without relying on critical or hazardous metals.

Methodology and Catalysis in Organic Chemistry

Aromatization-Driven Generation of Iminoboranes and Their Cycloaddition Behavior

Batya Blank¹, Dr Samer Gnaim¹

Molecular Chemistry and Materials Science, weizmann institute of science, Israel

Iminoboranes—molecules featuring a boron–nitrogen triple bond ($\text{RB}\equiv\text{NR}'$)—are high-energy intermediates isoelectronic with alkynes. Their synthetic potential has remained untapped due to the harsh conditions and kinetic instability associated with their formation. This work presents a mild, modular platform for the generation and in-situ functionalization of iminoboranes via a boranoanthracene-driven release strategy using rearomatization as a driving force. Two complementary nitrogen-atom transfer reagents, aryl azides and sulfilimines, enable practical access under mild thermal conditions. The nascent iminoboranes are efficiently trapped through [3+2] cycloadditions, with nitrones offering enhanced selectivity and synthetic value. The resulting fully characterized products confirm the successful formation and incorporation of the $\text{B}\equiv\text{N}$ motif. Together, these findings transform iminoboranes from fleeting curiosities into synthetically accessible intermediates, providing a general blueprint for exploring their reactivity and expanding boron–nitrogen chemistry within modern organic synthesis.

Methodology and Catalysis in Organic Chemistry

Catalysis of organic reaction under external electrical fields using ferroelectric particles

Ranu Dhale¹, Dr. Yuval Vidavsky², Prof. Charles Diesendruck³

¹*Faculty of Chemistry, Technion Israel Institute of Technology, Israel*

²*Space Environment Department, Soreq NRC, Israel*

³*Technion Israel Institute of Technology, Israel*

External electric fields offer a non-invasive and tunable means to control a chemical reaction. The reaction environment can be dynamically modulated just by adjusting the applied voltage. There are several theoretical predictions, particularly those involving oriented electric fields on reaction pathways and selectivities. However, experimental demonstrations are highly limited and rare. To date, most successful implementations of electric field catalysis have been achieved at the single molecule level using scanning tunneling microscopy (STM) or through interfacial (electrode-electrolyte) electric fields generated by surface charging. Moreover, these techniques are highly sophisticated and currently not scalable, with yields typically limited to the nanomolar scale.

The required electric field strength for affecting a chemical reaction is around 1V/nm, which is exceptionally large and likely impossible to achieve in bulk systems practically. In this project, we propose an approach to amplify local electric fields within a large reaction environment using ferroelectric materials dispersed in the reaction medium. Upon the application of an external electric field, ferroelectric domains can be temporarily aligned, creating a net polarization effect in molecules that later diffuse into the solution. In our study, we investigate a CoCl₂ catalyzed 1,3-rearrangement of O-acyl-N-arylhydroxylamines to O-acylated 2-aminophenol. The thermal reaction requires Ag⁺ salts under inert and anhydrous conditions to generate the catalytically active Co²⁺ species. We hypothesized that oriented domains of BaTiO₃ particles under an external electric field will induce the polarization of the electron cloud of CoCl₂ and assist in ionizing the pre-catalyst without the need for Ag⁺ salts.

Methodology and Catalysis in Organic Chemistry

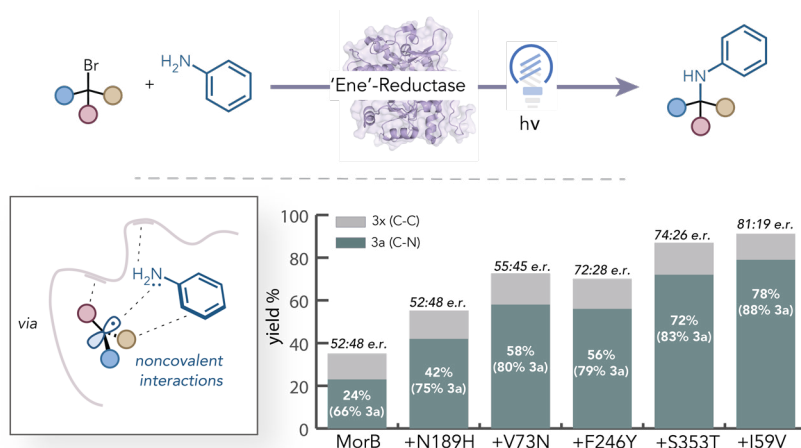
Intermolecular Nucleophilic Radical Substitution (SRN1) enabled by engineered photoenzymes

Dr Zayed Alassad¹, Prof. Todd Hyster¹
Chemistry, Princeton University, NJ, United States

Constructing C(sp³)–N bonds between tertiary alkyl electrophiles and unsubstituted anilines is a major synthetic challenge as conventional polar mechanisms are plagued by eliminations, while modern copper-catalyzed radical approaches favor addition to the arene π -system. Here, we report a biocatalytic strategy showing that flavin-dependent ene-reductases use visible light to generate and tame highly reactive tertiary radical intermediates, to achieve the direct N-alkylation, a transformation with no precedent in asymmetric synthesis.

Starting from a Morphinone reductase that provided the product in modest yield (22%), moderate chemoselectivity (66%) and no enantioselectivity, iterative protein engineering yielded a mutant that delivers the N-alkylated product in 78% yield, 88% chemoselectivity, and 82:18 e.r. with a broad substrate scope.

Mechanistic investigations, combining multivariate statistical modeling with DFT calculations and experiments, reveal that the enzyme's active site steer the reaction outcome through a synergistic combination of π -stacking and radical hyperconjugation with the aniline's nitrogen lone pair. This work establishes biocatalysis as a versatile platform for directing challenging radical reactivities toward valuable chiral amine scaffolds.



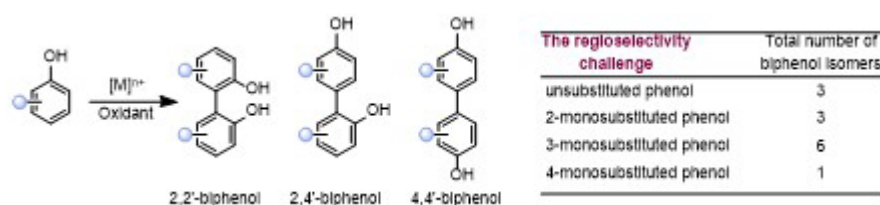
Methodology and Catalysis in Organic Chemistry

ortho-ortho Selective Oxidative Coupling of Phenols by Hydroxo Multicopper(II) Clusters^{1,2}

Omer Shaashua¹, Ratnadeep Bera¹, Prof. Doron Pappo¹
Chemistry, Ben-Gurion University of the Negev, Israel

2,2'-Biphenols are a crucial class of C₂-symmetric compounds valued across coordination chemistry, asymmetric catalysis, pharmaceuticals, and host–guest systems. Their direct, atom-economical synthesis via metal-catalyzed oxidative coupling of phenols is highly desirable, yet its practical utility is limited by persistent chemo-, regio- and stereoselectivity challenges. While the chemo- and stereoselectivity challenges have been tackled previously, the chemoselectivity challenge still remains unmet. For unsubstituted and monosubstituted phenols, the reaction typically yields unpredictable mixtures of 2,2'-, 2,4'-, and 4,4'-biphenol isomers, leaving these important precursors beyond the scope of the reaction.

This work reports an unprecedentedly ortho-ortho selective, one pot aerobic oxidative coupling of unsubstituted and mono-substituted phenols, providing a direct entry to desirable 2,2'-biphenols in moderate to good yields. The method utilizes readily available hydroxo multi-copper clusters, particularly the [Cu(tmeda)(μ-OH)]₂(ClO₄)₂ complex, in 1,1,1,3,3,3-hexafluoropropan-2-ol (HFIP). Our detailed mechanistic studies, employing Density Functional Theory (DFT) computations, high-resolution mass spectroscopy (ESI-MS), and Infrared photodissociation (IRPD) spectroscopy, rationalize the unique site selectivity, and open the gate towards specifically designed catalytic system tailored for the desired isomer.



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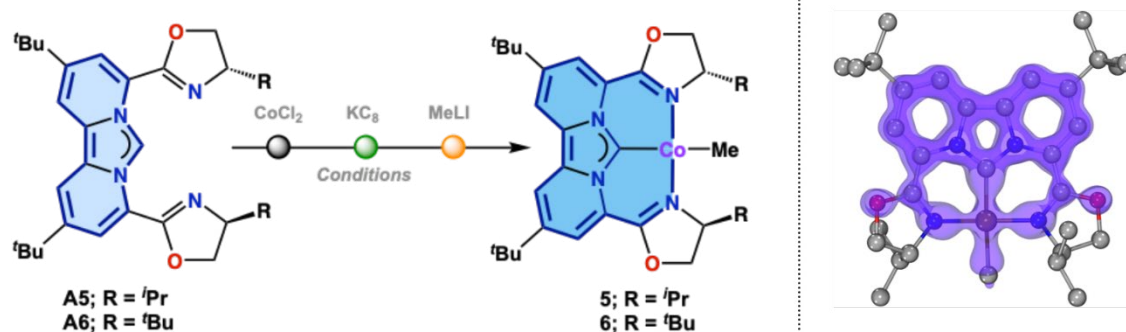
Methodology and Catalysis in Organic Chemistry

Redefining Metallaaromaticity of Cobalt Containing Macrocycles Through Dative Metal–Ligand Bonding

Sakthi Raje¹, Prof. Graham de Ruiter¹

Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Israel

Aromaticity is a foundational principle in chemistry, yet its extension to organometallic systems remains challenging due to the absence of straightforward strategies that enable through-metal π -delocalization. Conventional routes to metallaaromatic compounds typically rely on element-substitution approaches that form covalent metal–carbon bonds. In this work, we introduce a fundamentally different design paradigm: the construction of macrocyclic metallaaromatic complexes through dative metal–ligand coordination chemistry. By using such an approach, we are able to introduce a generalizable and modular platform in which dative metal–ligand interactions serve as active design operators to construct robust, extended macrocyclic frameworks with tunable aromatic character. The applicability of our approach is demonstrated by the synthesis of macrocyclic cobalt complex (5) that exhibits all the hallmarks of metallaaromaticity: energetic stabilization, magnetically induced ring currents, and global π -delocalization, as demonstrated by the highly downfield-shifted ¹H NMR resonances and corroborated by comprehensive computational analyses, including NICS, ISE, and SYSMOIC π -current integrations. Overall, these findings establish a generalizable platform for accessing metallaaromaticity through coordination chemistry, expanding the design principles of aromatic systems to include dative metal–ligand bonding, which will be further discussed in this poster.



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Methodology and Catalysis in Organic Chemistry

Developing Pyrido-Annulated Imbox(NCN) Pincer Complexes for Acceptorless Alkane Dehydrogenation

Ratan Debnath¹, Dr. Sakthi Raju¹, Prof. Alan S. Goldman², Prof. Graham de Ruiter¹

¹Israel Institute of Technology (Technion), Israel

²Rutgers, the State University of New Jersey, USA

The selective conversion of unreactive alkanes into the corresponding olefins represent a central challenge in modern catalysis. Olefins serve as versatile intermediates for downstream functionalization and for the synthesis of high-value chemicals. However, the dehydrogenation of alkanes is profoundly endothermic, and efficient catalysis requires thermally robust systems capable of sustaining high temperatures and delivering high turnover numbers. Recent advances, including the development of fluorinated Phebox iridium complexes, reported by Goldman and co-workers for acceptorless alkane dehydrogenation, have demonstrated that carefully tuned ligand frameworks can significantly enhance catalytic performance. In this context, we have synthesized a series of pyrido-annulated Imbox(NCN) ligands with the goal of creating highly stable metal pincer complexes. The unique steric and electronic features of these pyrido-fused carbene scaffolds are expected to provide strong σ -donation together with favorable π -acceptor properties, which should enhance both the thermal stability and the reactivity of the resulting complexes. Our ongoing work focuses on preparing the corresponding metal pincer complexes and evaluating their activity in acceptorless alkane dehydrogenation. In parallel, computational studies will be carried out to elucidate structure-reactivity relationships and guide further ligand optimization. This combined experimental and theoretical approach aims to establish pyrido-annulated NCN pincer systems as a new platform for efficient, high-temperature alkane dehydrogenation catalysis.

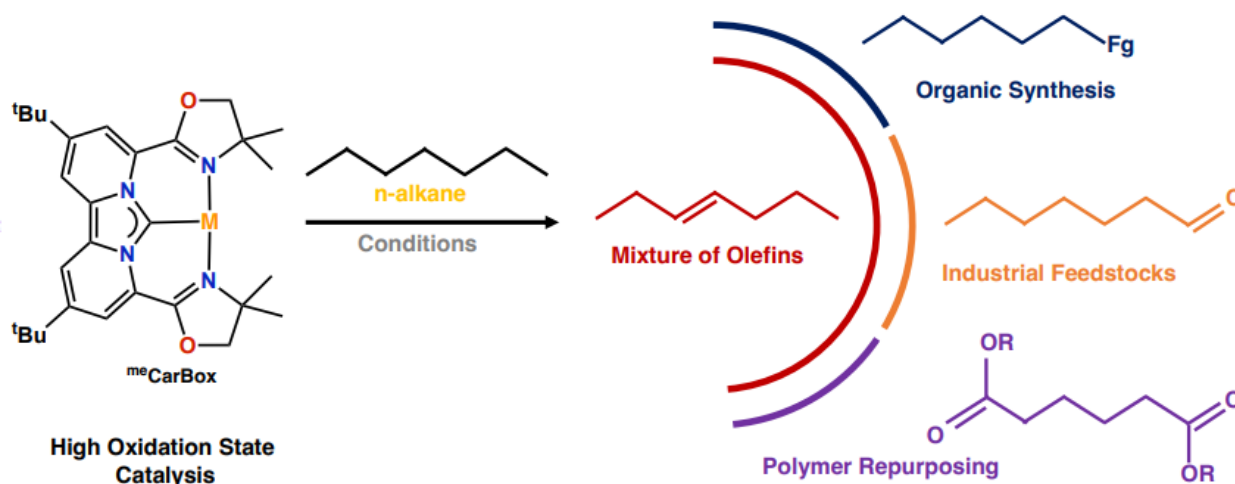


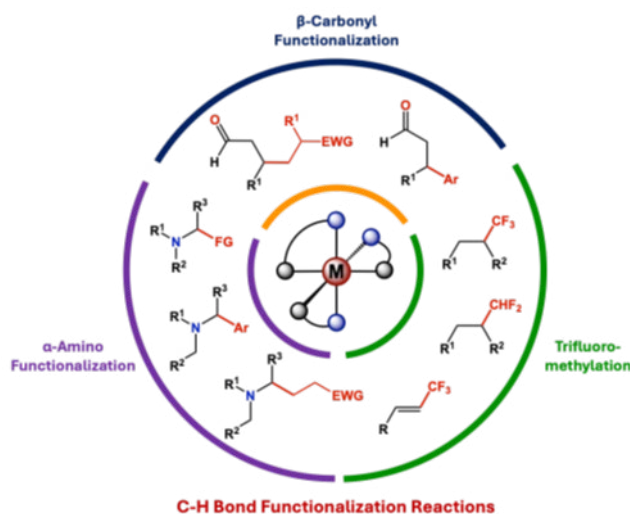
Figure 1: Alkane Dehydrogenation and Olefin Functionalization

Methodology and Catalysis in Organic Chemistry

Synthesis and Photophysical Studies of Cr (III) and Co (III) Complexes

Kritika Verma¹, Mr Ashutosh Mishra¹, Dr. Zeqing Chen¹, Prof. Graham de Ruiter¹
Chemistry, Technion Institute of Technology, Israel

During the past decade, photoredox catalysis has transformed the way we perform organic chemistry. Integral to these developments are the unique photophysical properties of 4d- and 5-d metals, which possess extended lifetimes for their metal-to-ligand charge-transfer (MLCT) excited states. However, these metals (e.g., Ru and Ir) are coincidentally some of the rarest on earth, necessitating the development of more environmental friendly and earth-abundant alternatives. Nonetheless, simply replacing 4d- and -5d-metals for their 3d-congeners is not trivial. The key to overcoming the limitations inherent to 3d-metals, such as (i) small ligand field splitting, (ii) short excited-state lifetimes, and (iii) small ionic radii, is bespoke ligand design. In this poster, we will demonstrate how we can harness the power of our previously explored imidazo [1,5-a] pyridine-3-ylidene ligands and pyrido[1,2-c;2',1'-e]-imidazolin-6-ylidene ligands which will be decorated with additional donor ligands that focus on introducing (i) strong σ -donors, (ii) strong π -acceptors, or (iii) strong π -donor moieties onto the PA-NHC framework. Furthermore, we have developed a pyridine (dicarbene) ligand with flanking phenyl substituents. The photophysical properties of the resulting cobalt and chromium complexes will be studied and their extended excited-state lifetimes will be tailored for photoredox catalysis. Reactions of interest are trifluoromethylation, C–H bond functionalization, and α -amino functionalization, amongst others (Figure 1).



Methodology and Catalysis in Organic Chemistry

Ligand-Stabilized Mn(I) Complexes as Sustainable Photocatalysts

Priya Mata¹, Ashutosh Mishra¹, Zeqing Chen¹, Prof. Graham de Ruiter¹
Schulich Faculty of Chemistry, Technion- Israel Institute of Technology, Israel

Recent developments in photoredox chemistry have demonstrated that complexes of first-row transition metals can approach, and in some cases match, the performance of noble-metal photocatalysts. Success in this area relies heavily on ligand architectures that stabilize long-lived charge-transfer states and promote efficient photochemical reactivity. Designing complexes that achieve this balance is therefore a key strategy for advancing sustainable photocatalysis. In this work, we introduce a Mn(I) complex supported by a CNC-type N-heterocyclic carbene ligand that was designed to enforce strong metal–ligand interactions. The ligand framework stabilizes the low-valent Mn center and promotes metal-centered reduction during complex formation, giving rise to a well-defined Mn(I) species. Structural characterization by single-crystal X-ray diffraction reveals a rigid coordination environment that supports the desired electronic configuration. The photophysical profile of the complex shows distinct absorption bands in the UV–Vis region that are absent in the free ligand, consistent with enhanced metal-to-ligand and ligand-to-metal charge-transfer character. Electrochemical studies further demonstrate reversible redox behaviour, indicating that the electronic structure of the Mn(I) center can be tuned through ligand design. Together, these features suggest that this CNC-supported Mn(I) complex offers a promising platform for visible-light-driven photocatalysis. The combination of earth-abundant manganese, a strongly binding carbene-based ligand, and accessible excited-state redox properties underscores its potential as a sustainable alternative to traditional noble-metal systems. This study highlights how rational ligand design can unlock photochemical reactivity in 3d metals and expand the toolbox of green photocatalytic technologies.

Methodology and Catalysis in Organic Chemistry

Enhanced Olefin Metathesis Selectivity via Ruthenium Diiodide Catalysts

Keren Iudanov¹, Dr Noy Nechmad¹, Dr Albert Poater², Prof N. Gabriel Lemcoff¹

¹*Department of Chemistry, Ben-Gurion University of the Negev, Israel*

²*Departament de Química Universitat de Girona c/ Maria Aurèlia Capmany, Institut de Química Computacional i Catàlisi, Spain*

Olefin metathesis, a powerful catalytic reaction forming new carbon-carbon double bonds from alkene rearrangement. The reaction's outcome is sensitive to substrate properties, reaction conditions, and catalyst structure.

We recently found that substituting chloride ligands with iodides in sulfur-chelated ruthenium catalysts significantly alters their selectivity. These diiodo catalysts have proven effective for challenging transformations, including the formation of strained rings through macrocyclization and depolymerization.

Crucially, we discovered that diiodo catalysts uniquely drive cross metathesis (CM) over ring-closing metathesis (RCM) for 1,5-dienes possessing a hindered terminus. This unexpected preference stems from the iodide ligands' ability to inhibit the coordination of the non-terminal olefin to the ruthenium center. While 5-membered ring formation (RCM) is usually entropically and enthalpically favored, the steric hindrance at the dimethyl terminus, forces the catalyst to favor CM.

We investigated this transformation using Density Functional Theory (DFT) calculations. The utility and scope of this unique CM reaction were demonstrated by the straightforward functionalization of several terpene natural products, yielding novel derivatives in a single step-a feat previously unattainable.

Current research focuses on establishing a structure-activity correlation to design catalysts with high activity for RCM while selectively suppressing other metathesis pathways. This involves applying data science and multivariate modeling to correlate catalyst steric and electronic parameters with predictive activity.

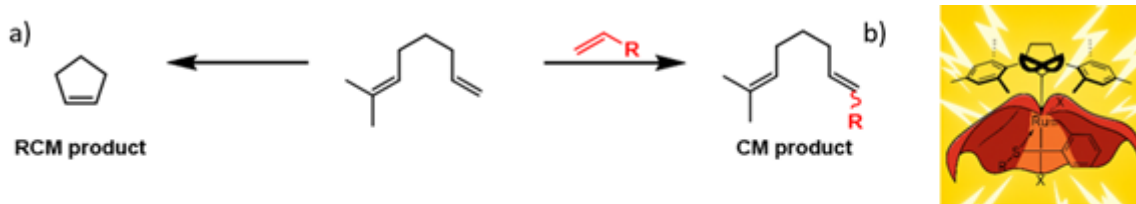


Figure 1. a) Sulfur-chelated ruthenium benzylidene “super” catalyst structure. b) Reaction scheme for RCM and CM of 1,5-diene.

Iudanov K.; Nechmad, N. B.; Poater, A.; Lemcoff, N. G. Selective Cross-Metathesis Versus Ring-Closing Metathesis of Terpenes, Taking the Path Less Travelled. *Angew Chem Int Ed Engl* **2024**, 63 (52), e202412430.

Methodology and Catalysis in Organic Chemistry

Toward Metal-Ion Fluorescent Sensing: A New Pyridyl syn-Bimane Platform

Anjali Soniwal¹, Mr. Nathaniel Chennattuparambil Roy¹, Prof. Flavio Grynszpan¹
Chemical Sciences, Ariel University, Israel

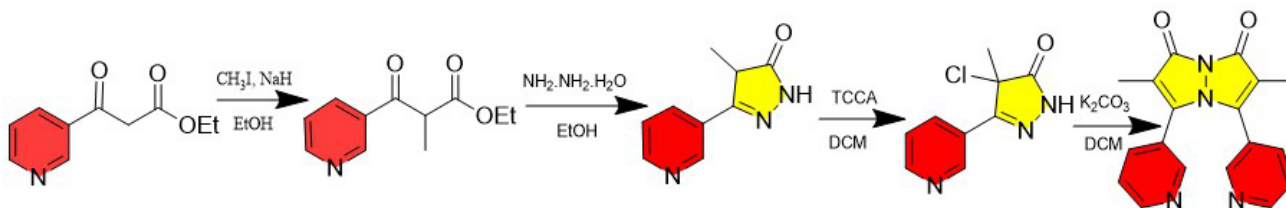
Bimanes are a compact and structurally versatile class of heterobicyclic fluorophores, that have played an important role in spectroscopy, chemical sensing, and bioimaging for more than five decades.[1] Their photophysical behavior can be readily tuned through α - and β -substitutions, enabling control over absorption, emission, and metal-binding properties. Building on our long-standing efforts to design bimanane-based sensors, we report the design, synthesis and preliminary photophysical characterization of a new bimanane derivative, 2,6-dimethyl-3,5-di(pyridin-3-yl)-1H,7H-pyrazolo[1,2]pyrazole-1,7-dione (Fig. 1).

Absorption and emission spectra of the compound were recorded in a range of solvents, with methanol producing the brightest fluorescence. The molecule displayed absorption within the 358–465 nm and emission in the 441–447 nm region. Its molar extinction coefficient (ϵ between 5200 and 5600 M⁻¹ cm⁻¹), is lower than expected for a bimanane derivative but consistent with other organic chromophores with robust $\pi \rightarrow \pi^*$ electronic transitions.

A preliminary metal-complexation study of the bimanane derivative with selected metal ions revealed fluorescence quenching, most notably in the presence of Pd(OAc)₂ and MgCl₂. Guided by these results, ongoing work is expanding the analysis to a broader panel of environmentally and industrially relevant metal ions. The DFT minimized structures, synthesis, complexation data and structure–response correlations will be presented.

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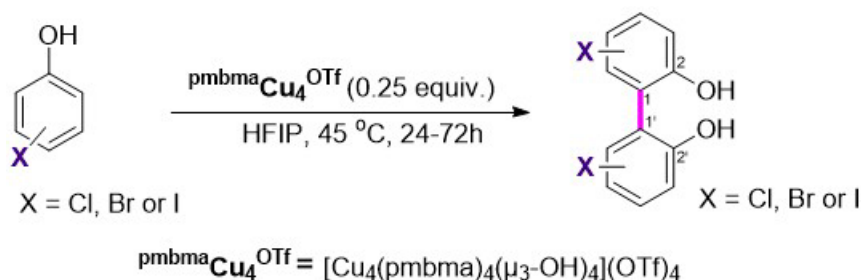


Methodology and Catalysis in Organic Chemistry

Dihalo-2,2'-biphenols: Ortho-ortho Selective Oxidative Coupling of Halophenols¹

Ratnadeep Bera¹, **Raja Kapaniaiah**¹, Prof. Doron Pappo¹
Chemistry, Ben-Gurion University of the Negev, Israel

2,2'-Biphenols are common structural motifs found in many biologically active natural products and serve as chiral ligands that are widely used in asymmetric catalysis and as building blocks for complex organic frameworks, which are utilized in a variety of applications. The metal-catalysed oxidative phenol coupling reaction provides a direct entry to 2,2' biphenols from simple and readily available phenolic units. Recently, Pappo² together with the Roithová group, demonstrated that the hydroxo multicopper clusters, such as [Cu(tmeda)(μ-OH)]₂(ClO₄)₂(tmedaCu₂ClO₄), mediate the oxidative coupling of unsubstituted and monosubstituted phenols with complete ortho-ortho coupling selectivity, affording 2,2'-biphenols as single products. Despite the remarkable discovery in controlling the selectivity in oxidative coupling reactions, the method remains underutilized for preparing complex 2,2'-biphenol structures. Herein, we report simple conditions for ortho-ortho selective oxidative coupling of halophenols using the [Cu₄(pmbma)₄(μ₃-OH)₄](OTf)₄ cluster (0.25 equiv) in HFIP (air, 45°C, 24–72 h). The method is applicable for preparing 3,3'-, 4,4'- and 5,5'- dihalo-2,2'-biphenols directly from commercially available chloro, bromo, and iodophenols. The single-step methodology offers an efficient alternative to key dihalo-2,2'-biphenol compounds, which typically require multiple steps to access.



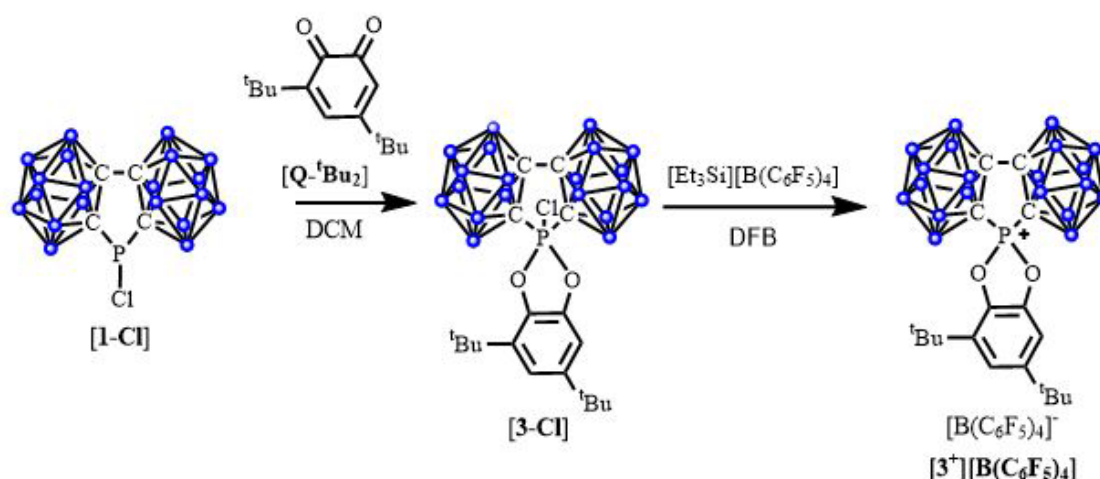
1. Ratnadeep Bera[‡], Raja Kapaniaiah[‡] and Doron Pappo^{*}. Dihalo-2,2'-biphenols: Ortho-ortho Selective Oxidative Coupling of Halophenols. [‡]These authors contributed equally. (manuscript under preparation)
2. Ratnadeep Bera, Omer Shaashua, Anna Libman, Max T.G.M. Derks, Bowei Yuan, Aleksandr Y. Pereverzev, Raja Kapaniaiah, Mor Ben Lulu, Lina Kertzman, Yulia Vainer, Yury V. Torubaev, Jana Roithová^{*}, and Doron Pappo^{*}. Selective Oxidative Coupling of Phenols by Hydroxo Multicopper(II) Clusters. *J. Am. Chem. Soc.*(doi: 10.1021/jacs.5c10379)

Methodology and Catalysis in Organic Chemistry

A new Lewis super acid: a Phosphonium cation Based on a Biscarborane-Catechol Framework.

Itay Raz¹, mr Mohanad Diab¹, Dr. Kuldeep Jaiswal¹, Prof. Roman Dobrovostky¹
school of chemistry, Tel aviv university, Israel

A new phosphonium cation featuring a biscarborane–catechol framework is presented. The phosphonium salt $[3^+][B(C_6F_5)_4]$ was synthesized using 3,5-di-tert-butyl-ortho-quinone and bis-oCbPCl. $[3^+][B(C_6F_5)_4]$ was found to be an exceptionally strong Lewis acid, confirmed by the Gutmann–Beckett method, as well as by computed fluoride and hydride ion affinities, which place $[3^+]$ among the strongest phosphonium-based Lewis acids reported. The catalytic abilities of $[3^+][B(C_6F_5)_4]$ were tested and found to efficiently catalyze the hydrosilylation of alkenes, dimerization of diphenylethylene, and polymerization of 1-hexene. These results highlight the biscarborane–catechol framework as a promising platform for designing novel main-group super Lewis acids with significant potential.



Methodology and Catalysis in Organic Chemistry

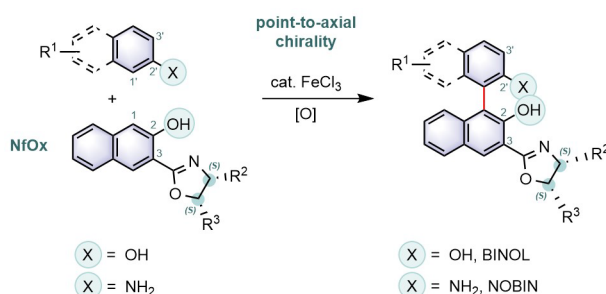
Transferring Point to Axial Chirality in Oxidative Coupling Reactions for the Synthesis of Novel Chiral NxOy Ligands

Hen Shalev¹, Prof. Doron Pappo¹
Ben-Gurion University of the Negev, Israel

1,1'-Bi-2-naphthols (BINOLs) and 2-amino-2'-hydroxy-1,1'-binaphthyls (NOBINs) belong to the axially chiral binaphthyl family. These privileged C₁- and C₂-symmetric molecules have significantly advanced asymmetric catalysis and related fields³. Consequently, there is an ongoing effort to develop efficient methods for their synthesis, starting from simple and readily available naphthalene units.

In a recent study, our group reported the transfer of point-to-axial chirality in the oxidative coupling between 2-aminonaphthalenes with a labile chiral auxiliary and 2-naphthol derivatives.⁴ This method enabled access to optically pure tailor-designed (*R_a*)- and (*S_a*)-NOBINs that are not attainable by any other means.

In this work, we investigate the possibility of inducing axial chirality from the 3-position of the 2-naphthol substrate to the newly formed biaryl bond. For this purpose, various chiral naphthol-oxazolines (NfOx) were synthesized and subjected to iron-catalyzed oxidative cross-coupling reactions with phenols, 2-naphthols, arenes, or 2-aminonaphthalenes. The products of these diastereoselective reactions serve as axially chiral NxOy-binaphthalene ligands for metals such as iron and vanadium.



Methodology and Catalysis in Organic Chemistry

Biomimetic Oxidative Phenol Coupling of Monolignols

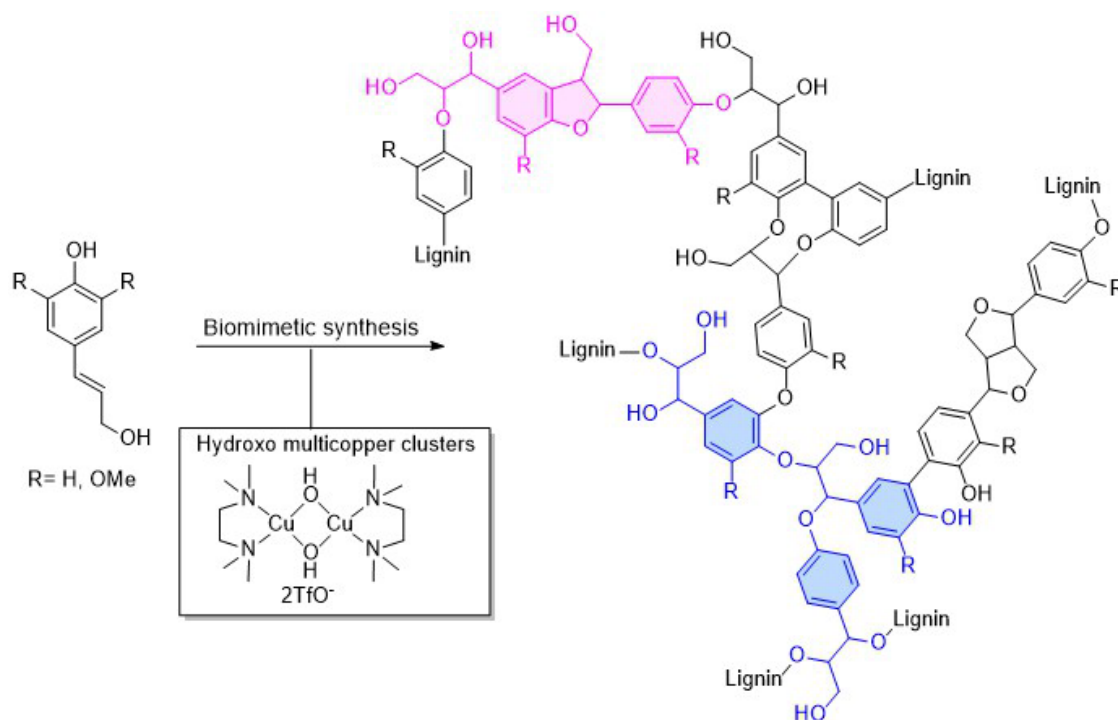
Mariana Awadalla¹, Prof. Doron Pappo¹

Chemistry, Ben-Gurion University of the Negev, Israel

Lignin, the second most abundant organic material on earth, is a highly complex natural polymer found in plant cell walls and synthesized via the dehydrogenative polymerization of monolignols such as p-coumaryl, coniferyl, and sinapyl alcohol. Lignin is essential for plant growth; it reinforces cell-wall rigidity, enhances hydrophobicity, facilitates mineral transport, and provides a protective barrier against insects and pathogens.

In plants, fungi, and bacteria, this dehydrogenative polymerization is catalyzed by laccase enzymes, which are multicopper oxidases that consist of four copper centers in the active site. Recently, our group developed hydroxo multicopper clusters that promote oxidative phenol coupling reactions.

Using one of these copper clusters, we successfully achieved a biomimetic oxidative homocoupling of monolignols (scheme 1), affording several of the coupling motifs present in lignin. This study offers insight into the mechanism of the formation of the growing lignin polymer.

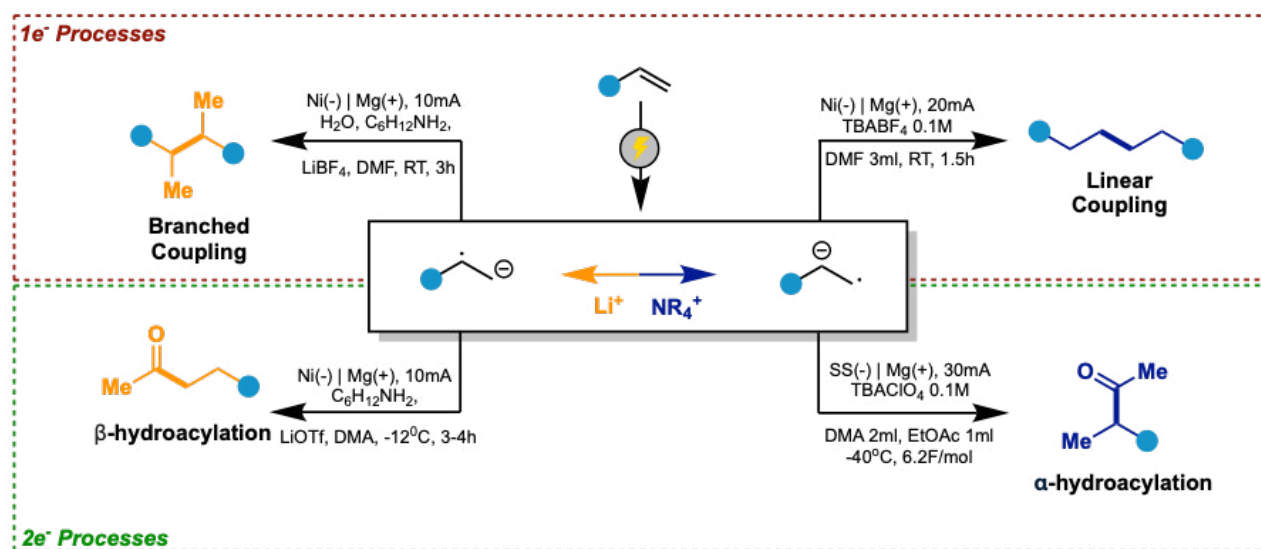


Methodology and Catalysis in Organic Chemistry

Electrolyte-Guided Selectivity Unlocks Pathway Control in Olefin Functionalization

Daniel Gordon-Levitan¹
Weizmann Institute of Science, Israel

The identity of electrolytes exerts a decisive yet underexplored influence on organic electrosynthesis. We show that switching the supporting cation toggles olefin coupling between exclusive linear and branched selectivity. Ammonium salts preserve the terminal spin bias of the styrene radical anion, promoting solution-phase Giese-type addition for linear products. Lithium salts instead form a Li-rich interphase that drives benzylic spin localization and channels surface-confined radical coupling to yield branched products. Radical probes, CV, SEM, ssNMR, EPR, and DFT clarify these distinct pathways. This platform streamlines access to pharmaceutical-relevant scaffolds and reveals previously untapped polar hydrofunctionalization of conjugated olefins. These findings establish electrolyte-controlled interfacial organization as a powerful lever to control product selectivity in organic electrosynthesis.

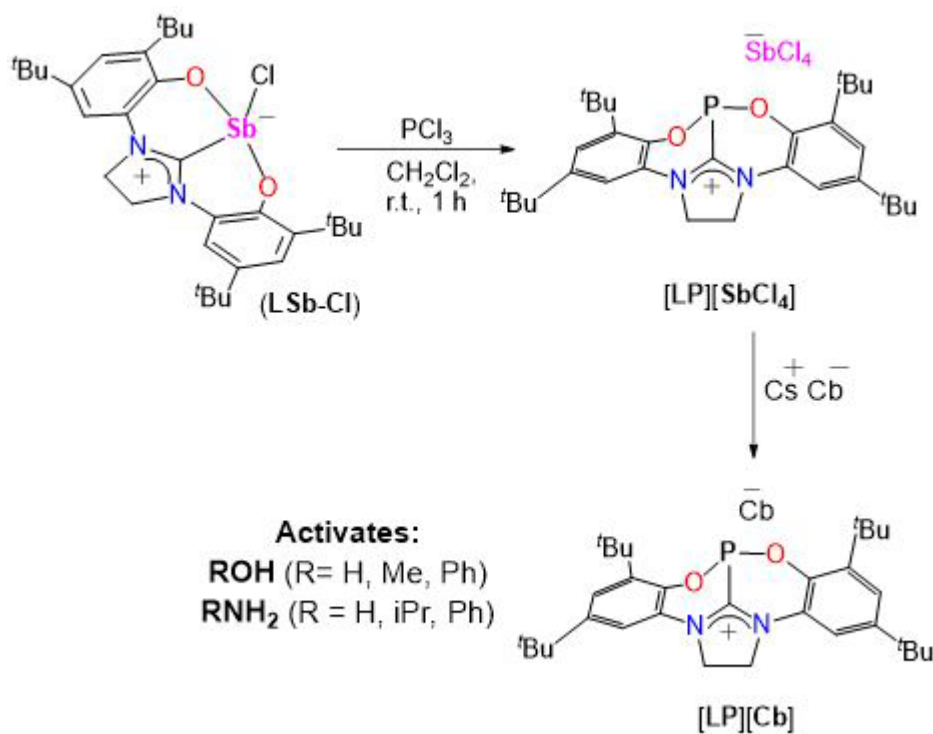


Methodology and Catalysis in Organic Chemistry

Sb-to-P Metathesis - A Direct Route to Structurally Constrained, Cationic P^{III} Compound

Irina Malahov¹, Dr. Deependra Bawari¹, Prof. Roman Dobrovetsky¹
Tel Aviv University, Israel

A cationic, structurally constrained P^{III} compound, [LP][SbCl₄], in *OCO* pincer-type ligand with a central carbene donor, was directly obtained through an Sb-to-P metathesis reaction between LSb-Cl and PCl₃. The reactivity of [LP][SbCl₄] with small molecules such as ROH and RNH₂ revealed that the [SbCl₄][−] anion actively participates in these reactions and is not chemically inert. By replacing the [SbCl₄][−] with [CB₁₁H₁₂][−] (Cb[−]) anion the reactivity was redirected towards the [LP]⁺ cation exclusively that activated E–H bonds in ROH (H, Me, Ph) and RNH₂ (R = H, iPr, Ph). The reactions with H₂O and NH₃ were irreversible, producing OA-type products in the case of NH₃, while H₂O activation led to a ring rearrangement process. Notably, the activation of PhOH and PhNH₂ was reversible under thermoneutral conditions, an important feature for advancing catalysis using main-group compounds.



Methodology and Catalysis in Organic Chemistry

on the structure, formation and reactivity of enolonium species

Bat-El Oded¹, Prof. Alex. M Szpilman¹

Chemistry, Ariel University, Israel

Mechanistic pathways of BF₃-assisted Umpolung α -functionalization of carbonyl compounds using hypervalent iodine (III) compound, [PhI(OH)OTs], to generate α -substituted aldehydes or ketones as the final products were examined using DFT. The reaction was explored in two separate processes: (i) enolonium species formation and [1,3]-sigmatropic rearrangement (ii) the nucleophilic attack and product formation. Our study revealed that the barrier for [1,3]-sigmatropic rearrangement is increasing with increasing temperature. Additionally, the enolonium species formation is promoted by BF₃ coordination, to yield OPh enolonium species. Moreover, the nucleophilic attack, can take place on the OPh or the CPh, depending on the nucleophile. The second route is taking place after OPh $\leftrightarrow$ CPh interconversion. This computational study supports our previous NMR experiments done at -78 °C and the observed species

Methodology and Catalysis in Organic Chemistry

Examination of Fenton-like reactions with various metal complexes

Maayan Weiss^{1,2}, Maksim Kolesnikov¹

¹*The Department Of Chemical Sciences, Ariel University, Israel*

²*Alpha Program, Future Scientists Center, Israel*

In recent years, the rapid development of industrial society has intensified water pollution concerns and increased the need for effective treatment methods. Among advanced oxidation processes, Fenton-like reactions have gained significant attention due to their high efficiency in removing pollutants. These reactions are considered key strategies for reducing toxic organic compounds in water sources, including drinking water and industrial effluents. Since the discovery of the original Fenton reaction, numerous variations have been introduced, yet their mechanisms remain only partially understood, highlighting the importance of continued research.

This study examined the decomposition efficiency of ethanol and dimethyl sulfoxide (DMSO) as model pollutants in nine different solutions, three of which were expected to undergo a Fenton-like reaction. The metal complex used included $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ as the transition metal, hexamethyltriethylenetetramine as the ligand, and H_2O_2 as the oxidizing agent.

UV spectrophotometry results showed that in the solutions intended for a Fenton-like reaction, nearly 50% of DMSO decomposed, confirming the occurrence of the reaction. In contrast, solutions containing only H_2O_2 or only the metal complex showed much lower decomposition levels of 10.4% and 3.5%, respectively. Additional analyses tested the influence of pH on reaction performance. LCMS results demonstrated that pollutant degradation occurs effectively and is most efficient at pH 7. Moreover, the oxidation level of the environment had only a minor impact on decomposition efficiency.

These conclusions indicate that the catalytic system studied can function efficiently under varying environmental conditions, offering a practical advantage for industrial water treatment processes where pH levels may fluctuate.

Methodology and Catalysis in Organic Chemistry

One-Electron Approach for Trans-Selective Alkyne Semi-Reduction via Cobalt Catalysis

Rakesh Mondal¹, Ms. Lior Galmidi¹, Dr. Samer Gnaim¹

Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

The diastereoselective semireduction of alkynes to alkenes is a powerful transformation in synthetic chemistry, yet catalytic methods for trans-selective (E) alkyne reduction remain limited. Herein, we introduce a fundamentally new approach for the highly selective trans-semireduction of internal alkynes, enabled by a cobalt-catalyzed electrochemical radical pathway. This method offers a broad substrate scope, accommodating alkynes with diverse electronic and steric profiles, and displays exceptional chemoselectivity and functional group tolerance. The methodology was extended to isotopically labeled trans-deuteration and demonstrated excellent chemoselectivity in substrates containing multiple alkyne motifs. Mechanistic studies, including cyclic voltammetry, UV–vis spectroelectrochemistry, and DFT calculations, support a dual catalytic cycle involving electrochemical Co–H formation and a subsequent organometallic radical pathway.

Methodology and Catalysis in Organic Chemistry

Strategic DMA-Assisted EDA Complex Activation for Mild and Metal-Free C(sp²)–X Bond Functionalization

Ashutosh Mishra¹, Dr. Sakthi Raje¹, Priya Mata¹, Prof. Graham de Ruiter²

¹*Technion Israel institute of technology, Israel*

²*Schulich School of Chemistry, Technion Israel Institute of Technology, Israel*

Electron donor–acceptor (EDA) complexes have emerged as powerful platforms for visible-light-driven radical chemistry. Their ability to undergo direct photoexcitation provides an appealing alternative to traditional photocatalysis, especially for activating strong carbon–halogen bonds. Yet many EDA systems are hampered by fast charge recombination, which limits their synthetic utility. Developing donor–acceptor pairs that favor productive charge separation remains a central challenge in this field. Here we present a visible-light arylation of pyrroles that operates through photoactive EDA complexes formed between N,N-dimethylaniline (DMA) and electron-poor haloarenes. Unlike many conventional EDA systems that suffer from rapid back electron transfer, this design promotes efficient single electron transfer from DMA and generates aryl radicals from aryl chlorides, bromides, and iodides under irradiation at 450 nm. The method enables activation of typically inert C–Cl bonds and proceeds under mild, metal-free conditions while supporting a wide range of functional groups. Representative aryl bromides that contain cyano, keto, or ester substituents provide consistently high yields in the coupling with N-methylpyrrole. Mechanistic studies that include UV-Vis spectroscopy, NMR titration, and cyclic voltammetry confirm the formation of the DMA–haloarene complexes and clarify their photochemical behavior. Taken together, these results establish a general and practical approach for direct carbon–halogen bond activation through visible-light excitation of donor–acceptor assemblies. The findings broaden the synthetic scope of EDA chemistry and highlight its potential for scalable, catalyst-free arylation reactions.

Methodology and Catalysis in Organic Chemistry

Reactivity of Novel Manganese PC_{NHCP} Pincer Complexes in Nitrile Hydration and α -Deuteration of Amides Chemistry

Rohit Kamte¹

Chemistry, Technion Israel Institute of Technology, Haifa, Israel, Israel

Transition metal complexes that contain pincer-type ligands have played a central role in homogeneous catalysis for the past five decades. Many of these systems rely on precious metals such as rhodium, ruthenium, and iridium, which are among the scarcest elements on earth. Replacing them with earth-abundant metals is a significant challenge that requires new ligand designs capable of stabilizing a wider range of oxidation and spin states. In this work, we describe the design and synthesis of a family of Mn(I) PC_{NHCP} pincer complexes developed for new catalytic C–C and C–N bond-forming reactions. We focus in particular on the ability of Mn(I) PC_{NHCP} complexes to mediate the hydration of nitriles. Mechanistic studies combined with computational analysis allowed us to identify key catalytic intermediates and map the kinetic features of the reaction. These insights provided a clear picture of the catalytic cycle and enabled the optimization of reaction conditions based on mechanistic understanding rather than empirical screening. The same catalyst also gives access to deuterated amides through subsequent H/D exchange with D₂O, providing a straightforward route to isotopically labeled products. The full scope of this reactivity, together with detailed mechanistic findings, will be presented and discussed in this poster.

Methodology and Catalysis in Organic Chemistry

Uncovering a New Reaction Hidden within 130-Year-Old Knoevenagel Conditions

Alon Amir¹, dr Natalie Pariente-Cohen¹
Bar-ilan University, Israel

This work describes the discovery, scope, and mechanistic elucidation of a previously unrecognized reaction pathway that occurs in parallel with the classical Knoevenagel condensation. Under standard Knoevenagel conditions, we identified an unexpected two-carbon-shortening transformation proceeding through a tandem Michael Addition and Carbon Chain Shortening (MACCS) process, achieving C-C σ -bond cleavage under metal-free conditions. Our comprehensive investigation combines synthetic, analytical (HPLC, LC-MS, NMR), and computational (DFT) approaches to delineate the mechanism and define the parameters controlling selectivity between the classical Knoevenagel and the newly uncovered MACCS reactions. We demonstrate that the MACCS reaction proceeds under orbital control, in contrast to the charge-controlled nature of the Knoevenagel pathway, and that the reaction outcome is profoundly governed by temperature and the nature of the electrophile and nucleophile. This study not only exposes an unexpected reactivity mode within one of the oldest and most widely used condensation reactions but also provides a conceptual advance in metal-free C-C σ -bond activation. The MACCS reaction establishes a promising foundation for the development of new organocatalytic C-C bond cleavage methodologies, as a sustainable alternative to conventional metal-catalyzed protocols.

Methodology and Catalysis in Organic Chemistry

olefin metathesis in flow with cyclic(alkyl)(amino) carbene-based ruthenium precatalysts

Nadir Rosenblat¹, Prof. Gabriel Lemcoff¹
Chemistry, Ben-Gurion University of the Negev, Israel

In recent years, the field of flow chemistry has experienced growing interest in both research and industry due to its highly desirable advantages. Fast reaction times, minimal side-product formation, and ease of scale-up have all contributed to its appeal. Olefin metathesis, an important and widely used tool for synthesizing alkenes, has also been investigated under continuous-flow conditions with varying degrees of success. One significant obstacle to its implementation in flow is the stoichiometric generation of ethylene, a known deactivator of olefin metathesis catalysts. While under batch conditions the reactor headspace allows the gas to escape, the confined environment of a flow reactor creates high-interface gas–liquid zones that accelerate catalyst decomposition. To circumvent this problem, we studied cyclic(alkyl)(amino) carbene (CAAC)-based ruthenium precatalysts, known to be resistant to ethylene deactivation, in benchmark olefin metathesis reactions under continuous-flow conditions and compared their efficiency with N-heterocyclic carbene (NHC)-ligated counterparts. These findings may bring us closer toward the incorporation of olefin metathesis as a more viable method in flow reactors, further expanding the chemist's toolset for producing a wide range of useful compounds with high efficiency and with more environmentally benign methodologies.

Methodology and Catalysis in Organic Chemistry

Developing Earth Abundant Metal Complexes for Ammonia Oxidation

Akhanda Gorai¹, Prof. Graham De Ruiter¹
Chemistry, Technion, Israel

Electrocatalytic oxidation and reduction of small molecules via homogeneous catalysis is a vibrant research area that has attracted much attention in the last decade. Naturally available molecules such as N₂, NH₃, CO₂, H₂O undergo a variety of chemical transformations either using biological catalysts (e.g., enzymes) or transition metal catalysts based on 3d-, 4d- and 5d-metals. The advantage of using transition metal catalysts lies in our ability to precisely tune their electronic structure resulting in highly efficient chemical processes relevant for developing a sustainable future. One of these transformations involves the reduction of dinitrogen to ammonia (NRR) and the reverse reaction oxidation of ammonia (AOR). Several homogeneous catalysts have been developed that are either based on ruthenium and iron.

In herein presented research, we describe the design and synthesis of bespoke iron complexes that show promising activity for ammonia oxidation under mild conditions. The metal complexes are based on our unique dipyrrodo-annulated N-heterocyclic carbene (PA-NHC) ligands that provide a robust coordination environment (Figure 2), while at the same time enable facile electron transfer to and from the metal center. We will discuss the electrochemical and spectrochemical behavior of these iron metal complexes and how their electrochemical properties can be used for efficient ammonia oxidation led to formation of H₂ and N₂.

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Methodology and Catalysis in Organic Chemistry

Iron-catalyzed aryl-aryl Cross-Coupling reactions: a mechanistic and computational investigation Jatin Panda,^[a] Michael Neidig,^[b] and Graham de Ruiter*^[a]

Jatin Panda¹, Prof. Graham de Ruiter¹
Technion IIT, Israel

The use of precious metals as catalysts in pharmaceutical processes is widespread, but their toxicity and limited availability are incentives to replace these precious metals with less-toxic and readily available alternatives. By focusing on earth-abundant 3d-metals, we aim to overcome these challenges and develop more sustainable alternatives. For example, by finding earth-abundant metal alternatives for palladium catalyzed cross-coupling reactions one cannot only improve the sustainability of one of the most frequently used chemical transformations in synthetic organic chemistry, but also eliminate the need for the removal of toxic palladium down to the part-per-million level. While significant progress has been made in the field of iron-based cross-coupling, it still lags behind its precious metal counterpart, primarily due to a lack of mechanistic understanding.

To address these challenges, we propose a mechanism driven approach towards facilitating the iron-catalyzed Kumada aryl-aryl cross-coupling, which remains underdeveloped despite the prevalence of C(sp²)–C(sp²) bonds in organic synthesis. In the herein presented work, we resolve the lack of mechanistic understanding by using a combination of NMR and ⁵⁷Fe Mössbauer spectroscopy, GC analysis, single crystal X-ray crystallography, and reactivity studies of in situ formed iron-PCNHCP intermediates observed during catalysis. In our studies, indicate that despite PCP Fe(0) and PCP Fe(II) are able to undergo reliable two-electron chemistry, a novel radical mechanism is at play that results in efficient aryl-aryl cross-coupling. Moreover, our studies also indicate the important role of small coordinating molecules (e.g., N₂) on the mechanism of the reaction, which is further discussed in this report.

Methodology and Catalysis in Organic Chemistry

Promoting entropically disfavored reactions in solid phases

Shira Dukarker¹

chemistry, ben gurion university, israel

The synthesis of HG-EDPP and HG-TPP catalysts via coordination of a phosphorous moiety to a Ru-alkylidene catalyst was recently reported by our research group. Notably, coordination did not occur under typical solution-phase conditions, but was serendipitously discovered while the mixture was in the solid state.

Unlike traditional solution-phase reactions, where molecules can freely diffuse in a solvent, solid-state reactions take place under highly restricted conditions with limited molecular motion. These constraints present both challenges and opportunities, allowing for transformations that may be difficult or even impossible in solution. Our working hypothesis is that in some reactions where the change in entropy is disfavored, a positive ΔG may be obtained, preventing reaction progress even with a favorable change in enthalpy. However, the entropy component is less significant in the solid phase, thus reducing the entropic component in the free energy and allowing the reaction to proceed toward the products. This unusual discovery may open the door to “solid-phase synthesis”.

Our goal is to explore several entropically favored/disfavored reactions by taking advantage of the unique environment of the solid phase. We will focus on synthesizing triphenyl phosphite derivatives bearing either electron-donating/withdrawing substituents on meta or para positions.

These derivatives will then be reacted with the HG-2 catalyst in solid solvent promoting solid-state conditions as previously reported.

This study will allow us to determine how the electronic nature of the substituents on the triphenyl phosphite affects the efficiency of coordination under solid-state conditions, and possibly extend this idea to other spheres.

Methodology and Catalysis in Organic Chemistry

Proline-Promoted Electrophilic Dichloromethylation of α -Enaminones via Stereochemically Gated Resolution

Elihay Kuniavsky¹, Dvora R. Levy¹, Prof. Dmitry Tselikhovsky¹
Institute for Drug Research, The Hebrew University of Jerusalem, Israel

Electrophilic β -dichloromethylation of carbonyl derivatives has remained unexplored due to the presumed incompatibility of closed-shell reagents with electron-poor systems. Here we describe a proline-promoted transformation in which α -enaminones, under ambient and non-radical conditions, undergo selective β -dichloromethylation with anti-stereochemistry. The reaction proceeds without metals, strong bases, light, or carbene intermediates—conditions previously thought incompatible with such transformations. Mechanistic analysis reveals a stereochemically gated resolution: one diastereomeric intermediate selectively evolves toward the product, while the other is diverted and fragmented to the parent amine. This bifurcation, supported by kinetic profiling, isotopic labeling, and crystallographic analysis, defines a unique resolution-type control mode that channels molecular topology into chemical outcome. Control experiments confirm that the intact α -enaminone scaffold is essential—neither enamine nor enone fragments react independently. The resulting dichloromethylated enaminones feature a triad of orthogonal functional groups, positioning them as synthetically versatile building blocks. This study establishes a conceptually distinct reactivity paradigm for α -enaminones and expands the synthetic repertoire for the direct incorporation of halomethyl groups.

Methodology and Catalysis in Organic Chemistry

Bis(Pyridino-*o*-Carboranyl) Phosphenium: A Platform for Dual-Site Reactivity in Small-Molecule Activation

Shiv Kumar¹, Deependra Bawari¹, Dr. Roman Dobrovetsky¹

School of Chemistry, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Israel

Phosphenium, $[L_2P^+][B(C_6F_5)_4]$, substituted by two bis(pyridino-ortho-carboranyl) groups, was prepared, fully characterized, and its preliminary reactivity with small molecules was studied. Surprisingly, cation $[L_2P^+][B(C_6F_5)_4]$ reacts differently with O–H and N–H bonds. With RO–H (R = H, Me, Ph), the reaction takes place at P center in $[L_2P^+][B(C_6F_5)_4]$, via hydrolysis or alcoholysis of the P–C bonds, leading to the carboranopyridinium salt ($[LH_2^+][B(C_6F_5)_4]$) and the complementary $(RO)_2P(O)H$. In contrast, the reaction of $[L_2P^+][B(C_6F_5)_4]$ with R_2N-H (Ph(H)NH, *i*Pr(H)NH, Et₂NH) does not proceed at the P center, but takes place at the ortho-carboranyl (oCb) moiety by deboronation, producing zwitterionic phosphenium ($L(L_{nido})P^+$), with significant reduction in the reactivity of the P-center compared to L_2P^+ . Remarkably, $[L_2P^+][B(C_6F_5)_4]$ reacts with SO₂ in MeCN at both sites, the P and oCb, stripping both oxygens from sulfur, leading to zwitterionic phosphonium sulfide ($L(L_{nido})P^+=S$).

Methodology and Catalysis in Organic Chemistry

Exciton trapping with a twist

Israa Shioukhi¹, Prof. Ori Gidron¹

The Hebrew University of Jerusalem, Institute of Chemistry, Israel

In electron donor-acceptor (D-A) molecules, the relative orientation of the donor and acceptor units is a key factor in the dictation of the photophysical behavior. However, the influence of the molecular curvature of the conjugated molecules is largely unexplored. In this study, we investigate how twisting of the aromatic core in symmetric, double branched D- π -A molecules affects the nature and dynamics of the lower singlet excited state. Our results demonstrate a strong correlation between the degree of twisting in the central donor unit and the chiroptical properties and the triplet yield. Furthermore, twisting facilitates excited-state symmetry breaking (ESSB) enabling exciton trapping on single D- π -A branch. This enhancement is attributed to the decrease in the interbranch coupling upon distortion. As a result, a smaller gain in solvation energy is required for coupling upon ESSB, allowing exciton localization even in less polar solvents. Consequently, distortion can be viewed as an additional tuning knob for controlling the localisation of electronic excitation in large conjugated systems.

Methodology and Catalysis in Organic Chemistry

Alternating behavior in furan-acetylene macrocycles reveals the size-dependency of Hückel's rule in neutral molecules

Yuval Rahav¹, Shinaj K. Rajagopal¹, Or Dishi¹, Benny Bogoslavsky¹, Prof. Ori
Gidron¹

Chemistry, The Hebrew University of Jerusalem, Israel

Hückel's rule predicts that planar rings with delocalized $(4n+2)$ π -electrons are aromatic, whereas those with $4n$ π -electrons are antiaromatic. However, global aromaticity is commonly observed in charged macrocycles, but rarely in their neutral state. For that reason, the maximal value of "n" to which Hückel's rule applies remains unknown.¹ Therefore, the significance and size dependency of global effects remains an open question with respect to neutral macrocycles.² A series of furan-acetylene macrocycles were synthesized, ranging from the pentamer to octamer, whose neutral states display alternating contributions from global aromatic and antiaromatic ring currents. We find that the odd-membered macrocycles display global aromatic characteristics, whereas the even-membered macrocycles display contributions from globally antiaromatic ring current. These factors are expressed geometrically (X-ray structures), electronically (oxidation potentials), optically (emission spectra), and magnetically (chemical shifts). The global characteristics are more pronounced for small macrocycles and are attenuated for larger members. Overall, the current work establishes furan-acetylene macrocycles as shape-persistent models for the study of global aromaticity.³

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Methodology and Catalysis in Organic Chemistry

Changing P to Its Big Brother Sb

Donia Toami¹, Dr. Deependra Bawari¹, Prof. Roman Dobrovetsky¹
Tel-Aviv University, Israel

Geometrical constriction of main group elements leading to a change in the reactivity of these main group centers has recently become an important tool in the main-group chemistry. A lot of focus on using this modern method is dedicated to group 15 elements and especially to phosphorus.

In this poster, our group's recent progress in the field of geometrically constrained pnictogenium (P, Sb) cations. Their synthesis, structure and chemistry with small molecules is discussed. Furthermore, the ability of these novel geometrically constrained cations to activate Si-H, Si-C and H-H bonds by an oxidative addition type reaction to the pnictogenium (P, Sb) center and their use in catalysis are shown.

Methodology and Catalysis in Organic Chemistry

Substituent Effects on Carborane Reactivity with CAAC

Nardeen Safadi¹, Prof. Roman Dobrovetsky¹, Dr. Vladimir Kampel¹
School of Chemistry - Exact Science, Tel Aviv University, Israel

ABSTRACT: The functionalization of carboranes, particularly at boron atoms, is a topic of extensive research. Here, we report the reactivity of ortho-carboranes (oCb) with cyclic (alkyl)(amino)carbene (CAAC) - a transformation that, surprisingly, has not been previously reported. We found that the substitution at the carbon atoms of the oCb strongly influences the reaction outcome. Unsubstituted oCb (H at carbon) reacts with CAAC via carbene insertion into the C-H bond. However, when the carbon atoms of the oCb are substituted, the reaction is dictated by the electronic nature of these substituents: electron-withdrawing groups (EWG) promote the formation of the nido-type products via the nucleophilic attack by CAAC at B3 (or B6) position, whereas electron-donating groups (EDG) favor insertion of CAAC into the B-H bonds at these positions. The explanation of this reactivity pattern, along with the proposed mechanism of these processes, is supported experimentally and by density functional theory (DFT) computations.

Methodology and Catalysis in Organic Chemistry

Green Chemistry with Pincer Catalysts: It all Begins with Dehydrogenation

Dr. Jie Luo¹, Dr. Lijun Lu¹, Dr. Shan Tang¹, Dr. Michael Rauch¹, Dr. Cai You¹, Dr. Sayan Kar¹, Dr. Quan-Quan Zhou¹, Yehoshua Ben-David¹, Dr. Yael Diskin-Posner²,
Michael Montag¹, Prof. David Milstein¹

¹*Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Chemical Research Support, Weizmann Institute of Science, Israel*

Traditional chemical processes often involve corrosive or toxic reagents, and generate byproducts that are discarded as chemical waste, which can itself be harmful. Although such processes are common and useful, they are inherently hazardous and inefficient, and when applied on a large scale in the chemical industry, can endanger both human health and the environment. Therefore, there is great current interest in developing “green” chemical reactions, i.e., environmentally-benign processes that maximize efficiency, while minimizing the use of toxic reagents and waste production. Over the past two decades, our group has introduced numerous pincer-ligated transition-metal-based homogenous catalysts, primarily those of ruthenium, manganese, iron and cobalt, which promote a host of industrially-important organic transformations. Many of these catalytic reactions utilize simple starting materials like alcohols, amines and water to generate the desired organic products, while avoiding noxious reagents and emitting H₂ as the only byproduct. The common catalytic motif of these systems is acceptorless dehydrogenation of the substrates to afford unsaturated reactive intermediates like aldehydes and imines, which react further to form the target products. Herein, we will explore recent examples of ruthenium- and manganese-catalyzed reactions that involve acceptorless dehydrogenation as an entryway to cleaner, more efficient methodologies for organic synthesis and hydrogen storage.

Methodology and Catalysis in Organic Chemistry

Sequential Coupling of Arenes and Aldehydes for the Synthesis of Unsymmetrical (Deuterated) 1,1-Diarylethylenes

Nicole Hanania¹, Amit Garti¹, Prof. Ahmad Masarwa¹

Institute of Chemistry, The Center for Nanoscience and Nanotechnology, and Casali Center for Applied Chemistry, Hebrew University of Jerusalem, Jerusalem, 9190401, (Israel)

Unsymmetrical (deuterated) 1,1-diarylethylenes are important scaffolds in synthesis, materials science, and medicinal chemistry, yet efficient and broadly applicable routes to access them remains challenging.^{1–3} Here, we present a programmable two-step platform based on readily available benzhydryl triarylphosphonium salts.^{4,5} The sequence involves regioselective formation of phosphonium salts from arenes and aldehydes, followed by a chemoselective Wittig-type olefination with (deuterated) formaldehyde, affording (deuterated) 1,1-diarylethylenes in good yields with high isotopic incorporation. Overall, the method offers a straightforward, practical, highly selective, and broadly applicable route to valuable (deuterated) diarylethylene frameworks from simple molecular building blocks.

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Methodology and Catalysis in Organic Chemistry

Bismetallated Cyclopropanes en-route to Fused Rings: Synthesis of Polysubstituted Housanes

Noam Orbach¹, Prof. Ilan Marek¹
Chemistry, Technion, Israel

In recent years the synthesis and ring opening of strain fused rings has emerged as a powerful tool for the construction of sp³-rich molecular backbones. Bicyclo[2.1.0]pentanes, known as housanes, have received little attention and currently there are limited number of methods to access them. Previously our group have developed the synthesis of spiro and fused rings through a carbometallation of cyclopropenes followed by a cyclization event. Applying this methodology for the synthesis of housanes would deliver the metal and the leaving group in an anti-relationship, preventing the cyclization step. Hence, we envisioned an alternative strategy utilizing gem-bismetallated cyclopropanes, where one of the metals would be syn to the leaving group. The bismetallated intermediates can be prepared through the well-established allyl zincation reaction by the addition of allylmagnesium bromide and zinc bromide to metallated cyclopropene. A subsequent cyclization provides metallated housanes that can be further functionalized by electrophile trapping or cross coupling reactions. This transformation allows the synthesis of polysubstituted housanes in a one-pot operation starting from cyclopropenes with high control over stereochemistry.

Methodology and Catalysis in Organic Chemistry

Metallo-Claisen Rearrangement a unique strategy for polysubstituted strained rings

Gautam Kumar Singh¹

Schulich faculty of chemistry, Technion, Israel

One challenging scaffold that has received less attention is bicyclo[2.1.0]pentanes, also known as housanes. We propose a unique strategy utilizing Gaudemar/Normant (G/N) coupling (metallo-Claisen rearrangement) to efficiently synthesize polysubstituted housanes and derivatives.

Gaudemar/Normant (G/N) coupling involves the formation of gem-bismetallated species by the addition of allylzinc bromide with vinyl or alkynyl organometallic species. The reaction proceeds through [3,3]-sigmatropic rearrangement known as metallo-Claisen rearrangement. The bismetallated species can be selectively functionalized in various transformations, such as Negishi cross-coupling and oxidation, to furnish versatile molecular frameworks.

We envisage to perform G/N Coupling on appropriately substituted cyclobutene to generate bismetallated cyclobutanes which undergo intramolecular nucleophilic substitution, providing polysubstituted housanes (Scheme 2). This method would not only provide non-trivial functionalization of cyclobutene but also direct method for housanes and other fused rings.

Methodology and Catalysis in Organic Chemistry

Nonclassical Carbocation-Mediated Access to Acyclic fragments via Stereoselective Rearrangements of Polysubstituted Cyclobutanes

Sayan Shee¹, Prof. Ilan Marek¹

Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Israel

Our goal is to develop stereoselective rearrangements of stereodefined cyclobutanes into acyclic products. We propose that a suitably polysubstituted cyclobutyl cation is most accurately represented by the corresponding cyclopropyl carbinyl cation (CPC). The latter is expected to undergo nucleophilic attack at the most substituted carbon center, furnishing. In the proposed strategy, the key challenge will be achieving a selective single bond migration to achieve a particular cyclobutyl cation. A competing elimination pathway leading to cyclobutene formation may also occur, and this pathway should be minimized. This transformation is synthetically appealing, as it enables nucleophilic addition to a four-membered ring, affording acyclic product with adjacent stereocenters in a single step and with complete selectivity control. A preliminary experiment shows that cyclobutanol provides homoallyl product in excellent yield and diastereoselectivity, presumably through the formation of CPC. Notably, the stereochemistry of the alcohol center of **1a** did not affect the reaction outcome, as this center is likely to become first a planar carbocation. A systematic investigation of the substrate scope will be undertaken to elucidate the parameters governing the stereochemical outcome of the C–C bond migration and its subsequent reactivity with nucleophiles.

Methodology and Catalysis in Organic Chemistry

Stereoinvertive Nucleophilic Substitution at Quaternary Stereocenters Enabled by Alkyne-Induced Cycloprolidene cation Rearrangement.

Rajan Kharwar¹

Chemistry, Technion – Israel Institute of Technology, Israel

Nucleophilic substitution reactions typically proceed through SN2 or SN1 pathways, leading to inversion or racemization of configuration, respectively. Achieving stereocontrol in SN1 reactions, particularly at tertiary centers, remains a major challenge. π -Participation offers a powerful solution by stabilizing developing carbocations and enforcing defined reaction trajectories. In homoallylic systems, neighboring π -bonds generate non-classical cyclopropylcarbinyl (CPC) cations that enable stereocontrolled substitution and skeletal rearrangement. Here, we report a stereoinvertive nucleophilic substitution of homopropargylic alcohols via an sp^2 -cyclopropylcarbinyl carbocation intermediate. Stabilization of this non-classical cation suppresses racemization and enables precise stereochemical control, expanding the synthetic utility of SN1-type mechanisms in complex molecule synthesis.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



NANOSCIENCE AND NANOTECHNOLOGY

Chair: Fernando Patolsky

Invited Lecture

Nanoscience and Nanotechnology

Excitons and multiexcitons in quantum dot molecules

Einav Scharf¹, Adar Levi¹, Rotem Liran¹, Prof. Dan Oron², **Uri Banin**¹

¹*Institute of Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel*

²*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

Colloidal semiconductor Quantum Dots (QDs), often considered as artificial atoms, have reached an exquisite level of control, alongside gaining fundamental understanding of their size, composition and surface-controlled properties, as recognized by the Nobel prize in Chemistry 2023. Their tuned characteristics and scalable bottom-up synthesis accompanied by the applicability of solution-based manipulations, have led to their wide implementation in displays, lasers, light emitting diodes, single photon sources, photodetectors and more.

For the next step towards enhancing functionalities of quantum dots, inspired by molecular chemistry, we introduce the controlled linking and fusion of two core/shell quantum dots creating an artificial molecule manifesting two coupled emitting centers. Accordingly, the coupled colloidal quantum dot molecules (CQDMs) present novel behaviors differing than their quantum dot building blocks. Utilizing single particle spectroscopy, especially a version of heralded spectroscopy, we distinguish between localized versus segregated multiexciton states.

Moreover, we have recently developed a new method to study multiexcitons in QD ensembles utilizing spectrally resolved time-gated heralded spectroscopy. With this approach we extract the biexciton binding energies and resolve energetics and dynamics of higher order multiexciton states. The approach can be further implemented in the characterization of the energies and lifetimes of multiexcitons in other QD systems to enable rapid characterization and understanding.

Invited Lecture

Nanoscience and Nanotechnology

Capacitance-based carbon dot photodetector

Raz Jelinek¹

bgu, israel

We developed and implemented an innovative optical sensing technology based on capacitance modulation induced by carbon dots (carbon nanoparticles) prepared from different molecular dyes, interspersed with a conjugated polymer. Interestingly, light absorbed by the carbon dots gives rise to electron excitation, with the excited electrons transiently migrating to the conjugated polymer network, thereby affecting significant capacitance changes. The new technology demonstrates sensitivity to wavelength in a broad spectral range, dependence upon light intensity and polarization, and constructed from simple and cost-effective organic materials. The technology may be implemented in optical encoding, imaging, diagnostics, and other applications.

Nanoscience and Nanotechnology

Enantioselective Guided Growth of Chiral Nanowires

Ernesto Joselevich¹, Noya Ruth Itzhak¹
Weizmann Institute of Science, Israel

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 heterostructures 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 studied the growth mechanism of the nanowires by advanced *in situ* electron microscopy, revealing how the nanowires nucleate and grow in real-time, 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. Our findings demonstrate the potential of enantioselective heterostructures for advanced optoelectronics and future spintronic devices.

Invited Lecture

Nanoscience and Nanotechnology

Seeing Depth in Color: Optical Encoding of Nanometric Axial Distances

Adi Salmon¹

chemistry, Bar Ilan University, ישראל

Molecular dipoles located near interfaces encode rich quantitative information about their nano-environment through their emission patterns. In particular, the refractive index of the surrounding medium and the axial distance of the emitter from the surface are imprinted in the angular and spectral distribution of the emitted light. Here, we introduce an optical strategy that translates nanometric axial distances into distinct optical colors, directly observable under a conventional optical microscope. By combining dipole-interface coupling with our newly developed full-color nano beads emitters, axial positions on the nanometer scale can be read out in a simple manner, without mechanical scanning or interferometry. This approach provides a visually accessible route to axial nanometrology at interfaces, with broad relevance to surface chemistry, soft matter, and biological imaging.

Invited Lecture

Nanoscience and Nanotechnology

Rewriting the Rules of 3D Tumor-Host Interactions with Precision Nanomedicine

Ronit Satchi-Fainaro¹

Physiology & Pharmacology, Tel Aviv University, Israel

Many drugs show promising results in laboratory research but eventually fail to show clinical benefit. One main reason for this translational gap is that the cancer models used are inadequate. Most models lack the complex interactions between tumor-stromal-immune cells and their tumor microenvironment (TME) that are required for progression. Conventional 2D models, where cells grow on rigid plastic plates mainly as mono-cultures, fail to recapitulate these complex interactions. Hence, we developed a vascularized, hydrogel-based 3D-bioprinted tumor model containing patient-derived cells. Our 3D models are based on our library of hydrogels as scaffolds for various tumor types, tailored to the mechanical properties of the tissue of origin, which dictate the proteo-genomic signature and, consequently, the response to different therapies. Using these unique high-throughput 3D models, we are currently validating their ability to mimic patient-specific tumors and TME to serve as a tool for predicting patient response to different treatments. To determine which therapies to test on our 3D platforms, we consider cancer-specific standard-of-care therapies, investigational therapies developed in our lab, and therapies proposed by an AI-based algorithm that uses H&E slides to generate individual drug response scores for targeted and immune therapies. To validate our models' ability to predict patient responses, we are currently conducting an 80-patient clinical trial at Sheba Medical Center, testing different treatments across 7 distinct cancer types. These unique 3D models have the potential to facilitate target discovery and drug development, as well as to serve as a reliable system for precision medicine.

Nanoscience and Nanotechnology

Smart Drug Release Platform for Facile In Vitro Testing of Therapeutic Effects

Mai Rose Malovany¹, Prof. Roy Shenhar¹, Prof. Meital Reches¹, Wade She², Dr. Mo-Yuan Shen², Prof. Hsiao-Hua (Bruce) Yu²

¹*Hebrew University of Jerusalem, Israel*

²*Academia Sinica, Taiwan*

Approving a new drug requires approximately 5 years as part of a total of 20 years of development because of the need to develop special formulations during the initial phase of drug discovery. Our research aims to create a new platform that will eliminate the need for these formulations and thus considerably shorten the time necessary to discover and develop new drug leads.

The platform, which we term ‘DrugBurst’, is composed of several layers that enable the on-demand release of incorporated drugs. The first layer is a block copolymer film serving as a nanopatterned template. Alternating deposition of biocompatible polycations, electroactive polyanions, and drug molecules furnishes polyelectrolyte multilayers which incorporate the drug. Applying a low voltage causes the disassembly of the multilayers, which releases the drug in a burst. Preliminary results of applying this approach to cells adsorbed onto the platform demonstrate highly efficient uptake, which enables testing the therapeutic effect of the drug on the cell without the need to develop special formulations.

This study focuses on expanding the utility of the DrugBurst platform to different drugs and testing them using different target cells. We aim to demonstrate the generality of our approach to anti-cancer, anti-inflammatory, and anti-bacterial drugs.

Nanoscience and Nanotechnology

Development of Hydroxyapatite-Loaded TiO₂ Nanotubes on CP-Ti for Improved Osseointegration

Elinor Zadkani Nahum^{1,2}, Dr Alexander Sobolev², Dr Svetlana Lugovskoy², Prof Alex Lugovskoy²

¹*Materials Engineering, Azrieli College of Engineering, Israel*

²*Chemical Engineering, Ariel University, Israel*

The demand for improved biomedical implant materials has increased significantly in recent years, leading to extensive research on surface modification methods that enhance biological performance. One of the key challenges in implant technology is achieving strong and stable integration between the implant surface and surrounding bone tissue. To address this, many studies focus on creating bioactive coatings capable of promoting hydroxyapatite (HAP) formation, as HAP is the main mineral responsible for bone attachment.

Commercially pure titanium (CP-Ti) is widely used in medical applications due to its mechanical reliability and excellent biocompatibility. However, its natural surface does not always provide optimal conditions for rapid osseointegration, making surface engineering essential. In this study, CP-Ti was modified through anodization to form highly ordered TiO₂ nanotubes, followed by heat treatment to stabilize the structure. These nanotubes were subsequently exposed to calcium-containing solutions and immersed in Hanks' balanced salt solution to encourage hydroxyapatite incorporation and growth.

A range of analytical techniques-including XRD, SEM, EDS, electrochemical measurements, and contact-angle analysis, were employed to characterize the coatings and assess their structural, chemical, and surface properties. The results confirm that the anodization process successfully produces a nanotubular oxide layer that supports hydroxyapatite formation while also improving surface wettability and corrosion resistance.

Overall, the findings highlight that combining anodization with controlled chemical treatments offers an effective and straightforward approach for producing bioactive coatings on CP-Ti. This method enhances the material's potential for successful integration within biological environments and contributes to the development of improved titanium-based implants.

Nanoscience and Nanotechnology

Near-infrared Optical Sensors Based on Carbon Nanoparticles

Yogev David Yehezkel¹, Dr Nitzan Shauloff¹, Prof Raz Jelinek¹
Chemistry, Ben-Gurion University of the Negev, Israel

Carbon dots (CDs) are versatile nanomaterials known for their adjustable optical properties, high photostability, and excellent biocompatibility, making them promising options for optical sensing and photonics applications. However, their limited response in the near-infrared (NIR) region restricts their use in technologies that rely on efficient NIR detection, such as biomedical imaging and advanced optoelectronic devices. This work presents a strategy to develop NIR-responsive carbon dots by combining them with cyanine dyes—organic chromophores recognized for strong absorption in the NIR range. Two complementary synthesis methods were employed: (i) incorporating the dye during precursor carbonization and (ii) electrostatically binding oppositely charged CDs and dye molecules. Spectroscopic analysis confirmed the successful formation of the hybrid, exhibiting increased and extended absorption between 750 and 850 nm, which indicates effective dye–carbon interactions. The hybrid cyanine–carbon dots were embedded in a polydiacetylene (PDA) polymer matrix and deposited on interdigitated electrodes to create a novel capacitive NIR photodetector. Under NIR illumination, the device exhibited rapid, reversible changes in capacitance with response times under a second, demonstrating efficient photoinduced charge transfer between the hybrid nanoparticles and the polymer network. The capacitance returned to baseline immediately after illumination stopped, indicating excellent stability and reproducibility. These results establish a new platform for light-responsive, carbon-based sensing materials that convert optical signals into measurable electronic outputs. Combining the structural and optical advantages of carbon dots with the strong NIR absorption of cyanine dyes, this approach offers a simple, cost-effective, and environmentally friendly pathway to next-generation NIR photodetectors and biocompatible optical sensors.

Nanoscience and Nanotechnology

Upcycling of Expired Amoxicillin into Dual-Function Fluorescent Sensors

Jiawei Liu¹, Prof. Mindy Levine¹

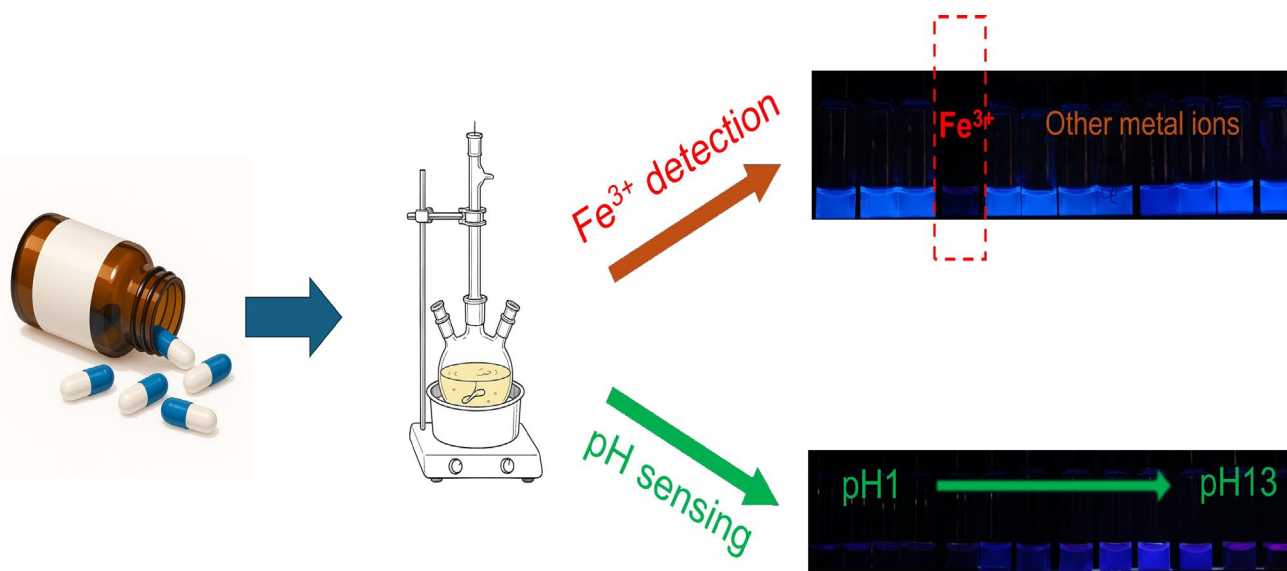
The Department of Chemical Sciences, Ariel University, Israel

The global accumulation and improper disposal of expired pharmaceuticals constitute a significant environmental and public health challenge, as up to 40% of prescribed drugs remain unused and ultimately enter ecosystems.^[1] Antibiotics in particular present significant hazards due to their disruption of microbial communities and their contribution to antimicrobial resistance.^[2] Developing strategies that transform expired pharmaceuticals into functional materials therefore represents a valuable approach to reducing pharmaceutical waste while enabling continued value.^[3]

A widely explored approach for repurposing pharmaceuticals involves high-temperature carbonization to generate carbon-based materials; however, this approach is energy-intensive and destroys key functional groups.^[4] In contrast, we report herein a mild upcycling strategy that converts expired amoxicillin into a transformation-derived fluorophore without carbonization.

The resulting fluorophore functions as a dual-mode sensor. It enables highly selective “turn-off” fluorescence detection of Fe³⁺ ions, demonstrating strong emission quenching and sensitivity in organic media. It also serves as a reversible pH sensor, with fluorescence enhancement under alkaline conditions suitable for monitoring wastewater.

This dual functionality—Fe³⁺ detection and reversible pH sensing—demonstrates a sustainable route for upcycling expired antibiotics into functional molecular architectures. The accessible synthesis and tunable photophysical properties of the resulting fluorophore highlight the broader potential of molecular upcycling as a platform for creating new sensing agents from pharmaceutical waste.



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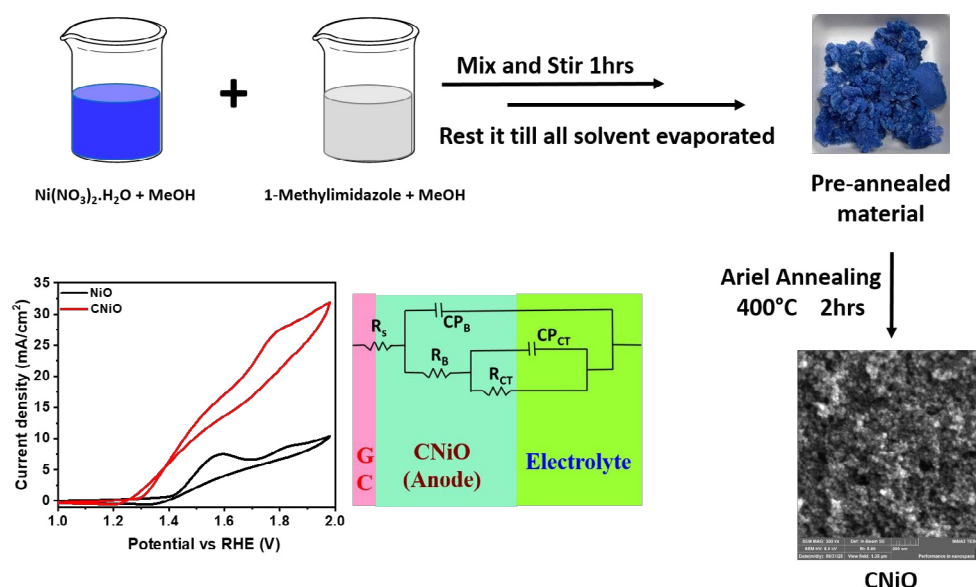
Nanoscience and Nanotechnology

NiO nanoparticles embedded on conductive carbon material as an efficient electrocatalyst for enhancing the urea oxidation reaction.

Devendra Sanke¹, Prof. Tomer Zidki¹
Chemical sciences, Ariel University, Israel

Waste water treatment and energy production are important fields of research to meet the current requirements of sustainable energy development and wastewater restoration.¹ Urea oxidation reaction (UOR) can be used for simultaneous environmental remediation and energy production on a priority basis. Nickel oxide (NiO) nanoparticles on conductive carbon material (CNiO) have been synthesized as an electrocatalyst by using a simple and easy aerial annealing method. Morphological analysis by Field Emission Scanning Electron Microscopy (FESEM) confirms the formation of CNiO. The electrochemical studies of CNiO nanocomposite reveal that it has better electrochemical activity and low onset potential with an $E_{onset} = 1.3$ V vs RHE and current density of 30 mA/cm² for a potential of 2.0 V vs RHE towards urea oxidation reactions. In urea oxidation studies, chronoamperometry (i-t) '95fwsz' and EIS analysis show that the proposed CNiO system has long-term stability and ultrafast electron transfer. This work showed a simple way for catalyst synthesis with enhanced electrochemical activity for urea oxidation, which is useful for sustainable energy production utilizing urea-rich wastewater.

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Nanoscience and Nanotechnology

Functional Assembly of Polycyclic Aromatic Hydrocarbons in Prebiotic Membranes

Yael Kapon¹, Dr Moran Frenkel-Pinter¹

Institute of Chemistry, the Hebrew University of Jerusalem, Israel

The transformation of matter into life required not only the availability of molecular building blocks but also their organization into protocells capable of compartmentalization and functions such as energy transduction(1). Simple amphiphiles capable of forming primitive membranes were likely present on early Earth(2,3) and in carbonaceous meteorites(4); yet key membrane functions in modern biology, such as light harvesting and electron transfer, are enabled by complex proteins that were unavailable in prebiotic systems.

Here, we explore an alternative, enzyme-free route to membrane functionality based on polycyclic aromatic hydrocarbons (PAHs), a class of molecules abundant in meteorites(4) and interstellar environments(5). PAHs possess extended π -conjugated systems that drive strong self-assembly into ordered, stacked structures, an ability widely exploited in synthetic materials chemistry but largely unexplored in prebiotic contexts.

We investigate the co-assembly of various environmentally available PAHs with simple lipids under aqueous, prebiotically relevant conditions. A conceptual framework (Figure A) illustrates how PAHs from the prebiotic inventory could embed within early membranes and form energy-active domains. Experimentally, we demonstrate the incorporation of PAH into decanoic acid–decanol vesicles (Figure B inset) and observe excimer emission in the fluorescence spectra, indicating dense molecular packing and ordered assembly within the membrane (Figure B). These results suggest that PAH–lipid co-assemblies could have endowed early membranes with primitive photo-active and charge-transport functionalities essential for protocell evolution.

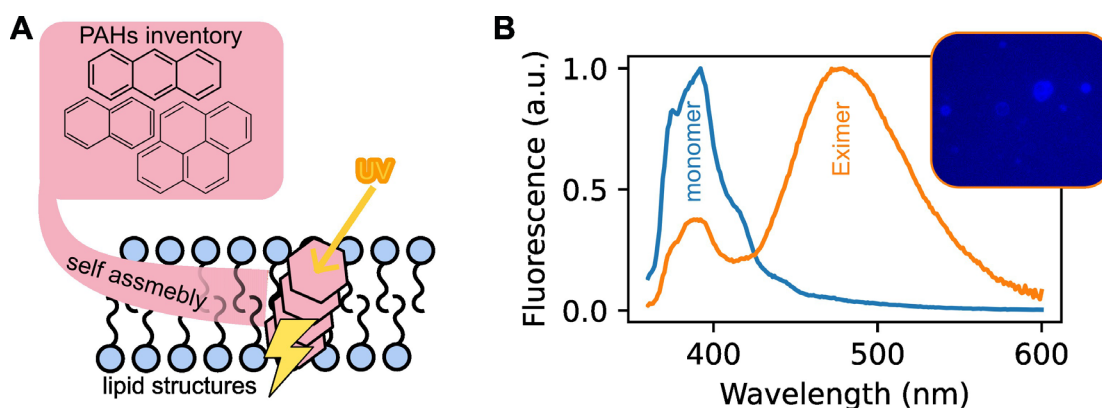
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Nanoscience and Nanotechnology

Tomo4D: 4D_STEM tomographic reconstruction

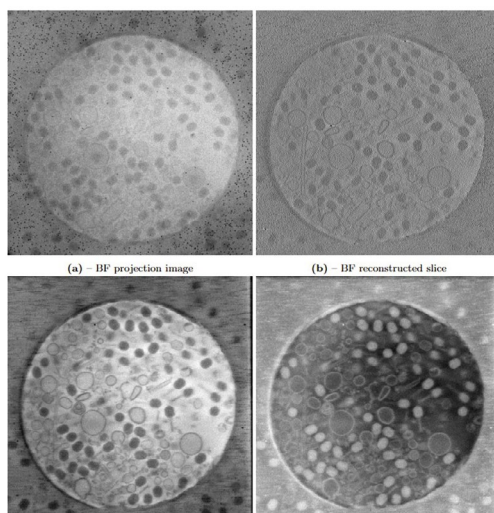
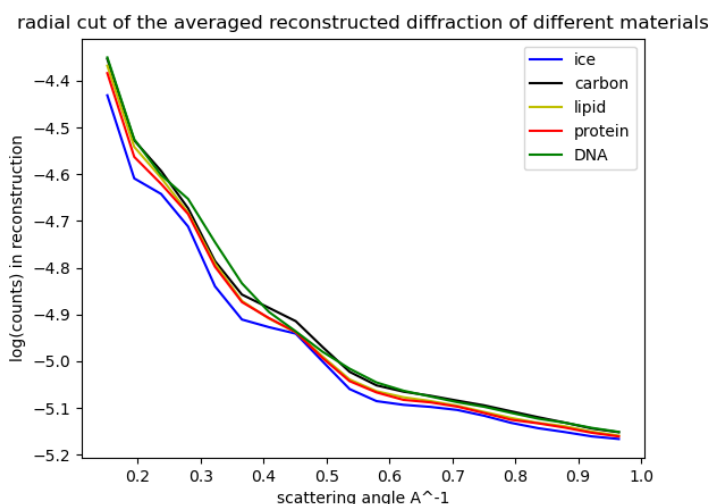
Shai Kiriati¹, Dr. Jose Jesus Fernandez², Prof. Michael Elbaum¹

¹Weizmann Institute of Science, Israel

²CSIS, Spain

4D-STEM records a 2D electron diffraction pattern using a pixelated electron detector, while scanning the electron probe in 2D across the specimen. Thus it captures the full diffraction pattern from each scan location. This technology has demonstrated uses in enhancing STEM image quality (Seifer, Elbaum 2024, Varnevides 2024) and has the potential to be used for quantitative analysis of the sample composition (Seifer, Houben 2024). 4D-STEM has further been adapted in our lab for cryo-tomography of biological specimens (Seifer, Elbaum 2024). However, conventional tomographic reconstruction addresses only a single measured intensity rather than a 2D array.

We have developed the Tomo4D pipeline to reconstruct a 2D diffraction pattern for each voxel (x,y,z) in the scanned sample. This provides depth resolution within the projected diffraction patterns. We demonstrate Tomo4D on a T4 Bacteriophage sample containing in addition gold nanoparticles for alignment, showing reconstructed diffraction patterns of both the disordered materials of the sample and the crystalline gold nanoparticles.



Nanoscience and Nanotechnology

Networking with a fluoro-iodo ligand and divalent zinc: metal coordination, hydrogen and halogen bonding

Elad Gaver¹, Christoph J. Vonnemann², Julian Stoesser², Linda J. W. Shimon³, Prof. Stefan M. Huber², Michal Lahav¹, Prof. Milko E. van der Boom¹

¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Organische Chemie II, Ruhr-Universität Bochum, Germany*

³*Department of Chemical Research Support, Weizmann Institute of Science, Israel*

Halogen-functionalized ligands offer opportunities for structural diversity in crystalline materials. Here, we report the synthesis and characterization of three distinct crystalline systems derived from a ligand with two carboxyl groups bearing both iodine and fluorine substituents - a combination rarely used for the formation 3D crystals such as metal-organic frameworks (MOFs). By varying crystallization conditions, the ligand assembles with bivalent zinc cations into: (i) a metal-containing hydrogen-bonded organic framework; (ii) a metal-organic framework; and (iii) one-dimensional metal-organic chains, in which coordination bonds are propagated via intermolecular halogen bonding (XB) and hydrogen bonding (HB) between adjacent chains. The latter crystals (iii) were obtained by using carbon disulfide as the crystallization medium. These results highlight the role of non-covalent interactions and halogen chemistry in directing crystal packing and connectivity. Our findings underscore the potential of uncommon solvent control in the design of structurally diverse crystalline materials formed from different supramolecular interactions.

Nanoscience and Nanotechnology

Cystamine-functionalized gold nanoparticles for high selectivity sensing of arsenic in water

Ayala Dredzen¹, Ms. Jenisha John Peter¹, Prof. Mindy Levine¹

Department of Chemical Sciences, Ariel University, Israel

Arsenic contamination remains a critical global health challenge, particularly in regions such as Bangladesh, Bengal, and parts of the United States. While numerous highly sensitive detection methods exist, such methods rely on expensive instrumentation and trained personnel, thus limiting their suitability for environmental monitoring. To provide a more practical alternative, this study developed a colorimetric arsenic sensor based on cystamine-functionalized gold nanoparticles (AuNPs). Cystamine introduces amine groups that modulate the nanoparticle surface charge under alkaline conditions and enable electrostatic interactions with arsenic species, promoting aggregation and a red-to-purple color change.

Cystamine-coated AuNPs were synthesized using a gold:cystamine ratio of 1:0.25 and characterized using UV-visible spectrometry, dynamic light scattering, zeta potential analysis, SEM and EDX. The exposure of the cystamine-AuNPs to increasing concentration of arsenite (As^{3+}) induced nanoparticle aggregation, a red-to-purple color transition, and red shifts in the plasmon absorption band, enabling a solution-state detection limit of 0.02 ppm. The sensor displayed high selectivity for arsenic, showing only weak responses to arsenate (As^{5+}) and negligible responses to other metal ions. Incorporation of the sensor into polyvinylidene fluoride (PVDF) membranes preserved its high selectivity in a solid-state format, providing a practical detection limit of 9 ppm.

The sensor produced accurate responses in tap and bottled water samples spiked with As^{3+} , highlighting its suitability for real-world analyses. Overall, this work presents a portable, selective, and operationally simple platform for arsenic detection with strong potential for field deployment.

Nanoscience and Nanotechnology

Repurposing expired omeprazole for the development of a cost-effective paper-based sensor for mercury(II) detection

Sharanya M. Karyadath¹, Ms. Ayala Dredzen¹, Mr. Jiawei Liu¹, Prof. Mindy Levine¹

Chemistry, Ariel University, Israel

Mercury contamination in drinking water poses a serious threat to human health and the environment due to its high toxicity and bioaccumulative nature. Industrial activities, improper waste management, and environmental release of mercury compounds are major sources of this contamination. In parallel, the improper disposal of expired pharmaceuticals generates chemical waste that further exacerbates environmental pollution.

In this study, we present a sustainable strategy that addresses both challenges by repurposing expired omeprazole, a widely used gastroenterological drug, for the colorimetric detection of mercury(II) ions. Silver nanoparticles (AgNPs) functionalized with omeprazole were synthesized and employed as an efficient sensing platform. Upon exposure to Hg^{2+} ions, the sensor exhibited a distinct color change from yellow to colorless. The system was further integrated into a paper-based format, and was used for effective detection of Hg^{2+} in spiked real-world samples, demonstrating both its analytical robustness and its potential as a practical, sustainable solution for environmental monitoring through pharmaceutical upcycling.

Nanoscience and Nanotechnology

From Centro-Symmetric Racemic Organic Crystals to Pyroelectric and Ferrielectric Analogues

Shir Abrahams Ben Harush¹, Prof. Igor Lubomirsky¹, Prof. Meir Lahav¹, Dr. David Ehre¹, Dr. Shiri Dishon Ben Ami¹, Noor Abo-Ahmad², Shaked Ezra-Brandwein³, Michal Hartstein⁴, Dr. Anna Eden Kossoy⁵, Dr. Linda J W Shimon⁵, Sergey Khodorov⁴, Dr. Isabelle Weissbuch⁴, Prof. Leeor Kronik⁴, Prof. Omer Yaffe³, Dr. Yonatan Calahorra², Prof. Michal Leskes⁴, Nitzan Livni⁴

¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Department of Materials Science and Engineering, Technion, Israel*

³*Department of Chemical & Biological Physics, Weizmann Institute of Science, Israel*

⁴*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

⁵*Department of Chemical Research Support, Weizmann Institute of Science, Weizmann Institute of Science*

Understanding how macroscopic material properties arise from microscopic structures remains a central challenge in materials science. Particularly for organic functional materials, whose unique properties are often difficult to achieve in their inorganic counterparts. Crystal symmetry governs many material properties: only 10 out of the 32 crystal classes are polar and thus expected to exhibit pyroelectric and piezoelectric behaviour. Among these, only a few are ferroelectric/ferrielectric. Here, we present a symmetry-reduction strategy that transforms enantiopolar centrosymmetric racemic crystals into polar quasi-racemic (PQR) structures through the selective modification of one enantiomer.

Following this approach a de novo PQR crystal designed, which exhibits ferrielectricity, with spontaneous polarization- P_s of $1 - 3 \cdot 10^{-9} \text{ C/cm}^2$

, remanent polarization- P_r of $0.2 - 1.4 \cdot 10^{-9} \text{ C/cm}^2$

and a low coercive field- E_c of $\sim 200 \text{ V/cm}$. This

crystal shows unexpected very enhanced pyroelectricity, ($4.3 \cdot 10^{-9} \text{ C/Kcm}^2$) leveling that of LiNbO_3 ($5 \cdot 10^{-9} \text{ C/Kcm}^2$) but minimal piezoelectricity. The new synthetic method and the unique properties in contrast to the racemic crystal will be describe in detail.

Nanoscience and Nanotechnology

The sol-gel metal-oxide skeleton affects the catalytic properties of in-situ formed metal nanoparticles

Kavya Vidyadharan¹, Dr. Yael Albo², Prof. Dan Meyerstein¹

¹*Chemistry, Ben-Gurion University of the Negev, Israel*

²*Chemical Engineering and Biotechnology, Ariel University, Israel*

The interaction between the mesoporous metal-oxide matrix and the adsorbed/entrapped active metal species attracts attention and curiosity due to its critical role in defining catalytic performance. Herein, the effects of TiO₂, Al₂O₃ and SiO₂ sol-gel matrices on the catalytic properties of encapsulated Cu and Ni species catalyzing the dehalogenation of the hazardous disinfection by-products, chloro and bromoacetic acids are reported. A pre-catalyst approach is employed in which a matrix is prepared by incorporating M(II) species into the pores of the sol-gel, which are later reduced to the active catalyst, M(0) during the reduction reaction by BH₄⁻. The synthesized pre-catalysts are thoroughly studied using BET isotherms, X-ray diffraction, X-ray fluorescence, X-ray photoelectron spectroscopy and scanning electron microscopy. The results point out that the relative effect of the metal-oxide environment on the adsorbed active metal speciesnanoparticle affects the process studied: for example, in the dechlorination of chloroacetic acid by Cu⁰-NPs, the order of activities is SiO₂ Al₂O₃ TiO₂; whereas for the analogous processes catalyzed by Ni⁰-NPs, the order of reactivities is Al₂O₃ SiO₂ TiO₂. For the other processes studied, other orders of activity are observed. Thus, the results indicate that the different sol-gel materials encapsulating the catalytic metals affect the reduction reactions differently.

Nanoscience and Nanotechnology

Near Infrared Emitting Carbon Dots as a Probe for Early Gastric Ulcer Detection

Zoe Agin-Peters¹, Ms Nila Nandha Kadamannil¹, Prof Raz Jelinek¹

Department of Chemistry, Ben Gurion University of the Negev, Israel

Helicobacter pylori (*H. pylori*) infection of upper gastrointestinal tract in human permanently damages the stomach lining due to chronic duodenal or gastric ulcers. These ulcers later develops into gastric carcinoma. Identifying *H. pylori* infection in earlier stages is crucial to direct effective treatments to counter these chronic developments. *H. pylori* colonization in gastric mucosa raises the gastric pH corresponding to the urease activity. Herein we develop an efficient non-invasive method to detect the growth of *H. pylori* using a pH sensitive Carbon dots (Cdots). Autoclave assisted solvothermal method is employed for the synthesis of cdots. The near infrared (NIR) emission of cdots is sensitive to pH; emission being stronger in lower pH values. Their fluorescence emission response is quantified across a physiologically relevant pH range to define sensitivity and dynamic window under gastric-like conditions. In vitro growth of *H. pylori* is monitored by analyzing the NIR emission intensities of cdots in the growth medium. NIR emission offers in vivo monitoring of *H. pylori* growth due to deep tissue penetration, low auto fluorescence, and high biocompatibility. Preliminary data support NIR pH-sensitive CDs as a minimally invasive optical platform for detecting and monitoring *H. pylori*–associated gastric microenvironment changes, with potential future application in in vivo endoscopic or oral diagnostic formats.

Nanoscience and Nanotechnology

Enhancing the Stability of CsSnBr₃ Nanocrystals via Aligned Growth and Core–Shell Encapsulation

Achiad Goldreich¹, Dr. Lena Yadgarov¹
Chemical engineering, Ariel University, ישראל

Lead-free perovskites, particularly cesium tin bromide (CsSnBr₃), have gained significant interest in optoelectronic applications due to their favorable bandgap and high carrier mobility.[1] However, their practical implementation is hindered by poor stability and rapid degradation under ambient conditions. [2] In this study, we aim to enhance the stability of the CsSnBr₃ using two different approaches: morphology control and core-shell encapsulation. We successfully synthesized CsSnBr₃ nanowires (NWs) through a controlled ligand-based approach. Although the synthesized NWs showed uniform morphology and characteristic optical behavior, their environmental stability remained insufficient.

To address this, we developed a CsSnBr₃/MoS₂ heterostructure, leveraging the passivating and electronic properties of MoS₂ to significantly enhance the stability and performance of CsSnBr₃ NCs. Structural (XRD, TEM) and optical (PL, absorption) analyses confirmed the successful formation of the heterostructure. The incorporation of MoS₂ not only improved the air stability of CsSnBr₃ but also created new opportunities for enhancing stability in optoelectronics. Furthermore, optoelectronic measurements revealed an enhanced absorption spectrum, while PL decay analysis implies charge transfer,[3] indicating a strong synergistic interaction between CsSnBr₃ and MoS₂.

Our findings demonstrate that MoS₂-based heterostructures offer a promising strategy to improve the stability and performance of lead-free perovskite materials. This work paves the way for further exploration of hybrid nanomaterials in next-generation optoelectronic devices.

Nanoscience and Nanotechnology

Engineering enzyme-responsive amphiphile based sensors.

Avichai Gabbay¹, Michal Brodsky¹, Shirel Kleiner¹, Prof. Gili Bisker¹, Prof.
Roey Amir¹
Tel Aviv University, Israel

Over the past few decades, stimuli-responsive amphiphilic block copolymers have attracted significant interest due to their ability to self-assemble into various nano-structures in aqueous media. These assemblies hold great promise for various applications, including drug delivery, tissue engineering, and sensors. In our group, we design amphiphiles composed of hydrophilic linear polymers and hydrophobic dendrons, which provide molecular precision that allows for systematic examination of how subtle structural differences affect their responsiveness toward enzymatic degradation. These amphiphiles can also serve to disperse single-walled carbon nanotubes (SWCNTs) by forming polymeric coronae around them in aqueous media. Because SWCNTs emit fluorescence in the near-infrared (NIR) region, they are widely used as biomedical sensors.

Designing hydrophobic enzyme-responsive dendrons as dispersing agents provides a high degree of control in tuning their interaction with the SWCNTs. Enzyme-responsive polymeric assemblies are particularly attractive since overexpression of specific enzymes is associated with various diseases, and many disease-causing pathogens produce specific enzymes, which are found in environmental samples such as soil, water, and food.

In this work, we developed a series of enzymatically degradable diblock amphiphiles with varying hydrophilic to hydrophobic ratios, achieved by modifying either of the two blocks. We characterized their self-assembly into micelles and evaluated their ability to disperse SWCNTs. This strategy enables controlled modulation of fluorescence spectra in response to enzymatic cleavage, advancing the development of SWCNT-based sensors.

Nanoscience and Nanotechnology

Investigation of Structural Effects in Methyl Radical Adsorption and Reactivity on Transition Metal (111) Surfaces (M = Pt, Ag, Au): A DFT Study

Bobby Solanki¹, Prof. Haya Kornweitz¹
Department of Chemical Sciences, Ariel University, Israel

Methyl radical interactions with transition metal surfaces are fundamental to heterogeneous catalysis. Building on previous DFT studies from our research group on pristine Pt(111), Ag(111), and Au(111) surfaces, this work systematically investigates how surface defects—including vacancies and step edges—modify adsorption and reactivity compared to ideal surfaces. Our DFT calculations demonstrate that defect sites substantially alter adsorption energetics and enhance radical binding strength relative to terrace sites. In certain cases, defects enable reaction pathways inaccessible on pristine surfaces. Comparative analysis across the three metals reveals metal-specific responses, where the electronic structure of each metal interacts uniquely with surface irregularities to create distinct reactivity patterns and varying sensitivity to structural perturbations. These results highlight the critical role of atomic-scale structural variations in catalytic performance and provide insights for rational defect engineering in nanostructured catalysts. By connecting fundamental surface science with practical catalyst design, this work advances our understanding of how surface morphology controls reactivity at the nanoscale.

Nanoscience and Nanotechnology

2D Metal Halide Perovskites: Synthesis and Characterization

Diksha Prabhu Gaonkar¹, Prof Efrat Lifshitz¹

Chemistry, Technion Israel Institute of Technology, Israel

2D metal halide perovskites (HPs) are recently emerging as promising materials for optoelectronic and spintronic applications, due to their structural versatility that allows tuning of their photophysical properties. In these HPs, inorganic and organic layers are alternately stacked, creating an electronic band structure that resembles classical multiple quantum wells. The mentioned electronic band structure can be manipulated by the change of the composition, either of the inorganic or the organic moieties. Furthermore, our laboratory has recently demonstrated that the heterogeneity of a soft structural nature enables a motion degree of freedom, which is responsible for breaking inversion symmetry and the consequent formation of the Rashba effect. The last is pronounced as a split emission band at a band-edge energy with opposing circular polarization, hence beneficial for spin-related technologies.

The present work explores the design and synthesis of lead-free two-dimensional (2D) hybrid perovskites by substituting lead with manganese, aiming to introduce magnetic functionality into the crystal lattice. By systematically altering both the inorganic framework and the organic spacer cations, the study focuses on tuning the local structural distortions within the layered perovskite architecture. These structural modifications are expected to directly influence the magneto-optical behaviour. Building on the group's earlier investigations of magnetic impurities in three-dimensional (3D) hybrid perovskites, where impurity–host carrier interactions and changes in the carrier g-factor were observed, this work extends the understanding to 2D systems.

Nanoscience and Nanotechnology

Writing amorphous and crystalline nanostructures with light

Dr. Ehud Greenberg^{1,2}, Keren Chaika^{1,2}, Dr. Nina Armon^{1,2}, Dr. Eitan Edri^{1,2}, Dr. Ilana Perelshtein², Dr. Maria Tkachev², Dr. Gal Radovsky², **Hagay Shpaisman**^{1,2}

¹*Chemistry Department, Bar-Ilan University, Israel*

²*Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel*

Additive manufacturing of metals at the microscale remains challenging due to fundamental limits in resolution and structural control imposed by particle-based inks and inefficient heat dissipation. In particular, existing approaches offer little ability to tune the internal phase of printed features, such as crystalline versus amorphous structure.

Here we introduce a laser-driven metal microprinting strategy that enables direct, localized conversion of metal ions into solid architectures while providing deterministic control over the resulting nanostructure. The process relies on photothermal reactions coupled to transient laser-induced microbubble formation, allowing metal growth to proceed through distinct, spatially controlled pathways.

High-resolution transmission electron microscopy and selected-area diffraction reveal that the position of the laser focus relative to the liquid, gas, and substrate interfaces governs phase formation. Focusing within the liquid phase promotes crystalline metal growth, whereas focusing at the liquid–gas interface favors amorphous structures due to rapid quenching and kinetic constraints. Printing at the substrate interface yields mixed-phase architectures, consistent with the coexistence of two parallel pathways: direct formation of crystalline nanoparticles and microbubble-mediated transport accompanied by amorphous metal generation.

By adjusting laser intensity, we tune the relative contribution of these pathways and thereby control the final phase composition of the printed structures. The method enables fabrication of sub-micron metal pillars and heterogeneous microstructures, establishing a versatile platform for phase-programmable metal microprinting.

Nanoscience and Nanotechnology

Tuning Magnetic Anisotropy and Magneto-Optical Response in $\text{Mn}_{1-x}\text{Fe}_x\text{PS}_3$ Alloys via FePS_3 -Derived Anisotropy

Kusha Sharma¹, Ellenor Geraffy¹, Prof. Efrat Lifshitz¹
Schulich Faculty of Chemistry, Technion-IIT, Israel

Layered transition metal phosphorus trichalcogenides, MPX_3 ($M = 3d$ transition metal such as Fe, Mn or Ni; $X = \text{S, Se}$), constitute an important family of van der Waals magnetic semiconductors. Their structure comprises layers built from a 2:1 arrangement of edge-sharing $[\text{MX}_6]^{2+}$ and $[\text{P}_2\text{X}_6]^{4-}$ octahedra, in which the metal cations form a honeycomb lattice. [1,2] Within this family, FePS_3 is distinguished by its pronounced intrinsic in-plane magnetic anisotropy. This anisotropy arises from lateral lattice distortions and spin–orbit coupling (SOC), which stabilize a zigzag-type AFM (z-AFM) ground state and give rise to strong spin–phonon coupling,[3] in clear contrast to the nearly isotropic behavior of MnPS_3 . [4]

We investigate the $\text{Mn}_{1-x}\text{Fe}_x\text{PS}_3$ alloy series as a model platform to bridge these limiting cases and to probe how structural and magnetic anisotropies govern the optical properties of MPX_3 -based two-dimensional magnets. By gradually increasing the Fe content, we embed the strong in-plane anisotropy of FePS_3 into the MnPS_3 matrix and monitor the evolution of the magnetic ground state and low-temperature photoluminescence. Polarization-resolved and magneto-optical measurements reveal the progressive emergence of SOC-induced, polarization-selective emission and anisotropic magnetic responses correlated with lattice distortions and spin texture. We, thus, aim to establish $\text{Mn}_{1-x}\text{Fe}_x\text{PS}_3$ as a chemically tunable platform for engineering anisotropy-controlled magneto-optical functionalities in van der Waals magnets.

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Nanoscience and Nanotechnology

Aromatic C-H Bond Activation in Mechanically Controllable Break Junction: A Theoretical Study

Alexandra Freidzon¹, Tal Klein², Prof. Leeor Kronik¹, Prof. Oren Tal²

¹*Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Chemical and Biological Physics, Weizmann Institute of Science, Israel*

Single-molecule junctions can promote chemical reactions, owing to the presence of metal tips, which are more active than pristine metal surfaces, and to the applied voltage that introduces additional electric field effects. Recently, the formation of benzene dimers from benzene precursors was observed in a mechanically controllable copper break junction at 4K. This result is unexpected, taking into account the strength of the C-H bond. Therefore, the mechanisms that facilitate this reaction require elucidation. Here, we present a computational study of the first step of this process, namely C-H bond activation and cleavage in a benzene molecule placed between the tips of copper electrodes. We demonstrate that: (1) the benzene molecule changes its position and orientation relative to the metal tips, as the inter-electrode distance is varied; (2) C-H bond activation and cleavage take place at short inter-electrode distances; and (3) an electric field applied in a certain direction allows C-H bond activation to proceed at larger distances. We further find that at short distances the reaction proceeds essentially without a barrier, which is a necessary condition at cryogenic temperatures.

Nanoscience and Nanotechnology

Stabilization of high valence first-row transition metals by SiO₂

Pnina Gorodishchev¹

Ariel University, Israel

Silicon dioxide (SiO₂) is widespread in modern technologies, including electronics, optics, and glass manufacturing. While crystalline silica is known for its severe health hazards, amorphous SiO₂ serves as an excellent and versatile substrate capable of forming stable interactions with transition metals. Its structural and chemical properties make it a promising matrix for stabilizing high oxidation states of first-row transition metals, which are often short-lived under ambient conditions. First-row transition metal-based catalysts, including Mn, Fe, Co, Ni, and Cu, exhibit outstanding electrocatalytic activity due to their variable oxidation states, high density of active sites, good electrical conductivity, and large surface area, achieving performances comparable to noble metal catalysts. The high porosity and optical transparency of amorphous silica nanoparticles provide a three-dimensional, non-interfering environment that preserves the intrinsic properties of the metal centers incorporated within them. By elucidating the stabilizing effect of amorphous SiO₂ on high-valence transition metal species, this study seeks to advance the fundamental understanding of metal–support interactions and to contribute to the rational design of efficient, stable, and noble-metal-free electrocatalysts. Specifically, this research aims to investigate the role of amorphous SiO₂ in stabilizing high-valence first-row transition metals following oxidation. Preliminary results obtained for copper indicate that its bonding to SiO₂ significantly prolongs the lifetime of Cu(III), suggesting enhanced stability and potential applicability of such high-valence species. Building on these findings, pulse radiolysis will be employed to systematically probe the formation, stability, and decay kinetics of high-valence states of transition metals embedded in a SiO₂ matrix

Nanoscience and Nanotechnology

Fe–Zn electrocatalysts for electrochemical CO₂ reduction to syngas Lama Younis, Bibhudatta Malik, Alina Sermiagin, and Hannah-Noa Barad Department of Chemistry, Institute of Nanotechnology & Advanced Materials, Bar Ilan University

Lama Younis¹, Bibhudatta Malik¹, Alina Sermiagin¹, Hannah-Noa Barad¹

Mitigating CO₂ emissions while producing value-added chemicals under mild conditions is an important route to a sustainable future. Electrochemical CO₂ reduction (CO₂RR) is a promising method for this, with products such as syngas, a mixture of CO and H₂. Syngas is particularly attractive for wide industrial applications, especially when the H₂/CO ratio can be controlled. Therefore, the development of electrocatalysts capable of generating syngas with tunable compositions is highly desirable. Different transition metals show distinct selectivity toward CO₂RR and the hydrogen evolution reaction (HER), producing CO and H₂. For example, Zn favors CO production, due to its moderate CO binding strength, facilitating CO desorption, while iron exhibits high (HER) activity. Combining these metals is expected to balance the CO/H₂ ratio, enabling the direct formation of tunable syngas. Based on this Fe–Zn systems were selected as potential candidates for producing syngas.

In this study, bimetallic Fe–Zn electrocatalysts were designed with varying compositions and synthesized via electrodeposition on different substrates, carbon paper and titanium foam. The morphology and elemental composition of the catalysts were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). Electrochemical evaluations under CO₂-saturated conditions were performed, including product analysis through mass spectrometry (MS) to determine syngas ratios across various compositions and operational conditions. Given the abundance and low costs of Fe and Zn, this research contributes to the development of efficient, sustainable, and economically viable electrocatalysts for CO₂ conversion, supporting global efforts toward a cleaner energy future.

Nanoscience and Nanotechnology

Transition metal (molybdenum, tungsten, and manganese) doping of nickel phosphide nanoparticles for enhanced electrocatalytic activity toward the methanol oxidation reaction.

Amit Ben Zeev¹, Dr Rupesh Mandal¹, Dr Alevtina Neyman¹, prof. Maya Bar Sadan¹
Chemistry, Ben-Gurion University of the Negev, Israel

The development of non-precious metal electrocatalysts is critical for sustainable energy technologies, particularly direct methanol fuel cells. Nickel phosphides (Ni-P) have emerged as highly active, stable, and cost-effective alternatives to noble metal catalysts for various oxidation reactions. Here, we report the synthesis of transition metal (Mo, W and Mn) doped nickel phosphide nanoparticles (Ni-P NPs) via a colloidal synthesis. The systematic incorporation of these dopants was performed to tune the electronic structure and surface properties of the catalytic interface. Structural characterization confirms the successful doping into the bulk phase of the Ni-P NPs. Electrocatalytic screening revealed that the chosen dopants significantly enhanced the Methanol Oxidation Reaction (MOR) activity compared to the undoped Ni-P. Specifically, the Mn-Ni-P system achieved the lowest overpotential of 1.48 V vs RHE at 20 mA/cm² current density, representing an 80 mV reduction compared to the pure Ni-P catalyst (1.57 V). In contrast, the Mo-Ni-P catalyst demonstrated a maximum current density of 194 mA/cm² at 1.72 V vs RHE, more than tripling the 58 mA/cm² achieved by the pure Ni-P, suggesting a distinct role for each dopant in optimizing MOR kinetics and capacity. This work provides a general route for designing next-generation, high-performance, non-precious metal catalysts for sustainable energy applications.

Nanoscience and Nanotechnology

Synthesis and Optical Investigation of 2D Perovskite-Quantum Dot Hybrid Materials

Delaila Martins¹, Prof Efrat Lifshitz¹
Schulich Faculty of Chemistry, Technion, Israel

The 3D Metal Halide Perovskite (MHP) is known to be highly beneficial for solar cell applications. They are, however, unstable in the environment and undergo degradation easily. 2D MHPs are more stable than the 3D counterparts, showing high quantum efficiency, high Photoluminescence Quantum Yield (PLQY), and being relatively defect-free. Unfortunately, they possess high exciton binding energy, which hampers charge transfer, and they do not expand in the infrared spectral regime. Semiconductor QDs can change their optical properties by varying their size and composition, letting them absorb in the UV-Vis or IR region of the electromagnetic spectrum. We suggest hetrostructuring of QDs with optical activity in NIR and MHP with optical activity in the visible to form hybrid structures. We expect that this hetrostructuring will endow the QD/HPs heterostructure with a wider spectral range for absorption, with a benefit for a solar cell.

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THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



POLYMER AND SUPRAMOLECULAR CHEMISTRY

Chair: Charles Eliezer Diesendruck

Invited Lecture

Polymer and Supramolecular Chemistry

Toward bimetallic nanowires:
Insights from the co-impregnation of block copolymer films

Ofer Burg¹, Carmel Cohen¹, **Roy Shenhar¹**

*Institute of Chemistry and the Harvey M. Krueger Family Center for Nanoscience
and Nanotechnology, Hebrew University of Jerusalem, Israel*

Bimetals and alloys often display synergistic effects that give rise to non-linear properties at specific composition ranges. Confining these materials in nanowires is particularly beneficial for applications in catalysis, magnetism, and sensing owing to the high surface area and nanoscale confinement effects.

To date, ordered arrays of mono-metallic nanowires have been obtained by employing block copolymer films as sacrificial templates. In this approach, periodic arrays of nanoscale domains formed by phase separation are selectively impregnated by metal precursors. Subsequent plasma treatment eliminates the polymer film, and the metal precursors are reduced in situ into metallic nanostructures in the process. Selective co-impregnation with two metal precursors in solution seems like the next logical step toward obtaining bimetallic nanowires. However, the need to tune their composition to a desired range poses a challenge, because the resulting metal composition seldom matches the ratio of metal precursors in the impregnating solution.

In the presentation, I will describe the intricate competitive-cooperative mechanisms of impregnation that were unraveled by a deep exploration into the nature of interaction between pairs of three metal precursors (Pd, Pt, and Co) and the functional groups in the block copolymer domains. The different behaviors were successfully modelled using a single equation, which provides intuitive physical insights into the interplay between the metal precursors as they compete over binding sites.

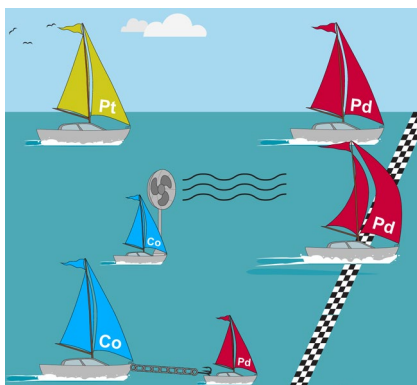


Illustration of the competitive-cooperative co-impregnation mechanism

O. Burg, C. Cohen, R. Shenhar, *Angew. Chem. Int. Ed.*, **2025**, 64, e202512695 (“Hot paper”).

Invited Lecture

Polymer and Supramolecular Chemistry

Photoswitchable latent monomers as a new paradigm for latency in metathesis polymerization

Yossi Weizmann¹

Chemistry, Ben-Gurion University of the Negev, Israel

Spatiotemporal control over olefin metathesis polymerization is commonly pursued via switchable catalysts, yet catalyst drift, decomposition, and background reactivity often limit storage stability and reproducibility. Here we present a complementary paradigm in which latency is encoded directly in the monomer. Using the norbornadiene/quadracyclane (NBD/QC) photoswitch, we design a family of latent monomers where QC is a dormant, metathesis-inactive isomer and NBD is a highly reactive ring-opening metathesis polymerization (ROMP) monomer. Activation of QC is achieved thermally or via photothermal heating with silica-encapsulated gold nanobipyramids that convert near-infrared light into a local plasmonic heat source, driving QC-to-NBD retrocycloaddition and initiating ROMP with ruthenium initiators. QC/ruthenium/gold nanobipyramid formulations remain unchanged for at least seven weeks at 4 °C yet polymerize efficiently on demand, with photothermal triggering providing faster kinetics and lower apparent activation temperatures than conventional bulk heating. We demonstrate the generality of this latent-monomer platform with multiple diester NBD derivatives and both a benchmark Hoveyda–Grubbs II catalyst (HG II) and a thermally latent bis-CAAC initiator, exploiting the unique latency to access macromolecular architectures that are difficult to realize with catalyst-based strategies. These include a one-pot ROMP diblock copolymer formed by combining an active NBD monomer with a QC latent monomer, as well as a Janus-type monomer that undergoes linear acyclic diene metathesis (ADMET) polymerization followed by on-demand crosslinking upon QC activation. Finally, masked photothermal activation of thin films affords spatially patterned polymer structures, underscoring the potential of monomer-encoded latency for light-driven curing and three-dimensional printing applications.

Invited Lecture

Polymer and Supramolecular Chemistry

Synthesizing water filtration polymer membranes, one monolayer at a time

Assoc. Prof. Tamar Segal-Peretz¹

Chemical Engineering, Technion- Israel Institute of Technology, Israel

Developing high-performance nanofiltration (NF) and reverse osmosis (RO) membranes is essential for addressing global water and resource challenges. Conventional thin-film composite (TFC) membranes, fabricated by liquid-phase interfacial polymerization (IP), suffer from structural and compositional variability that limits performance and fundamental understanding of transport mechanisms.

Here, we introduce Molecular Layer Deposition (MLD), a vapor-phase, layer-by-layer polymerization route that provides Angstrom-level control over film thickness, composition, and architecture. Using MLD, we grew ultrathin, ultrasmooth, and highly cross-linked aromatic polyamide selective layers directly on porous supports, achieving tunable, Angstrom-level controlled thickness in the 2–30 nm range.

MLD-based membranes exhibited exceptional uniformity and defect-free structure, yielding high selectivity for ions and uncharged molecules such as boric acid. By modulating the MLD layers' chemistry and stacking sequence, MLD enabled tunable ion-ion and ion-molecule selectivity in both NF and RO regimes. In addition, the precise control allowed us to probe the intrinsic transport properties of the polymers, decoupled from the heterogeneities inherent to IP-based membranes. For example, in polyamide films thinner than the ions' Bjerrum length, salt permeability increases sharply, defining a fundamental lower bound on the selective layer thickness.

Beyond enhanced performance, MLD provides a powerful experimental platform for probing structure–composition–transport relationships with unprecedented precision. This approach opens new pathways toward rational design of polymer layers, building one molecular layer at a time.

Invited Lecture

Polymer and Supramolecular Chemistry

semiaza-Bambusurils as Versatile Macrocycles for Anion Transport and Sensing

Ofer Reany¹

Natural Sciences, The Open University of Israel, Israel

Chloride and related anions are central to cellular homeostasis, biological signaling, disease mechanisms, and environmental chemistry, yet their controlled transport and detection remain a major challenge. *semiaza*-Bambusurils (*semiaza*-BUs) have emerged as modular supramolecular platforms that enable innovative solutions for anion recognition, transport and sensing. This lecture will explore four complementary strategies that demonstrate the versatility of these macrocycles.

First, tailored *semiaza*-BUs function as synthetic anion carriers, enabling efficient and selective chloride transport across lipid bilayers through principles of lipophilicity, with promising therapeutic applications for chloride channelopathies.^[1] Second, their incorporation into α -hemolysin nanopores transforms non-selective channels into stochastic chloride sensors, allowing real-time single-molecule detection in biologically relevant environments.^[2] Third, surface-confined electrochemical sensors based on self-assembled monolayers on gold electrodes provide robust, highly selective perchlorate sensing via electrochemical impedance spectroscopy, creating a stable, tunable platform for environmental monitoring.^[3] Finally, photo-switchable ion channels derived from azobenzene-functionalized macrocycles act as light-controlled ion gates, enabling reversible chloride flux in liposomes and living cells, with potential anticancer applications through organelle disruption.^[4]

Together, these approaches illustrate how *semiaza*-BUs bridge molecular recognition, membrane transport, and interfacial sensing, paving the way for next-generation diagnostics, therapeutics, and environmental technologies.

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Invited Lecture

Polymer and Supramolecular Chemistry

Polymer Upcycling and Recycling: Insights from NMR Methodology

Shira Haber¹

Department of Chemistry, Bar-Ilan University, Israel

Despite global efforts, plastic recycling rates remain near 15%, necessitating innovative upcycling strategies to transform discarded polymers into high-value materials. Amidation of polyethylenes (PE) offers a pathway to materials with enhanced surface and bulk properties; however, the impact of these functional groups on the resulting polymer microstructure remains poorly understood.

In this work, we employ multi-nuclear ¹H and ¹³C solid-state nuclear magnetic resonance (NMR) spectroscopy, relaxometry, with complimentary X-ray scattering to quantitatively characterize the phase compositions and chain dynamics of amide-modified PEs. Our findings indicate that overall crystallinity decreases with increasing functionalization. By utilizing NMR relaxation techniques to probe the chain mobility of the crystalline, amorphous, and interphasial regions, we demonstrate that the grafted amidyl groups specifically partition into the rigid amorphous fraction (RAF), the constrained region between the crystalline and amorphous domains.

The chemical specificity of solid-state NMR allows for precise mapping of functional groups localization within the polymer morphology. By correlating microstructure with macroscopic material behavior, we provide a mechanistic understanding of how chemical modification enhances the performance of functional PEs. These insights into the structural underpinnings of amide-containing polyolefins establish a critical foundation for the rational design of next-generation upcycled materials with tailored mechanical and chemical properties.

Polymer and Supramolecular Chemistry

Macrocyclic Diacetylene based multifunctional soft nanostructures

Nila Nandha Kadamannil¹, Raz Jelinek^{1,2}

¹*Department of Chemistry, Ben Gurion University of the Negev, Israel*

²*Ilse Katz Institute for Nanoscale Science and Technology, Be Gurion University of the Negev, Israel*

Hierarchical supramolecular assemblies constitute an important class of functional materials exhibiting diverse structural features and applications. Polydiacetylene (PDA) are a class of conjugated polymers formed by the 1,4- addition of diacetylene (DA) units. Herein we discuss the design and construction of diverse hierarchically organized macrocyclic diacetylene (MCDA) based nanostructures. Self-assembled hollow nanotubes formed by the photopolymerized of MCDA amphiphilic monomers, as revealed by single-particle cryo-electron microscopy (cryo-EM) and tomographic analysis shows tubes consisting of six pairs of covalently bonded filaments held together by hydrophobic interactions. The hollow MCDA nanotubes efficiently scavenge amphiphilic pollutants in water and subsequently photodegrade the guest species. Hierarchically coassembled nanotoroids comprising MCDA and 8-anilino-1-naphthalene sulfonate (ANS) shows nanofibers formed by stacked DA monomers as the basic units, which are further bent and aligned into toroids by electrostatic and hydrophobic interactions with the ANS. The amine moieties on the nanotoroids surface are employed for deposition of gold nanostructures – Au nanoparticles or Au nanosheets – which constitute effective platforms for photocatalysis and surface enhanced Raman scattering (SERS)-based sensing. Modulating noncovalent interactions between the MCDA, anthraquinone DA, and carbon dots facilitates formation of thin films exhibiting a long-range, uniform “honeycomb” pore structure. Wavelength- induced coassembly plays a key role by both initiating interactions between the carbon dots and the anthraquinone moieties and giving rise to the topotactic polymerization of the DA network. Macroporous films were used as photocatalytic platforms for the degradation of water pollutants and as potential supercapacitor electrodes, leveraging the films high surface-area, and porosity.

Polymer and Supramolecular Chemistry

development of peo-brush-peo for lithium-ion batteries.

Alisa Bouketov¹, Prof. Charles E. Diesendruck¹

Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Israel

Li-ion batteries (LIBs) are amongst leading energy storage technologies due to their high energy density and long cycle-life.¹ LIBs performance and safety strongly depend on electrolyte properties, responsible for Li-ion transfer between electrodes to balance the electron charge. Among commercial LIBs, the emblematic system is based on a liquid electrolyte composed of lithium salts, functional additives and organic solvents.² These electrolytes present high operating voltage and ionic-conductivity, good wettability and easy processability, all contributing to its widespread use. Despite these advantages, liquid electrolytes pose safety challenges, particularly due to their volatility and flammability.³

A broadly used solution is to exchange the organic solvent by lithium-conductive polymers such as polyethylene oxide (PEO). Polymers have low vapor-pressure and therefore are significantly less flammable. Yet, they are also less conductive and therefore are typically plasticized with the same organic solvents and/or operated at high temperatures. In this project, we address this issue by synthesizing PEO-brush-PEO. This new polymer presents ion-conductive groups in the backbone and side-chains while remaining liquid even at high molecular weights. Such polymers combine the higher ionic-mobility and ion-transfer of liquid electrolytes with improved thermal and electrochemical stability of a polymer. This new material shows strong potential for stable Li-ion coordination with high ionic-conductivity, providing a pathway towards safer and high-performance LIBs.

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Polymer and Supramolecular Chemistry

Amyloid-Based Catalysis of BHET Hydrolysis Toward Sustainable PET Biodegradation

Elinor Slavsky¹, Sisira Mambram Kunnath¹, **Shahar Blecher¹**, Prof. Raz Jelinek¹
chemistry, Ben Gurion university of the negev, israel

The global accumulation of polyethylene terephthalate (PET) waste highlights the urgent need for efficient and sustainable degradation technologies. While enzymatic PET hydrolases such as cutinases and PETases have advanced the field, challenges remain in stability, cost, and large-scale applicability. In this work, we explore a new class of minimalist, bio-inspired catalysts: amyloid-like peptide fibrils capable of promoting ester hydrolysis. We demonstrate that short synthetic peptides, upon self-assembly into β -sheet-rich fibrillar structures, exhibit esterase-mimicking activity toward bis(2-hydroxyethyl) terephthalate (BHET), a key intermediate in PET degradation. The fibrils catalyze the conversion of BHET to mono-(2-hydroxyethyl) terephthalate (MHET) and terephthalic acid (TPA) under mild aqueous conditions, without requiring complex protein scaffolds or metal cofactors.

Kinetic studies reveal that fibril morphology, hydrophobicity, and accessible catalytic residues strongly influence hydrolytic efficiency. The ability of these assemblies to perform selective bond cleavage suggests a functional analogy to natural esterases, yet with enhanced robustness and tunability. Our findings position amyloid-like fibrils as promising next-generation biomimetic catalysts for PET depolymerization pathways. This peptide-based approach offers a modular, low-cost, and potentially scalable platform for plastic biodegradation and circular recycling strategies.

Polymer and Supramolecular Chemistry

Self-healing Formulations based on Light-triggered Frontal Metathesis Polymerization

Sandra Idelman¹, prof Charles Diesendruck¹

Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, israel

Self-healing materials present a promising avenue for enhancing material longevity and reducing maintenance demands. A key challenge in self-healing systems is energetics - whether sufficient energy is embedded or provided for the healing chemistry to propagate throughout the fill volume in the damage site. Building on the light-triggered frontal ring-opening metathesis polymerization (FROMP) of dicyclopentadiene (DCPD) developed by Moore et al.,¹ we test this established chemistry as a formulation in self-healing epoxy composites, using embedded optical fibers to detect damage and trigger light-activated self-healing, which is capable to expand beyond the light-exposed volume. The photo-latent Grubbs catalyst remains inert under ambient conditions and is activated by light, providing precise spatial and temporal control over the initiation of polymerization. By integrating the photochemical FROMP formulation into microvascular networks, this approach allows localized, on-demand healing over extended regions while maintaining material stability before activation. This strategy could pave the way for next-generation composites capable of rapid, targeted repair under remote activation conditions, offering a pathway toward more durable and sustainable materials for aerospace, structural, and defense applications.

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Polymer and Supramolecular Chemistry

Metal-Organic Nanolayers for Patterning and Controlling the Properties of Electrochromic Coatings

Noga Levinson¹, Nadav Moav^{1,2}, Dr. Michal Lahav¹, Prof. Milko E. van der Boom¹

¹*Weizmann Institute of Science, Israel*

²*Tel Aviv University, Israel*

Electrochromic (EC) materials, which reversibly change color under applied voltage, are key components in energy efficient technologies such as smart windows and color displays. Realizing advanced EC displays requires both broad spectral tunability and spatial control of the active material, for segmented or pixelated designs. Our group has developed a family of polypyridyl-based metal-organic complexes that form thin films via layer-by-layer deposition on transparent conductive oxides (TCOs). These complexes exhibit high optical contrast, excellent stability, and tunable coloration across the visible range by varying the ligand and metal center. Here, we introduce assemblies of cobalt polypyridyl complexes to create insulating layers. The cobalt complexes are colorless and electrochemically inactive on TCOs, forming a nanoscale barrier to electron transfer. It is isostructural with the active EC complexes, differing only by the metal center, and can be deposited using the same solution-based methods. These assemblies allows spatial modulation of electron transfer, enabling both pattern formation and control over color. Our approach provides a versatile route to scalable, patterned EC displays.

Polymer and Supramolecular Chemistry

Functionalization of Supramolecular Polymers Using Phosphate Derivatives

Lior Hamu¹, Nawal Fahoum¹, Prof. Roy Shenhar¹

The institute of Chemistry, The Hebrew University of Jerusalem, Israel

Supramolecular polymers are dynamic materials composed of monomers bound together via reversible, non-covalent interactions, such as hydrogen bonds. The non-covalent nature of binding imparts unique properties such as self-healing ability and environmental responsiveness. The degree of polymerization can be regulated by introducing monofunctional molecules that compete with the supramolecular monomers on the supramolecular interaction and cap the chain ends. Organic anions can serve as efficient "chain cappers" for hydrogen bonding-based supramolecular polymers. In addition to shortening the supramolecular chains, they can also be used for chain-end functionalization.

This study focuses on phosphate derivatives as chain cappers for bisurea-based supramolecular polymers, and focuses on the level of protonation as a knob to fine-tune their capping efficiency. Interestingly, self-diffusion measurements showed that partially neutralized phosphate favors the formation of a "triad" structure when present alone in solution. However, our results revealed that in the presence of the supramolecular polymer, the "triad" disassembles into an anion-cation pair and neutral phosphate. Both the anionic and neutral phosphates co-diffuse with the supramolecular chain, confirming their integration into the supramolecular polymer structure. The data evidence that the anionic species is a more efficient chain capper than the neutral phosphate.

Polymer and Supramolecular Chemistry

Silver Nanowires Organized in Periodic Arrays

Ofer Burg¹, Prof. Roy Shenhar¹

*The Institute of Chemistry and the Harvey M. Krueger Family Center for Nanoscience
and Nanotechnology, The Hebrew University of Jerusalem, Israel*

Silver nanostructures, such as nanoparticles and nanowires, exhibit remarkable properties that arise from their nanoscale confinement, which give rise to plasmonic behavior. Silver nanowires, in particular, support plasmon propagation and exhibit polarization-dependent response that varies with the angle between the long axis of the wire and the polarization angle of the incident light.

While numerous methods for the synthesis of silver nanowires are known, arranging them in ordered arrays is challenging. Hence, instead of organizing pre-formed silver nanowires, obtaining ordered arrays is usually accomplished by employing subtractive lithography schemes, which are both expensive and material-inefficient. As an alternative, templated synthesis using block copolymer films offer a versatile platform for fabricating periodic nanostructure arrays through selective infiltration of anionic metal precursors followed by plasma treatment. Yet, applying silver precursors to this method posed a challenge, as silver typically forms cationic aquo complexes that cannot infiltrate the polymer film. Additionally, silver nanostructures tend to oxidize under ambient conditions, leading to a loss of their plasmonic properties over time.

In this work we demonstrate our solution for the creation of ordered arrays of silver nanowires using block copolymer films, including different methods for countering the silver oxidation. Using patterned substrates, we achieved highly aligned nanowires, and begun exploring their optical properties.

Polymer and Supramolecular Chemistry

Cascade Mesophase Transitions of Polymeric Formulations

Keerthana Mulamukkil^{1,2,3}, Mr. Orr Sarid⁴, Ms. Shahar Tevet^{1,2,5}, Prof. Roey J. Amir^{1,2,3,5}

¹*School of Chemistry, Faculty of Exact Sciences, Tel Aviv University, Israel*

²*The Center for Physics and Chemistry of Living Systems, Tel Aviv University, Israel*

³*Center for Nanoscience and Nanotechnology, Tel Aviv University, Israel*

⁴*The Future Scientists Center–Alpha Program at Tel Aviv Youth University, Israel*

⁵*ADAMA Center for Novel Delivery Systems in Crop Protection, Tel Aviv University, Israel*

Polymeric systems capable of undergoing multiple mesophase transitions are highly intriguing and hold significant promise as next-generation materials for advanced drug delivery applications. While many reported systems achieve such behavior by incorporating multiple stimuli-responsive functionalities, micellar formulations composed of diblock (DBA) and triblock amphiphiles (TBA) provide a simpler and more modular alternative. Owing to their distinct enzymatic degradability, co-assembled DBA/TBA micelles can undergo a sequence of well-defined mesophase transitions upon enzymatic activation: initially transforming from mixed micelles into TBA-rich hydrogels or microgels and eventually degrading further into soluble hydrophilic polymer fragments.

In biological environments, these assemblies are exposed to numerous proteins that may significantly alter their performance. Thus, evaluating the impact of non-specific protein-polymer interactions on both enzymatic degradation and subsequent mesophase transitions is crucial. To investigate this, we examined the effects of varying concentrations of the activating enzyme, porcine liver esterase (PLE), and bovine serum albumin (BSA), a model protein known to form non-specific interactions with hydrophobic domains. Our findings revealed that higher enzyme concentrations accelerated DBA degradation, resulting in faster transition to the hydrogel mesophase. Increasing BSA concentration also accelerated DBA degradation and significantly shifted the mesophase transition to occur at a DBA to TBA ratio that was approximately 30% higher than in the absence of BSA. These results underscore the crucial role of both specific and non-specific protein-polymer interactions in dictating mesophase transitions, providing fundamental insights into the mechanisms governing the structural transformations of such mesophase-shifting polymeric formulations under biologically relevant conditions.

Polymer and Supramolecular Chemistry

Rheological Behavior of Branched Supramolecular Polymers

Carmel Cohen¹, Isay Columbus¹, Roy Shenhar¹

Institute of Chemistry and the Center for Nanoscience and

Nanotechnology, The Hebrew University of Jerusalem, Israel

Supramolecular polymers represent a unique family of polymers, in which the repeat units are connected by non-covalent interactions such as hydrogen bonds. This virtue makes them specifically intriguing, because under certain conditions they could disassemble into individual molecules and give rise to low viscosity solutions, whereas under different conditions they behave like conventional polymeric chains that tend to entangle, resulting in elastic materials. Environmentally responsiveness and self-healing are thus part of their identity.

We recently introduced branching – a fundamental aspect in polymer science – into supramolecular polymers, and showed its dramatic influence on the solution viscosity. In this work, we studied the rheological behavior of branched supramolecular polymers and compared it to the known behavior of linear supramolecular polymers. Interestingly, we found that branching leads to an unusual frequency-dependent response of the storage and loss moduli, which raises the possibility for a complex relaxation mechanism that is unique to branched supramolecular systems.

Polymer and Supramolecular Chemistry

Edible Coatings Integrating Cold-Adapted Bio-Preservatives as a Natural Approach to Improve Food Safety and Storability

Sheizaf Stav¹

*Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem,
Israel*

Both chemical and biological strategies play a critical role in developing advanced food preservation technologies. We propose to design edible coatings based on modified polysaccharides (MPs) and psychrophilic (cold-adapted) bacterial bio-preservatives to enhance food safety and reduce postharvest losses. Since most foods are stored under refrigeration, cold-adapted bacteria are ideal bio-preservatives, as they maintain activity at low temperatures. Polysaccharide-based edible coatings are considered promising natural solutions for maintaining food quality; however, their application is limited by safety concerns associated with conventional chemical modifications.

In this study, modified polysaccharides, including carboxymethyl chitosan (CMCS), a water-soluble chitosan derivative, were synthesized through a safe Schiff base reaction using only edible reagents. The resulting CMCS-N-alkylimine derivatives were comprehensively characterized by FT-IR and NMR spectroscopy to confirm imine formation and molecular modification, while thermal, physicochemical, and surface analyses (TGA, contact angle, CAC, and zeta potential) were used to assess their functional properties.

Next, these optimized matrices will be combined with psychrophilic bacterial bio-preservatives, both obtained from ATCC and isolated during this study, to create multifunctional edible coatings capable of supporting microbial activity under refrigeration. We hypothesize that cold-adapted bacteria will colonize the food surface, forming a protective barrier by outcompeting spoilage microorganisms, while the MP matrix will stabilize and enhance bio-preservative activity.

This research aims to develop a safe, sustainable, and cost-effective platform for food preservation, addressing current gaps that limit the practical adoption of edible coatings and microbial bio-preservatives in the food industry.

Polymer and Supramolecular Chemistry

Gating Covalent Mechanochemistry with Supramolecular Interactions: H-bonds Effects on Mechanophore Activation at a Heterointerface.

Nawal Fahoum¹, Prof Charles Diesendruck¹
Chemistry, Technion, Israel

Mechanophores undergo specific chemical transformations under mechanical force, offering opportunities for stress-sensing and adaptive materials. While mechanophore activation in thermoplastics and covalent polymer networks is well-established, the role of supramolecular interactions in modulating mechanochemical reactivity remains largely unexplored. This research aims to investigate whether strong hydrogen bonding networks can induce enough force for covalent bond scission, using trityl-based mechanophores.

For that goal, we are using solid-phase organic synthesis (SPOS), based on chlorotriptyl chloride (CTC) resin to introduce mechanophores at interfaces. Our synthetic strategy involves functionalizing CTC resin with 1,4-butanediol, creating mechanically sensitive C-O ether bonds, followed by conjugation with 2-ureido-4[1H]-pyrimidinone (UPy) units. UPy moieties form exceptionally strong quadruple hydrogen bonds, creating robust supramolecular assemblies adjacent to the mechanophore site.

This molecular design positions the trityl ether mechanophore at a critical heterointerface between the solid resin support and the supramolecular hydrogen bonding network. Upon mechanical stimulation, cleavage of the mechanophore will be monitored via its distinct mechanochromic response — a color change indicating the formation of a stabilized carbocation or radical. By systematically applying controlled mechanical stress, we aim to determine whether supramolecular forces can be transmitted across the interface to facilitate covalent C-O bond cleavage.

This work addresses a fundamental question in mechanochemistry: can covalent bond activation occur in supramolecular networks, where non-covalent interactions are transmitting the force between molecules? Demonstrating supramolecular modulation of mechanophore thresholds would establish new design principles for adaptive materials with tunable mechanical responses, advancing applications providing crucial design principles for next-generation, force-responsive systems.

Polymer and Supramolecular Chemistry

Light-fueled transient catalytic amyloid-like fibrils for antibiotic degradation

Shubhra Kanti Bhaumik¹, Ms. Sisira Mambram Kunnath^{1,2}, Dr. Elad Arad^{1,2,3}, Dr. Itamar Kass², Dr. Einat Nativ-Roth², Dr. Arunavo Chatterjee¹, Dr. Albert Batushansky², Prof. Hanna Rapaport⁴, Prof. Raz Jelinek^{1,2}

¹*Department of Chemistry, Ben-Gurion University of the Negev, Israel*

²*Ilse Katz Institute (IKI) for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Israel*

³*Department of Chemical Engineering, Columbia University in the City of New York, USA*

⁴*Department of Biotechnology Engineering, Ben-Gurion University of the Negev, Israel*

Short peptides that self-assemble into highly ordered fibrillar structures like amyloid fibrils have gained enormous interest in recent years. Amyloid fibrils are linear polypeptide aggregates that are linked to a variety of neurodegenerative diseases. Despite their toxicity, amyloid and amyloid-like fibrils have attracted considerable attention in the fields of catalytic hydrolysis of esters and phosphor-esters, lipid degradation, and catecholamine oxidation. Herein, we present light-fueled transient amyloid-like fibrils from a short peptide with a highly organized structure in water. We employed PFK (PKFKFKFKFKFKP), a short amphiphilic and cationic peptide, and MCH, a short-lived photoswitch in water, for this purpose. Co-mixing of PFK and MCH (1:2 molar ratio) in water under dark conditions results in small random aggregates. However, quite surprisingly, upon light irradiation, within 10 minutes, highly organized fibrils are formed as evidenced by cryo-TEM. MCH transforms into SP, having an aromatic ring and a pendant sulfonate group, which might interact with the peptides non-covalently to form amyloid-like fibrils under light. Such fibril formation is transient, and the formed fibrils dissociate once the light source is removed. The light-fueled peptide fibrils are further tested towards catalytic degradation of β -lactam antibiotics, an expanding health and environmental risk in wastewater that helps propagate antibiotic-resistant bacterial strains. These light-fueled catalytic fibrils formed under light can hydrolyze nitrocefin, a chromogenic β -lactam antibiotic, and penicillin G, a non-chromogenic antibiotic, demonstrating a novel approach for the degradation of antibiotics in water, providing solutions for tackling this significant environmental and health issue.

Polymer and Supramolecular Chemistry

New Biocompatible Additives for Bioplastic Based on Soybean Oil

Adi Ticher^{1,2}, Dr Elena Poverenov¹

¹*Food Science, Agricultural, The Volcani Institute, Israel*

²*Biochemistry, Food Science and Nutrition, The Hebrew University of Jerusalem, Israel*

Poly(lactic acid) (PLA) is a biodegradable bioplastic widely used in industrial composting applications due to its renewable origin and environmentally friendly nature. However, its brittleness and limited mechanical flexibility restrict its use in demanding applications. To address these challenges, PLA was combined with polysaccharides and plasticizers derived from renewable sources, specifically soybean oil, to improve its mechanical properties and biodegradability. Plasticizers, defined as small molecules that interact with polymers to improve flexibility, reduce brittleness, and enhance processability, were synthesized and modified with lactate group and 6- or 8-carbon chains. Comprehensive analyses using NMR and FT-IR confirmed the successful synthesis and structure of these soybean oil-based plasticizers. When incorporated into PLA, the lactate-modified soybean oil exhibited remarkable improvements in mechanical performance, achieving a 100-fold increase in elongation at break compared to unplasticized PLA. This substantial enhancement demonstrates the ability of tailored plasticizers to significantly alter polymer behavior. A practical experiment further illustrated the material's applicability: PLA threads containing lactate-modified soybean oil successfully supported tomato seedlings, maintaining their integrity under stress, while threads made of unmodified PLA failed. These results emphasize the importance of selecting plasticizers compatible with the polymer matrix to achieve superior performance. The use of biocompatible, renewable plasticizers like soybean oil not only improves the functionality of PLA but also expands its potential applications, from agriculture to packaging, contributing to the development of more sustainable and versatile bioplastic solutions.

Polymer and Supramolecular Chemistry

Force induced selective scission of N-N single bond in the 6-membered ring mechanophore

Lixin Yang¹, Prof. Charles Diesendruck¹
Chemistry, Technion, Israel

Over 100 mechanophores, force sensitive functional groups, have been developed since the concept inception in the early 2000s. In addition of providing a chemical to approach to mechanoresponse, mechanophores are helpful in studying elemental questions about the chemical bond. Using chemical design supported by the power of modern computational modeling, bigger understanding, as well as new functions are provided as new mechanophores are developed.

In 2006, one of the first mechanophores was developed, in which a C-N bond around an azo moiety was mechanically cleaved using ultrasonication to apply mechanical stress to the chains. Additional C-N bonds were shown to be mechanochemically active since: dicyanocyclobutane, aziridines, and 4-membered ring mechanophores with C-N or N-N bonds. Looking at these examples, one could think that perhaps, C-N bonds will always cleave prior to N-N bonds. Yet, C-N and N-N bonds have the same length, but C-N bond has higher enthalpy. Therefore, N-N bonds should be easier to break, and not only thermally but also mechanically. In this work, we designed a 1,2-diazinane mechanophore - a 6-membered ring bearing N-N single bond, which we connected to the center of a linear polymer chain the nitrogen atoms. Ultrasonication was employed to stress the chains in solution and GPC and NMR analysis supported the functional group added acted as a mechanophore. NMR indicated a symmetric scission, supporting the N-N bond scission, and quantum computation using ab initio steered molecular dynamics provided further support.

Polymer and Supramolecular Chemistry

Influence of Peripheral Halogenation on Axial Phenoxylation Kinetics of Boron Subphthalocyanines

Reshma Jose¹, Dr Alexandra Freidzon¹, Erika Remigio², Prof Leeor Kronik¹, Prof Timothy P. Bender²

¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Department of Chemical Engineering and Applied Chemistry, University of Toronto, Canada*

We investigate the effect of peripheral fluorination and chlorination on the rate of axial phenoxylation of boron subphthalocyanines (BsubPcs), with Br and Cl as axial ligands, specifically Br-BsubPc, Br-F12BsubPc, Br-Cl12BsubPc, Cl-BsubPc, and Cl-F12BsubPc. For this study, we use various solvents at their reflux temperature to acquire conversion of axial phenoxylation and obtain kinetic data. We found the experimentally observed reactivity of the BsubPcs used in this study followed Br-BsubPc > Cl-BsubPc > Br-F12BsubPc ≈ Br-Cl12BsubPc > Cl-F12BsubPc. This shows that peripheral fluorination or chlorination inhibits the rate of axial phenoxylation and confirms the axial B–Br bonds to be more reactive than B–Cl bonds. Density functional theory (DFT) calculations confirm the observed kinetic data and suggest that phenoxylation proceeds primarily via the Torres mechanism and solvent polarity facilitates the reaction.

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Polymer and Supramolecular Chemistry

Amyloid-Based Catalysis of BHET Hydrolysis Toward Sustainable PET Biodegradation

Elinor Slavsky¹, Sisira Mambram Kunnath¹, Shahar Blecher¹, Prof. Raz Jelinek¹
chemistry, Ben Gurion university of the negev, israel

The global accumulation of polyethylene terephthalate (PET) waste highlights the urgent need for efficient and sustainable degradation technologies. While enzymatic PET hydrolases such as cutinases and PETases have advanced the field, challenges remain in stability, cost, and large-scale applicability. In this work, we explore a new class of minimalist, bio-inspired catalysts: amyloid-like peptide fibrils capable of promoting ester hydrolysis. We demonstrate that short synthetic peptides, upon self-assembly into β -sheet-rich fibrillar structures, exhibit esterase-mimicking activity toward bis(2-hydroxyethyl) terephthalate (BHET), a key intermediate in PET degradation. The fibrils catalyze the conversion of BHET to mono-(2-hydroxyethyl) terephthalate (MHET) and terephthalic acid (TPA) under mild aqueous conditions, without requiring complex protein scaffolds or metal cofactors.

Kinetic studies reveal that fibril morphology, hydrophobicity, and accessible catalytic residues strongly influence hydrolytic efficiency. The ability of these assemblies to perform selective bond cleavage suggests a functional analogy to natural esterases, yet with enhanced robustness and tunability. Our findings position amyloid-like fibrils as promising next-generation biomimetic catalysts for PET depolymerization pathways. This peptide-based approach offers a modular, low-cost, and potentially scalable platform for plastic biodegradation and circular recycling strategies.

Polymer and Supramolecular Chemistry

Development of hydrogel-Forming Microneedles for Sustained Transdermal Delivery in Cutaneous Fungal Infections

Hala Dawud¹, Prof Roey J amir¹, Prof Aiman Abu Ammar²

¹*Organic Chemistry, Tel Aviv University, Israel*

²*Pharmaceutical Engineering, Azrieli College of Engineering Jerusalem, Israel*

Hydrogel forming microneedles (HFMNs) are solid MNs that transform into hydrogel upon absorption of skin interstitial fluid, whereas dissolving MNs (DMNs) dissolve upon insertion, releasing the encapsulated drug.

Using tri-block polymeric amphiphiles based on linear PEG, as the hydrophilic block, and dendrons with enzymatically cleavable end-groups, as the hydrophobic blocks, we developed a promising platform for a new type of MNs – mesophases shifting microneedles (MSMNs). The mesophase shifting mechanism is based on the tendency of these amphiphiles to form (i) hydrogels upon contact with water, and subsequently undergo a transition into (ii) hydrogel microparticles, which can then be degrade into (iii) soluble hydrophilic polymers in the presence of target enzymes that cleave the hydrophobic end-groups of the dendrons. By varying the hydrophobic end-group lengths in the triblock amphiphiles, we assessed their effect on MSMN drug release, integrity, and mechanical performance. The developed MSMN arrays, were loaded with an antifungal agent and demonstrated high drug content, sufficient strength, and excellent insertion ability. Testing the MSMNs using porcine skin, demonstrated their ability to penetrate and undergo complete dissolution. To further study their therapeutic potential, these MSMNs were tested against *Candida albicans* and exhibited prolonged inhibition of growth.

Showing that the ability of these MSMNs to undergo mesophase transition combines advantages of both HFMNs and DMNs, potentially enabling localized and more effective treatment by increasing the residence time of the drug at the target site, by better penetration and sustainable delivery for an extended period.

Polymer and Supramolecular Chemistry

Bio-Inspired Hydrolysis of Phthalates Using Catalytic Amyloid Fibrils

Shahar Blecher¹, Elinor Slavsky¹, Sisira Mambram Kunnath¹, Prof. Raz Jelinek¹
chemistry, Ben Gurion university of the negev, Israel

Phthalate esters (PAEs) are widespread plasticizers whose persistence and potential toxicity raise significant environmental concerns. Enzymatic degradation offers a sustainable route for their removal, yet natural esterases often suffer from limited stability under harsh environmental conditions. In this work, we present amyloid-based catalytic fibrils as robust esterase mimics for the hydrolysis of common phthalates. Short synthetic peptides designed to self-assemble into β -sheet-rich amyloid fibrils were evaluated for their ability to promote ester bond cleavage via surface-exposed catalytic residues. The fibrillar assemblies exhibited high structural stability, retained activity across a broad pH and temperature range, and demonstrated selective hydrolysis of representative phthalates such as DEP, DMP, and DnOP. Kinetic analyses revealed rate enhancements consistent with microenvironment-mediated catalysis, highlighting the role of the ordered fibrillar scaffold in facilitating substrate binding and activation. These findings position amyloid fibrils as promising, tunable platforms for bio-inspired degradation of persistent plasticizers and contribute to the development of sustainable strategies for environmental remediation.

Polymer and Supramolecular Chemistry

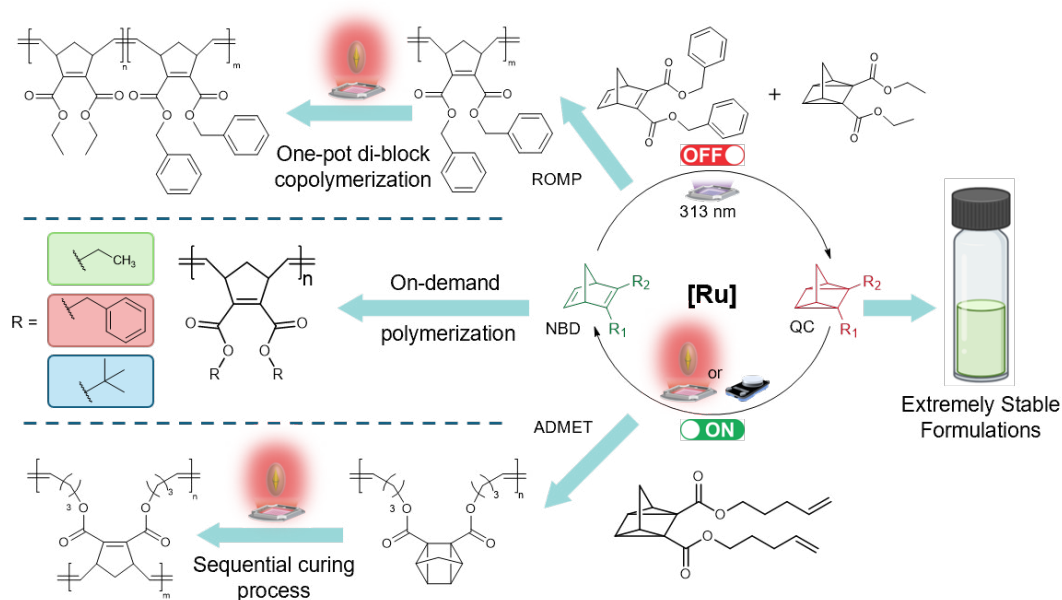
Photoswitchable olefins as latent metathesis monomers for controlled polymerization

Nir Lemcoff¹

Chemistry, Ben-Gurion University of the Negev, Israel

Our understanding of polymers has given rise to fundamental changes in society. Nonetheless, there is much room for progress in developing and improving creative techniques enabling advanced materials. Among the frontiers of this endeavor is the development of switchable catalysts aimed at providing spatiotemporal control over polymerizations. In our work,¹ we present an alternative to the conventional catalyst-centered approach by utilizing the quadricyclane/norbornadiene isomerization as a switchable ROMP monomer. The on-demand polymerization of four norbornadiene derivatives was achieved using two different ruthenium-based olefin metathesis initiators. The latent quadricyclane isomer generated remarkably stable formulations upon mixing with ruthenium initiators, unchanged for up to seven weeks. In addition to conventional heating, the latent monomer could also be activated by the photothermal response of gold bipyramids, enhancing the retrocycloaddition back to norbornadiene and leading to highly efficient polymerizations amenable to 3D printing techniques. Finally, a one-pot di-block copolymerization strategy and a sequential curing process inaccessible by traditional methodologies were developed based on the monomers' exceptional latency.

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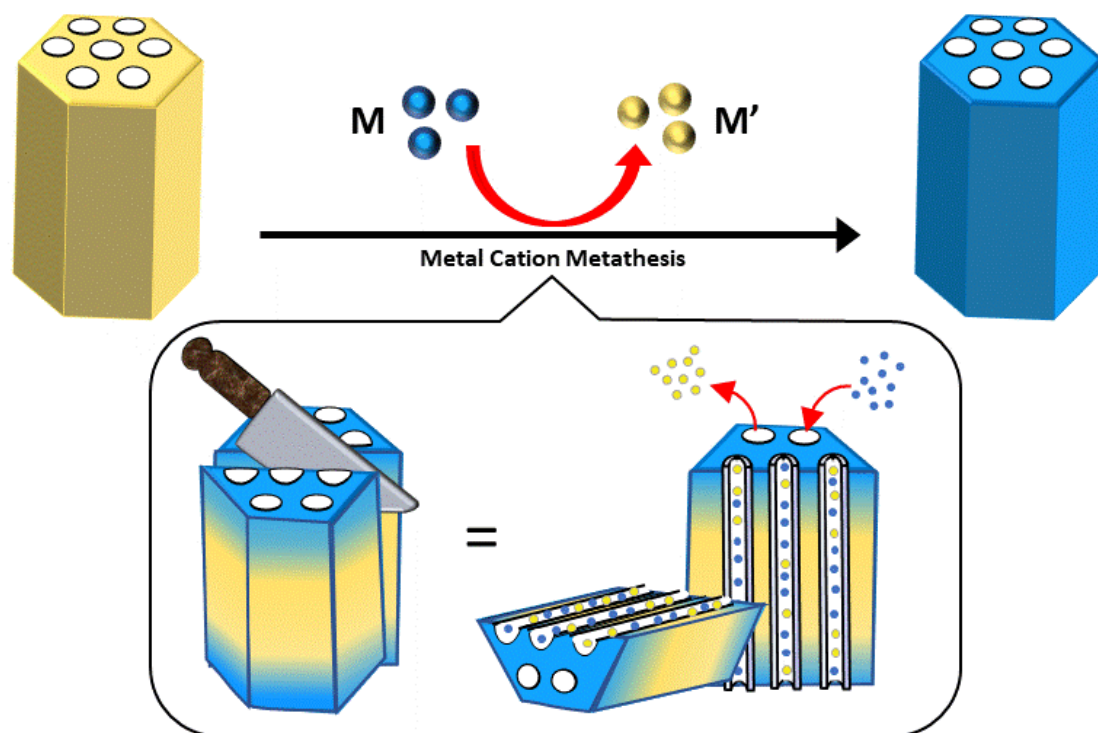
Polymer and Supramolecular Chemistry

Directing the Morphology, Packing, and Properties of Chiral Metal–Organic Frameworks by Cation Exchange

Hadar Nasi¹, Dr. Maria Chiara di Gregorio¹, Dr. Qiang Wen¹, Dr. Linda J. W. Shimon², Dr. Ifat Kaplan-Ashiri², Dr. Tatyana Bendikov², Dr. Gregory Leitus², Dr. Miri Kazes¹, Prof. Dan Oron¹, Dr. Michal Lahav¹, Prof. Milko E. van der Boom¹
¹*Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel*

²*Department of Chemical Research Support, Weizmann Institute of Science, Israel*

We show that metal–organic frameworks, based on tetrahedral pyridyl ligands, can be used as a morphological and structural template to form a series of isostructural crystals having different metal ions and properties. An iterative crystal-to-crystal conversion has been demonstrated by consecutive cation exchanges. The primary manganese-based crystals are characterized by an uncommon space group (*P622*). The packing includes chiral channels that can mediate the cation exchange, as indicated by energy-dispersive X-ray spectroscopy on microtome-sectioned crystals. The observed cation exchange is in excellent agreement with the Irving–Williams series (Mn Fe Co Ni Cu Zn) associated with the relative stability of the resulting coordination nodes. Furthermore, we demonstrate how the metal cation controls the optical and magnetic properties. The crystals maintain their morphology, allowing a quantitative comparison of their properties at both the ensemble and single-crystal level.



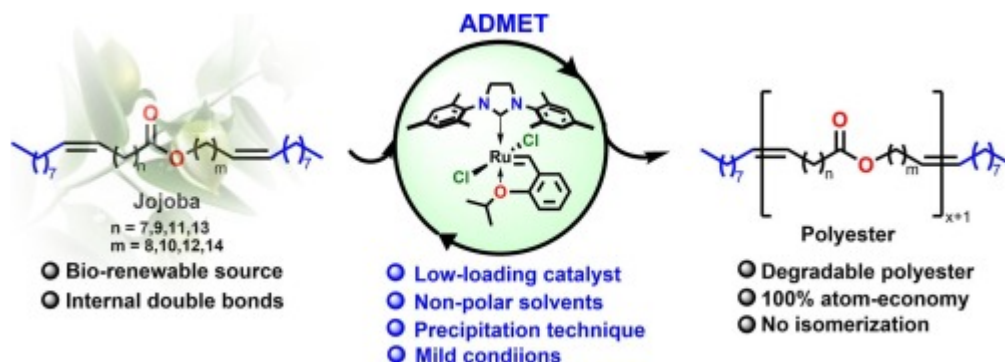
Polymer and Supramolecular Chemistry

Precipitation driven ADMET polymerization of jojoba oil for recyclable biorenewable polymers

Koushik Sarkar¹

Chemistry, Ben Gurion University of the Negev, Israel

Unsaturated natural oils, waxes, and their associated fatty acids represent promising starting materials for sustainable polymer synthesis due to their abundance and propensity to participate in metathesis reactions. In this work, the polycondensation polymerization of jojoba oil to produce high molecular weight polymers and valuable 9-octadecene as the condensate is efficiently achieved through an atom-efficient catalytic process under mild conditions. The fundamental breakthrough in the complete conversion of jojoba oil to the corresponding polyester was achieved by separating the polymer from 9-octadecene via an iterative precipitation technique. The resulting high-molecular-weight polyesters could be readily deconstructed under basic hydrolytic conditions and repolymerized by acid-catalyzed esterification of the resulting degradation products. These findings underscore the potential of jojoba-derived polyesters for closed-loop recycling, where polymers can be chemically broken down and reassembled into new materials. The technology developed in this study can be further expanded to produce a wide range of useful bio-renewable polymers from other natural oils and waxes in an environmentally accountable manner.



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Polymer and Supramolecular Chemistry

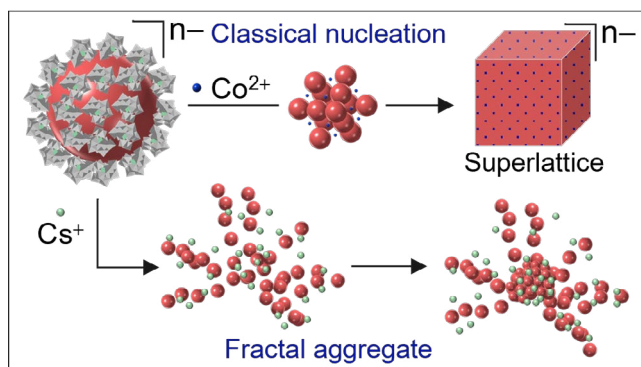
Polyoxometalate-Engineered Assembly of a Small-Ion Superlattice

Shubasis Roy¹, Nitai Leffler¹, Dr. Mark Baranov², Dr. Arti Joshi¹, Dr. Alevtina Neyman¹, Prof. Ira A. Weinstock¹

¹Chemistry, Ben Gurion University of the Negev, Israel

²Ilse Katz Institute for Nanotechnology Science, Ben-Gurion University of the Negev, Israel

The assembly of charged nanoparticles (NPs) with much smaller, oppositely charged ions has recently emerged as a rational strategy for designing multidimensional nanostructured materials, including superlattices (SLs).^{1,2} Herein, we demonstrate that negatively charged polyoxometalate (POM) protected 4 nm gold (Au) NPs³ can be reversibly assembled into face-centered cubic (FCC) SLs through electrostatic interactions with Co^{2+} aq in water. Disassembly into individual Au NPs shows that electrostatically-stabilized POM protecting-ligand shells remain intact during SL formation, after which the small mobile ions may diffuse rapidly through the lattice. Additional insight into the criteria that must be met to obtain well-defined SL assemblies was provided by investigating the effects of POM charge and the nature and valence of counteranions. Collectively, these findings establish a strategy in which POM cluster anions enable rational control over the structure and morphology of well-defined NP assemblies.



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Polymer and Supramolecular Chemistry

Self-Limiting Assembly of a Keggin-Ion Complexed Metal-Oxide into Multifunctional Nanocrystal Gel

Arti Joshi¹, Nitai Leffler¹, Dr. Shubasis Roy¹, Dr. Einat Nativ-Roth²

¹Department of Chemistry, Bgu, Israel

²Ilse Katz Institute for Nanotechnology Science, Ben-Gurion University of the Negev, Bgu, Israel

The design of functional materials via supramolecular or nanoparticle gelation is a growing frontier in nanochemistry.[1-2] Metal-oxide nanocrystals (NCs) offer unique optical, electronic, and catalytic properties, but conventional sol-gel approaches typically compromise these attributes through irreversible metal speciation and amorphous phase formation. Herein, we report a new type of gel formed by [PSnW₁₁O₃₉]³⁻-O₂- (PSnW₁₁)-complexed SnO₂ NCs, synthesized in aqueous media without organic ligands. Unlike conventional sol-gel methods, this approach yields dynamic, reversible gels that retain the phase and properties of the constituent NCs. Cryo-SEM imaging reveals a percolated structure composed of self-limiting, negatively charged gel walls enclosing interconnected aqueous nanocavities. The gels exhibit self-healing and cation-exchange behavior, as demonstrated by solution-state NMR spectroscopy and confocal microscopy, confirming dynamic ion mobility within the network. The PSnW₁₁-SnO₂ gel exemplifies a new class of functional, porous nanomaterials based on POM-mediated assembly.

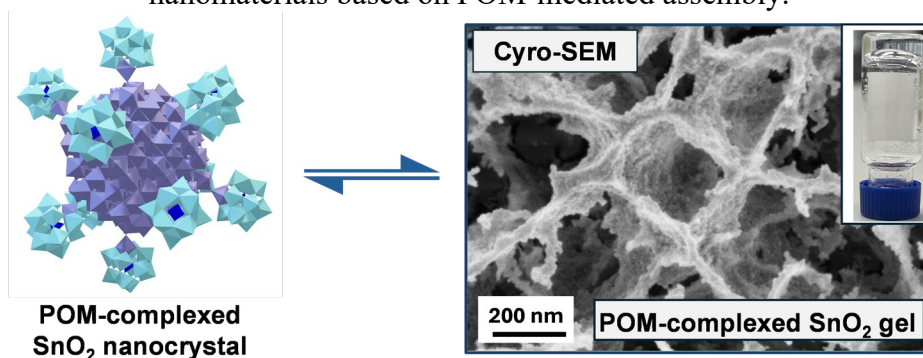


Figure caption: Representation of a [PSnW₁₁O₃₉]³⁻-O₂- ligated SnO₂ NC. The SnO₂ core is in light-violet, and the [PSnW₁₁O₃₉]³⁻-O₂- oxo-donor ligands are in teal blue color. The cryo-SEM image at right shows gel walls that surround water-filled cavities.

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Polymer and Supramolecular Chemistry

Hydrogen-Bond-Directed Active-Template CuAAC Enables High-Yield Synthesis of Handcuff Rotaxanes

Arjun Veliyl Prakash¹, Mr Helal Metawi¹, Dr. Abed Saady¹
Chemical Sciences, Bar Ilan University, Israel

Mechanically interlocked molecules (MIMs)¹ offer powerful platforms for controlling molecular motion, topology, and cooperative function, yet synthetic access to higher-order architectures such as handcuff rotaxanes remain limited.²

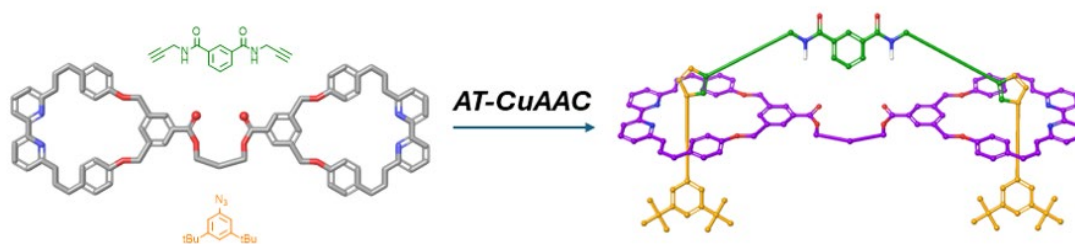
Here, we report a hydrogen-bond-directed active-template CuAAC (AT-CuAAC) strategy that enables the efficient and high-yielding synthesis of handcuff rotaxanes using a 2,2'-bipyridine-based bis-macrocycle. The bis-macrocycle is designed to act simultaneously as a dual catalytic pocket and a supramolecular template. Strategic incorporation of ester hydrogen-bond acceptors promote preorganisation of amide-containing bis-alkyne axles through directional hydrogen bonding, biasing the system toward dual threading and suppressing competing single-threaded pathways.

Under mild AT-CuAAC conditions, this cooperative preorganisation enables simultaneous covalent capture of two axle termini, delivering [2]handcuff rotaxanes in consistently high isolated yields. Spectroscopic analysis confirms the dual-threaded architecture and reveals that hydrogen-bonding interactions dominate the binding landscape, overriding classical triazole-centered recognition. Variation of macrocycle linker length shows minimal impact on reaction efficiency, highlighting the robustness and generality of the design.³

This hydrogen-bond-directed AT-CuAAC approach provides one of the most efficient routes to handcuff rotaxanes reported to date, and establishes a broadly applicable supramolecular design principle for constructing complex, mechanically interlocked architectures. The methodology opens new opportunities for the development of functional MIMs with cooperative host-guest behaviour, redox activity, and controlled molecular motion.

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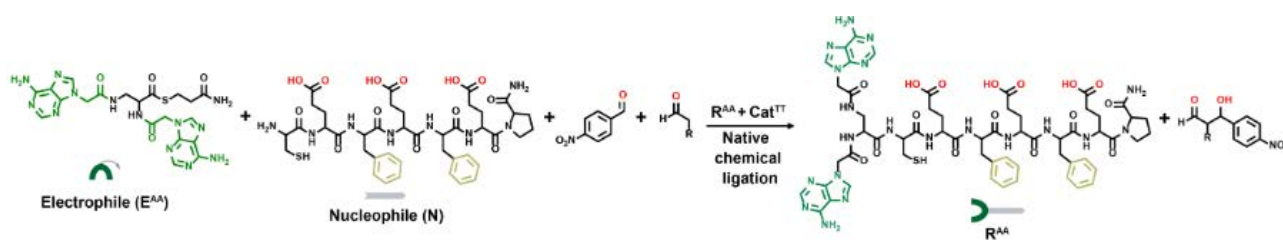
Polymer and Supramolecular Chemistry

Mutualistic Interplay Between Replication and Catalysis in Nucleopeptide Systems

Suman Maji¹, Saurabh Yadav¹, Dr Zehavit Dadon¹, Prof Gonen Ashkenasy¹
Chemistry, Ben Gurion University of the Negev, Israel

Early life likely required molecules that combined genetic information storage with catalytic functions. Modern biology separates these roles into nucleic acids for information storage and proteins for catalysis. However, this division likely did not exist in the earliest stages of life. Instead, primitive life may have relied on simpler molecules capable of performing both functions simultaneously. Such molecules are crucial in models of life's origin because they bridge the gap between prebiotic chemistry and the sophisticated biochemistry we observe today.

Nucleopeptides are of great interest in studies on the origin of life because they provide a plausible model for the transition from simple prebiotic molecules to complex biomolecules capable of both information storage (like nucleic acids) and catalytic activity (like peptides). This dual functionality makes nucleopeptides attractive candidates for early biomolecules. They may have served as "protocatalysts" facilitating their own replication or other chemical reactions critical for early life, while also preserving and transmitting genetic-like information. Their hybrid nature suggests they could represent intermediates or foundational molecules in the evolution of life. In our study, an adenine-based thioester (EAA) underwent native chemical ligation with a β -sheet-forming peptide (N) to form RAA, exhibiting autocatalytic behavior. A thymine-containing peptide enhanced this process through base-pairing interactions. To demonstrate functional output, we engineered CatTT, featuring a di proline glutamic acid motif for aldol catalysis and a thymine domain for template recognition. We further explored the mutual catalytic influence between RAA and CatTT, revealing cooperative behavior.



Polymer and Supramolecular Chemistry

Steroid-functionalized *semiaza*-bambusuril macrocycles as channel-like ditopic $\text{Na}^+/\text{K}^+-\text{Cl}^-$ transporters with cytotoxic activity

Suresh Saini¹, Prof. Ehud Keinan², Prof. Ofer Reany¹

¹Department of Natural Sciences, The Open University of Israel, Israel

²The Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Israel

Transmembrane anion transport is a fundamental process that underpins cellular homeostasis, which is responsible for numerous systemic physiological processes. Understanding the mechanisms of ion transport, including channelopathies and other pathological conditions, could lead to the design of non-protein synthetic ion transporters capable of replacing defective channels and natural carriers, with clinical implications. Herein, we introduce a new class of *semiaza*-bambusurils (*semiaza*-BUs) bearing triazole-containing side chains and steroid-derived lipophilic end groups designed to promote membrane insertion and ion conduction (Figure 1).

In unilamellar vesicles, compounds 1–3 showed activity in HPTS (pH dissipation) and SPQ (chloride influx) assays, whereas 4 was inactive, consistent with excessive hydrophobicity/poor solubility. Dose–response analysis revealed nanomolar potency with Hill coefficients ~ 1 , supporting unimolecular transport. Anion selectivity followed the Hofmeister series.

Under gluconate conditions that suppress anion flux, 1 and 2 unexpectedly mediated Na^+/H^+ and K^+/H^+ exchange with minimal K^+/Na^+ discrimination. Chloride-selective electrode measurements supported electroneutral Na^+/Cl^- and K^+/Cl^- cotransport (1 2 3). Channel-like behavior is supported by cholesterol-insensitive transport (30% cholesterol), preserved membrane integrity, and planar bilayer electrophysiology showing compound-induced currents.

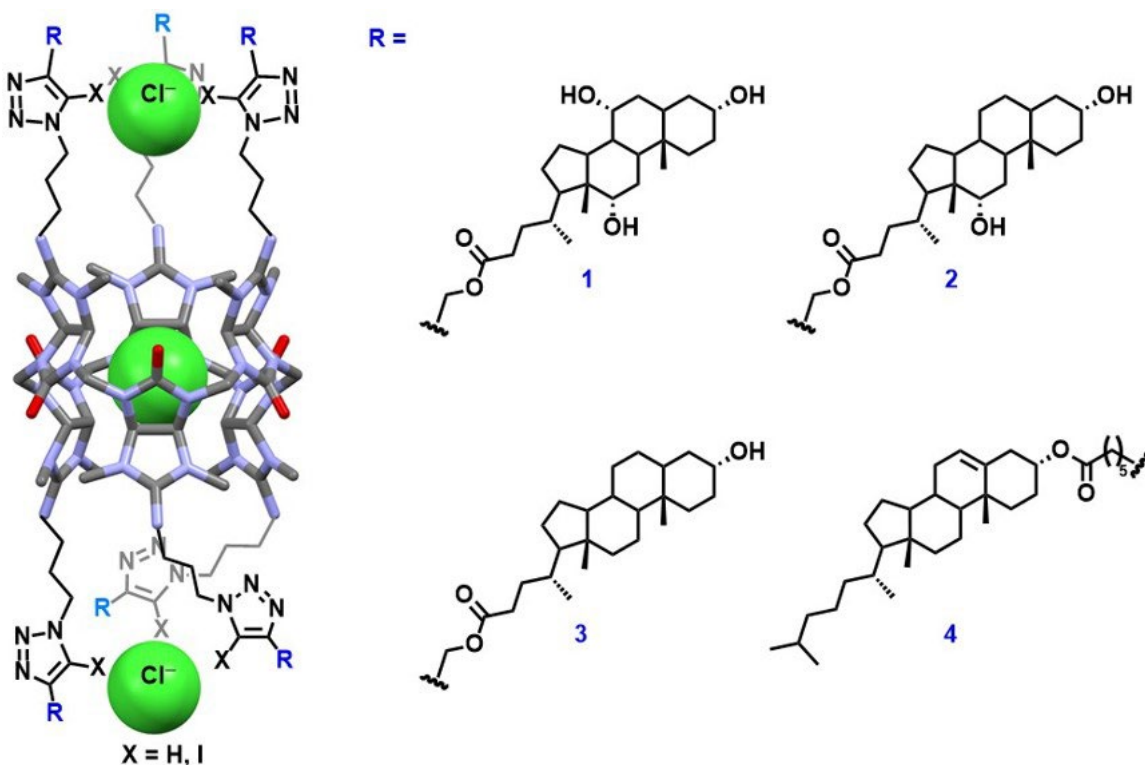


Fig.1: Novel steroid-based *semiaza*-BUs as channel-like ditopic $\text{Na}^+/\text{K}^+-\text{Cl}^-$ transporters.

Polymer and Supramolecular Chemistry

Novel simple method for chitin quantitative determination in BSF (Black Soldier Fly)

Alexander Laskavy¹, Inbal Domb Joseph¹

Department of Food Science, Agriculture Research Organization, The Volcani Institute, Israel

Industrial interest in *Hermetia illucens* (black soldier fly, BSF) has expanded considerably over the past two decades. BSF larvae can be efficiently cultivated on a wide range of organic waste substrates originating from domestic, agricultural, and food-processing sectors, providing a cost-effective and environmentally sustainable source of nutrients. In particular, BSF larvae constitute a novel and renewable source of proteins, lipids, and chitin.

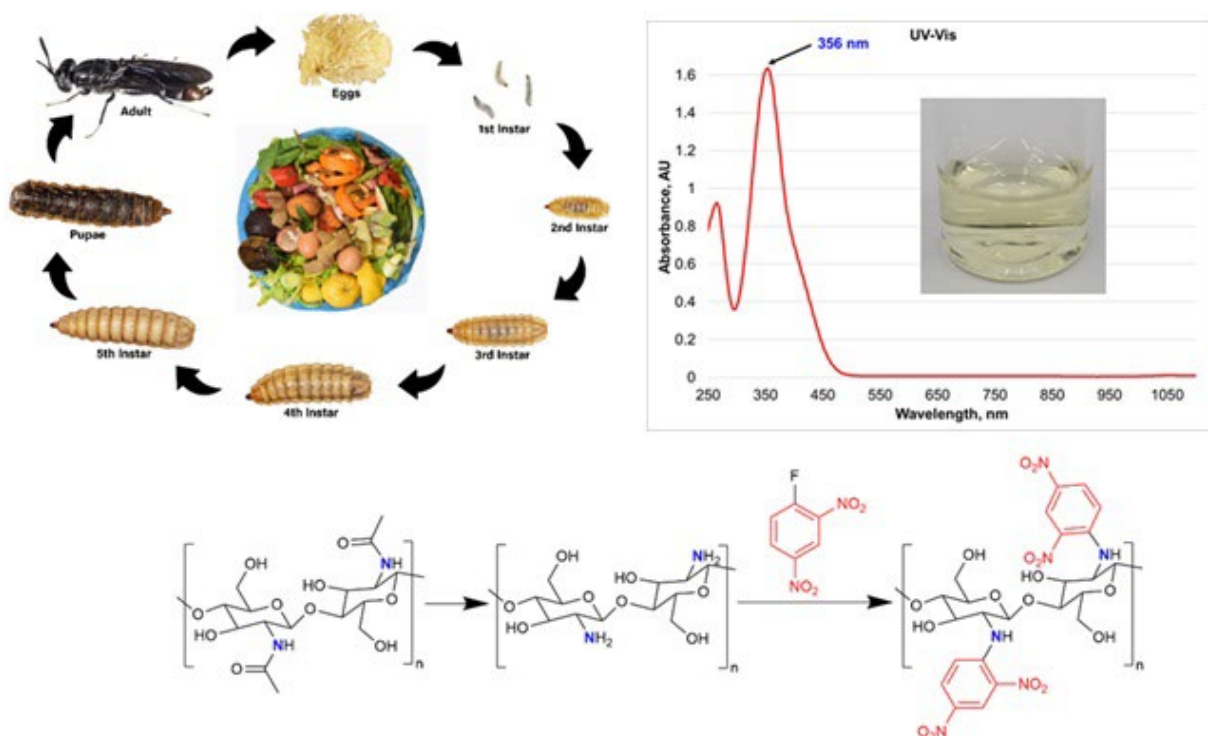
A major limitation in the direct utilization of BSF larvae or derived protein fractions is the presence of chitin, a structural polysaccharide that is indigestible in the mammalian gastrointestinal tract. Consequently, accurate quantification of residual chitin in defatted and de-chitinized BSF protein isolates remains a challenging analytical task.

During the development of a reliable method for the quantitative determination of chitin, we investigated the selective reactivity of Sanger's reagent (1-fluoro-2,4-dinitrobenzene, DNFB) toward primary amino groups in amino acids of proteins.

For the implementation of this approach, chitin must be purified to remove mineral residues, proteins, and lipids, which may interfere with quantitative analysis. In addition, the chitin must undergo deacetylation to chitosan, thereby exposing reactive amino groups.

Upon reaction with purified chitosan, Sanger's reagent forms a yellow chromophore derivative that can be quantified spectrophotometrically using UV-Visible detection.

The proposed method offers high sensitivity, simplicity of operation, and low analytical cost. It does not require specialized instrumentation, expensive reagents, or highly trained personnel, making it a practical alternative for the routine quantification of chitin in BSF-derived materials.



Polymer and Supramolecular Chemistry

Sequence-Dependent Mesophase Cascades in Dual-Responsive Polymeric Micelles

Michal Brodsky¹, Dr Nicole Edelstein-Pardo¹, Prof. Roey J. Amir¹
Chemistry, Tel Aviv University, Israel

In recent years, stimuli-responsive nanostructures have attracted significant attention for their ability to undergo structural and physical property changes upon exposure to specific stimuli, such as pH, temperature, or enzyme presence. These stimuli can induce morphological transitions between self-assembled states, enabling dynamic control over structure and function. Tuning these transitions through precise chemical modifications of the amphiphilic building blocks provides a valuable step towards the design and performance of responsive delivery systems.

Our group recently reported a novel strategy for programming polymeric micelles to undergo sequential mesophase transitions into hydrogel and, later, into degraded, soluble polymers, demonstrating how molecular architecture and enzyme specificity can be used to control these transitions. These more complex systems, which can undergo multiple mesophase transitions, can serve as advanced drug delivery platforms: carriers in their micellar state can be readily injected and circulate in the body, then, upon enzymatic stimulation, they can form soft hydrogels that serve as drug depots. After cargo release, the polymers can be further degraded into soluble polymers that can be readily cleared.

In this work, we extend our modular strategy into a general approach for designing polymeric formulations capable of undergoing sequential mesophase transitions by mixing diblock and triblock amphiphiles with orthogonal stimuli-responsive groups. We demonstrate how their distinct responsiveness provides a generic molecular tool for programming cascades of mesophase transitions that depend not only on the type of responsive groups but also on the sequence of activation.

Polymer and Supramolecular Chemistry

London dispersion between confined alkyl groups

Dr. Itai Massad¹, James T. F. Dobson¹, Paula C. P. Teeuwen¹, Tanya K. Ronson¹,
 Jonathan R. Nitschke¹

Department of Chemistry, University of Cambridge, United Kingdom

London dispersion forces between alkyl groups can give rise to “steric attraction”—a promising design element in organic chemistry. However, the scope and magnitude of this attraction are subject to intense debate, along with its ability to outweigh competing effects. Here, we describe a system of four tetrahedral $M_4L^R_4$ cages ($M=Fe^{II}$ or Zn^{II} , $R=Me$ or Et), each confining twelve R groups within its cavity. The cages display trends in stereochemistry and stability—both in solution and in the gas phase—which violate intuitive notions of steric hinderance, strain, solvophobic effects, and metal-ligand bond strength. Instead, the observed trends align with the optimization of London dispersion between the confined alkyl groups, even at the expense of other driving forces in the system. These differences in stability are manifested in the self-sorting of a mixture containing both metals and both ligands into the cages that feature optimal alkyl-alkyl contacts, despite the entropic preference for a statistical mixture. Overall, this work establishes coordination cages as a promising platform to study London dispersion forces.

Polymer and Supramolecular Chemistry

The Solubility of Chitin in Aqueous Solution and DESs Solvent

Ahmad Tanbuz¹, Prof Daniel Harries¹
Institute of Chemistry

The Fritz Haber Research Center, hebrew university, israel

Chitin, a linear polysaccharide composed of (1–4)-linked 2-acetamido-2-deoxy- β -D-glucopyranose units, is the second most abundant polymerized carbon source in nature, with roughly 10 billion tons produced annually by crustaceans, insects, fungi, algae, and related organisms. Its low toxicity, biodegradability, and biocompatibility make it valuable for biomaterials and biorefinery applications, though its poor solubility has limited broader use. This study explores two solvent systems to improve chitin dissolution: aqueous NaOH/urea and KOH/urea solutions, and thymol-based deep eutectic solvents (DES). DES, formed from hydrogen bond donors and acceptors, offers low toxicity, biodegradability, and tunable properties, while thymol provides hydrophobic, antimicrobial, and antioxidant characteristics. Using alkaline urea solutions, up to 5% chitin could be dissolved; although dissolution occurs without urea, the polymer rapidly precipitates, indicating urea's role in stabilizing the solution.

Polymer and Supramolecular Chemistry

pH-Dependent Autocatalysis of Nucleopeptides: Implications for Prebiotic Chemistry

Saurabh Yadav¹, Dr. Suman Maji¹, Prof. Gonen Ashkenasy¹
Chemistry, Ben Gurion University of the Negev, Israel

Many essential cellular and viral processes, including replication and translation, rely on highly coordinated systems in which nucleic acids and proteins/peptides operate synergistically. Substantial experimental evidence suggests that the precursors of both nucleic acids and peptides could have been synthesized under plausible prebiotic conditions. In our previous work, we demonstrated the selective replication of nucleopeptide chimeras, uncovering mechanisms that favor one product over another. Specifically, we investigated two nucleobase-containing replicators, R^{AA} and R^{TT} , synthesized via native chemical ligation of di-nucleobase thioesters with a cysteine-containing peptide (N). Both replicators exhibited significantly enhanced replication rates in template-seeded reactions compared to template-free controls, with cross-catalysis outperforming autocatalysis. Building on this foundation, our ongoing research has examined the replication behavior of cytosine-based nucleopeptides. We identified a nucleopeptide chimera (R^{CC}), generated through the native chemical ligation of a cysteine based nucleophile (N) with cytosine-containing electrophiles (E^{CC}), which is capable of undergoing autocatalysis under specific pH and temperature conditions. We hypothesize that under mildly acidic conditions, selective hemi-protonation of cytosine enhances base-pairing interactions, thereby stabilizing the formation of R^{CC} and promoting autocatalysis. We propose that this autocatalytic system is highly relevant to origin-of-life studies, as it illustrates how molecular assemblies could self-sustain, amplify, and ultimately evolve toward increasing complexity.

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Polymer and Supramolecular Chemistry

Multifunctional, Multipolymer Porous Systems

Lynn Cohen¹, Prof. Michael S. Silverstein¹
Materials Science and Engineering, Technion, Israel

The design of multifunctional porous polymers is of great interest for applications ranging from environmental remediation to biomedical engineering. This study focuses on synthesizing multipolymer porous systems through dual-phase polymerization within high internal phase emulsions (HIPEs), employing both water-in-oil and oil-in-water inverse systems. Hydrophobic matrices based on styrenic monomers and hydrophilic networks derived from anionic monomers were successfully polymerized in parallel phases.

The resulting PolyHIPEs exhibited interconnected macroporous structures with tunable pore morphology and density, strongly influenced by the monomer composition and phase ratio. Structural and thermal characterization (FTIR, SEM, DSC, DMTA) confirmed successful polymer formation and crosslinking.

These results present a versatile approach for fabricating dual-polymer porous materials with controllable architecture and functionality, bridging synthetic polymer chemistry and materials engineering.

Polymer and Supramolecular Chemistry

Dually Selective Polymeric Membrane for Charge-Specific and Solvent Transport Using Diversely Structured Copolymers

Layla Namaa¹, Prof. Charles E. Diesendruck², Prof. Lucy Liberman¹

¹*The Wolfson Department of Chemical Engineering, Technion Israel Institute of Technology, Israel*

²*Schulich Faculty of Chemistry, Technion Israel Institute of Technology, Israel*

Polymeric membranes are essential for selective transport in electrochemical and separation technologies. However, most current membranes target the transport of a single molecular species, typically in one direction. This study aims to develop a copolymer-based membrane capable of dual selectivity, where ions and neutral solvents are transported through distinct polymer phases in opposite directions.

The proposed membrane design integrates a quaternary ammonium (QA)-functionalized block for hydroxide ion conduction with a triethylene glycol (TEG)-containing block for water/methanol transport, leveraging their distinct hydrophilicity and Flory–Huggins interaction parameters. Using reversible addition–fragmentation chain transfer (RAFT) polymerization, we synthesized homopolymers, random copolymers, and block copolymers with controlled composition and molecular weight to investigate how polymer composition influences self-assembly, ionic conductivity, and solvent transport, both independently and simultaneously.

Characterization through gel permeation chromatography (GPC), nuclear magnetic resonance (NMR), and small-angle X-ray scattering (SAXS) is employed to correlate molecular structure with morphology and transport behavior. This work is expected to provide new insights into the design of multifunctional membranes that enable coupled charge and solvent transport, with potential applications in fuel cells, sensing, and water management systems. In addition, it will provide fundamental understanding on how transport in opposite directions affect each other.

THE 89TH ANNUAL MEETING OF **FEBRUARY 10-11, 2026**
THE ISRAEL CHEMICAL SOCIETY SMOLARZ AUDITORIUM, TEL AVIV UNIVERSITY



TRANSLATIONAL COLLOID SCIENCE: BRIDGING MATERIALS, MEDICINE, AND AGRICULTURE

Chair: Guy Mechrez

Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Engineered Supramolecular Nanostructures for Tissue Regeneration

Lihi Adler-Abramovich¹

*Department of Oral Biology, The Goldschleger School of Dental Medicine, Gray
Faculty of Medical & Health Sciences, Tel Aviv University, Israel*

Advances in regenerative medicine require materials that provide precise control over nanoscale organization, mechanical behavior, and biological function. We develop bioinspired supramolecular scaffolds based on short aromatic peptides that undergo solvent-regulated self-assembly and polymorphic phase transitions, allowing for the fine-tuning of crystalline structure, rigidity, and bioactivity. Co-assembly of complementary dipeptides yields exceptionally rigid hydrogels that support cell mechanotransduction and osteogenic differentiation. The incorporation of biopolymers, such as hyaluronic acid and gelatin, yields injectable and 3D-printable composite hydrogels that exhibit thixotropic behavior and enhanced calcium mineralization. These materials result in substantial bone regeneration *in vivo*.

Expanding their functionality, we fabricate patient-specific, bioactive titanium implants via additive manufacturing and design conductive peptide-MXene hybrid hydrogels that function as piezoresistive sensors for real-time tissue monitoring and electrical stimulation. Furthermore, we developed an autologous electrospun polymer-peptide skin equivalent for treating severe burn injuries, demonstrating accelerated wound closure and a reduction of T_{50} from 12 to 4 days.

Together, these studies establish a modular platform that integrates mechanical tunability, printability, and sensing capabilities to fabricate multifunctional biomaterials and hybrid bioelectronic interfaces. This supramolecular approach enables the design of personalized regenerative systems with translational potential across soft and hard tissue repair.

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Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Polymorphism in agrochemical formulations: A case study

David Mocatta

ADAMA

Formulation science is an inherently multidisciplinary field that translates fundamental chemistry and materials science into robust, scalable products for consumers. At ADAMA, formulation chemists routinely integrate concepts from a large array of subjects—for example, solubility, emulsion and polymer science, rheology, comminution, and many more—to develop novel products that deliver exceptional pest control. In this presentation, I will focus on how crystallography and solid-state control come into play in formulation development.

Using a commercial herbicide product as a case study, I will describe how, using a combination of powder X-ray diffraction and ATR-FTIR, a polymorphic transition was identified as the cause of a serious product failure mode, and how understanding the physical system at play allowed us to direct a transition to the more favored polymorph.

The solution restored manufacturability and shelf-life without changing the product composition, demonstrating how industrial crystallography can be used pragmatically to make more robust products for the agrochemical market. Beyond the specific case, the talk will highlight the type of applied research conducted at ADAMA and the opportunities it provides for chemists interested in combining rigorous science with tangible impact on global food production.

Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Solid lipid nanoparticles for the delivery of lipophilic drugs

Abraham Domb¹

School of Pharmacy-Faculty of Medicine, Hebrew University of Jerusalem, Israel

Lipid nanoparticles have been prepared and used for various applications, particularly as carrier for the delivery of various agents. They have been used for the delivery of lipophilic agents in medicine, food, and agriculture, where the active agent is solubilized within the lipid phase to allow dispersion in water.

Formulations that spontaneously form nanoparticles when added to aqueous media have been developed for the delivery of cyclosporin and other agents. These liquid formulations are composed of surfactants, lipids, and a solvent loaded in a soft gelatin capsule for oral delivery. Cannabinoids having a log P of 6-7 have been incorporated into such formulations, and they have shown improved bioavailability.

Insecticides and herbicides are generally water insoluble, thus they require formulation for improved absorption in plant and/or extended release formulations for long action. Pickering emulsions have been extensively applied for the delivery of these agents. These emulsions have limited stability and are in liquid form, therefore limiting their use. A new type of particles has been developed, termed "Solid Pickering," in which a solid lipid core is decorated with nanoparticles to form spherical particles for controlled delivery of agents. These Solid Pickering particles have been used for formulating lipophilic drugs, food additives, and insecticides for extended release for weeks.

Various lipid formulations and their applications in medicine and agriculture will be discussed.

Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Hierarchical structure of self-assembled peptide-polymer hybrids

Ronit Bitton¹

BGU, Israel

Self-assembled membranes that form at the interface between oppositely charged aqueous solutions of polyelectrolytes and self-assembling peptides provide a versatile platform for three-dimensional cell culture. Despite their promise, however, the ability to rationally control their structure and mechanical properties remains limited.

Here, we present a systematic investigation of the formation mechanisms and key design parameters governing peptide–polysaccharide interfacial membranes. Using β -sheet-forming cationic peptides from the PFX family in combination with negatively charged polysaccharides—including alginate, hyaluronic acid (HA), and carrageenan—and integrating scattering techniques with electron microscopy across multiple length scales, we show that membrane formation is dictated by coupled reaction–diffusion and self-assembly processes at the aqueous–aqueous interface. Depending on the balance between interfacial complexation and peptide assembly kinetics, the membranes evolve into either hierarchically organized structures with oriented fibrous domains or thicker, more homogeneous morphologies lacking long-range order.

Importantly, we demonstrate that subtle variations in peptide chemistry or polysaccharide chain characteristics—even in systems with identical net charge—profoundly influence interfacial interactions, assembly pathways, and the resulting membrane hierarchy. Extending these principles beyond planar interfaces, we further show that spherical membrane architectures with tunable size and mechanical stability can be reproducibly generated by controlling assembly conditions and material properties.

Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Burn Rate Enhancement by In-Situ Catalytic Metathesis Reaction

Levi Gottlieb¹

M4230, RAFAEL, Israel

One of the major areas of focus in propellant engineering is high burn rate propellants. High burning rates provide the ability to generate high thrust levels without the need for elaborate grain designs. An extensive amount of work devoted to burn rate enhancement utilize various systems including nanometric materials tested with aim to modify the reaction rate of the major component in solid propellants formulations, the oxidizer, ammonium perchlorate (AP).

It occurred to us that if we can deliberately induce the degradation of Hydroxyl Terminated Poly Butadiene (HTPB) fuel-matrix in the these composites an enhancement of the rate of volatilization of the organic matrix will occur. A degradation reaction will produce lower molecular weight fragments not only increasing the rate of gasification (where the major energy producing combustion occurs), but also the increase thermal energy feedback to the unreacted solid composite, increasing the matrix temperature, resulting in an overall increased burn rate. We have envisioned that if a cross-metathesis (CM) reaction (1) can be induced in the burning sub-surface the mass flux would be increased thus increasing burn rate. A rational choice of catalyst and a double bond donor (CM donor) have resulted in an increase of 20-35% in burn rate (figure) without the need to use nanometric or other materials that effect viscosity and workability.

Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Pharmaceutical Formulations: From API to Therapeutic Impact

Sivan Antler¹

R&D, Teva Pharmaceutical LTD., Israel

The development of pharmaceutical formulations is a critical step in transforming active pharmaceutical ingredients (APIs) into safe, effective, and patient-friendly dosage forms. This presentation provides a comprehensive overview of formulation science, starting with the key pre-formulation considerations, including API physicochemical properties, therapeutic requirements, and patient-centric factors. It explores formulation design principles such as dosage form selection, excipient functionality, and manufacturing feasibility, highlighting the pivotal role of excipients in achieving bioavailability, controlled drug release and stability. Advanced techniques for improving the solubility and bioavailability of poorly soluble drugs will be discussed alongside mechanisms for modulating drug release within the gastrointestinal tract. The session also addresses stability and shelf-life considerations including manufacturing challenges for successful product development and its commercialization. Attendees will gain insights into various strategies and practical approaches that drive formulation excellence and ensure therapeutic success.

Invited Lecture

Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Engineered Alternative Casein Proteins for Drug Delivery

Prof. Dganit Danino¹

*Cryo-EM Laboratory of Soft Matter, Department of Biotechnology and Food
Engineering, Technion, Israel*

Casein proteins are intrinsically disordered and amphiphilic. In nature, they collectively assemble into milk micelles; when isolated, however, they spontaneously self-organize into classical, well-defined soft core–shell micelles of nanometric dimensions.

We previously developed β -casein (bCN) micelles as delivery carriers, demonstrating high drug-loading capacity, excellent colloidal stability, and improved bioavailability of highly hydrophobic therapeutic compounds. Despite these advantages, the clinical translation of natural proteins is constrained by regulatory considerations.

To overcome these limitations, we now employ precision fermentation to produce a sustainable, animal-free, and functional casein analogue. This engineered protein preserves the key self-assembly and drug-encapsulation properties of native bCN and, through rational sequence modifications enables further optimization of pharmaceutical performance. The resulting platform offers a versatile and scalable delivery system for poorly soluble bioactives. This system can additionally function as a nanoscale bioreactor for drug reshaping, supporting advanced formulation strategies with translational and clinical potential.

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Europium Doped CsPbBr₃ Nano Crystals

Ayelet HaShachar Wallach^{1,2}, Hila Shalom¹

¹*Department of Chemical Engineering, Ariel University, Israel*

²*Alpha program, Future Scientists Center, Israel*

CsPbBr₃ is a useful halide perovskite metal. It has drawbacks, such as low photoluminescence (PL) efficiency and a short lifetime. Doping CsPbBr₃ with rare earth elements, specifically europium (Eu), improves CsPbBr₃'s characteristics. We hypothesized that changing the percentage of Eu doping will affect these characteristics. Our goal was to synthesize CsPbBr₃ nano crystals (NCs) and to check how the percentage of Eu doping affects the optical parameters and the PL stability of the NCs.

We used the hot injection technique to synthesize and dope CsPbBr₃ NCs with four different concentrations of Eu. The NCs were characterized in different manners. The size and shape of the NCs were characterized using Transmission Electron Microscopy and X-ray diffraction. The optical parameters and PL stability of the NCs were measured using a Spectrophotometer and a Spectrofluorometer.

The positive effect of Eu doping increases as the doping concentration increases. In CsPbBr₃ NCs 2.5 wt% Eu the doping effect was negligible. In CsPbBr₃ NCs 5 wt% Eu the doping was not successful. In CsPbBr₃ NCs 10 wt% Eu the doping effect on the optical parameters and PL stability was particularly pronounced. The PL intensity was twice the PL intensity of CsPbBr₃, the energy gap was wider, and the PL stability was significantly improved.

Our study provides insights into the effect of Eu doping on the optical parameters of CsPbBr₃ NCs. In addition, our study is the first to examine the effect of Eu doping on PL stability, opening the door for further research in this field.

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Impact of Hydrocarbon Chain Ligands on the Stability of Dispersed Small Nanoparticles

Yehonatan Levy¹, Daniel Harries¹

Fritz Haber center for molecular dynamics, Israel

Semiconductor nanoparticles (NPs) play crucial roles in many applications. A persistent challenge is stabilizing NPs in apolar solvents, where colloidal stability is often limited and rigorous theoretical descriptions are scarce. A common strategy is to modify the grafted ligands, yet longer chains do not always improve stability, in some cases, shortest ligands are most stabilizing. Our experiments show a non-monotonic dependence of stability on chain length for CdSe NPs: both short and long linear chains can destabilize particles, while intermediate lengths give the best stability. Here we propose to determine the effective interactions between NPs in solution as a function of ligand type by combining high-precision X-ray scattering with all-atom molecular-dynamics simulations.

In this performed systematic X-ray measurements across concentration and temperature to refine the effective interaction potentials and extract virial coefficients. In parallel, we use MD simulations to compute potentials of mean force between ligand-coated nanoparticles in explicit solvent. Our emphasis here is on the ligand's net effect on NP–NP repulsion and overall colloidal stability in apolar media. The combined experimental and computational approach should clarify how hydrocarbon ligand architecture controls stability and suggest simple design rules for robust NP dispersions. Ultimately, this study aims to bridge molecular-scale ligand properties with macroscopic phase behavior in relevant dispersions.

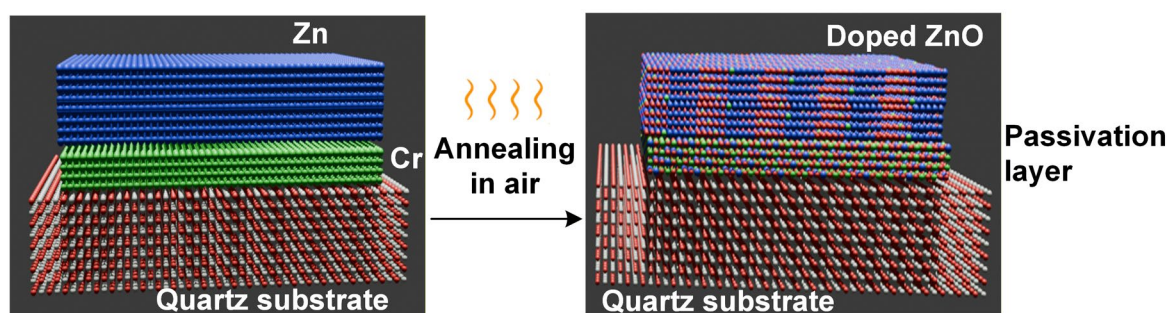
Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Defect–interface co-engineering in Cr-doped ZnO films

Men Guo¹, Dr. Gilad Orr¹, Prof. Paul Ben Ishai¹, Dr. Xia Zhao², Mr. Shlomo Glasser¹

¹Department of Physics, Ariel University, Israel

²Department of High Voltage, China Electric Power Research Institute, China



Defect–interface co-engineering in Cr-doped ZnO films

ZnO films are promising transparent electrodes in flexible and wearable electronics¹. However, it is still challenging to simultaneously improve the transmittance, conductivity, and stability^{2,3}. In order to improve the stability while maintaining higher optoelectronic properties of ZnO films, we proposed a new but feasible method, that is, annealing Cr-Zn layers deposited via DC magnetron sputtering in air. Microstructures of the films were investigated using X-ray diffraction, scanning electron microscopy, and atomic force microscopy, intrinsic point defects were identified via photoluminescence spectroscopy, and optical and dielectric properties were analyzed using a UV-vis spectrophotometer and dielectric spectrometer, respectively. It was found that the average grain sizes decrease (56.34~39.50 nm), the band gap increases (3.18~3.23 eV), and the transmittance (at 600 nm) decreases (91%~83%) with increasing Cr. Two activation energies of conduction increase after doping Cr, indicating enhanced temperature stability. With optimal doping, a higher transmittance and a lower resistivity are maintained, despite the passivation layer. Interestingly, Hall effect measurements also suggest that the carrier type can be tuned by varying Cr sputtering time. This method can be extended to other doped ZnO films, e.g., by further introducing Al, to achieve simultaneous improvements in transmittance, conductivity, and stability for flexible and wearable applications.

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Translational ColloidScience: Bridging Materials, Medicine, and Agriculture

Hydrophobic-hydrophilic Janus Meshes for Improved Directional Liquid Transport

Yarin Shiloni¹

School of Mechanical Engineering, Tel Aviv University, Israel

Fog harvesting is the process of collecting liquid water suspended in the air. Yet, in order to collect significant amounts of water, the transport of condensed water should be improved. The gain is twofold: greater overall water yield and continuous renewal of the surface area for further droplet capture.

Inspired by unique properties of asymmetric wettability found in nature, such as evident in insects, this study aims to enhance and improve fog collection by meshes engineered with different properties of hydrophobicity and hydrophilicity on each side (Janus faces), specifically designed for this study.

The current approach employs copper coating to establish hydrophobicity gradients and as a bedding for fluorosilanes that impart superhydrophobic behavior.

Droplets are therefore expected to accumulate on one side of the mesh, and once they reach a critical size, transition to the opposite side and then be directed downward, due to gravity, into a reservoir.

Meshes surfaces are characterized by contact angles and adhesion forces of liquid droplets to the solid surface a quantitative analysis of the condensation and transport dynamics of water on them. This will provide guidelines for the structural design and interfacial properties of meshes for fog harvesting.

