

# IVS-IPSTA 2023

## 40<sup>th</sup> Annual Conference

March 2<sup>nd</sup> • Nanocenter, Bar-Ilan University

### BOOK OF ABSTRACTS

**Sponsors:**

**Exhibitors:**

**PROGRAM**

9:00-9:30	Registration & Gathering <b>Introduction &amp; Welcome: Prof. Arie Zaban, BIU President &amp; Prof. Daniel Nessim (BIU) IVS President</b>
9:30-9:50	<b>Plenary session I: Avi Domb (HUJI, Israel Chief Scientist)</b>
9:50-10:25	<b>“Innovation, Science and Technology in Israel”</b>
10:25-10:50	Coffee Break
10:50-13:00	Morning Parallel Sessions
13:00-14:50	Lunch with Poster Presentations
14:50-17:00	Afternoon Parallel Sessions
17:00-17:20	Coffee Break
17:20-17:55	<b>Plenary session II: Prof. Zeev Zalevsky (BIU) IVS Research Excellence Award</b>
17:55-18:15	Conclusions / prizes
18:15-18:30	IVS General assembly
18:30	Speakers lab visit & dinner (by invitation only)

---

The Organizing Committee:

Daniel Nessim (BIU) | Amos Bardea (HIT) | Gary Eliad (BIU) | Irit Rosenhek-Goldian (WIS)

---

## Contents

<b>Program</b>	<b>4-5</b>
<b>Posters abstracts</b>	<b>6-103</b>
<b>Energy and Sustainability: Materials, Methods, and Breakthroughs (ES)</b>	<b>6-32</b>
<b>Surface Science (SS)</b>	<b>33-49</b>
<b>Frontiers in Nano Photonics (NP)</b>	<b>50-56</b>
<b>Bio Applied Surfaces and materials (BI)</b>	<b>57-65</b>
<b>Nanomaterials (NM)</b>	<b>66-78</b>
<b>Smart and Multifunctional Materials and Devices: Transducers, Sensors and Actuators (SM)</b>	<b>79-88</b>
<b>Computational Modeling and Data Science for New Materials (CM)</b>	<b>89-93</b>
<b>Nanoscience for future quantum technologies: novel materials, devices, and characterizations (NS)</b>	<b>94-97</b>
<b>Plasma Science (PS)</b>	<b>98-103</b>

## MORNING SESSIONS

Keynote  
Invited  
Contributed

**Bio Applied Surfaces and Materials**  
Chair: Christopher Arnusch (BGU)

- 10:50 Han Zuilhof (The Netherlands), The light way to polymer brushes  
 11:15 Axel Rosenhahn (Germany), Amphiphilic coatings for marine antifouling applications  
 11:40 Meital Reches (HUJI), Biodegradable and environmentally-friendly peptide-based functional coatings  
 12:00 Zvi Yaari (HUJI), AI-Guided Optical Sensors for The Early Detection of Gynecologic Cancers  
 12:20 Camilah Powell (BGU), Laser-induced Graphene Capacitive Killing of Bacteria  
 12:33 Aneena Lal (Ariel University), Laser-processed Direct Coating of Graphene-Based Films on Plastic Substrates with Anti-Bacterial Properties  
 12:46 Adi Hendler-Neumark (TAU), Near-infrared fluorescent single-walled carbon nanotubes for In vivo imaging within C. elegans nematodes

**HALL Energy and Sustainability: Materials, Methods, and Breakthroughs**  
Chair: Hannah Noa Barad (BIU)

- 10:50 Peter Strasser (TUB), Electrocatalytic materials, interfaces, and devices for the production of e-fuels and e-chemical  
 11:15 Iris Visoly-Fisher (BGU), Surface science for sustainability: Pb leaching from halide perovskites  
 11:40 Idan Hod (BGU), Molecular manipulation of heterogeneous electrocatalytic CO<sub>2</sub> reduction using metal-organic frameworks  
 12:00 Michal Leskes (WIS), Elucidating the structure and function of the electrode-electrolyte interface by new solid state NMR approaches  
 12:20 Maya Bar-Sadan (BGU), Complex bimetallic and monometallic phosphides as catalysts  
 12:33 Gideon Segev (TAU), Operando characterization of charge extraction and recombination profiles in solar cells with nanoscale resolution  
 12:46 Ortal Lidor-Shalev (BIU), Molecular layer deposition of alucone thin film on LiCoO<sub>2</sub> to enable high voltage operation

**Nanomaterials**

Chair: Ronen Gottesman (HUJI)

- 10:50 Uri Banin (HUJI), Coupled Colloidal Quantum Dot Molecules  
 11:15 Daniel Mandler (HUJI), From Nano to Nano: A Different Approach for the Formation of Thin Films of Nanomaterials  
 11:40 Menny Shalom (BGU), Photo- and electrocatalyst development for catalytic oxidation of organic molecules to value-added chemicals  
 12:00 Gil Markovich (TAU), Anisotropic Optical Activity in Chiral Tellurium Nanocrystals  
 12:20 Arie Borenstein (Ariel U.), Recent progress in Laser Processing of Carbon nanomaterials  
 12:33 Rotem Azoulay (Technion), Spatially Controlled Atomic Layer Deposition within Polymer Templates for Multi-Material Nanorods and Nanowires Fabrication  
 12:46 Iris Berg (HUJI), Selective Deposition of N-Heterocyclic Carbene Monolayers on Designated Au Microelectrodes Within an Electrode Array

**Nanoscience for Future Quantum Technologies: Novel Materials, Devices, and Characterizations**

Chair: Assaf Ben-Moshe (BIU)

- 10:50 Efrat Lifshitz (Technion), Magnetic-electronic coupling in semiconductor nanostructures  
 11:15 Amos Sharoni (BIU)  
 11:40 Eran Maniv (BGU), Antiferromagnetic switching driven by the collective dynamics of a coexisting spin glass  
 12:00 Tal Schwarz (TAU), From enhanced diffusion to ultrafast ballistic motion of hybrid light-matter excitations  
 12:20 Salma Khaldi (HUJI), Vapor Phase Deposition of Chiral Thin Films by Atomic and Molecular Layer Deposition Showing Spin Selective Transport  
 12:33 Ora Bitton (Weizmann), Plasmonic cavities and individual quantum emitters in the strong coupling limit  
 12:46 Gili Scharf (TAU), Pressure Tuning of Berry curvature in CrGeTe<sub>3</sub>

**Plasma**

Chair: Prof. Yosi Pinchasi (Ariel U.)

- 10:50 Aharon Friedman (Ariel U.), First Observation of Superradiant TeraHertz Radiation at the Israeli Free Electron Laser  
 11:20 H. Strauss (HRS Fusion, Jerusalem, Israel), Disruptions in the ITER Tokamak  
 11:40 A.S. Kesar (Soreq NRC), Fast solid-state switches at Soreq NRC  
 12:00 D. Maler, (Technion), Supersonic water jets as point-like sources of extremely high pressure  
 12:20 Yosef Golovachev (Jerusalem College of Technology), The Propagation of Ultra-Wideband Modulated Pulses in Plasma Media  
 12:40 T. Miller (Rafael Advanced Defense Systems), RF plugging of multi-mirror machines

Keynote  
Invited  
Contributed

**Surface Science**  
Chair: Ilan Goldfarb (TAU)

- 14:50 Edward Bormashenko (Ariel University) Quantification of Ordering in 2D Patterns
- 15:15 Moshe Ben Shalom (TAU), Ladder Ferroelectrics by vdW Sliding
- 15:40 Beena Kalisky (BIU), Imaging quantum materials with scanning SQUID microscopy
- 16:00 Igor Rahinov (Open U) Steric hindrance of NH<sub>3</sub> diffusion on Pt(111) by co-adsorbed O-atoms
- 16:20 Adva Ben-Yaacov (WIS) On the interaction of hydrogen with ceria in ambient conditions: hydride formation VS hydroxylation of the surface
- 16:33 Alexandr Leontev (Technion) Analyzing and modeling of microrheological and adhesive properties of soft hydrated surfaces by AFM and flow cell tests
- 16:46 Tatyana Bendikov (WIS) Charge Transport across Biomolecular Electronic Junctions. Ultraviolet and X-ray Photoemission Spectroscopy Studies

**Frontiers in Nanophotonics**  
Chair: Nir Shitrit (BGU)

- 14:50 Nir Davidson (WIS), Solving computational problems with coupled lasers
- 15:15 Marco Sampietro (Politecnico di Milano) Electronics into a photonic chip: Technological challenges and functional advantages in dense photonic architectures
- 15:40 Boubacar Kante (UC Berkeley) tbd
- 16:00 Ofer Kfir (TAU) Electron-photon coupling: From fundamentals to quantum correlated nanoscopy
- 16:20 Hodaya Klimovsky (BIU) Smart surfaces enable near-field detection by simple far-field optic
- 16:33 Raghendra P. Chaudhary (BGU) Observation of the orbit-orbit interaction of light in plasmonics
- 16:46 Sivan Tzadka (BGU), Antireflective structures directly imprinted on chalcogenide glasses

**Smart and multifunctional materials and devices: transducers, sensors, and actuators**  
Chair: Yonatan Calahorra (Technion)

- 14:50 Elisabetta Comini (U. Brescia), Metal oxide nanostructures as building blocks for energy and environmental applications
- 15:15 Esti Segal (Technion), Self-Reporting Porous Silicon Arrays as a Playground for Microorganisms
- 15:40 Roei Yerushalmi (HUJI) Novel Device Concepts using Nano-Florets Metal-SC Hybrid Nanosystems
- 16:00 Alla Zak (HIT) WS<sub>2</sub> & MoS<sub>2</sub> from 3D to 1D structures: Curvature and chirality induced properties of nanotubes
- 16:20 Ronen Verker (Soreq) Infrared Irradiated Reversible Shape Memory Polymers - Mechanisms and Applications
- 16:33 Shiran Ziv Sharabani (TAU) Messy or ordered? Multi-scale mechanics dictates shape-morphing of hierarchical 2D fiber-networks
- 16:46 Daniel Kaufmann (BGU) Novel bioelectronic interface based on mucin-modified electrodes

**Computational modeling and data science for new materials**  
Chair: Ilya Grinberg (BIU)

- 14:50 Leeor Kronik (WIS), Defects, defect tolerance, and self-healing in lead halide perovskites: a first principles perspective
- 15:15 Dan Major (BIU), Computational studies of structure, composition, and electrochemical behavior of Li-ion battery components
- 15:40 Oswaldo Dieguez (TAU), Trends of the mean inner potential of solids from computations using density-functional theory
- 16:00 Eli Kraissler (HUJI), Potentials in density functional theory (DFT): exact properties and advanced approximations
- 16:20 Long Nguyen (BGU), Structural prediction of group IV monochalcogenides and their phase transitions mechanism: Evolutionary algorithm and ab-initio calculations
- 16:33 Hillel Kugler (BIU), Network-Based Biocomputation Circuits
- 16:46 María Camarasa-Gómez (WIS), Transferability of screened range-separated hybrid functionals for layered materials

**Plasma**  
Chair: Yosi Pinchasi (Ariel U.)

- 14:50 Samuel A. Cohen (Princeton), Physics of Field-reversed Configuration (FRC) Fusion Reactors
- 15:20 Adva Ben-Yaacov (WIS), On the interaction of hydrogen with ceria in ambient conditions: hydride formation VS hydroxylation of the surface
- 15:40 Eli Gudinetsky (HUJI & Nuclear Research Center), Autoresonant ash removal in magnetic mirrors
- 16:00 Anat Itzhak (BIU), Reactive sputtering of nickel nitride passivation layers Improves halide perovskite P-LN solar cells
- 16:20 Yossi Rabinovich (Ariel U.),
- 16:40 Asher Yahalom (Ariel U.), Non-ideal Magnetohydrodynamics – a Comparative Study

**Energy and Sustainability: Materials, Methods, and Breakthroughs**

**(ES)**

# Engineering of solid oxide fuel cell's electrode containing a heterogeneous catalyst for simultaneous ammonia synthesis and energy conversion

Or Rahumi<sup>1</sup>, Manasa Kumar Rath<sup>1</sup> and Konstantin Borodianskiy<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, Ariel University, Ariel, Israel.

Solid oxide fuel cells (SOFC) are prominent electrochemical devices for directly converting chemical energy into electricity due to their fuel flexibility and high conversion efficiency, at a high-operating temperature range of 600–800°C [1]. Alongside the generated electrical power, rarely SOFC's operation can be expanded also to the coproduction of desired chemical components during the cell's operation as a valuable byproduct [2,3].

Ammonia (NH<sub>3</sub>) is one of the most demanded chemicals in the world. Up to these days, ammonia is being produced through the well-known Heber-Bosch process, which requires strict operating conditions and involves high greenhouse gas emissions and high energy consumption [4]. Therefore, the co-production of electricity and ammonia using a SOFC operation is an innovative and cost-efficient approach.

In this study, manganese-nitride modified Ni-ScSZ supported SOFC was fabricated for simultaneous ammonia synthesis and energy conversion. X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) analysis revealed the chemical stability of the nitride catalyst under H<sub>2</sub> and N<sub>2</sub> atmospheres at cell operating conditions, and the nitrogen reduction reaction (NRR) over the Mn<sub>4</sub>N active sites was confirmed. Electrochemical impedance (EIS) analysis revealed improved activity toward hydrogen oxidation reaction and NRR during cell operation. The catalyst-modified cell exhibited peak power densities of 539 and 374 mW·cm<sup>-2</sup> for humidified H<sub>2</sub> and dry N<sub>2</sub>/H<sub>2</sub> (1:1) mixture, respectively. Furthermore, a significantly high rate of ammonia production  $1.63 \times 10^{-9}$  mol cm<sup>-2</sup> s<sup>-1</sup> combined with a power density of 348 mW cm<sup>-2</sup> was achieved at 800°C.

- [1] N. Q. Minh, *Solid State Ionics*, **174**, 271–277, 2004.
- [2] K. Panagi, C. J. Laycock, J. P. Reed, and A. J. Guwy, *Appl. Energy*, **255**, 113854, 2019.
- [3] A. Perna, et. al., *Appl. Energy*, **231**, 1216–1229, 2018.
- [4] J. W. Erisman, et. al., *Nat. Geosci.*, **1**, 636–639, 2008.

## Carbon nanodots for all-in-one photo(electro)catalytic performance

**B. Jana**\*<sup>1,2</sup>, **Y. Reva**,<sup>1</sup> **Alejandro Cadranel**<sup>1</sup>, **Lilac Amirav**<sup>2</sup> and **Dirk M. Guldi**\*<sup>1</sup>

<sup>1</sup>Department of Chemistry and Pharmacy & Interdisciplinary Center for Molecular Materials (ICMM), Physical Chemistry I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

<sup>2</sup>Technion – Israel Institute of Technology, Schulich Faculty of Chemistry, Technion, 3200008 Haifa, Israel

Dual functionalized carbon nanodots (CNDs) were photochemically altered to produce dihydrogen from seawater under light irradiation without any external photosensitizer or co-catalyst. Record hydrogen evolution reaction activity of  $19.70 \text{ mmol (H}_2\text{) g(catalyst)}^{-1} \text{ h}^{-1}$  was obtained after 1 hour of  $75 \text{ mW/cm}^2$  Xe lamp illumination. [1] Subsequently, the photoelectric performance of electron-rich, yellow CNDs (yCNDs) obtained by the *in-situ* addition of NaOH during synthesis, while otherwise electron-deficient, red CNDs (rCNDs) were inscribed. [2] The catalytic mechanism is comprehended through a full-fledged physicochemical investigation based on an arsenal of steady-state and time-resolved spectroscopic characterizations together with microscopy and electrochemistry (Fig. 1).

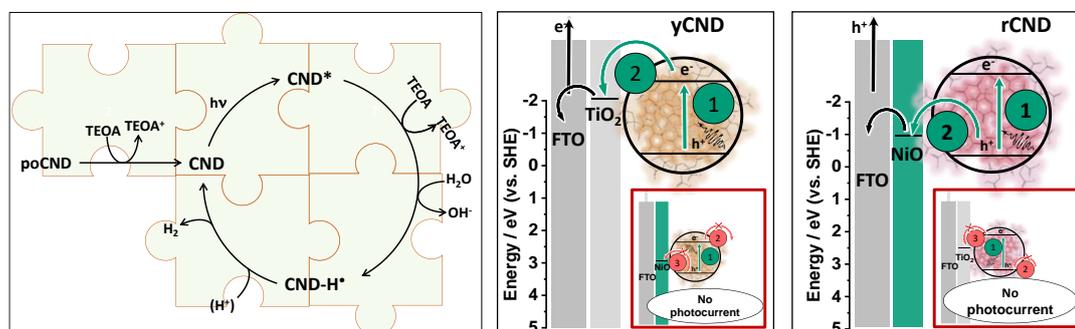


Fig. 1: Photo(electro)catalytic mechanism.

[1] B. Jana\*, Y. Reva, T. Scharl, V. Strauss, A. Cadranel\*, D. M. Guldi\*, J. Am. Chem. Soc. 2021, **143**, 20122 (2021).

[2] Y. Reva,<sup>‡</sup> B. Jana,<sup>\*‡</sup> D. Langford, M. Kinzelmann, Y. Bo, P. R. Schol, T. Scharl, X. Zhao, R. W. Crisp, T. Drewello, T. Clark, A. Cadranel,\* D. M. Guldi\*, Small, **Accepted** (2023) (<sup>‡</sup> contributed equally).

# Electrochromic Metallo-Organic Films: Spray-Coating, On-Surface Self Assembly, and Laminated Devices

Naveen Malik, Michal Lahav and Milko E. van der Boom

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

Email: naveen.malik@weizmann.ac.il

Electrochromic materials (ECMs) reversibly change their optical properties when applying a potential. ECMs can find extensive applications in smart windows, sunglasses, anti-glare mirrors, display technology, etc. Various ECMs based on organic polymers, metallo-organic polymers, polyelectrolytes, transition metal oxides (TiO<sub>2</sub>, ZnO, WO<sub>3</sub>, etc.) have been studied for several decades.<sup>[1]</sup> A combination of various factors still limit the large-scale commercial implementation of electrochromic windows, including fabrication cost, optical contrast, stability, low switching speed, and scalability. Recently, our group investigated the electrochromic properties of molecular assemblies formed from iron, ruthenium and osmium polypyridyl complexes using layer-by-layer (LBL) dip-coating or spin-coating methods.<sup>[2]</sup>

In this study, we demonstrate spray-coating for the formation of homogeneous and uniform electrochromic assemblies on transparent-conductive oxides (TCOs) on both rigid and flexible substrates with surface areas of up to 36 cm<sup>2</sup>. This fast and versatile process is suitable for the on-surface production of self-assembled 3D-networks with a high chromophore density using polypyridyl complexes and a metal salt. These films have been integrated into laminated electrochromic devices (ECDs) containing a gel electrolyte and a conductive polymeric layer as the charge storage layer. The ECDs have attractive ON/OFF ratios (50%) and electrochemical stabilities up to >1000 redox cycles. In this study, we also observed that, the performance/stability of the ECDs depends on the type of counter anion of the gel electrolyte.<sup>[3]</sup>

## References

[1] McConnell, A. J.; Wood, C. S.; Neelakandan, P. P; Nitschke, J. R. *Chem. Rev.* **2015**, *115*, 7729.

[2] Lahav M. and van der Boom M. E. *Advanced Materials*, **2018**, *30*, 1706641.

[3] (a) Malik, N.; Singh, V.; Shimon, L.; Houben, L.; Lahav, M.; van der Boom, M. E. *J. Am. Chem. Soc.* **2021**, *143*, 16913. (b) Malik, N.; Dov, N. E.; de Ruiter, G; Lahav, M; van der Boom, M. E. *ACS Appl. Mater. Interfaces* **2019**, *11*, 22858.

## A combinatorial approach to the exploration of multi-metallic gradient libraries for the oxygen evolution reaction

**Anagha Usha Vijayakumar, Hannah Noa Barad\*, David Zitoun\***

*Department of Chemistry and Bar-Ilan Institute for Technology and Advanced Materials (BINA), Bar-Ilan University, Ramat Gan 5290002, Israel.*

*\*e-mail: uv.anagha@gmail.com , David.Zitoun@biu.ac.il*

A sustainable future based on hydrogen fuel rests its faith on the rapid advancement of non-precious metal catalysts for the oxygen evolution reaction (OER). Nickel based systems are the most studied catalysts for OER in alkaline media and various multicomponent systems involving Fe, Co, V, Cr *etc*, have been explored, although a systematic investigation is lacking and there are discrepancies as to which formulations make the best catalyst. We demonstrate the efficient utilisation of time and effort in the analysis of a vast compositional space of binary NiFe and ternary NiFeV and NiFeCo alloys for OER using a combinatorial method<sup>[1]</sup>. This approach thrives on the principle of parallel processing which makes it much more efficient than the linear traditional

approach by accelerating material discovery, offering higher data fidelity and an increased access to a broader range of materials<sup>[2]</sup>. We synthesised the gradient libraries using spray pyrolysis and physical vapour deposition techniques and their electrochemical activity was analysed using an automated scanning droplet cell (SDC) set up

composition-activity relationship. We establish the reliability and efficiency of this combinatorial approach whilst also providing insights into the design of high performing OER catalysts.

### References

1. Vijayakumar, A. Usha, et al. "Combinatorial Synthesis and Screening of a Ternary NiFeCoO<sub>x</sub> Library for the Oxygen Evolution Reaction." *ACS Applied Energy Materials* 5.4 (2022): 4017-4024.
2. Barad, Hannah-Noa, et al. "Combinatorial growth of multinary nanostructured thin functional films." *Materials Today* 50 (2021): 89-99.

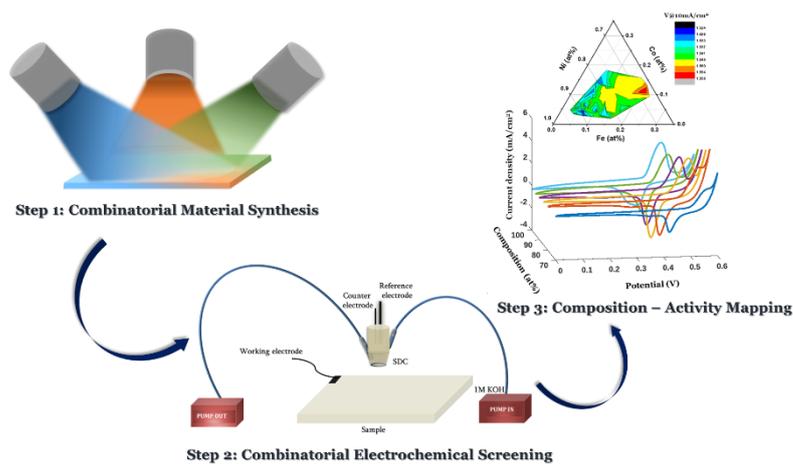


Fig 1. Schematic representation of work execution

## Diverging expressions of anharmonicity in halide perovskites

Adi Cohen<sup>1</sup>, Thomas M. Brenner<sup>1</sup>, Johan Klarbring<sup>2</sup>, Rituraj Sharma<sup>1</sup>, Douglas H. Fabini<sup>3</sup>, Roman Korobko<sup>1</sup>, Pabitra K. Nayak<sup>4</sup>, Olle Hellman<sup>2</sup>, and Omer Yaffe<sup>1,\*</sup>

<sup>1</sup>Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot 76100, Israel

<sup>2</sup>Theoretical Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden

<sup>3</sup>Max Planck Institute for Solid State Research, Stuttgart 70569, Germany

<sup>4</sup>TIFR Centre for Interdisciplinary Sciences, Tata Institute of Fundamental Research, Hyderabad 500046, India

Lead-based halide perovskite (PbHaP) crystals were shown to have strongly anharmonic structural dynamics. This behavior is important because it may be the origin of their exceptional photo-voltaic properties. The double perovskite,  $\text{Cs}_2\text{AgBiBr}_6$ , has been recently studied as a lead-free alternative for optoelectronics applications. However, it does not exhibit the excellent photo-voltaic activity of the PbHaPs.

Therefore, to explore the correlation between the anharmonic structural dynamics and optoelectronic properties in PbHaPs, we investigate the structural dynamics of  $\text{Cs}_2\text{AgBiBr}_6$  and compare it to its lead-based analog  $\text{CsPbBr}_3$ . Using temperature-dependent Raman measurements, we find that both materials are indeed strongly anharmonic. Nonetheless, the expression of their anharmonic behavior is markedly different.

The anharmonicity in  $\text{Cs}_2\text{AgBiBr}_6$  is expressed by a displacive phase transition, and yet has well-defined normal modes throughout the measured temperature range. However,  $\text{CsPbBr}_3$  shows fluid-like inelastic light scattering, leading to a complete breakdown of the normal mode picture at elevated temperature. Our results suggest that the specific expression of fluid-like motion is imperative for the superior electronic properties in perovskites.

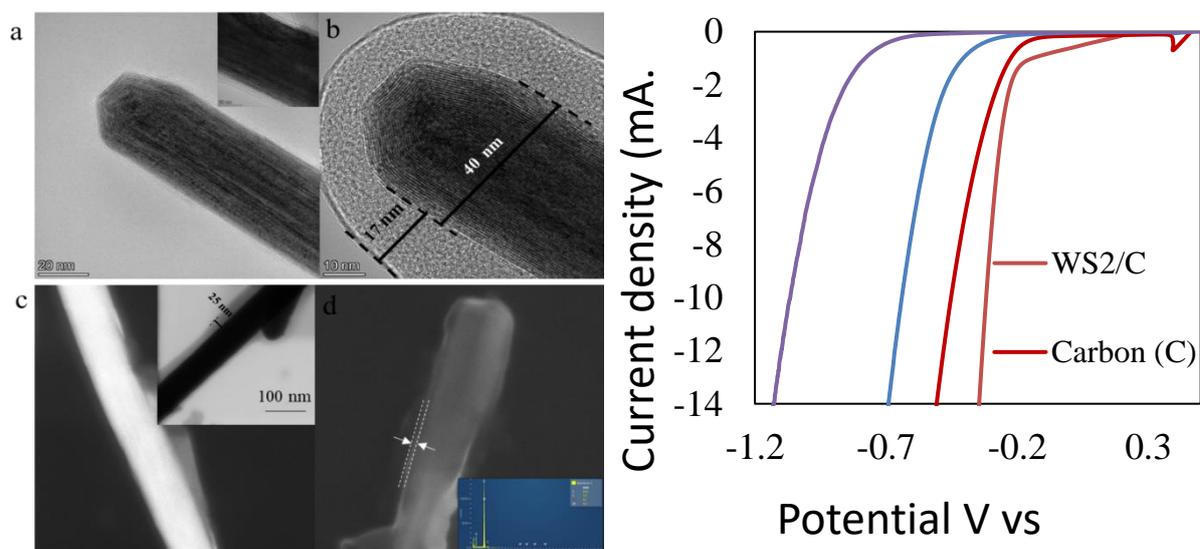
## Innovative N-doped carbon coated WS<sub>2</sub> nanotubes for efficient hydrogen evolution reaction (HER)

A. Dutta<sup>1</sup>, A. Borenstein<sup>1</sup>

<sup>1</sup>Department of Chemical Sciences, Ariel University, Israel

Hydrogen energy is considered to be an excellent potential and a an alternative of fossil fuels energy source owing to the merits of large [energy density](#), high calorific value, environmental friendliness with zero carbon footprints . Two-dimensional transition metal dichalcogenides (TMDCs) are an emerging class of materials with properties for applications ranging from nanoelectronics and nanophotonic to sensing. Most of the research groups is mainly focused on others forms of WS<sub>2</sub> structure (Bulk, flakes, sheets) due to increased edge site density relative to bulk crystals where the majority of atoms remain chemically inactive for HER. We report patching of WS<sub>2</sub> nanotube with carbon. The added carbon with WS<sub>2</sub> after annealing at high temperature (800<sup>0</sup>C) in presence of N<sub>2</sub> inert atmosphere create a thin layer around the tube which apparently can adjust the electronic state of the surface of the tube. Moreover, addition of carbon helps to increase the intrinsic conductivity, which leads to improve electrochemical performances. We can modify the tubes however does not change the original active form of the tube. Compare with the tube, tube modified with carbon exhibits excellent HER performance under both acidic and alkaline conditions. Under acidic conditions, the overpotential is 0.282 mV at 10 mA cm<sup>-2</sup> and under alkaline conditions, the overpotential at 10 mA cm<sup>-2</sup> is 0.353 mV, all of which have excellent catalytic stability.

We introduce carbon doped WS<sub>2</sub> as a HER electrochemical catalyst, which may provide new opportunities for discovering high surface activity and low-cost doped WS<sub>2</sub> as water-splitting materials.



## Static and Dynamic Disorder in Formamidinium Lead Bromide Single Crystals

**Guy Reuveni<sup>1</sup>, Yael Diskin-Posner<sup>2</sup>, Christian Gehrman<sup>3</sup>, Shravan Godse<sup>3</sup>, Giannis G. Gkikas<sup>4</sup>, Isaac Buchine<sup>5</sup>, Sigalit Aharon<sup>1</sup>, Roman Korobko<sup>1</sup>, Constantinos C. Stoumpos<sup>4</sup>, David A. Egger<sup>3</sup>, Omer Yaffe<sup>1</sup>**

<sup>1</sup> Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel

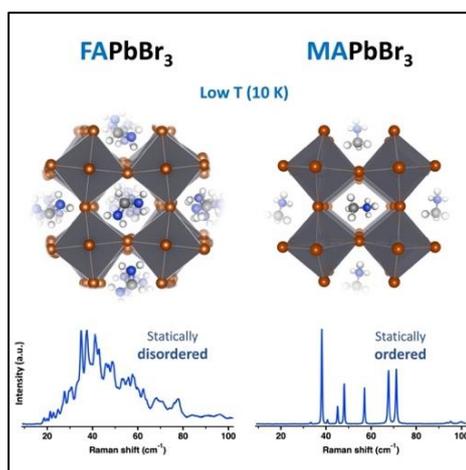
<sup>2</sup> Chemical Research Support, Weizmann Institute of Science, Rehovot, Israel

<sup>3</sup> Department of Physics, Technical University of Munich, 85748 Garching, Germany

<sup>4</sup> Department of Materials Science and Technology, University of Crete, Voutes Campus, Heraklion, Greece

<sup>5</sup> Department of Chemistry and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat Gan, Israel

We show that formamidinium-based are distinct from methylammonium-based halide perovskite crystals because their inorganic sub-lattice exhibits intrinsic local static disorder that co-exists with a well-defined average crystal structure. Our study combines terahertz-range Raman scattering with single-crystal X-ray diffraction and first-principles calculations to probe the evolution of inorganic sublattice dynamics with temperature in the range of 10–300 K. Our findings suggest that the static disorder at low temperatures is related to the bulky FA molecule and demonstrate that it augments the dynamic disorder present at higher temperatures in  $\text{FAPbBr}_3$ . The temperature evolution of the Raman spectra shows that low-temperature, local static disorder strongly affects the crystal structural dynamics and phase transitions at higher temperatures. Our results potentially have significant implications for the optoelectronic and thermal stability properties of FA-based lead halide perovskites.



*Fig. 1: Comparison between  $\text{FAPbBr}_3$  and  $\text{MAPbBr}_3$  at 10 K. Top: schematic representation of the structures. Bottom: terahertz Raman scattering showing a plethora of lattice vibrations of  $\text{FAPbBr}_3$ , compared to that of  $\text{MAPbBr}_3$ , demonstrating the relaxation of Raman selection rules due to a high degree of static disorder.*

[1] Reuveni, Guy, et al. "Static and Dynamic Disorder in Formamidinium Lead Bromide Single Crystals", *J. Phys. Chem. Lett.* 2023, 14, 5, 1288–1293. doi:10.1021/acs.jpcllett.2c03337.

## AZ31 Magnesium Alloy Foils as Thin Anodes for Rechargeable Magnesium Batteries

A. Maddegalla<sup>1</sup>, A. Mukherjee<sup>1</sup>, J.A. Blázquez<sup>2</sup>, E. Azaceta<sup>2</sup>, O. Leonet<sup>2</sup>, A. R. Mainar<sup>2</sup>, A. Kovalevsky<sup>3</sup>, D. Sharon<sup>1,4</sup>, J-F. Martin<sup>5</sup>, D. Sotta<sup>5</sup>, Y. E. Eli<sup>6,7</sup>, D. Aurbach<sup>1</sup>, and Malachi Noked<sup>1</sup>

<sup>1</sup> Department of Chemistry, Bar Ilan University, Ramat Gan, Israel

<sup>2</sup>CIDETEC, Basque Research and Technology Alliance (BRTA), Sebastian, Spain

<sup>3</sup>Israel Institute of Metals, Technion R&D Foundation, Technion City, Haifa, Israel

<sup>4</sup>Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

<sup>5</sup>CEA-LITEN, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France

<sup>6</sup>Department of Materials Science and Engineering, Technion-Israel Institute of Technology, Haifa, Israel

<sup>7</sup>Grand Technion Energy Program (GTEP), Technion-Israel Institute of Technology, Haifa, Israel

Recently, Rechargeable Magnesium Batteries (RMBs) emerged as promising next - generation energy storage technologies based on abundant elements, as the use of thin Mg foils as anodes that enables to develop high energy densities batteries.[1] Most RMB studies concentrate on the development of novel electrolyte systems, while only few studies have focused on the practical feasibility of using pure metallic Mg as the anode material. Though pure Mg metal anodes are useful to understand fundamentals of non-aqueous Mg electrochemistry, commercialization of ultrathin Mg foils ( $< 100\mu\text{m}$ ) has a disadvantage due its low ductility. We demonstrate herein the feasibility of processing ultrathin Mg anodes in electrochemical cells by using AZ31 Mg alloys (3% Al; 1% Zn). [2] Thin film Mg AZ31 anodes present reversible Mg dissolution and deposition behavior in complex ethereal Mg electrolytes solutions that is comparable to that of pure Mg foils. Moreover, we demonstrated that secondary Mg battery prototypes comprising ultrathin AZ31 Mg alloy anodes ( $\approx 25\mu\text{m}$  thick) and  $\text{Mg}_x\text{Mo}_6\text{S}_8$ -Chevrel phase cathodes exhibit cycling performance that is equal to that of similar cells containing thicker pure Mg foil anodes. The possibility of using of ultrathin processable Mg metal anodes is an important step in the realization of rechargeable Mg batteries.

[1] D. Aurbach, Y. Gofer, Z. Lu, A. Schechter, O. Chusid, H. Gizbar, Y. Cohen, V. Ashkenazi, M. Moshkovich and R. Turgeman, *J. Power Sources*, **97**, 28 (2001).

[2] J.Niu, Z. Zhang, and D. Aurbach, *Adv. Energy Mater.*, **10**, 1 (2020).

## High entropy: an emerging prospect for design of Na-ion battery cathode

Akanksha Joshi, Sankalpita Chakrabarty and Malachi Noked

*Department of Chemistry, Institute of Nanotechnology and Advanced Materials,*

*Bar-Ilan University, Ramat Gan 5290002, Israel*

*E-mail: akanksha1991joshi@gmail.com*

Li ion batteries have already electrified our present and future. However, declining Lithium resources have pushed the researchers to explore its alternative and here comes in the picture “Sodium ion battery” because of the abundancy of sodium resources [1]. In theory, it seems easy to replace lithium by sodium thanks to their similar chemical properties, but random disclosures are often found due to unknown interaction of host structure depending on sodium and lithium intercalation/de-intercalation. To compete with the Li ion batteries, it is needed to develop efficient cathode materials that are able to accommodate larger sodium ions without structure degradation and that too without cobalt in view of some serious concern [2]. Recent studies have reported that the entropy stabilized oxides are able to accommodate larger sodium ions with high structural stability [3, 4].

Keeping in view the above mentioned concerns and studies, here we report a multiple cation and anion high entropy cathode that delivers reversible initial discharge capacity of 109 mAh g<sup>-1</sup> (90% retention up to 200 cycles) and 144.7 mAh g<sup>-1</sup> (70% retention up to 130 cycles) within 2-4V and 2-4.3V respectively. This study paves a way to design the efficient stable cathode for Na ion batteries.

### References:

1. Dongliang Chao et al., Roadmap for advanced aqueous batteries: From design of materials to applications, Chao et al., *Sci. Adv.* 2020; 6 : eaba4098.
2. Water Science School. U.S. Geological Survey. [https://www.usgs.gov/special-topic/water-science-school/science/acid-rainand-water?qt-science\\_center\\_objects=0#qt-science\\_center\\_obj](https://www.usgs.gov/special-topic/water-science-school/science/acid-rainand-water?qt-science_center_objects=0#qt-science_center_obj).
3. A. Sarkar, L. Velasco, D. Wang, Q. Wang, G. Talasila, L. de Biasi, C. Kgbel, T. Brezesinski, S. S. Bhattacharya, H. Hahn, B. Breitung, *Nat. Commun.* 2018, 9, 3400
4. C. Zhao, F. Ding, Y. Lu, L. Chen, and Y. Hu, *Angew. Chem. Int. Ed.* 2020, 59, 264–269.

## The effect of the amount of residual sodium in the active material NMC 532 after an innovative recycling process

Yakir Kabalo and Malachi Noked <sup>1</sup>

<sup>1</sup> Department of Chemistry, The Institute for Nanotechnology, Advanced Materials Bar-Ilan University, Ramat-Gan, Israel, Ramat Gan, 5290002, Israel

Following the increase in the use of lithium-ion batteries in recent years, the amount of battery waste has also increased. The waste includes toxic and expensive transition metals such as cobalt and nickel. Therefore, battery recycling is necessary to protect the environment and make better use of the resources at our disposal.

In this work, we demonstrated the difference between NMC 532 cathode active materials containing different amounts of sodium after an innovative recycling process that includes the use of hydrobromic acid HBr. The samples in which NaOH was used in the precipitation process presented an initial specific capacity that depends on the amount of residual sodium, as the amount of sodium decreased the initial specific capacity increased. On the other hand, the stability of these samples (78-83%) is less than samples whose precipitation process uses LiOH instead of NaOH (89-94%) over 100 cycles as can be seen in Figure 1.

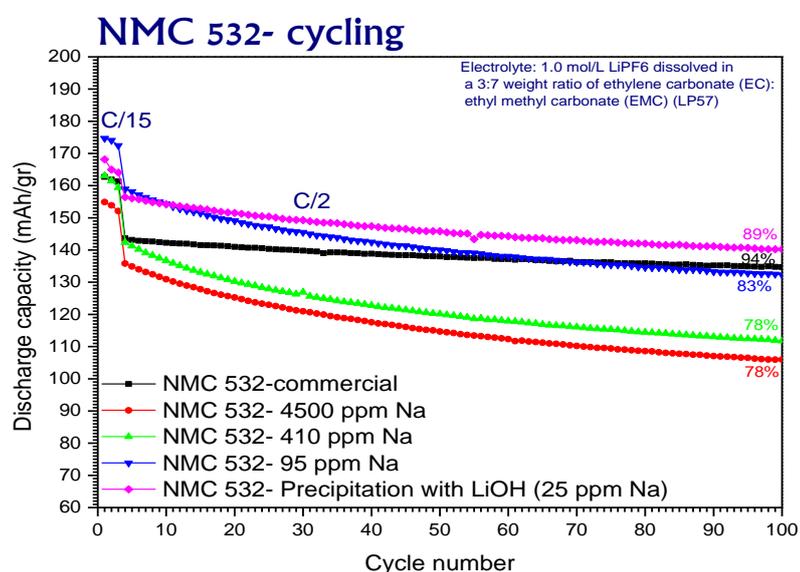


Fig. 1. The effect of the amount of sodium and the precipitation process on the specific capacity over 100 cycles.

## Unusual Surface Texture: Multidomain Single Crystal and Chirality

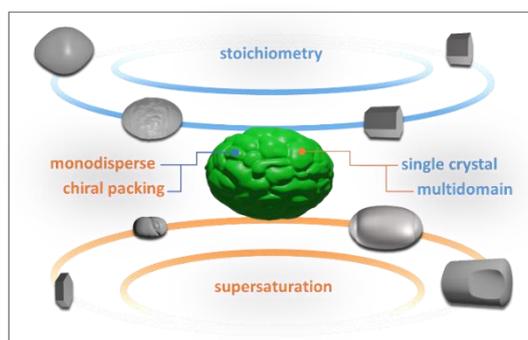
V. Singh,<sup>1</sup> L. Houben,<sup>2</sup> L. J. W. Shimon,<sup>2</sup> S. R. Cohen,<sup>2</sup> Y. Feldman,<sup>2</sup> O. Golani,<sup>3</sup> M. Lahav<sup>1</sup> and M. E. van der Boom<sup>1</sup>

<sup>1</sup>Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot, Israel

<sup>2</sup>Department of Chemical Research Support, Weizmann Institute of Science, Israel

<sup>3</sup>Department of Life Sciences Core Facilities, Weizmann Institute of Science, Israel

Metal-organic frameworks (MOFs) are among the most studied crystals because of their many different possible applications.<sup>[1-3]</sup> However, the factors that influence the growth of such crystals are not very well understood. Controlling dimensions and morphology is a challenge in these materials.<sup>[4]</sup> Moreover, homogeneity of morphology and crystallographic phase with monodispersity is difficult to achieve and predict. In this work, we show a unique MOF where the multidomain appearance and the crystallographic structure contradict.<sup>[5]</sup> These monodispersed micron-sized crystals have a “brain-like” morphology. Remarkably, our X-ray diffraction and electron diffraction studies prove that these structures are single-crystals and homochiral. The porous framework has helical hexagonal and triangular channels. Interestingly, different reaction conditions generate a series of isostructural and monodispersed crystals. These results indicate that there are hidden rules to be discovered for fascinating single crystals expressing multidomain morphologies.



**Fig. 1.** Multidomain chiral single crystals using achiral building blocks.

- [1] O. Yaghi, *J. Am. Chem. Soc.*, **138**, 15507–15509 (2016).
- [2] Z. Chen, K. O. Kirlikovali, P. Li, O. K. Farha *Acc. Chem. Res.*, **55**, 579–591 (2022).
- [3] N. Zigon, V. Duplan, N. Wada, M. Fujita *Angew. Chem., Int. Ed.*, **60**, 25204–25222 (2021).
- [4] N. Malik, V. Singh, L. Houben, L. Shimon, M. Lahav and M. E. van der Boom *J. Am. Chem. Soc.*, **143**, 16913–16918 (2021).
- [5] V. Singh, L. Houben, L. Shimon, S. Cohen, O. Golani, Y. Feldman, M. Lahav and M. E. van der Boom, *Angew. Chem., Int. Ed.* **60**, 18256–18264 (2021).

## Solid electrolyte membrane preparation using casting in different solvents

Gayathri Peta, Miryam Fayena-Greenstein, and Doron Aurbach

Chemistry Department, Bar-Ilan University, Ramat-Gan 5290002, Israel

The prevailing method today for preparing an organic solid electrolyte is through casting. With this method, all the components of the electrolyte must be dissolved or suspended in a solvent and then cast on a Teflon dish. For decades, acetonitrile has been widely used, a solvent that is not environmentally friendly and its exposure to alkali metals such as sodium and lithium results in a rapid reaction to form highly toxic substances such as cyanide [1,2]. In this study, we present the possibility of switching to environmentally friendly solvent instead of acetonitrile. Characterization and comparison of a membranes produced with and without acetonitrile environments are presented in the article and include spectral measurements [3], electrochemistry of symmetric cells under stable and under dynamic conditions as well as electrochemistry of all solid-state batteries. The results show that there is no visible difference in the tools at our disposal between the two membranes and if the anodic voltage in the battery does not exceed 3.5 V vs. Na it is certainly possible to use membranes of this type and surprisingly even get better electrochemical performance.

- [1] Mankovsky, D.; Lepage, D.; Lachal, M.; Caradant, L.; Aymé-Perrot, D.; Dollé, M. *Chem. Commun.*, 56 (70), 10167–10170 (2020).
- [2] Zhang, X.; Zhou, L.; Wang, Y.; Zhou, Q. Influence of Humidity on the Complex *Polym. Sci. - Ser. A* 60 (1), 50–56 (2018).
- [3] Harris, C. S.; Rukavina, T. G.. *Electrochim. Acta* 40 (13–14), 2315–2320 (1995).

## Stability of Perovskite Solar Cells with Copper Thiocyanate as Hole-Transport Material

**D. Kishore Kumar<sup>1</sup> and Iris Visoly-Fisher<sup>1,2</sup>**

<sup>1</sup>National Solar Energy Center, Swiss Institute for Dryland Environmental and Energy Research, Blaustein Institutes for Energy Research, Ben-Gurion University of the Negev, Israel

<sup>2</sup>Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Israel

Email: kishorek@post.bgu.ac.il

For efficient photo-generated charge transport, the choice of interfacial layers is important for improving the performance of perovskite solar cells (PSCs). In recent years, copper thiocyanate (CuSCN) is being utilized as a low-cost, inorganic hole transport material (HTM) for n-i-p PSCs. It possesses high hole mobility, wide band-gap, chemical and thermal stability and can be solution processed.

In this work, the role of CuSCN as HTM in triple cation PSCs in the cells photostability is studied. Triple cation PSCs with the architecture FTO/c-TiO<sub>2</sub>/m-TiO<sub>2</sub>/Perovskite/CuSCN/Au are tested for indoor and outdoor photostability under MPPT condition. While the PSCs output power showed monotonous decline under constant illumination indoors, their performance dynamics were drastically affected by the light/ dark cycling and solar spectrum variations outdoors. The efficiency of the PSCs was observed to increase during the day (light soaking effect), decrease with decreasing illumination intensities in the evening, and recover during the night, resulting in increased morning PCE followed by a quick degradation. The effect of CuSCN on the degradation and recovery dynamics of PSCs is currently under investigation.

[1] K. Domanski, B. Roose, T. Matsui, M. Saliba, S.-H. Turren-Cruz, J.-P. Correa-Baena, C. R. Carmona, G. Richardson, J. M. Foster, F. De Angelis, J. M. Ball, A. Petrozza, N. Mine, M. K. Nazeeruddin, W. Tress, M. Grätzel, U. Steiner, A. Hagfeldt A. Abate, *Energy Environ. Sci.*, 10, 604 (2017)

[2] N. Arora, M. Ibrahim Dar, A. Hinderhofer, N. Pellet, F. Schreiber, S. M. Zakeeruddin, Michael Grätzel, *Science* 358, 768 (2017)

## Stabilizing High-Voltage Lithium-Ion Battery Cathodes Using Functional Coatings of 2D Tungsten Diselenide

**Hadar Sclar,<sup>1</sup> Sandipan Maiti,<sup>1</sup> Rajashree Konar,<sup>1</sup> Judith Grinblat,<sup>1</sup> Michael Talianker,<sup>2</sup> Maria Tkachev,<sup>1</sup> Xiaohan Wu,<sup>3</sup> Aleksandr Kondrakov,<sup>3</sup> Gilbert Daniel Nessim,<sup>1</sup> and Doron Aurbach<sup>1</sup>**

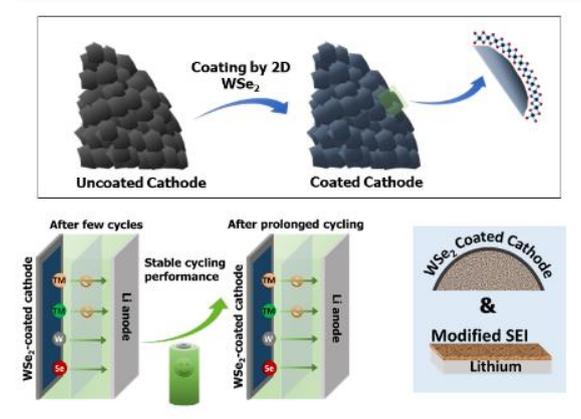
<sup>1</sup>Department of Chemistry and Institute of Nanotechnology & Advanced Materials (BINA), Bar-Ilan University, Ramat-Gan 5290002, Israel

<sup>2</sup>Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva 8410501, Israel

<sup>3</sup>BASF SE, Carl-Bosch-Straße 38, 67063 Ludwigshafen am Rhein, Germany

E-mail: hadar.sclar@biu.ac.il

Functional surface coatings were applied on high-voltage spinel ( $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ; LNMO) and Ni-rich ( $\text{LiNi}_{0.85}\text{Co}_{0.1}\text{Mn}_{0.05}\text{O}_2$ ; NCM851005) NCM cathode materials using few-layered 2H tungsten diselenide ( $\text{WSe}_2$ ). Simple liquid-phase mixing with  $\text{WSe}_2$  in 2-propanol and low-temperature ( $130^\circ\text{C}$ ) heat treatment in nitrogen flow dramatically improved electrochemical performance, including stable cycling, high-rate performance, and lower voltage hysteresis in Li-coin cells at 30 and  $55^\circ\text{C}$ . Significantly improved capacity retention at  $30^\circ\text{C}$  [Q401/Q9 of 99% vs. 38% for LNMO and Q322/Q23 of 64% vs. 46% for NCM851005] indicated efficient functionality. TEM and XPS clarified the coating distribution and coordination with the cathode surface, while post cycling studies revealed its sustainability, enabling lower transition metal dissolution and minor morphological deformation/microcrack formation. A modified and stable SEI was apparently formed owing to W and Se deposition on the Li anode during cycling. The synergistic functionalization provided a significant dual benefit of cathodic and anodic stability.[1]



*Fig 1: Schematic illustrations demonstrating the surface coating of cathode materials and their positive impacts on cathodes' electrochemical behavior.*

[1] S. Maiti, R. Konar, H. Sclar, J. Grinblat, M. Talianker, M. Tkachev, X. Wu, A. Kondrakov, G. D. Nessim, and D. Aurbach, *ACS Energy Lett.* 7 (2022) 1383-1391.

### **Synergistic Effect of Copper Corrole and Iron Porphyrin in Porphyrrole Aerogel for the Electrocatalysis of Oxygen Reduction Reaction**

*Yeela Persky<sup>1,2</sup>, Łukasz Kielesiński<sup>3</sup>, Noam Zion<sup>1,2</sup>, Ariel Freidman<sup>1,2</sup>, Hilah C. Honig<sup>1,2</sup>, Beata Koszarna<sup>3</sup>, Michael J. Zachman<sup>4</sup>, Daniel T. Gryko<sup>3\*</sup> and Lior Elbaz<sup>1,2\*</sup>*

<sup>1</sup>Chemistry Department, Bar-Ilan University, Ramat-Gan 5290002, Israel.

<sup>2</sup>Bar-Ilan Center for Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 5290002, Israel.

<sup>3</sup>Institute of Organic Chemistry of Polish Academy of Sciences, Warsaw 01-224, Poland.

<sup>4</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA.

The development of bio-inspired catalysts for oxygen reduction reaction is one of the most prominent pathways in the search for active materials to replace Pt-based catalysts in fuel cells. Herein, we report new bio-inspired catalyst which based on Cytochrome C Oxidase using a directed synthetic pathway to create Cu and Fe sites next to each other. This new catalyst is composed of a covalent three-dimensional framework in an aerogel form. Aerogels are high surface area and porous hierarchical structures, that can allow the formation of ultra-high active site density and optimized mass transport of reactants and products to and from the catalytic sites. The catalyst exhibited excellent performance in half-cell in 0.1 M KOH, with an onset potential of 0.94 V vs. RHE, high selectivity towards the 4-electron reduction of oxygen to hydroxide, and very good durability. These results are translated very well in anion exchange membrane fuel cell (AEMFC), reaching an open circuit potential of 0.97 V and I-R corrected peak power density of 0.51 W cm<sup>-2</sup>.

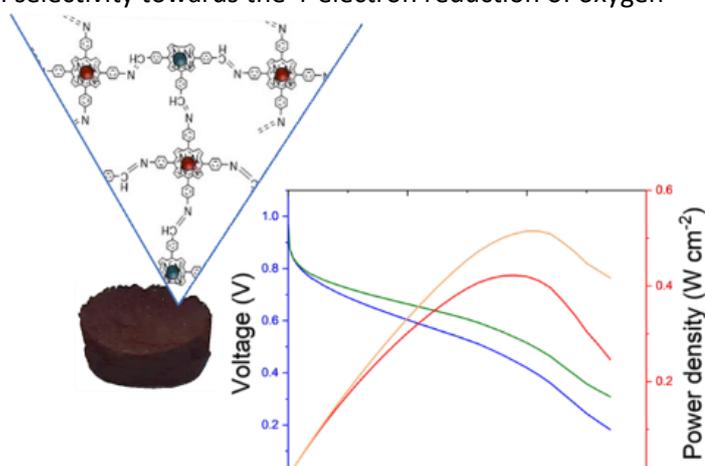


Figure 2: The obtained aerogel, its chemical structure and its AEMFC measurement

## Dual atom electrocatalysts for hydrogen oxidation and oxygen reduction reaction

*Manoj Shanmugasundaram and David Zitoun\**

E-mail: [manosp1996@gmail.com](mailto:manosp1996@gmail.com), and [David.zitoun@biu.ac.il](mailto:David.zitoun@biu.ac.il)

Department of chemistry, Bar-Ilan Institute of Nanotechnology and Advanced Research, Bar-Ilan University, Ramat Gan, Israel

The growing concerns over climate change and energy security have stimulated the use of renewable energy in lieu of fossil fuels. Hydrogen is an attractive alternate fuel and electrolyzers and fuel cells are important for its production and utilisation. Precious metal based electrocatalysts for HOR and ORR, e.g., platinum group materials, usually shows better performance, favourable stability, recyclability and can significantly reduce activation energy barrier. However, due to inefficient utilization of active sites, high cost and poor selectivity of Pt-based catalysts greatly hinders the large-scale application. Recently, subatomic scale level of electrocatalysts such as single atom (SAEs) and dual atom (DAEs) electrocatalysts are getting more attention. It has opened up new way for the development of advanced electrocatalysts to achieve maximum atom utilization efficiency, excellent stability and high catalytic activity. In this context, we have developed effective DAMs electrocatalysts encapsulated in heteroatom doped carbon matrix for HOR. Our work delves into the following questions: 1. How DAs are encapsulated into the carbon matrix to avoid agglomeration/sintering, and to study which active sites take part during electrolysis process, 2. Mass transport limitation in the rotating disk electrode (RDE) setup. We take help from advanced spectroscopic and electrochemical tools such as in situ/operando X-ray absorption spectroscopy (XAS) and floating electrodes to address them.

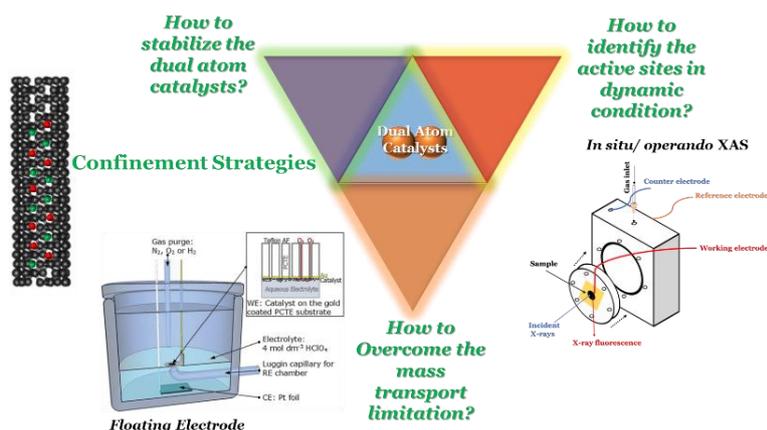


Fig.1. Schematic representation of scientific motivation

[1] Hardisty et al, Single atom Pt electrocatalysts inside carbon nanotubes for selective catalysis, *Carbon energy*, in press

## **Investigating The Effect Of PGM-Free Catalysts' Loading On The ORR Activity In PEFC**

Or Rimon, Rifael Z. Snitkoff-Sol, Yan Yurko & Lior Elbaz

Polymer electrolyte fuel cells are a growing interest and an integral part of energy production shift to clean sources. Extensive research efforts were made in order to replace the cathode catalyst which is the most expensive PEFC component. The development of highly active, durable, and cheap precious-group metal-free (PGM-free) has the potential to reduce the price of fuel cells considerably and enable sustainable widespread commercial integration. The most active and well-researched PGM-free catalyst comprises Fe ions coordinated to several nitrogen atoms embedded in a carbonaceous matrix in a structure of  $\text{FeN}_x\text{C}_y$ . These catalysts have shown increasing activity and durability but still lack in both. In order to obtain power densities comparable to the PGM-based cathode's performance, the cathode demand higher loading which leads to a much thicker order of magnitude. While this increase the available power (at the kinetic zone in particular) it's a major source of mass transport and ohmic resistance which limit the available power that can be produced by the cell at high currents.

In this study, we investigate the effect of the thickness on ORR activity by using FTacV to acquire Quantitative knowledge of the electrochemical active site density (ESAD), and DRT in order to understand the ORR resistance at different cell potentials. By using those methods it enables us to better understand the activity in a more knowledgeable method and enables us to optimize the electrode loading, a crucial parameter for the utilization of the catalyst.

## **Quantifying the electrochemical active site density of precious metal-free catalysts in situ in fuel cells**

**Rifael Z. Snitkoff-Sol and Lior Elbaz**

Department of Chemistry, Bar-Ilan Center for Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 5290002, Israel  
rafisnitkoff@gmail.com

The rising interest in polymer electrolyte fuel cell (PEFC) technology, is accompanied by efforts to drive down the cost of this technology, focusing primarily on the cathode catalyst, the most expensive PEFC component. While platinum-group metals (PGMs) continues to be the materials of choice for oxygen reduction reaction (ORR) catalysts, use of these materials in PEFCs must be significantly reduced or eliminated without a penalty in the overall cell performance for PEFC technology to become fully viable.

The most promising class ORR catalysts that do not utilize PGMs (i.e., PGM-free catalysts), involve first-row transition metals (e.g., Fe, Co), incorporated in a nitrogen-doped carbon (M-N-C catalysts). While advancements in M-N-C activity have been impressive, the much sought-after improvement in durability has been impeded by limited information on changes in the PGM-free catalyst active site density, activity and its degradation rate during fuel cell testing. Currently, degradation of PGM-free catalysts during fuel cell operation is often quantified using the low-current region of polarization curves. While this approach is well established, it neglects complications from such factors as catalyst pore structure, membrane conductivity, ionomer content, nature of the support, and the inhomogeneity of active sites. Hence, there exists a critical need for a method with high specificity towards catalytic activity.

In this poster we will report for the first time on the use of Fourier-transform alternating current voltammetry (FTacV) as an electrochemical method for accurately quantifying the electrochemically active site density of PGM-free ORR catalysts and following their degradation in situ during operation of polymer electrolyte fuel cells. Using this method, we were able to detect changes in performance of electrochemically active species (electrocatalytic centers in this case), allowing us to calculate the electrochemical active site density (EASD) for the first time, which is necessary to elucidate the degradation mechanisms of PGM-free ORR catalysts that occur in situ fuel cells. large-amplitude FTacV, a well-established electrochemical method with distinct advantages over dc methods, was utilized to quantify the electrochemically active site density of PGM-free FeNC catalysts in situ in PEFC. First, we will demonstrate that an accurate measurement of the EASD can be made using this method. To further emphasize the strength of the technique, we will present our findings during degradation of commercial FeNC catalysts in operating PEFC. The peak currents from higher harmonics produced by this method are correlated to the fuel cell performance, and decrease after durability tests in a manner that indicates EASD loss may not be the only catalyst degradation mechanism, thus inviting further studies of yet-unknown degradation pathway(s).

## **Developments of Transition multi-Metal Oxide catalysts for Alkaline Electrolyzers**

**Michal Mizrahi<sup>1</sup> and Lior Elbaz<sup>1</sup>**

<sup>1</sup>Department of Chemistry, Bar-Ilan University, Ramat Gan, Israel

The most efficient and clean technologies today are fuel cells coupled with electrolyzer technologies, given that the energy is produced from renewable, green resources, such as wind and solar power. Fuel cells convert chemical energy, into usable electrical energy from the reaction of Hydrogen and oxygen gas. Electrolyzers are based on the back reaction of Fuel Cells: splitting water into Hydrogen and Oxygen gas. Additionally, electrolyzers solve one of the biggest challenges towards sustaining a clean, green energy economy: energy storage. This technology can use the, otherwise wasted, renewable energy to produce green Hydrogen. The Hydrogen can then be used in fuel cells to convert the stored chemical energy into usable electrical energy.

My research focuses on optimizing the catalytic materials needed for water splitting. Two reactions must occur for water to split: Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER). The HER is relatively easy to perform, leaving OER as the bottleneck. For OER to occur at peak efficiency, precious metal catalysts are used, such as Iridium and Ruthenium. While these allow the OER to happen efficiently, they are not cost efficient. Therefore, there is a rising interest to find alternative, cheaper, Platinum-group metal free (PGM-free), catalysts for OER.

To switch to PGM-free materials, novel alkaline electrolyzers are being developed. The most common OER PGM-free catalysts are first-row transition metals in their oxyhydroxide forms. Specifically, nickel iron oxyhydroxides (NiFeOOH), have shown promising results, allowing the electrolyzer to split water at low over potentials and high activity. My research is focusing on maximizing these materials' efficiency. This is being achieved by synthesizing NiFeOOHs as nanoporous structures to maximize their surface area and by adding additional transition metals which has been proven to increase the catalytic activity. The material is made in the form of aerogels, one of the lowest density solids, composed of 99.9% void volume. This allows for almost every particle to be exposed and therefore catalytically active. Cobalt (Co) was chosen to be the first transition metal added to the NiFeOOH in hopes to increase its catalytic abilities. Co is chosen given its similar properties to Fe and Ni.

## **Efficient and stable perovskite solar cells enabled by amino acids additives**

**S. Kassou<sup>1</sup>, H. Peled<sup>2</sup>, N. Ashkenasy<sup>2,3</sup>, and I. Visoly-Fisher<sup>1,3</sup>**

<sup>1</sup> Solar Energy Center, Swiss Institute for Dryland Environmental and Energy Research, Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Midreshet Ben-Gurion 8499000, Israel.

<sup>2</sup> Department of Materials Engineering, Ben-Gurion University of the Negev, Be'er Sheva, Israel

<sup>3</sup> Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of the Negev, Be'er Sheva, Israel

Despite the remarkable progress in the performance of perovskite solar cells (PSC) with power conversion efficiencies (PCE) of 25.7%, mitigating performance degradation remains a great challenge for their commercialization. Surface and interface engineering using molecular additives has proven to be an effective strategy to ensure further advances in charge extraction, interface recombination, and device stability. Here, we utilized amino acids with different functional groups as additives to modify interfaces in n-i-p perovskite solar cells to improve devices' PCE and operational photostability. Amino acids were chosen because of their diversity, enabling, for example, introducing amino and carboxyl functional groups known to bind to perovskite surface defects. We found that modifying the perovskite/HTL interface with an optimized amount of amino acids (1 mg/ml) has the greatest effect on device performance, compared to grain boundaries' and ETL/perovskite interface modification. Modification with glutamic acid (with carboxylic acid functional groups) and tryptophan (with indole functional group) were found to improve both efficiency and photostability of the devices compared to control devices and devices modified with lysine (with amine functional group). Peptides can be *de-novo* designed based on the functional behavior of the amino acids, providing an easy platform for engineering the perovskite interface. We, therefore, postulate that the efficiency and stability of perovskite solar cells can be improved by introducing peptides rich in carboxylic acid and indole at the perovskite/HTL interface.

# A Study Towards Preventing The Shuttle Effect of Polysulfides in Sulfur Aqueous Batteries: The Detection of Polysulfides via Scanning Electrochemical Microscopy (SECM)

Nevo Cohen and Daniel Mandler\*

Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

nevo.cohen@mail.huji.ac.il

Category: Surface science (SS)

Sulfur aqueous batteries (SABs) offer much interest in today's world and are considered to be the next generation of rechargeable batteries due to their high energy density and capacity. However, several technical issues currently prevent these batteries from being commercially available. One of the major issues is referred to as "the shuttle effect", which is associated with the discharge of sulfide because of diffusion. This study aims to serve as a step towards solving this issue. Our goal is to detect the release of polysulfides from a sulfur-covered electrode and study how to control or prevent their release. We use scanning electrochemical microscopy (SECM) and its feedback and generation-collection modes to approach and study the behavior and release of polysulfide at the interface.

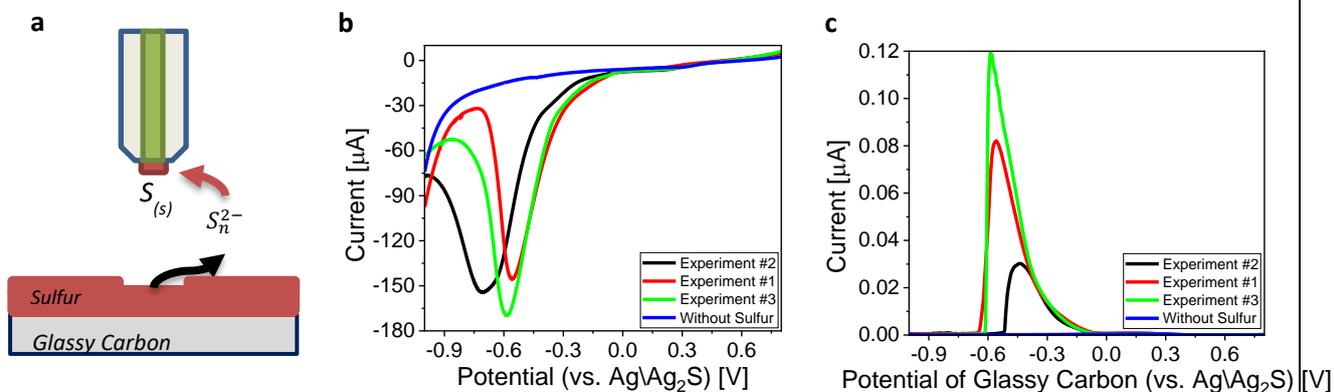


Figure 1: Generation-collection of polysulfides to sulfur. (a) Illustration of the release of polysulfide from a sulfur-covered glassy carbon and its oxidation (collection) to sulfur atop the microelectrode. (b) Linear sweep voltammetry of the sulfur-covered glassy carbon from 0.8 to  $-1$  V. (c) Oxidation at the microelectrode tip at 0.8 V.

[1] Liu, J., Zhou, W., Zhao, R., Yang, Z., Li, W., Chao, D., ... & Zhao, D. (2021). Sulfur-based aqueous batteries: electrochemistry and strategies. *Journal of the American Chemical Society*, 143(38), 15475-15489.

[2] Bard, A. J., & Mirkin, M. V. (2001). *Scanning electrochemical microscopy*. CRC Press.

## **Combinatorial Vacuum-Deposition of Wide Bandgap Perovskite Films and Solar Cells**

**Adi Kama<sup>1</sup>, Isidora Susic<sup>3</sup>, Lidón Gil-Escrig<sup>3</sup>, Chris Dreessen<sup>3</sup>, Francisco Palazon<sup>3</sup>,  
David Cahen<sup>1,2</sup>, Michele Sessolo<sup>3</sup>, Henk J. Bolink<sup>3</sup>**

<sup>1</sup>Department of Chemistry and Bar-Ilan Institute for Nanotechnology &  
Advanced Materials Bar-Ilan University, Ramat Gan, Israel

<sup>2</sup>Department of Molecular Chemistry and Materials Science  
Weizmann Institute of Science, Rehovot, Israel

<sup>3</sup>Instituto de Ciencia Molecular Universidad de Valencia, Paterna, Spain

The development of vacuum-deposited perovskite materials and devices is partially slowed down by the minor research effort in this direction, due to the high cost of the required research tools. But there is also another factor, thermal co-deposition in high vacuum involves the simultaneous sublimation of several precursors with an overall deposition rate in the range of few  $\text{\AA s}^{-1}$ . This leads to a deposition time of hours a single perovskite composition. Here we report the combinatorial vacuum deposition of wide bandgap perovskites using 4 sources and a non-rotating sample holder. By using small pixel substrates, more than 100 solar cells can be produced with different perovskite absorbers in a single deposition run. The materials are characterized by spatially resolved methods, including optical, morphological, and structural techniques. By fine-tuning of the deposition rates, the gradient can be altered and the best-performing formulations in standard depositions with rotation can be reproduced. This is viewed as an approach that can serve as a basis to prototype other compositions, overcoming the current limitations of vacuum deposition as a research tool for perovskite films.

# Control System for a Novel Hydrogen Generator

Y. Ayalon, M. Sassoon and G. Golan

Department of Electrical & Electronic Eng., Ariel University, Ariel, Israel

## Abstract [1]

Recently, there has been a growing need for sustainable energy sources that don't harm the environment. One of the most promising options is hydrogen gas, which doesn't produce greenhouse emissions. However, currently, its production isn't cost-effective. In this context, a control and management system has been created to carefully control the production of hydrogen gas and test a new electrode system. This system aims to make the production process more efficient and reliable.

The control and management system that has been developed for the hydrogen generator is based on the Internet of Things (IoT) and is responsible for monitoring a range of data points related to the generator's operation. These data points include temperature, voltage/current, flow rate, liquid level, and static pressure. All of this data is collected in real-time and can be accessed and analyzed by various means in a remote application (including web dashboard), LCDs, and SD-card.

The control and management system functions as intended. All sensors are providing accurate results and the data is being transmitted successfully to the Arduino Mega. The Arduino Mega then sends the data to various displays including LCDs, Blynk cloud, a remote application, and a web dashboard. Additionally, the data is also being recorded onto an SD-card-based data logger for future reference. Overall, the system is working well and providing valuable information.

The results obtained by the new measuring system can be attributed to several factors. First, the system utilizes high-quality sensors and measurement technologies that can accurately and reliably capture data on the various process variables. This is essential for the proper functioning of the control system, as any errors or inconsistencies in the data could lead to incorrect control decisions. In addition, the measuring system has been severely calibrated and tested to ensure that it is operating within its specified range and accuracy limits. This is important for maintaining the overall accuracy and reliability of the system, as well as for detecting any potential issues that may arise. Overall, the good results achieved by our measuring system demonstrate the effectiveness of the control and management system as a whole. The accurate and reliable data collected by the measuring system allows the operator to make better decisions and maintain a stable operation of the hydrogen generator, resulting in improved efficiency and reliability.

- [1] Y. Manoharan, "Hydrogen fuel cell vehicles; current status and future prospect," Applied Sciences, 2019.

## Nanoparticles of WS<sub>2</sub> towards Stabilization of Halide Perovskite Solar Cells

**A. Goldreich<sup>1</sup>, P. Immanuel<sup>1,2</sup>, A. Sadova<sup>1</sup>, L. Yadgarov<sup>1</sup>**

<sup>1</sup>Department of Chemical Engineering, Ariel University, Ariel, Israel

<sup>2</sup>Department of Mechanical Engineering, National Taiwan University of Science and Technology, Taipei 106, Taiwan

Perovskite solar cells (PSCs), due to their high efficiency, versatility, and affordable processing, are drawing significant attention. However, long-term stability is still a major issue and must be solved. In this work, the WS<sub>2</sub> nanoparticles (NPs) are successfully implemented in the halide PSCs, based on methylammonium lead iodide (MAPbI<sub>3</sub>), without compromising the properties and crystalline structure of MAPbI<sub>3</sub>. These NPs are active centers in the interface between the compact TiO<sub>2</sub> and MAPbI<sub>3</sub>. The main functions of the WS<sub>2</sub> NPs in the PSCs are the transport of electrons, acting as nucleation sites, and a stabilizing agent. The electron extraction by the WS<sub>2</sub> NPs from the adjacent MAPbI<sub>3</sub> is efficient and results in a higher current density. In addition, the absorption, grain size, and shelf life of the MAPbI<sub>3</sub> layers are increased. The application of the NPs instead of the commonly studied flakes significantly reduces the time fabrication of the PSCs. Our results demonstrate the potential of the WS<sub>2</sub> NPs in the long-term stabilization of the PSCs.

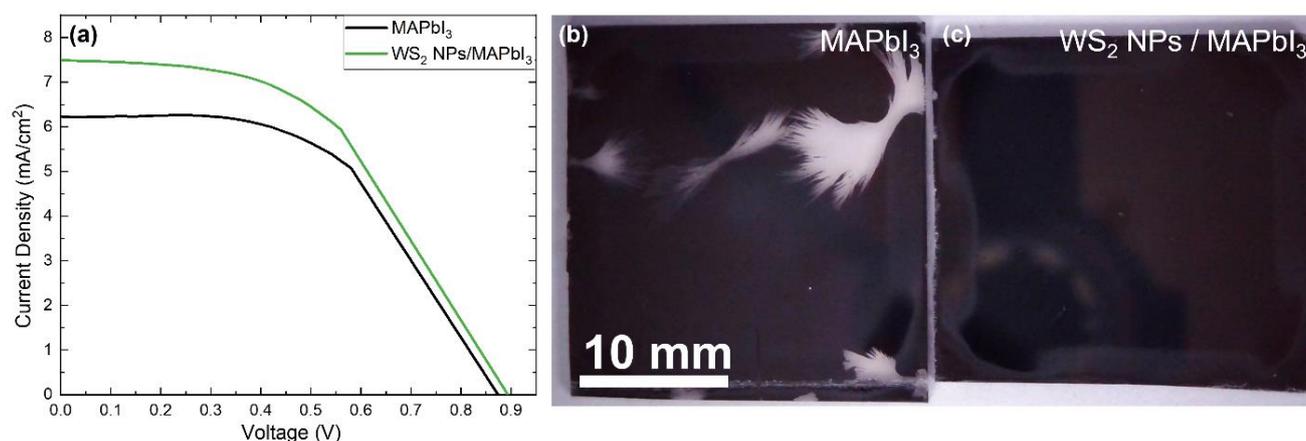


Fig 1: (a) *J-V* characteristics of the PSCs without (MAPbI<sub>3</sub>) and with WS<sub>2</sub> NPs and (b) MAPbI<sub>3</sub> and (c) WS<sub>2</sub> NPs/ MAPbI<sub>3</sub> layers on top of the FTO glass substrate after the exposure to air.

- [1] H. S. Jung and N. Park, "Perovskite solar cells: from materials to devices," *small*, vol. 11, no. 1, pp. 10–25, 2015.
- [2] L. Yadgarov et al., "Strong light–matter interaction in tungsten disulfide nanotubes," *Phys. Chem. Chem. Phys.*, vol. 20, no. 32, pp. 20812–20820, 2018.

## Superior photocatalytic activity of cesium lead bromide/tungsten disulfide hybrid nanocomposite

*Prilusky, J.<sup>2</sup>, Immanuel, P.N.<sup>1,2†</sup>, and Yadgarov, L.<sup>2\*</sup>*

<sup>1</sup>Department of Mechanical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan.

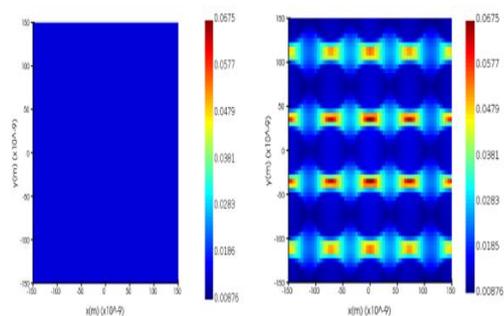
<sup>2</sup>Department of Chemical Engineering, Ariel University, Ariel, 4076414, Israel.

Photocatalytic processes are among the prime means for mitigating the pollution caused by toxic effluents. In this context, photocatalysis presents a promising path and undergoing rapid evolution. Halide perovskites (HPs) are excellent candidates due to their negative conduction band minimum and the low work function that are essential for photocatalysis. Interestingly, HPs performance significantly improves by introducing transitional-metal dichalcogenides as a co-catalyst, which enables suppressed charge recombination. Here we investigate the photocatalytic performance of  $\text{Cs}_4\text{PbBr}_6/\text{WS}_2$  nanocomposites towards organic dye degradation under visible light illumination. We found that the  $\text{Cs}_4\text{PbBr}_6/\text{WS}_2$  nanostructures significantly increase the degradation rate of methylene blue compared to pristine  $\text{Cs}_4\text{PbBr}_6$  nanocrystals. The transient absorption measurements reveal charge transfer from  $\text{Cs}_4\text{PbBr}_6$  to  $\text{WS}_2$ . The results of our study imply that the boosted photocatalytic performance of the nanocomposites is due to the reduced carrier recombination. Our findings pave the way for the implementation of  $\text{Cs}_4\text{PbBr}_6/\text{WS}_2$  nanocomposites as superior photocatalysts.

Photoluminescence (PL) measurement shows rapid intensity quenching for the nanocomposites. The quenching is caused by the rapid charge transfer between  $\text{Cs}_4\text{PbBr}_6$  and  $\text{WS}_2$ . We also used XRD, TEM.

In order to study this phenomenon we simulated using FDTD commercial software, we designed the model geometry and simulated it.

*Fig. 1: FDTD simulations Results .Electric field enhancement with  $\text{WS}_2$  compared to  $\text{Cs}_4\text{PbBr}_6$*



## Dual-Passivation Strategy for Improved Ambient Stability of Perovskite Solar Cells

**Ritesh Kant Gupta,<sup>1,2</sup> Rabindranath Garai,<sup>3,4</sup> Iris Visoly-Fisher,<sup>1,5</sup> and Parameswar Krishnan Iyer<sup>2,4</sup>**

<sup>1</sup>National Solar Energy Center, Swiss Institute for Dryland Environmental and Energy Research, Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Israel

<sup>2</sup>Centre for Nanotechnology, Indian Institute of Technology Guwahati, India

<sup>3</sup>Department of Physics, Indian Institute of Technology Roorkee, India

<sup>4</sup>Department of Chemistry, Indian Institute of Technology Guwahati, India

<sup>5</sup>Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Israel

Email: guptar@post.bgu.ac.il/ritesh110990@gmail.com

Minimizing the bulk and surface defects of perovskite films has been a major challenge towards the development of stable perovskite solar cells. In this work, dual-passivation of MAPbI<sub>3</sub>-based perovskite using p-toluenesulfonic acid (PTSA) in the bulk and hydrophobic polystyrene (PS) at the surface of the perovskite significantly diminishes the trap-density and improves the device performance substantially. The sulfonic acid functional group of PTSA interacts with the defects in the perovskite and passivates the trap-states, while PS repairs the surface defects and increases the moisture resistance. Improvement in perovskite crystallinity and formation of larger grain size occurs because of the passivation, thereby enhancing the power conversion efficiency (PCE) to 20.62% from 15.14% of the device without passivation. The modified device showcases reduced hysteresis and a steady-state PCE of >20%. The dual-passivated device also exhibited higher photogenerated charge densities, lower charge recombination, reduced trap-density, and better charge transport than the control device. Finally, the modified device displays superior ambient stability compared to the control device and retained 93% of the initial PCE after 1000 h.

[1] R. K. Gupta, R. Garai, P. K. Iyer, ACS Appl. Energy Mater., **2021**, 4, 9, 10025–10032.

**Surface Science**  
**(SS)**

## Synthesis of aluminum oxide surface using plasma electrolytic oxidation in ternary eutectic molten salt

Y. Yuferov<sup>1</sup> and K. Borodianskiy<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, Ariel University, Ariel, Israel

Aluminum alloys are usually coated to achieve a required wear, corrosion, and other functional properties. One of the most beneficial method to form such a surface is metallic oxidation using plasma-electrolytic oxidation (PEO) in aqueous solution [1]. Recently, PEO in binary eutectic molten salt  $\text{NaNO}_3\text{-KNO}_3$  (45.7 and 54.3 wt. %) was suggested as method to form impurity-free coatings on aluminum [2]. However, this method has several restrictions such as high processing temperature, difficulty to incorporate additional functional components and low capability of variation of phase composition. In current work application of a ternary molten eutectic salt of  $\text{NaNO}_3\text{-KNO}_3\text{-Ca(NO}_3)_2$  (17, 42 and 41 wt. %) as electrolyte in PEO process was studied. This composition allows to decrease processing temperature from 280 to 160 °C which tends to increase the addition of functional compounds into electrolyte in the form of ions or charged particles. Here, aluminum oxide surface was synthesized in the mentioned ternary salt using various current frequencies as shown in Figure 1a. The morphology of the surface was examined by SEM (Figure 1b), and almost a common porous structure of surface, traditionally fabricated by PEO, was obtained. The XRD analysis detected impurity-free  $\gamma\text{-Al}_2\text{O}_3$  phase, which further may be modified by heat-treatment approach.

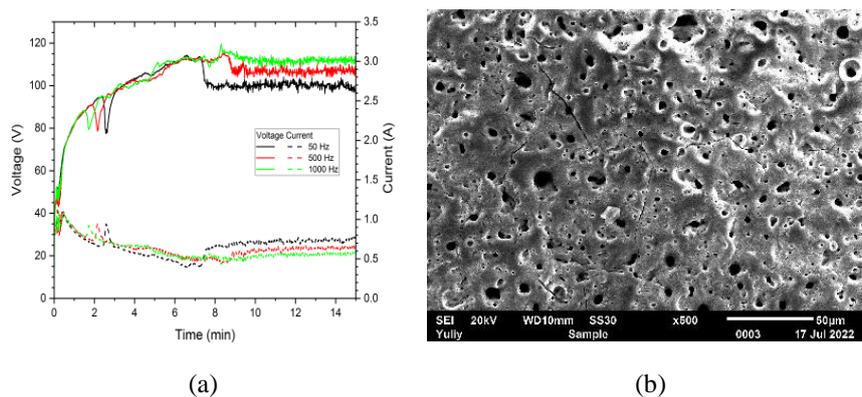


Fig. 1: a) Current-time and voltage time transients of PEO process on aluminum substrate at various frequencies and b) SEM-image of obtained alumina surface.

[1] M. Aliofkhazraei, et.al, Appl. Surf. Sci. Adv., **5**, 100121 (2021).

[2] Sobolev, A.; Bograchev, D.; Zinigrad, M.; Borodianskiy, K. Ceram. Int, **48**, 10990–10998 (2022).

## Polymer Thin Films: What is Happening During Molecular Layer Deposition?

B. C. Welch<sup>1,2</sup>, E. N. Antonio<sup>3</sup>, T. Chaney<sup>4</sup>, O. M. McIntee<sup>2</sup>, J. Strzalka<sup>5</sup>,  
V. M. Bright<sup>2</sup>, A. R. Greenberg<sup>2</sup>, M. F. Toney<sup>3,4</sup> and S. M. George<sup>6</sup>

<sup>1</sup> Department of Chemical Engineering Technion, Israel Institute of Technology, Haifa, Israel

<sup>2</sup> Department of Mechanical Engineering, University of Colorado, Boulder, CO, USA

<sup>3</sup>Department of Chemical and Biological Engineering, University of Colorado, Boulder, CO, USA

<sup>4</sup>Materials Science and Engineering, University of Colorado, Boulder, CO, USA

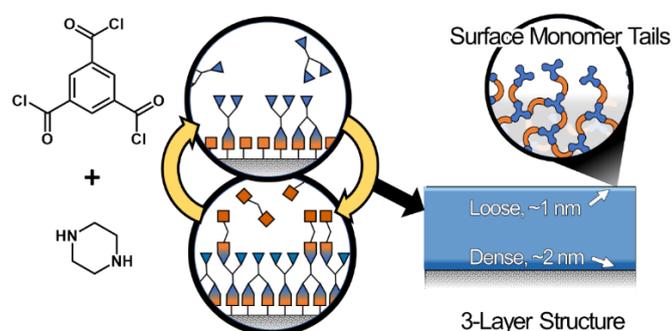
<sup>5</sup>X-ray Science Division, Argonne National Laboratory, Lemont, IL, USA

<sup>6</sup> Department of Chemistry, University of Colorado, Boulder, CO, USA

Flexible, organic films made by molecular layer deposition (MLD) have many applications in energy storage, flexible moisture barriers, and polymeric membranes [1]. MLD is based on the prolific atomic layer deposition (ALD) process: isolated exposure to a vapor precursor deposits a single layer of material on the substrate, producing new functional groups. A second precursor is then used in the same manner. This stepwise process may be repeated until the desired film thickness is achieved with sub-nanometer precision. MLD has nuanced behaviors due to the macromolecular nature of the film. Unlike ALD, the “reaction sites” of MLD do not have a fixed location on the surface, per se. Rather, film growth propagates at the functional end groups of polymer segments.

Using grazing-incidence x-ray scattering, x-ray reflectivity and ellipsometry, we have developed an understanding of how reactions at the surface occur during MLD. This work sheds light on unique behaviors which occur with changes in temperature and film thickness and explores the nuances between crosslinked and un-crosslinked films. We found that the surface of crosslinked organic MLD films is likely comprised of short polymer tails which are connected to a dense, crosslinked bulk layer. These segments are susceptible to thermal motion and double reactions, affecting film growth. These insights aid us in our development of MLD applications such as desalination membranes.

### Molecular Layer Deposition



*Fig. 1: Example of the structure and surface of a crosslinked polymer film made by molecular layer deposition*

[1] X. Meng, Journal of Materials Chemistry A, **5**, 18326–18378 (2017).

## Electro-freezing of water as induced by hydrated Al and Mg ions without supercooling

Leah Fuhrman Javitt<sup>1</sup>, Shiri Dishon Ben Ami<sup>1</sup>, David Ehre<sup>1</sup>, Hagai Cohen<sup>1</sup>, Meir Lahav<sup>1</sup>, and Igor Lubomirsky<sup>1</sup>

<sup>1</sup>Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot, Israel

Water molecules in the liquid state can be arranged in numerous different ways, however, in order for ice nucleation to occur, the water molecules must be arranged in ice like hexagons [1]. In bulk water the ice like architectures are a minority with respect to the many others that can form. For this reason water can be supercooled homogeneously down to  $-48^{\circ}\text{C}$  without freezing. The temperature of icing of super-cooled water is vital in controlling the climate, it affects rain precipitation, controls food preservation etc. This temperature may be controlled heterogeneously by performing the icing experiments on surfaces or by the applications of electric fields.

We recently demonstrated icing experiments on charged surfaces of pyroelectric crystals can be influenced by specific ions that are concentrated in the interfacial water layers near the charged surfaces. We found that trigonal planar ions can self-assemble, near the charged surfaces, with water molecules to form stable "ice-like nuclei" that are stabilized by covalent bonds rather than dissociable hydrogen bonds [2]. Based on this, we hypothesized that ions with other geometries with the ability to order water molecules through hydrogen bonding of OH groups might also create "ice-like" structures and raise the temperature of ice nucleation.

The transition metal ions of the periodic table create stable hydrate in aqueous solutions, which can take a variety of different geometries such as octahedron, tetrahedron, or trigonal bipyramid. In addition, the coordinated water molecules of those hydrates are highly polarized and acidic. Therefore, the interaction of those water molecules with interfacial water molecules should create near their surfaces more stable aggregates, in comparison than those formed in bulk water solutions. Here we report that the , hydrated ions of Aluminum and Magnesium induce water freezing without supercooling under the two following set-ups:- when those ions are dissolved within Galvanic cells in solution using Nickel cathodes, or when Aluminum electrodes are used as anodes or Mg either as anodes or cathodes.

- [1] Yu, H. and W.F. van Gunsteren, *Charge-on-spring polarizable water models revisited: From water clusters to liquid water to ice*. The Journal of chemical physics, 2004. **121**(19): p. 9549-9564.
- [2] Javitt, L.F., et al., *Chemical Nature of Heterogeneous Electrofreezing of Supercooled Water Revealed on Polar (Pyroelectric) Surfaces*. Accounts of Chemical Research, 2022.

## Determination of the Diffusion Coefficients of Silver in Thermoelectric Lead Telluride Compounds

D. Muhamed<sup>1</sup> and Y. Amouyal<sup>1</sup>

<sup>1</sup>Department of Materials Science and Engineering, Technion, Haifa, Israel

Lead telluride (PbTe) is a useful compound for thermoelectric (TE) power generation at mid-range temperatures. Ag diffusion in PbTe dictates the microstructure evolution rate, which is critical for the device operation. Herein, we optimize sample preparation procedures in terms of the TE power factor (PF). Remarkably, we obtained bulk density values as high as ca. 97% of the theoretical density, regardless of their processing conditions. To quantify Ag diffusion in PbTe we deposited a 300 nm Ag layer on PbTe surface and performed heat treatments. We applied secondary ion mass spectroscopy (SIMS) to analyze the diffusion profiles for undoped and 1 at. % Bi doped PbTe, and derived the temperature dependent Ag bulk diffusion coefficients, Fig. 1.

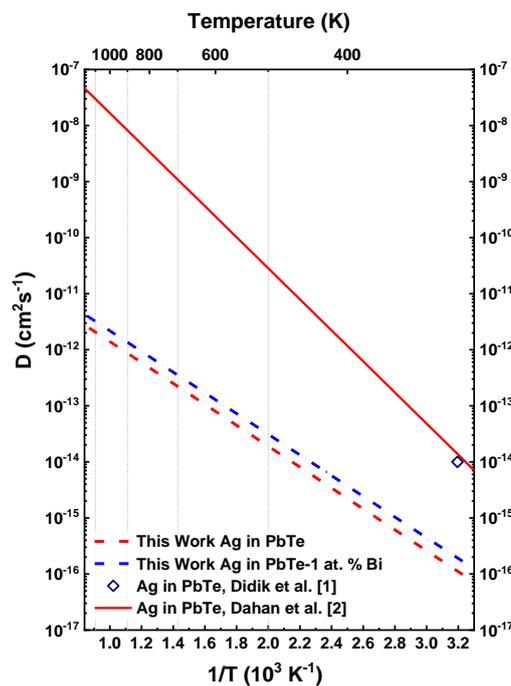


Fig. 1: Arrhenius diagrams presenting the bulk diffusion coefficients of Ag in PbTe and PbTe- 1 at. % Bi evaluated using SIMS. For reference, we add the Ag diffusion coefficients in PbTe and values calculated from first-principles [1,2].

[1] V. A. Didik, R. S. Malkovich, & E. P. Savin. *Fizika Tverdogo Tela*, 21(8), 2475-2477 (1979).

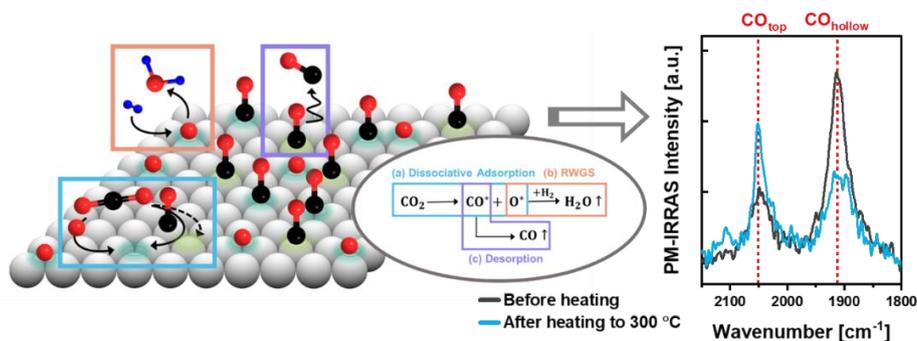
[2] M. H. Dahan, A. Baranovskiy, Y. Natanzon, & Y. Amouyal. *Acta Materialia*, 202, 243-254 (2021).

## CO<sub>2</sub> Activation on Ni(111): A Competitive Adsorption between Carbon Monoxide and Atomic Oxygen

**R. Ben David<sup>1</sup>, A. Ben Yaacov<sup>1</sup> and B. Eren<sup>1</sup>**

<sup>1</sup>Department of Biological and Chemical Physics, Weizmann Institute of Science, Rehovot, Israel

The dissociative adsorption of CO<sub>2</sub> on Ni surfaces is an important reaction step in CO<sub>2</sub> conversion processes, such as the Sabatier reaction and the dry methane reforming. However, the interface chemistry of Ni and CO<sub>2</sub> gas at ambient conditions is still poorly understood today with controversial results in the literature. Here, we study the interaction of CO<sub>2</sub> with metallic and oxidized Ni(111) model catalysts under 1 mbar CO<sub>2</sub> pressure in the temperature range of 25-300 °C using surface-sensitive infrared and Auger electron spectroscopies. At 25 °C, dissociative adsorption of CO<sub>2</sub> on Ni(111) produces CO and atomic oxygen; two strongly bound species which compete for the same preferred adsorption sites, namely the hollow sites. At this temperature, the produced CO adsorbs mainly on hollow sites, and small part adsorbs on top sites. At higher temperatures, the CO occupancy on top sites increases, as more atomic oxygen is produced and blocks the hollow sites. Overall, the surface temperature determines the site occupancy of the CO product during CO<sub>2</sub> dissociation on Ni(111) (see Fig.1). On oxidized surface, CO<sub>2</sub> dissociation is rather inactive at 25 °C, however, heating the surface to higher temperatures ( $\geq 200$  °C) reduces the oxide layer and exposes metallic Ni. Thus, both bare and oxide-covered Ni(111) surfaces have the same equilibrium chemical state and adsorbate coverage after heating to elevated temperatures. We attribute the reduction of the oxide layer to residual hydrogen impurities, which efficiently convert atomic oxygen into water vapor.



*Fig. 1: Schematics of the surface processes during CO<sub>2</sub> activation on Ni(111) and their effect on the temperature-dependent site occupancy of CO (i.e., the dissociation product).*

## X-ray photoelectron spectroscopy of solid-liquid interfaces under electrochemical control

Miguel A. Andrés<sup>1</sup>, B.-O. Shalom<sup>1</sup>, A. Head<sup>2</sup>, Y. Yu<sup>2</sup>, B. Eren<sup>1</sup>

<sup>1</sup>Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel

<sup>2</sup>Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, United States

X-Ray photoelectron spectroscopy (XPS) is arguably one of the most powerful techniques for probing solid-liquid interfaces. However, this element-specific and surface sensitive technique requires high vacuum conditions. Over the last two decades, ambient pressure XPS (AP-XPS) has been developed helping to extend the operating range to the mbar region [1]. Still, this technique alone is not sufficient to allow working with liquids and gases. To this end, few approaches have been developed, including the dip-pull method and graphene-capping approach. The first requires hard X-rays and synchrotron radiation, whereas the later can be used in lab X-ray sources, making it more versatile. Moreover, the graphene-capping approach can also be easily used under *operando* conditions: graphene is strong enough to sustain the large pressure difference but still thin enough to allow sufficient photoelectrons to pass through.

In this contribution, we demonstrate the successful application of the graphene-capping approach in a micro-electrochemical reactor [2]. In this reactor, Pt is used both as a counter and reference electrode and graphene acts as a working electrode (Fig. 1, right). Cu NPs are deposited on the backside of graphene and used as model system to monitor the changing oxidation state in a mildly alkaline aqueous solution under electrochemical control. The sensitivity of XPS to the chemical state and environment of the sample allows us to differentiate the oxidation/reduction of Cu and graphene (Fig. 1, left). These proof-of-concept experiments showed that similar signal-to-noise ratio can be obtained in comparison to other studies in the literature that use synchrotron radiation, making our approach more versatile and easily adaptable to any lab-based X-ray source facility and many model reactions.

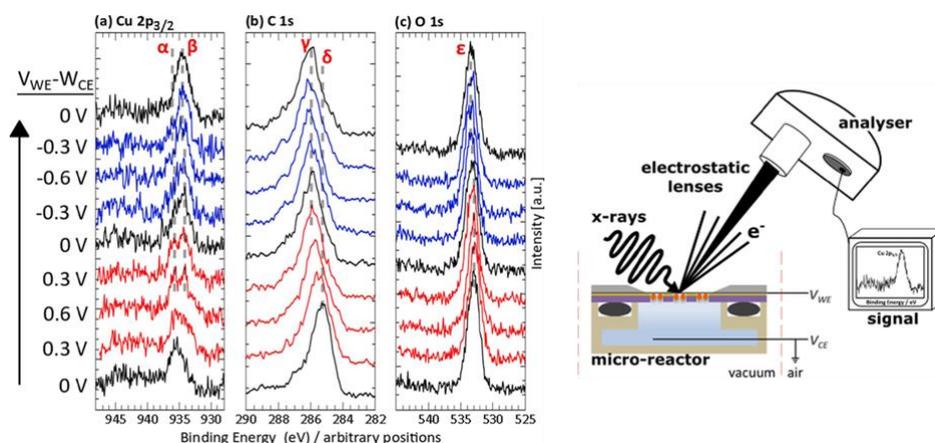


Fig. 1: Left: XPS spectra of Cu2p<sub>3/2</sub>, C1s and O1s acquired under electrochemical control. Right: Schematic of our micro-electrochemical reactor.

[1] M. Salmeron *et al.*, Surf. Sci. Rep., **63**, 169 (2008).

[2] B.-O. Shalom *et al.*, Electrochem. Commun., **142**, 107375 (2022)

## Enhancement of Polymer Thin Film Solvent Resistance Using Sequential Infiltration Synthesis

Gilad Sasson<sup>1</sup>, Brian C. Welch<sup>1</sup>, Tamar Segal Peretz<sup>1</sup>

<sup>1</sup> Department of Chemical Engineering Technion, Israel Institute of Technology, Haifa, Israel

We demonstrate the enhanced solvent resistance of polystyrene-random-polymethyl methacrylate (PS-r-PMMA) copolymer thin films modified with sequential infiltration synthesis (SIS). Through SIS copolymer samples were first exposed to trimethylaluminum then water in prolonged isolated steps, similar to the atomic layer deposition process. The long exposure times allowed the precursors to diffuse into the free volume of the polymers, nucleate, and grow inside the polymer matrix. Repeated cycles of trimethylaluminum and water led to increased Al<sub>2</sub>O<sub>3</sub> content within the samples.

SIS growth is typically controlled via exposure time, pressure and temperature. Herein, we investigated a different approach to control the mass growth: varying concentrations of PMMA in the random PS-r-PMMA samples. Using quartz crystal microbalance measurements, we found that increasing the PMMA content from 0 – 100% led to a nonlinear trend between the alumina growth and the PMMA% in the samples. This is due to the PMMA's functional group that are more reactive to trimethylaluminum precursor than the PS functional group<sup>1</sup> and the mechanism in which the alumina grows during the SIS process. Fourier transformation infrared spectroscopy, ellipsometry, and scanning electron microscopy were used to analyze the resilience of copolymer samples in liquid and vapor toluene environments. Pure PS samples lacked functional groups and remained susceptible to solvation after SIS treatment. However, PS-r-PMMA samples with as little as 9% PMMA displayed excellent resistance to toluene after SIS. Samples with less than 9% PMMA were susceptible to dissolution due to the insufficient mass of alumina grown in the samples free volume. This work expands our

understanding of the SIS process and may prove instrumental for applying the benefits of SIS modification to unreactive materials such as PS.

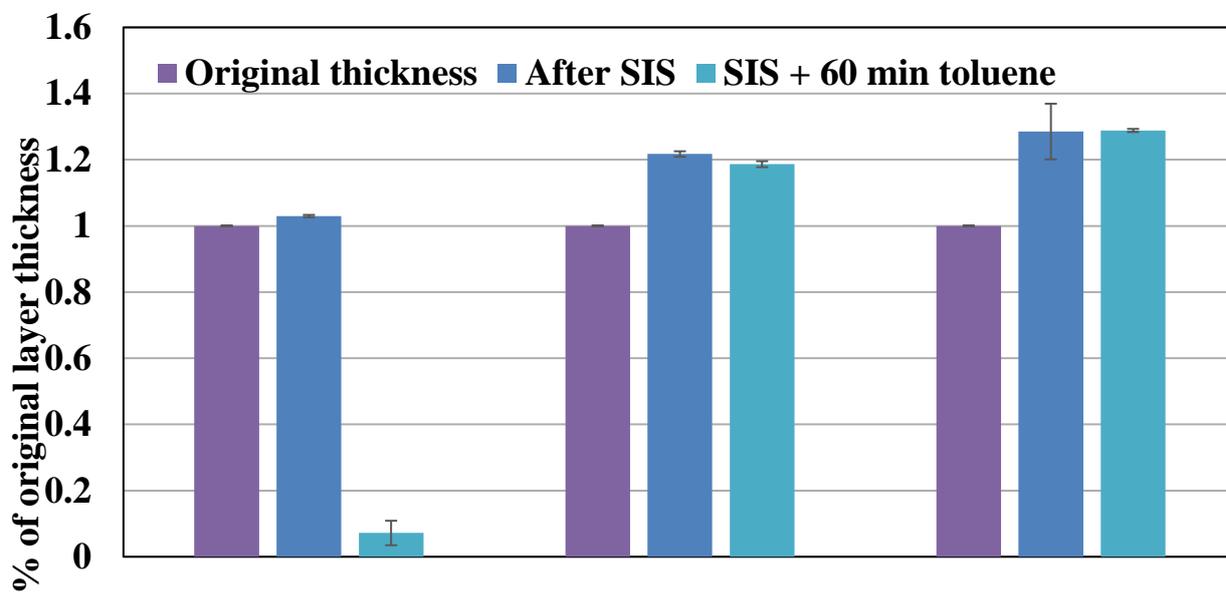


Fig. 1: changes in film thickness after SIS treatment and solvent exposure for 60 min

1. Peng, Q., Tseng, Y.C., Darling, S.B. and Elam, J.W., 2010. Nanoscopic patterned materials with tunable dimensions via atomic layer deposition on block copolymers. *Advanced materials*, 22(45), pp.5129-5133.

## **X-Ray Photoelectron Spectroscopy for Surface Characterization:**

### **Interesting new results**

**Kamira Cohen-Weinfeld**

Surface Science Laboratory, Solid State Institute, Technion, Haifa, Israel

The X-Ray Photoelectron Spectroscopy is a powerful technique that provides detailed information about the surface atomic composition and very valuable information about the chemical environment of the elements.

The XPS VersaProbe III- PHI Physical Electronics is equipped with several complementary analysis techniques making it a powerful platform for surface analysis of bulk and powder materials:

- Scanning X-ray Beam induced Secondary Electron Images (SXI) with a field of view of  $700 \times 700 \mu\text{m}^2$ ,
- Chemical State Imaging and Mapping of surface sample (lateral resolution of  $4\text{-}5 \mu\text{m}$ ),
- In situ sample cooling (down to  $-140^\circ\text{C}$ ) or heating (up to  $800^\circ\text{C}$ ).
- Ultra Violet integrated source allowing Ultra-Violet Photoelectron Spectroscopy (UPS) analysis for Valence Band and a direct measurement of Work Function of materials,
- Depth profiling materials by three different methods:
  - Angle Resolved XPS (AR-XPS) analysis for depth profile by tilting the sample without damaging the surface, up to approximately  $15\text{nm}$  depth,
  - Monoatomic  $\text{Ar}^+$  Ion Gun Sputtering for depth profiling semiconductor materials or metal oxide
  - Cluster  $\text{Ar}_{3000+}$  Ion Gun Sputtering (GCIB) for depth profiling organic based structures,

Some specific examples will be presented showing ability to determine the oxidation state of metals, presence of particles embedded in the material and presence of particular chemical functions could be identified by XPS analysis.

## Elucidating the mechanisms involved in Cr(VI) removal by activated carbon cloth

**Maurício N. Kleinberg<sup>1</sup>, Chidambaram Thamaraiselvan<sup>2</sup>, Camilah D. Powell<sup>1</sup>, Avner Ronen<sup>1</sup> and Christopher J. Arnusch<sup>1</sup>**

<sup>1</sup>Department of Desalination and Water Treatment, Zuckerberg Institute for Water Research, The Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede-Boqer Campus, Midreshet Ben-Gurion 84990, Israel

<sup>2</sup>Interdisciplinary Centre for Energy Research, Indian Institute of Science, Bangalore, 560012, India

In industrial effluents, hexavalent chromium [Cr(VI)] is toxic to living organisms, including humans, and can negatively affect the ecosystem. Typical electrodes used for the electrochemical reduction of Cr(VI) to less toxic trivalent chromium [Cr(III)] are made of metals or carbon. Effective electrode materials and energy-efficient methods are required to eliminate high concentrations of Cr(VI) contaminants from industrial waters. Here we show activated carbon cloth (CC) as a commercial high-surface-area carbon material that can adsorb Cr(VI) and also reduce Cr(VI) to Cr(III). We investigated the use of unmodified CC to remove 35 ppm Cr(VI) from an acidic solution, which could be similar to the condition found in wastewater from the electroplating industry. The CC used as a cathode removed Cr(VI) faster than without applied electricity. Noticeably, a further decrease in the cathodic potential of CC did not result in faster Cr(VI) removal. We investigated using XPS the mechanisms of Cr(VI) removal by CC used with or without applied electricity, and we elucidated the role of the hydroxyl groups present on CC on adsorption of Cr(VI) and reduction of Cr(VI) to Cr(III). This work could lead to strategies for modifying CC or other carbon materials to increase their effectiveness for Cr(VI) removal.

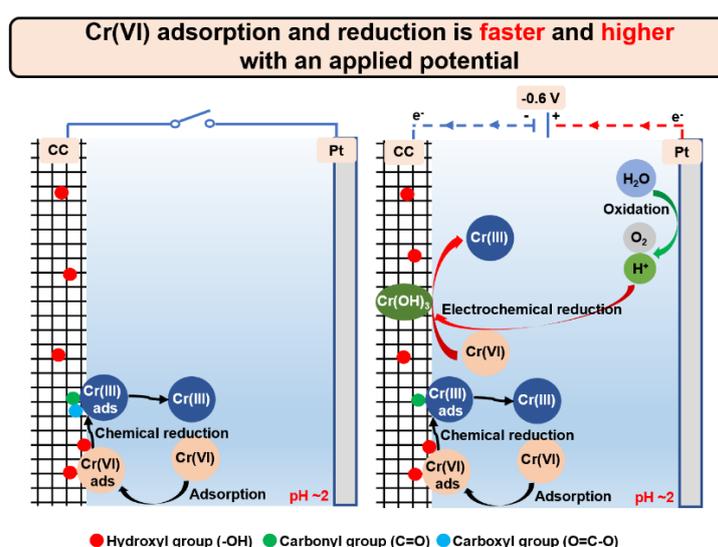


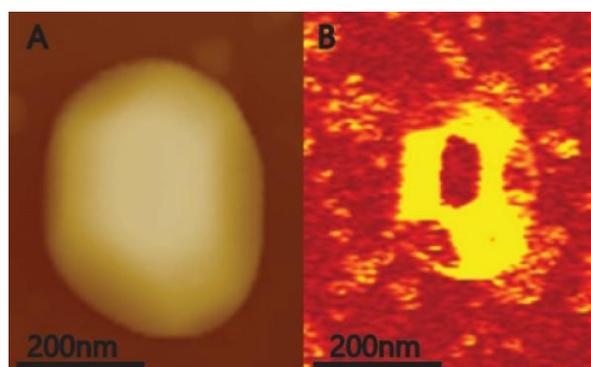
Fig. 1: Schematic illustrating the processes involved in the Cr(VI) adsorption and reduction in the absence or presence of an applied potential.

## Identifying reactivity variations on different facets in single Au nanocrystals.

**L. Rikanati<sup>1</sup>, E. Gross**

<sup>1</sup>Department of Chemistry, The Hebrew University of Jerusalem, Israel

Metal nanoparticles play an essential role in heterogeneous catalysis. However, catalytically-active metal nanoparticles are heterogeneous in their nature and even within the simplest particles, structural differences exist and affect the overall performances of a catalyst. Fundamental understanding of the facet-dependent reactivity requires analysis at the single-particle level. This study identifies, using AFM-IR (Atomic Force Microscopy Infrared) mapping and 4-Nitrobenzenethiol (p-NTP) as probe molecule, the chemical reactivity on different facets in single Au nanocrystal. IR mapping revealed that p-NTP coverage is facet-dependent and higher coverage was identified on (110) facets, while lower coverage was detected on (111) facets (Figure.1). Exposure of the sample to reducing conditions resulted in complete nitro-to-amine reduction on the (110) facets while on (111) facet both N-O and N-H vibrations were detected, implying that only partial reduction was achieved on these sites.



*Fig 1. (a) AFM topography of Au nanocrystal coated with p-NTP, (b) IR mapping at 1336 cm<sup>-1</sup> (correlated NO symmetric stretch), of the nanocrystal that is shown in a.*

## Structure and poisoning effects on hydrogen sorption affinity in single Pd nanoparticles

**Mazal Kostan<sup>1</sup>, Iwan Darmadi<sup>2</sup>, Athanasios Theodoridis<sup>2</sup>, Christoph Langhammer<sup>2</sup>, Elad Gross<sup>1\*</sup>**

<sup>1</sup>Institute of Chemistry, The Hebrew University of Jerusalem, Israel

<sup>2</sup>Department of Physics, Chalmers University of Technology, Göteborg, Sweden

To minimize the long-term consequences of a changing climate, large scale CO<sub>2</sub> emissions must be reduced using alternative technologies such as hydrogen sources. However, at concentration above 4%, H<sub>2</sub>-air mixtures are highly flammable [1]. Therefore, effective H<sub>2</sub> monitoring systems must be developed, which remain selective even under humidity and acidity conditions. Due to highly H<sub>2</sub> selectivity and unique way of interaction to form hybrid, Pd nanoparticles (NPs) can be used as Pd-based hydrogen sensors.

Our goal is to understand how structure and sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) poisoning, affect the hydrogen sorption affinity to Pd NPs. *In-situ* AFM-IR enable to characterize the Pd to Pd hybrid (Pd-H) transformation in single nanoparticle. Hence, AFM topography uses for the structural changes, IR mapping determine the H<sub>2</sub>SO<sub>4</sub> poisoning regions and KPFM analyze the effect of H<sub>2</sub> sorption on the Pd work function.

The current results reveal that Pd NPs with defined facets exhibit more homogeneous H<sub>2</sub> sorption resulting in homogenous Pd-H formation, while NPs with undefined amorphous morphology, display heterogeneous sorption. After exposure to H<sub>2</sub>SO<sub>4</sub> Pd NPs showed differences in the poisoning sites. Defined Pd NPs adsorb H<sub>2</sub>SO<sub>4</sub> uniformly to the surface, resulting limited H<sub>2</sub> sorption and homogenous Pd-H formation. However, H<sub>2</sub>SO<sub>4</sub> adsorb at the periphery of the amorphous particles, causing differences in Pd-H formation on the center and the edge of the NPs.

Consequently, better understanding the way structure and poisoning affects the H<sub>2</sub> sorption affinity in Pd NPs, will further improve the development of tolerant H<sub>2</sub> sensors.

[1] I. Darmadi, FA. Nugroho, C. Langhammer, *ACS Sens.*, 5, 11, 3306–3327 (2020).

# Electron induced chemistry of nitrous oxide-water co-adsorbed film ( $N_2O@H_2O$ ) as a model study of astrochemistry in the interstellar medium

Ahmad Nawaz<sup>1\*</sup>, Roey Sagi<sup>1</sup>, Hiley Iny<sup>1</sup> and Micha Asscher<sup>1</sup>

<sup>1</sup> Institute of Chemistry, Faculty of Science, The Hebrew University of Jerusalem, 91904, Israel

\*Corresponding Email: - ahmad.nawaz@mail.huji.ac.il

## Abstract

The desorption kinetics of  $N_2O@H_2O$  film deposited on a Ru (0001) surface under ultra-high vacuum (UHV) environment ( $2 \times 10^{-10}$  Torr) has been investigated as a model study for electrons-induced reactivity that takes place in the interstellar medium, using temperature-programmed desorption (TPD) measurements, at substrate temperature of 35K. The TPD spectra of all the prominent product masses were well detected by the QMS, employing a 3D-TPD analysis. The  $N_2O$  molecules, embedded within ASW as the host matrix, decompose upon exposure to electrons at kinetic energies of 10eV and 50 eV. This leads to the formation of new molecular products at  $m/z$  values of 28 ( $N_2$ ) and 30 (NO) as the primary products. Typical TPD spectra of the parent  $N_2O$  molecules, while embedded in ASW layer (15 ML) are shown in Figure 1a and product formation is shown in Figure 1b. Here, the primary  $N_2O$  TPD peaks appear at  $\sim 82$ K, while some of these molecules are trapped within the water film and desorb together with the main ASW film at  $\sim 160$ K. Decomposition cross sections for the various electron-induced products will be discussed in the main poster.

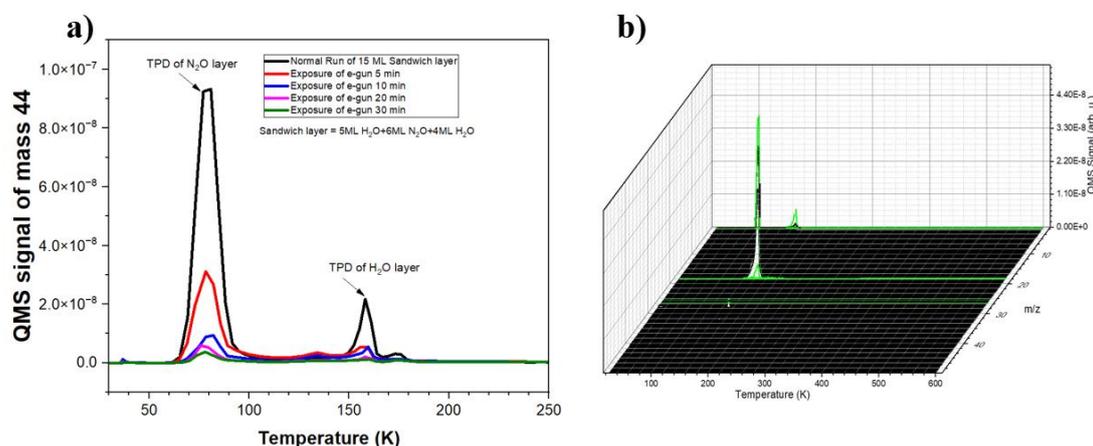


Fig. 1: a) TPD of 15 ML sandwich layer [5ML  $H_2O$ +6ML  $N_2O$  + 4ML  $H_2O$ ] with its multilayer peak at 82K and trapped molecules in ASW desorb at 160K and b) 3D TPD of 15 ML sandwich with product formation.

## References

- [1] G.Toker and M. Asscher, Phys.Rev.Lett., **107**, 167402 (2011).
- [2] A. Paldor, G. Toker, Y. Lilach and M. Asscher, Phys. Chem. Chem. Phys., **12**, 6774 (2010).

## **Nanospectroscopy mapping of supported molecular catalyst for CO<sub>2</sub> electroreduction to methanol**

**H. Shema and E. Gross\***

Institute of Chemistry and the Center of Nanoscience and Nanotechnology, The Hebrew University of Jerusalem

Electroreduction of CO<sub>2</sub> to methanol is a highly desired process for converting greenhouse gas to a bio-fuel building block. It was recently demonstrated that Cobalt phthalocyanine (CoPc) supported on carbon nanotubes (CNTs) is highly effective electrocatalyst, reaching 40% selectivity towards methanol formation.[1] In this work, we correlated the distribution of CoPc and the resulting reactivity by conducting high spatial resolution IR nanospectroscopy measurements. Atomic force microscopy infrared nanospectroscopy (AFM-IR) was utilized in order to map CoPc distribution on the CNTs. Comparison between the Catalytically-active hybrid structure and a physical mixture of CoPc and CNT, revealed a more homogeneous distribution of CoPc on the hybrid structure, while mostly aggregates of CoPc were detected in the physical mixture. These spectroscopic measurements show the crucial impact in the formation of a uniform monolayer of the molecular CoPc catalyst for its optimal catalytic functionality.

- [1] Y. Wu, Z. Jiang, X. Lu, Y. Liang, and H. Wang, "Domino electroreduction of CO<sub>2</sub> to methanol on a molecular catalyst," *Nature*, vol. 575, no. 7784, pp. 639–642, 2019.

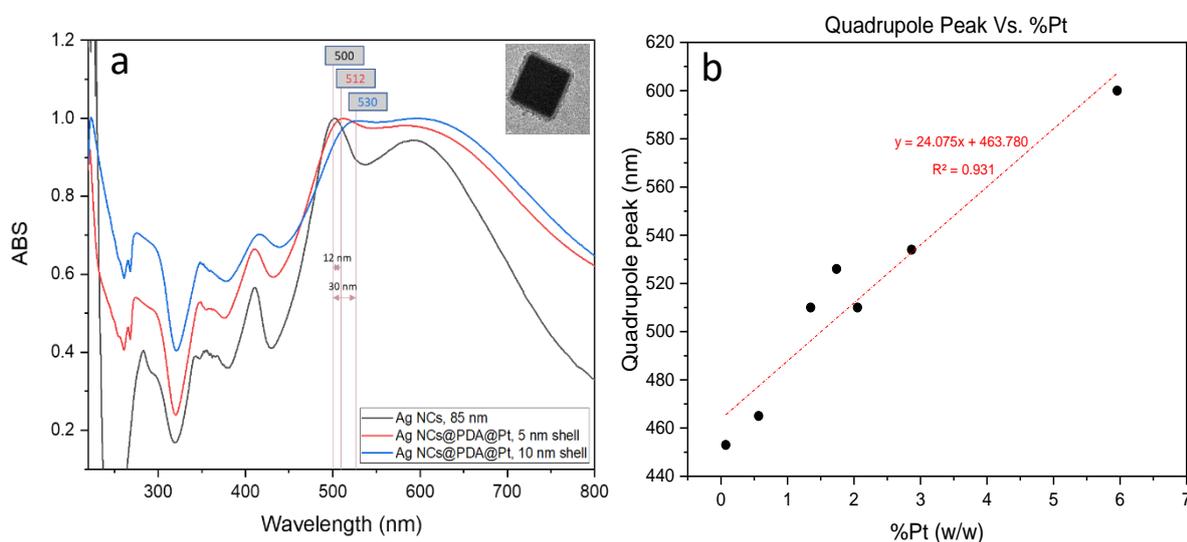
## Complexation of Platinum on the Surface of Shape-defined Plasmonic Nanoparticles

**Avi Huri<sup>1</sup>, Yaakov Mandelbaum<sup>1,2</sup>, Anya Muzikansky<sup>1</sup>, Mike Rozenberg<sup>1</sup>, and Davis Zitoun<sup>1</sup>**

<sup>1</sup>Department of Chemistry and Bar Ilan Institute of Nanotechnology and Advanced Materials (BINA), Bar Ilan University, Ramat Gan, Israel

<sup>2</sup>Department of Applied Physics/Electro-Optics Engineering, Advanced Lab for Electro-Optics Simulations (ALEO), Lev Academic Center, Jerusalem, Israel

The use of plasmonic particles, specifically, localized plasmonic resonance (LSPR), may lead to a significant improvement in the electrical, electro-chemical and optical properties<sup>[1,2]</sup>. For this, it is necessary to control the size, shape, composition and its dielectric environment. Many studies have dealt with the changes to the LSPR through chemical environment modification of metallic nanoparticles<sup>[3]</sup>. In this research, we investigated the change of the LSPR by modifying the chemical environment of metallic nanoparticles (NPs) through the introduction of metal cations: Pt(IV) complexes. This study was carried out by measuring the shift of the plasmon dipole peak of silver nanocubes (NCs)<sup>[4]</sup> (and nanowires (NWs)) of differing sizes upon coating the NCs surface with a layer of polydopamine (PDA)<sup>[5]</sup> and Pt(IV) complexes. The red shift (fig 1a) depends linearly on the thickness of the PDA:Pt(IV) layer and the Pt(IV) content (fig 1b). Additionally, we calculated the dielectric constant of the surrounding medium by a numerical method.



*Fig. 1: a) UV-Vis spectrum of 85 nm coated with platinum and uncoated nanocubes. b) Graph of Pt concentration influence on plasmon quadrupole peak*

- [1] M. A. Garcia, M. A. García, J Phys D Appl Phys 2011, 44, 283001.
- [2] M. Kim, J. Lee, J. Nam, Advanced Science 2019, 6, 1900471.
- [3] M. A. Mahmoud, M. Chamanzar, A. Adibi, M. A. El-Sayed, J Am Chem Soc 2012, 134, 6434.

- [4] H. I. Sang, T. L. Yun, B. Wiley, Y. Xia, *Angewandte Chemie - International Edition* 2005, 44, 2154.
- [5] A. Kitayev, M. Zysler, S. Hardisty, M. Page, E. Tal-Gutelmacher, D. Zitoun, *Energy Technology* 2021, 9, DOI 10.1002/ente.202100546.

**Frontiers in Nano Photonics**

**(NP)**

**Highly effective anti-reflective structures for polymer optics**<sup>1,2</sup>S.Tzadka, <sup>3</sup>I.Kalyan, <sup>1,2</sup>E.Toledo, <sup>3</sup>Y.Sivan, <sup>1,2</sup>M. Schwartzman

<sup>1</sup>Department of Materials Engineering and <sup>2</sup> Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of the Negev, P.O. Box 653, Beer-Sheva 84105, Israel

<sup>3</sup>Department of Electrical Engineering, Ben-Gurion University of the Negev, P.O. Box 653, Beer-Sheva 84105, Israel

Optical polymers are attractive for lightweight and cost-effective refractive optical components, yet they reflect part of the incident light. Traditional vacuum-deposited anti-reflective films purely adhere to polymers and suffer from mechanical stresses due to the difference in the thermal expansion coefficients. Alternatively, reflection can be reduced by moth-eye structures, yet, their efficiency strongly depends on their optical characterization matching with the optical substrate, which has not been demonstrated so far. Here, we introduce a new approach to engineering highly effective anti-reflective structures on the surface of the optical polymer, with an unprecedented ability to reduce the surface reflection from 5% to 0.1 %. The structures were produced by high-throughput nanoimprint lithography, and their superior optical performance was achieved due to the precise matching of their optical characterization to that of the underlying substrate. We further applied these structures on different polymers and showed that their anti-reflective effect correlates with index matching. We demonstrated that these structures could be applied on flat surfaces and curved lenses and produce high surface hydrophobicity. Overall, our work paves the way to an efficient and scalable anti-reflective solution for polymer optics.

## Characterization of nanometric thin films with far-field light

*Hodaya Klimovsky<sup>1,2</sup>, Omer Shavit<sup>2,3</sup>, Carine Julien<sup>3,4</sup>, Ilya Olevsko<sup>1,2</sup>, Mohamed Hamode<sup>1,2</sup>, Yossi Abulafia<sup>1</sup>, Hervé Suaudeau<sup>3</sup>, Martin Oheim<sup>3</sup>, and Adi Salomon<sup>1,2,\*</sup>*

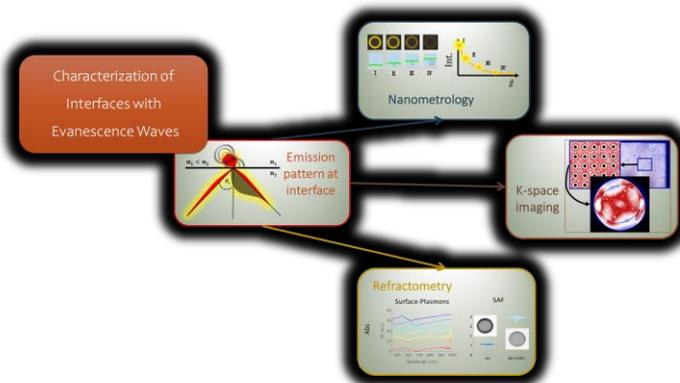
<sup>1</sup> Institute of Nanotechnology and Advanced Materials (BINA), Bar-Ilan University, Ramat-Gan, Israel;

<sup>2</sup> Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

<sup>3</sup> Université Paris Cité, CNRS, Saints Pères Paris Institute for the Neurosciences, F-75006 Paris, France;

<sup>4</sup> Université Paris Saclay, Ecole Normale Supérieure Paris-Saclay, CNRS, PPSM, F-91190 Gif-sur-Yvette, France.

Characterization of dielectric thin-films is paramount for various opto-electronic materials, coatings and photonics. As thin films within the nanoscale range (10-250 nm) can mimic an interface region, we introduce and validate a contact-less, all-optical characterization method for nanometric transparent films using far-field optics. The ability to fabricate nanometric, smooth and homogeneous layered samples enable us to position fluorescent layers in a controlled sub-wavelength manner above the layer surface. Thus, using super-critical-angle fluorescence (SAF)<sup>1-3</sup> microscopy, we recorded fluorophore the samples emission pattern at the fluorophore Near-Field (NF) transformed at the back-focal-plane (BFP) of the microscope objective by Furrier simple optics. We developed a quantitative image analysis to perform in-operando measurements of the refractive index, film homogeneity and to estimate axial fluorophore distances at a sub-wavelength scale with a precision of a few of nanometers. Our results compare favorably to those obtained through more complicated and involved techniques. Applications in nanometrology and axial super-resolution imaging are presented. We Our approach is cheap, versatile and it has applications in various field of photonics.



*Fig. 1: Evanescence Field Characterization using Far-Field optics*

1. Brunstein, M., Salomon, A. & Oheim, M. Decoding the information contained in fluorophore radiation patterns. *ACS Nano* **12**, 11725–11730 (2018).
2. Oheim, M., Salomon, A. & Brunstein, M. Supercritical angle fluorescence microscopy and spectroscopy. *Biophysical Perspective* **118**, 2339–2348 (2020).
3. Axelrod, D. Evanescent excitation and emission in fluorescence microscopy. *Biophysical Journal* **104**, 1401–1409 (2013).

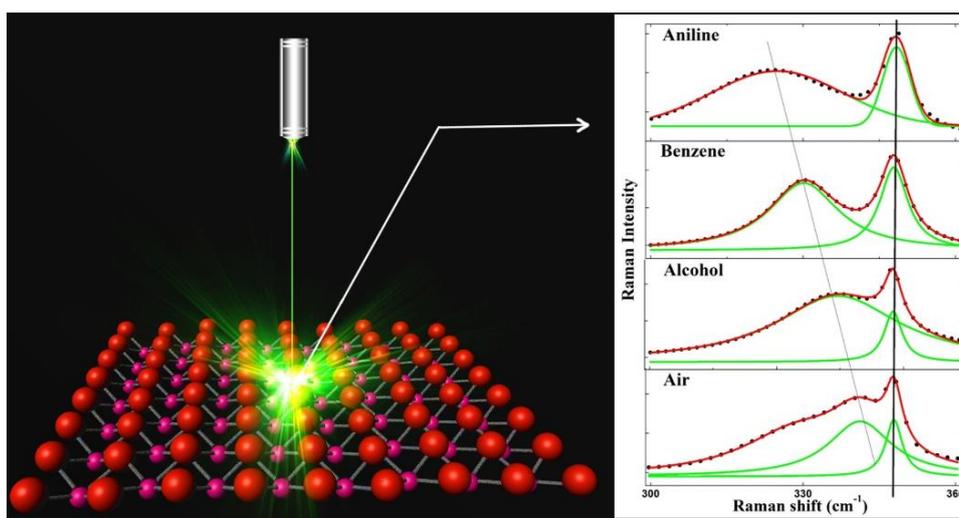
## Synthesis and formation mechanism of different phases and morphologies of polar ZnS nanostructures: morphology identification using Raman spectroscopy

**N. Prasad<sup>1,2</sup> and L. Yadgarov<sup>1</sup>**

<sup>1</sup> Department of Chemical Engineering, Ariel University, Ariel, Israel

<sup>2</sup> Department of Physics, National Institute of Technology, Tiruchirappalli, India

In general, field emission scanning electron microscopy (FE-SEM)) and transmission electron microscopy (TEM) are the advanced technologies used for characterizing nanomaterials morphology. Apart from these techniques, the present work proposes Resonant and non-resonant Raman spectroscopy to identify and morphology of the polar zinc sulfide (ZnS) nanostructures. Herein, poly (vinylpyrrolidone) (PVP) -capped stable cubic and hexagonal phases of ZnS nanostructures are successfully synthesized through simple co-precipitation and single-step hydrothermal method at low temperatures [1]. The role of the capping agent and formation mechanism is studied in detail [2]. The appearance of surface optical (SO) phonon modes in nanorods and nanowires from non-resonant Raman studies confirms the morphology of the samples. The appearance of SO mode is monitored by the SO peak position in accordance with the different dielectric mediums [3]. An approximate dielectric continuum (DC) model is used in this work to understand the SO modes and its dispersion relation.



[1] N. Prasad, and B. Karthikeyan, *J. Appl. Phys.*, **124**, 045702 (2018)

[2] N. Prasad, and B. Karthikeyan *Nanotechnology* **30**, 485702 (2019)

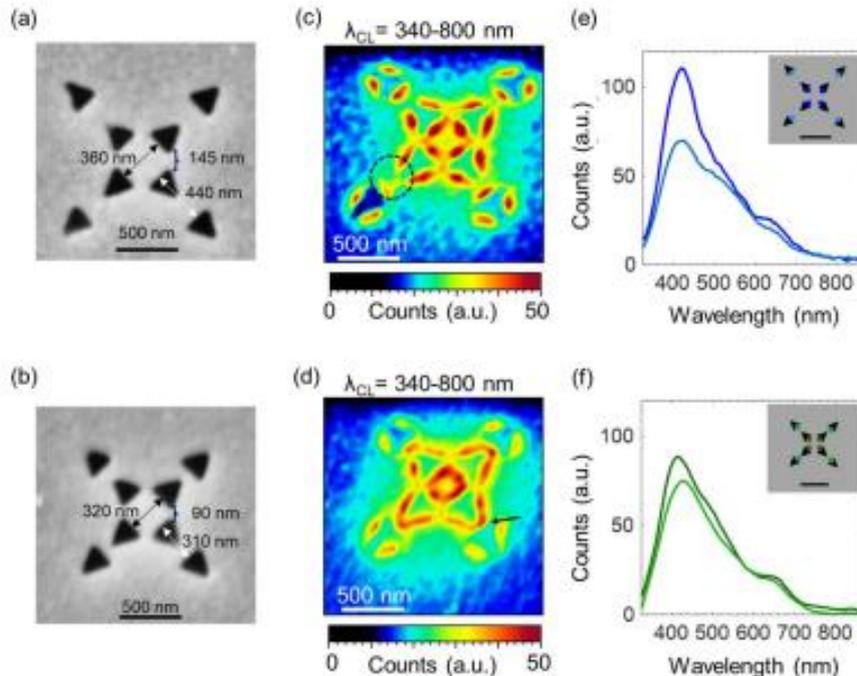
[3] C. H. Ho, P. Varadhan, H. H. Wang, C.Y. Chen, X. Fang and J. H. He *Nanoscale*, **8**, 5954-5958 (2016)

## Nanoscopy of Aluminum Plasmonic Cavities by Cathodoluminescence and Second Harmonic Generation

Tchiya Zar, Racheli Ron, Omer Shavit, Alon Krause, David Gachet and Adi Salomon

### Abstract

We study centrosymmetric aluminum plasmonic structures composed of triangular cavities and visualize their long-range coupling by cathodoluminescence (CL) nanoscopy. Four different plasmonic structures containing the same sub-unit are studied. The plasmonic modes of the individual triangular sub-units are localized at the triangle sides rather than at the vertices, in agreement with other studies. Yet, upon strong interaction between the cavities a redistribution of the electromagnetic field is observed such that it delocalizes around the cavities in the form of a contour, providing a mode enhancement and a pronounced nonlinear response as observed by second harmonic generation (SHG). Comparison between plasmonic structures made of either silver or aluminum reveals that the metal dielectric function plays an important role in the interaction between the cavities. Our study provides a rationale for designing plasmonic structures with enhanced nonlinear.



**Figure 1:** Hybridization and delocalization in quadrupolar plasmonic structures. (a, b) SEM images of two quadrupolar structures made of the same eight sub-units having different inter-unit distances. (c, d) Mapping of CL emission (340-800 nm) from the structure in (a), and from the structure in (b), respectively. (e, f) CL spectra extracted from the inner and the outer triangular cavity bases (see insets) of the structures shown in (a) and (b), respectively. Scalebars are 500 nm

## **Switching of photocurrent polarity in electrochemical cells with light via an excited state proton transfer mechanism**

**A. Yuchnovsky<sup>1</sup> and Y. Shlosberg<sup>2</sup>**

<sup>1</sup>Department of Chemistry, Technion, Haifa, Israel

<sup>2</sup>Department of Chemistry, Technion, Haifa, Israel

Light is a common source of energy in sustainable technologies for photocurrent generation. To date, in such light-harvesting applications, the excited electrons are generating the photocurrent. Here, we introduce a new mechanism for photocurrent generation that is based on excited state proton transfer (ESPT) of photoacids and photobases that can donate or accept a proton, respectively, but only after excitation. We show that the formed ions following ESPT can either serve as electron donors or acceptors at the electrodes, which are dependent on the application of an electric potential, or modify the properties of the electrochemical interface, both resulting in photocurrent generation. We further show the control of the current polarity by switching the irradiation between the photoacid and the photobase. Our study represents a new approach in photoelectrochemistry by introducing ESPT processes, which can be further utilized in light-responsive energy production or energy storage.

## **FDTD simulations of exciton-polariton resonances in WS<sub>2</sub> nanotubes**

**H. Shalom<sup>1</sup>, S. Sekhar Sinha<sup>2</sup> and L. Yadgarov<sup>1</sup>**

<sup>1</sup>Department of Chemical Engineering, Ariel University, Ariel, 4076414, Israel

<sup>2</sup>Department of Chemistry and Biochemistry, Jackson State University, Jackson, Mississippi 39217, United States

Transition metal dichalcogenides (TMDs) have visible or near-infrared and layer-dependent bandgaps, hence they have been shown a variety of intriguing optical and electronic phenomena. Two-dimensional (2D) layered TMDs like WS<sub>2</sub> nanotubes are one of the prime foci of this field in the last 30 years. The semiconducting WS<sub>2</sub> nanotubes have strongly bound excitons and high oscillator strength. They are as a unique class of quasi 1D-material, these materials can sustain exciton-polaritons (EPs) in ambient conditions, i.e., strong coupling of excitonic resonances to the optical cavity. Finite Difference Time Domain (FDTD) simulation permits to the investigation of the interactions between the excitons and the cavity mode with their effect on the extinction spectrum of these nanostructures. Moreover, controlling the radius of the nanotube allows for the manipulation of the EPs. These findings open up possibilities to incorporate the nanotubes in advanced quantum, polaritonic, and optoelectronic devices.

**Bio Applied Surfaces and materials**

**(BI)**

## Molecular Scale Spatio-Chemical Control of the Activating-Inhibitory Signal Integration in NK Cells

Esti Toledo<sup>1,2\*</sup>, Guillaume Le Saux<sup>1,2\*‡</sup>, Avishay Edri<sup>4</sup>, Maor Rosenberg<sup>1,2</sup>, Viraj Bhingardive<sup>1,2</sup>, Olga Radinsky<sup>4</sup>, Uzi Hadad<sup>2</sup>, Ana-Sunčana Smith<sup>3,5</sup> Angel Porgador<sup>4</sup>, Mark Schwartzman<sup>1,2‡</sup>

<sup>1</sup>Department of Materials Engineering, <sup>2</sup>Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of the Negev, Beer-Sheva, 8410501, Israel.

<sup>3</sup>Department of Physics, IZNF, FAU Erlangen-Nürnberg, Erlangen 91058, Germany, <sup>4</sup>The Shraga Segal Department of Microbiology, Immunology, and Genetics, Faculty of Health Science, Ben-Gurion University of the Negev, Beer-Sheva, Israel

\* Equally contributing authors ‡ Corresponding authors

Innate immune system is based on natural killer (NK) cells – lymphocytes that distinguish between healthy and diseased cells, and attack tumor. The activity of NK cells regulate through a delicate balance between activating and inhibitory signals delivered by a multitude of activating and inhibitory receptors. The role of juxtaposition of activating and inhibitory receptors in signal inhibition of cytotoxic lymphocytes remains strongly debated. The challenge lies in the lack of tools that allow simultaneous spatial manipulation of signaling molecules. Recently, biomimetic devices have been limited to control only receptor of one type, and thus could not be used to study signal integration between different receptors. To circumvent this, we produced a nanoengineered multifunctional platform with molecular scale spatial control of ligands. This platform was fabricated by an “out-of-the-box” fabrication approach, in which were included nanoimprint lithography with double angle evaporation. This approach was allowed to produce bimetallic nanoarrays registered with nanoscale accuracy using only one lithographic step, and with no need for alignment between different nanodots. We first patterned a thermal nanoimprint resist on a Si substrate and transferred the imprinted pattern into a resist by angle deposition of a metallic protection mask, resist over-etch by plasma, two sequential metal evaporations, Au and Ti/Cr in, and liftoff. This platform was conceived by bimetallic nanodot patterning with molecular-scale registry, followed by a ternary functionalization with distinct moieties. We found that a 40-nm gap between activating and inhibitory ligands provided optimal inhibitory conditions. This highly versatile approach provides an important insight into the spatial mechanism of inhibitory immune checkpoints, which is essential for the rational design of future immunotherapies.

## **Experimental and computational design of hybrid peptide self-assembled universal nanocarriers for cancer drug delivery**

Vijay Bhooshan Kumar<sup>1</sup>, Anastasia Vlachou<sup>2</sup>, Phanourios Tamamis<sup>2,3\*</sup> Ehud Gazit<sup>1,3\*</sup>

<sup>1</sup>The Shmunis School of Biomedicine and Cancer Research, George S. Wise Faculty of Life Sciences, Tel Aviv University, Tel Aviv, 6997801, Israel

<sup>2</sup>Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas, 77843-3122, USA

<sup>3</sup>Department of Materials Science and Engineering, Texas A&M University, College Station, Texas, 77843-3003, USA

<sup>4</sup>Department of Materials Science and Engineering, Iby and Aladar Fleischman Faculty of Engineering, Tel Aviv University, Tel Aviv, 6997801, Israel

### **Abstract**

Cancer is one of the most complex diseases that require complex therapies. However, conventional chemotherapy has some shortcomings, including low bioavailability, high dose requirements, adverse side effects, low therapeutic indices, development of multiple drug resistance, and non-specific targeting. In order to address these delivery-related problems, extensive efforts have been made to create drug delivery vehicles that transport drugs to the desired sites of therapeutic action while minimizing adverse effects. Designing novel cancer drug nanocarriers is of utmost importance in the framework of cancer therapeutics. Self-assembling peptides constitute an emerging novel class of materials with highly promising applications in drug delivery, as they can be used to facilitate drug release and/or stability while reducing side effects. The purpose of this work is to present experimental and computational designs of new universal peptide self-assembled nanocarriers for the delivery of different cancer drugs (polar, nonpolar, highly polar) and stabilization of their structures. Using cyclo-histidine-histidine (cyclo-HH) peptide-based nanocarriers that incorporate cancer drugs via self-encapsulation (core/shell) or encapsulation in mixed pattern grooves. TEM has been used to determine and characterize the self-assembly properties, as well as UV-VIS and fluorescence spectroscopy to determine the loading capacity of each cancer drug. The release of drugs for successful Cyclo-HH-Zn nanocarriers occurs at slightly acidic pH levels (6.0), whereas the release of drugs at neutral pH levels is slower. Based on cell viability studies, self-assembled structures of cyclo-HH-Zn-drugs structures are excellent cytocompatibility at concentrations of 1-2  $\mu\text{g/mL}$ . Self-assembled cyclo-HH-Zn-containing drugs (Dox, Epi, Mit C, Csp, 5FU, and Mtr) are capable of passing through cell/tissue membranes and can be used for drug delivery. As a result of the intrinsic advantages of this novel classis of single or multicomponent cancer drug delivery systems incorporating these materials may emerge.

## Electrochemical Exploration of Biofilm Using Micro Electrodes Array

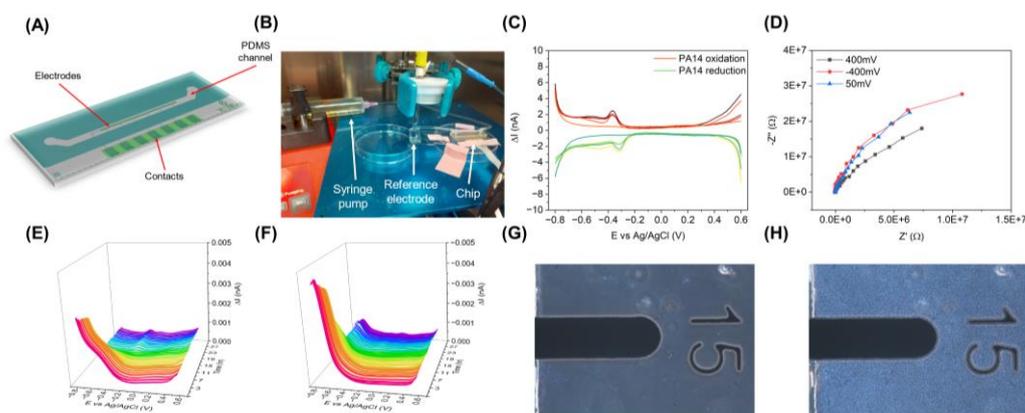
**Oriya Belous Maruani<sup>1,2</sup>, Anat Milo<sup>1</sup> and Hadar Ben-Yoav<sup>2\*</sup>**

<sup>1</sup>Department of Chemistry, Ben-Gurion University of the Negev, Beer Sheva, Israel

<sup>2</sup>Department of Biomedical Engineering, Ben-Gurion University of the Negev, Beer Sheva, Israel

Biofilm is the natural form of bacterial population and it composed of the bacteria encapsulated in secreted extracellular polymeric substances. The biofilm as a physical barrier provides protection from environmental changes and therefore found to increase bacterial antibiotic resistance up by 1,000 times. Therefore, analytical platforms that mimic the behavior of biofilms in nature and can investigate their response to various treatments will advance our understanding of these biosystems. Electrochemical lab-on-a-chip micro-systems enable monitoring biofilm formation over time in controlled environments. However, these micro-systems are based on single 2D electrodes that are limited in their ability to measure the 3D complex formation of the biofilm [1]. Here, we present a lab on a chip integrated with an array of microelectrodes that can be further modified with various partially selective coatings. The micro-system is designed and fabricated using conventional photolithography and lift off techniques, and it includes five gold disk working electrodes ( $\phi=70\mu\text{m}$ ), gold rectangle counter and an Ag/AgCl reference electrode (Figs. 1A&1B). The array of microelectrodes was bonded with a microfluidic channel made of polydimethylsiloxane. As proof-of-concept study to monitor the biofilm's formation and functionality, we grew *Pseudomonas aeruginosa*, a pathogenic bacterium that secretes electroactive molecules phenazines once it reaches high cell density. Then, we monitored the biofilm's formation for 30 hours by repetitively measuring the electrochemical signal using differential pulse voltammetry (DPV) (Fig. 1C) and electrochemical impedance spectroscopy (EIS; 1-hour frequency) at DC potentials of -400, +50, and +400 mV vs Ag/AgCl (Fig. 1D). Monitoring the oxidative (Fig. 1E) and reductive (Fig. 1F) currents revealed an increasing oxidation peak at -0.25V vs Ag/AgCl after 18hr that can be attributed to phenazines oxidation. Moreover, both oxidation and reduction signals showed a reduction in the peak current at negative potentials (-0.6 - -0.8 vs Ag/AgCl) that can be correlated to the bacteria growth. By integrating the developed micro-system with a fluorescent microscope, real-time and direct monitoring of the biofilm's formation can be achieved.

Figure 1. (A) Lab-on-a-chip illustration. (B) Experimental setup. (C) DPV of *pseudomonas aeruginosa* PA14 after two nights incubation at 37°C in Luria broth 2%(LB) measured on fives



electrodes on chip. (D) EIS of PA14 on chip using different DC potentials (50mV, 400mV and -400mV). DPV of PA14 on chip over 30hr (E) oxidative and (F) reductive modes while fresh LB 2% flow in chip. Change in bacteria density on chip at (G) 0hr and (H) 8hr.

[1] Estrada-Leypon, O. et. al, *Bioelectrochemistry* **2015**, 105, 56–64.

## Lubrication by PClated Polymers, Assemblies and Gels

**N. Kampf<sup>1</sup>, W. Lin<sup>1</sup>, M. Kluzek<sup>1</sup>, S. Angayarkanni<sup>2</sup>, N. Iuster<sup>1</sup>, E. Shimoni<sup>2</sup>, R. Goldberg<sup>3</sup> and J. Klein<sup>1</sup>**

<sup>1</sup>Department of Molecular Chemistry and Materials Science, WIZMANN Institute of Science, Rehovot, Israel

<sup>2</sup>Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Tamil Nadu, India

<sup>3</sup>Liposphere Ltd, Givat-Shmuel, Israel

About 20% of the world's total energy consumption spent to overcome friction. Friction is also present in biological systems such as in hips and joints, and correlated with joint diseases such as osteoarthritis. Due to the molecular complexity of the biological systems, the mechanism of lubrication is still not clear. Apart from our efforts to find the major components acting as biolubricants in biological systems, we also try to exploit nature's solution for lubricating interfaces such as cartilage by mimicking nature's strategies of boundary lubrication, which lead to an extreme reduction of friction in aqueous environments. I will present several examples of bio-inspired lubrication by polymers, liposome-polymer assemblies and in polymer gels. We carried out systematic investigations from the molecular to the macroscopic level, demonstrating excellent lubrication by polymer assemblies [1] and hydrogel composites [2], attributed to the hydration lubrication mechanism acting at highly-hydrated boundary layers.

[1] S. Angayarkanni et al., *Langmuir*. **35**, 48. (2019).

[2] W. Lin et al., *Science*. **370**, 6514 (2020).

## **Nanofabricated patterns for the control of T cell receptor clustering**

Y. Segal<sup>a</sup>, S. Naaz, A. Pandey<sup>a</sup>, S. Tzadka<sup>a</sup>, E. Toledo<sup>a</sup>, M. Iraqi<sup>b</sup>, O. Radinsky<sup>b</sup>, A. Porgador<sup>b</sup>, G. Le Saux<sup>a</sup>, M. Schwartzman<sup>a</sup>

<sup>a</sup> Department of Materials Engineering, Ben-Gurion University of the Negev, P.O. Box 653, Beer-Sheva, 84105, Israel.

<sup>b</sup> Genetics Faculty of Health Sciences, Ben-Gurion University of the Negev, P.O. Box 653, Beer-Sheva, 84105, Israel.

Cytotoxic T cells are the sentinels of our immune system, which directly attack pathogens and cancer cells by either cytotoxic or lytic mechanism. T cells have a distinct ability to distinguish between healthy cells and their targets, using T cell receptors (TCRs) that bind to specific ligands expressed by the targets, and initiate cascade of signaling events that determine T cell immune response. Although the biochemical aspects of TCR activation have been well studied, little is known about its biophysical aspects. Super-resolution microscopy revealed that during the activation of T cells, TCR receptors and costimulatory receptors CD 28 form highly regulated nanoscale clusters. However, the role of the cluster size and distribution in the signaling and activation of T cells is still unclear.

Here, we have prepared a research platform aimed at studying the effect of the size of activating nanoclusters on the signaling immune response of T cells. The platform consisted of a Silicon surface patterned with the nanoscale clusters of the antibodies for TCR and costimulatory receptors CD28, in which the cluster size was controllably varied within the range of 40 nm to 250 nm. The platform was fabricated using colloidal lithography, by depositing a monolayer of polystyrene nanoparticles of varying sizes (100nm to 500nm) using the Langmuir-Blodgett method. The monolayer formation was followed by plasma etching to reduce the nanoparticles by half, evaporation of gold, and liftoff. The resulting Silicon "holes" within the gold mesh were then functionalized with (3-Aminopropyl) triethoxysilane (APTES), following the attachment of COOH-PEG-Biotin, to which an even mix of Anti CD3 and Anti CD28 was selectively immobilized via neutravidin bridge. The surrounding Au area was passivated with PEG thiol to prevent non-specific interaction with T cells. To verify the selectivity of the functionalization, the surfaces were imaged by a confocal microscope. Here, green labeled Neutravidin was used as marker for the antibody-functionalized areas, clearly revealing that the antibody immobilization was indeed specific for the Silicon.

The fabricated surfaces were used as artificial microenvironment for T cell activation. To that end, primary CD8+ T-cells were isolated from a healthy donor, and incubated on the surfaces for different times. To probe the effect of the cluster size on the early signaling of T cells, TCR phosphatase was immunostained, and its intensity was quantified vs. the cluster size and compared to negative and positive control areas that consisted of continuous Poly-L-lysine and anti-CD3/anti-C28 mix, respectively. To probe the effect of the cluster size on the late signaling, nuclear translocation of NF-kB was quantified by NF-kB immunostaining. Finally, the immune response of T cells was quantified by ELISA of interferon-gamma. In summary, our work paves the way to nanotechnological platforms that can control the spatial clustering and segregation of T cell receptors with the nanoscale resolution. Such control can allow extensive research aimed at revealing the biophysical mechanism of the interaction of T cell receptors with their environment. Understanding this mechanism is fundamentally important, and critical for the rational design of future immunotherapies.

## Mechanism of stiffness induced contact guidance

**Carlos Ureña Martín, Lital Pevzner, Yuval Segal, Guillaume Le Saux, Mark Schwartzman**

1Department of Materials Engineering, 2Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of the Negev, Beer Sheva, Israel.

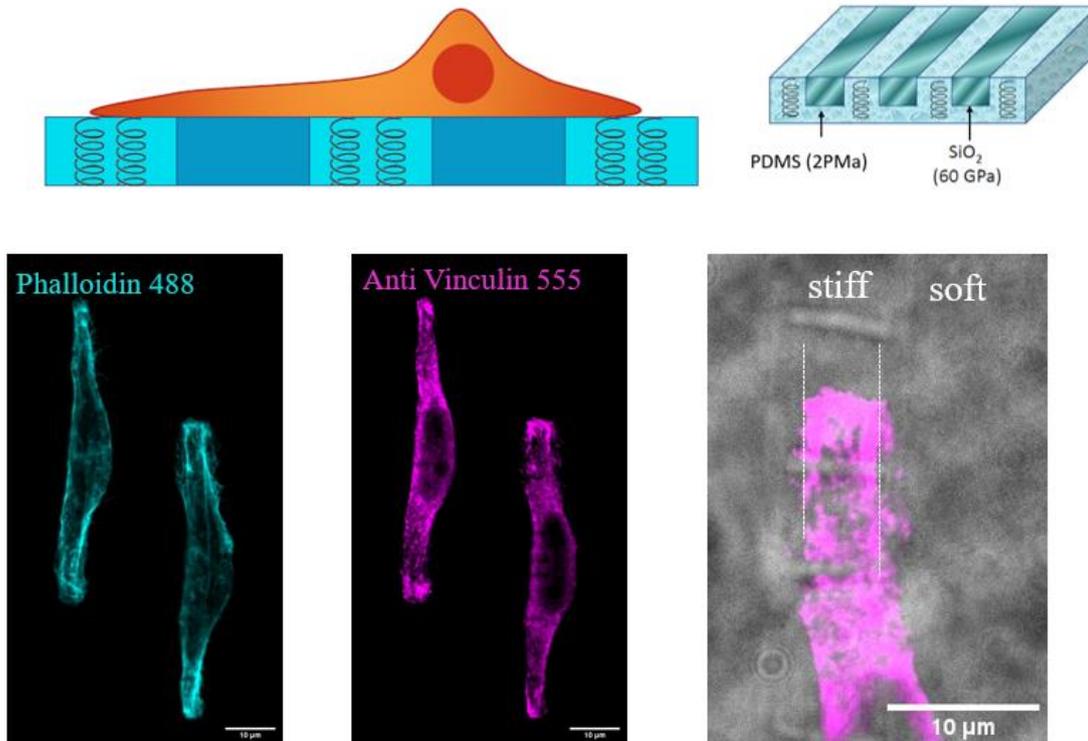


Fig 1. HeLa cells and focal adhesion are aligned to the stiffness pattern

Previously, it has been shown how cells response to gradients of extracellular adhesion molecules, topographical features or stiffness of the substrate by orientating their movement towards them. Moreover, anisotropic cues of these parameters (except stiffness) had been shown to align cellular migration and directionality to them.

In the present work we show how, with a new methodology relying on photolithography and vapour deposition, both single and groups of epithelial cells are able to align and migrate on the axis of stiffness intermittent linear features at the micron scale. For further study we will aim to define the distance threshold where the cells will stop feeling the directionality and thus the dissipation of the stiffness cues on the soft substrate, and define both physical and cellular mechanisms involved in this phenomenon

## Lithographic platform for reference-free traction force microscopy

B. Maman, E. Toledo, S. Tzadka, C. Ureña-Martin, G. Le Saux, M. Schwartzman  
 Department of Material Engineering, Ilse Katz Institute for the Nanoscale Science and  
 Technology, Ben Gurion University, Beer-Sheva, Israel

The mechanical communications between cells and their surroundings, such as other cells and extracellular matrix, is fundamental to regulating complex biological processes during tissue development, repair or pathology. Quantifying the forces cells produce and sense is essential for understanding cellular function. The most common way to identify these forces is Traction Force Microscopy<sup>[1]</sup>, by which cells are placed on an elastomer surface with embedded fluorescent nanoparticles, whose displacement indicates the force direction and magnitude. However, traditional traction force microscopy has three main limitations: (i) The initial position of randomly distributed nanoparticles must be recorded before the cell experiment to detect their displacement, (ii) The random nanoparticle location in z direction makes some of them out of focus, and produce uncertainty in their lateral displacement, and (iii) the nanoparticle displacement can be tracked with limited resolution, usually above 1 micron.

To circumvent these limitations, we engineered a novel platform for traction force microscopy, in which the fluorescent markers with arbitrary size and distribution are controllably positioned in ordered arrays, with the resolution down to the nanometric scale. To fabricate such a platform, we coated the Silicon wafer with a sacrificial film of Au. We patterned it on top of it fluorescently colored epoxy resin (SU-8) by either negative-tone photo- or e-beam lithography. Then, we poured on top of it liquid elastomer (PDMS), cured it, and separated it from Si by etching the Au. This way, we produced elastomer surfaces with arrays of various fluorescent markers sized down to 400 nm. We functionalized the surface with an adhesion molecule (RGD motif of fibronectin) to allow cell adhesion. To verify the feasibility of our platform, we seeded NIH 3T3 mouse fibroblast cells, demonstrating that the fluorescent arrays faithfully indicate the force distribution within and around the individual cells. Our new platform paves the way for numerous studies to understand cells' mechanical activities, focusing on the nanoscale force distribution at the cell-matrix interface.

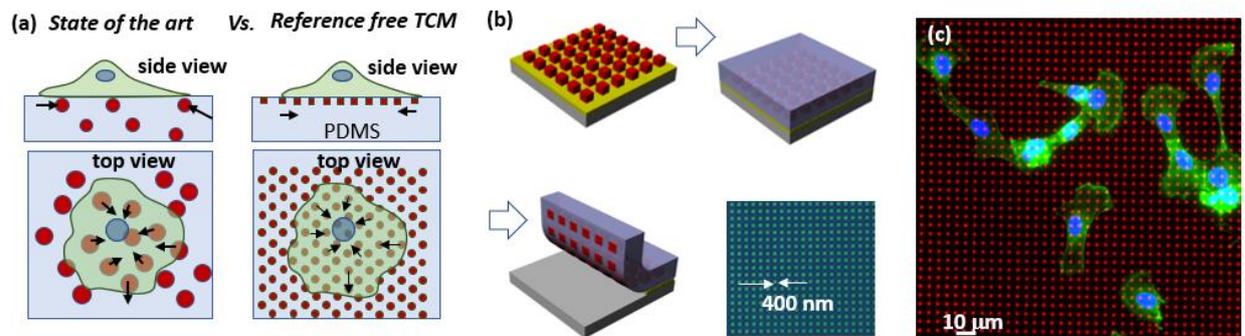


Fig. 1. (a) Commonly used traction force microscopy vs. reference free traction force microscopy demonstrated in this work. (b) Fabrication proves flow and a pattern with 400 nm fluorescent markers. (c) Cells spread on a pattern for reference free traction force microscopy.

## Photo and electrically activated antibacterial and antiviral laser-induced graphene surfaces and composites

**Chetan Prakash Sharma, Abhishek Gupta, and Christopher J. Arnusch**

Dept. of Desalination and Water Treatment, Zuckerberg Institute for Water Research, The Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, 8499000 Midreshet Ben Gurion, Israel

### **Abstract:**

Graphene-based photo- and electronic devices can potentially be useful for various antibacterial, and antiviral applications because of its electrical, optical, and surface properties. Laser-induced graphene (LIG) is an exciting technology for the preparation of porous graphene materials with high precision, fast processing time and mask free, environmentally friendly methodology. Substrate materials, laser parameters, and environmental conditions during LIG fabrication can result in various chemical and physical surface properties, and the graphene can be used “as is” or be transferred to other substrates for composites with photo- and electronic properties. Here we show the photo and electronic effects of LIG for decontamination of bacteria, and viruses in air and water. LIG was first fabricated on a polyimide (PI) non-woven air filter and the electrically conductive air filter resulted in ~99% removal of *Pseudomonas aeruginosa*, and 100% T4 virus in air at a very low applied voltage of ~0.3 V.[1] Also, we demonstrate an electrically conductive LIG composite double-sided adhesive tape (LIGC-tape), prepared via delamination of LIG from its substrate, which could inactivate bacteria on contact, as well as exhibiting excellent electrothermal properties with a maximum temperature >120 °C at 10 V. Also, a temperature rise >70 °C under 120 mW/cm<sup>2</sup> solar irradiation was seen, and enhanced bacterial sterilization up to 99.99% at ~3.5 V in 3 minutes was observed because of the combination of electro- and photothermal effects.[2] These two examples of photo- and electrothermal effects of LIG composites with biological effects indicate that LIG can immediately and easily be incorporated into products with diverse applications.

### **References:**

- [1] A. Gupta, C. P. Sharma, C. Thamaraiselvan, L. Pisharody, C. D. Powell, and C. J. Arnusch, “Low-Voltage Bacterial and Viral Killing Using Laser-Induced Graphene-Coated Non-woven Air Filters,” *ACS Appl. Mater. Interfaces*, vol. 13, no. 49, pp. 58253–59592, Dec. 2021, doi: 10.1021/acsami.1c20198.
- [2] C. P. Sharma and C. J. Arnusch, “Laser-induced graphene composite adhesive tape with electro-photo-thermal heating and antimicrobial capabilities,” *Carbon N. Y.*, vol. 196, no. February, pp. 102–109, 2022, doi: 10.1016/j.carbon.2022.04.041.

**Nanomaterials**

**(NM)**

## Block Copolymer Templated HfO<sub>x</sub> Nanostructures – from Fundamental Understanding to Rational Design

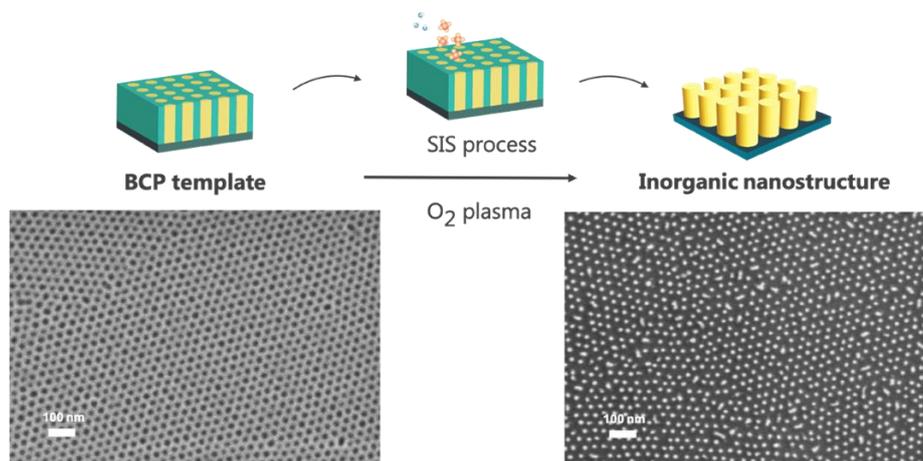
**R. K. Cai<sup>1</sup>, T. Segal-Peretz<sup>2</sup>**

<sup>1</sup>Interdepartmental Program of Polymer Engineering, Technion, Haifa, Israel

<sup>2</sup>Department of Chemical Engineering, Technion, Haifa, Israel

Hafnium oxide (HfO<sub>2</sub>) is an attractive material for optoelectronic applications and high- $\kappa$  dielectrics in semiconductor devices due to its advantageous properties- high dielectric constant, wide band gap, and high stability. However, hafnium oxide nanostructure fabrication currently relies on complex nanofabrication processes. Sequential infiltration synthesis (SIS)- a method derived from atomic layer deposition (ALD), in which vapor phase precursors diffuse into polymers and react with them to form hybrid material, can provide a simple and cost-effective alternative for these processes.

In this study, we demonstrate the formation of hafnium oxide nanostructures within block copolymers (BCPs) templates. BCP were self-assembled into highly ordered and periodic nanostructures. In SIS, selective interactions between the hafnium organometallic precursor and the polar block of the BCP resulted in selective growth within the polar block domains. Following the growth, the BCP template was removed to yield hafnium nanostructures templated by the BCP morphology. We explored the precursor-polymer interactions in various homopolymers using quartz crystal microbalance (QCM) microgravimetric measurements. This knowledge was further applied in finding a suitable BCP for templating HfO<sub>2</sub> inorganic nanostructure.



*Fig. 1: Schematic illustration of HfO<sub>x</sub> nanostructure fabrication process and the corresponding SEM images using PS-*b*-Epoxidized PI as template.*

## **On the Development and Atomic Structure of ZnO Crystals Grown in Polymers from Vapor Phase Precursors**

**I. Weisbord,<sup>1</sup> M. Barzilay,<sup>1</sup> A. Kuzmin,<sup>2</sup> A. Anspoks,<sup>2</sup> E. Welter,<sup>3</sup> T. Segal-Peretz<sup>1</sup>**

<sup>1</sup>Department of Chemical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

<sup>2</sup>Institute of Solid State Physics, University of Latvia, Riga, Latvia

<sup>3</sup>Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

Sequential infiltration synthesis (SIS), an ALD-derived method for growth of inorganic materials inside polymeric structures, is an emerging technique for hybrid materials and inorganic nanostructure fabrication which can be utilized in a wide array of applications. In this work, we study the development of ZnO crystalline particles within SU-8, polymethacrolein (PMCHO), and polymethyl methacrylate (PMMA) at the atomic scale. We probe the growth throughout diethyl zinc (DEZ)/H<sub>2</sub>O SIS cycles, as well as after polymer removal. The crystalline ZnO structure is deciphered by combining two powerful methods: extended x-ray absorption fine structure (EXAFS) and high-resolution scanning transmission electron microscopy (HR-STEM). Synchrotron-based EXAFS provides large-scale statistical information on the crystals' long-range order and predicts their Wurtzite structure. HR-STEM of the hybrid polymer-ZnO films corroborates the predicted structure and allows for precise analysis of crystal size, orientation, and existing defects, as well as the dispersion of the particles inside each polymer. Significantly, the polymer matrix allows us to probe the growth, cycle-by-cycle, providing insights to ZnO atomic growth mechanism inside different polymers and extending our understanding of SIS. In addition, the methodology developed for such high-resolution imaging of hybrid films will allow future studies of additional hybrid systems.

## **Anisotropic Microparticles through Periodic Autofragmentation of Amphiphilic Triblock Copolymer Microfibers**

**Nicole Edelstein-Pardo**<sup>1,2,3</sup>, Maya Molco<sup>2,3</sup>, Parul Rathee<sup>1,3</sup>, Gil Koren<sup>3,5</sup>, Roy Beck<sup>3,5</sup>, Roey J. Amir<sup>1,3,4</sup>, Amit Sitt<sup>2,3</sup>

<sup>1</sup>*Department of Organic Chemistry, School of Chemistry, Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv, Israel*

<sup>2</sup>*Department of Physical Chemistry, School of Chemistry, Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv, Israel*

<sup>3</sup>*Tel Aviv University Center for Nanoscience and Nanotechnology, Tel-Aviv University, Tel-Aviv, Israel*

<sup>4</sup>*The ADAMA Center for Novel Delivery Systems in Crop Protection, Tel-Aviv University, Tel-Aviv, Israel*

<sup>5</sup>*School of Physics and Astronomy, Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv, Israel*

Fracture formation due to drying is a common process in a range of systems, from mud cracks to thin polymeric films. Controlling the position and size of the fractures can be a beneficial patterning tool for different applications, however, in most systems, it is almost impossible to attain.

Here, we present a novel mechanism, based on spontaneous transverse periodic fracturing of drying of polymeric microfibers, for the formation of anisotropic microparticles of custom-made dendron-PEG-dendron amphiphilic tri-block copolymers. Upon drying of the fibers on a glass substrate, they spontaneously fracture into relatively uniform microscale tubular particles. The fracture frequency and the average fragment length are dictated by the diameter of the fibers. Furthermore, we show that the tri-block copolymer exhibits lamellar ordering in the fibers, as is indicated by X-ray scattering measurements. Fine-tuning of the hydrophobicity of the dendrons by modifying their end-groups can significantly alter the swelling and dissolving of the microparticles, hence providing control over their degradation rate.

This new method for creating anisotropic polymeric microparticles with controlled lengths and degradation times may pave the way for the simple formation of PEG polymeric particles for different applications.

[1] Edelstein-Pardo N.; Molco. M; Rathee. P; Koren. G; Tevet. S; Sharabani. S. Z; Beck. R; Amir. R. J.; and Sitt. A. Chem. Mater. 2022, 34, 6367-6377.

## **Laser-induced 3D Patterned Graphene Composites on Curved Surfaces for Fog Harvesting**

**Haeyoung Park<sup>1</sup>, Jonathan Switzer<sup>2</sup>, Camilah D. Powell<sup>1</sup>, Kyoo-Chul Park<sup>2</sup>, and Christopher J. Arnusch<sup>1</sup>**

<sup>1</sup>Department of Desalination and Water Treatment, Zuckerberg Institute for Water Research, The Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede-Boqer Campus 84990, Israel

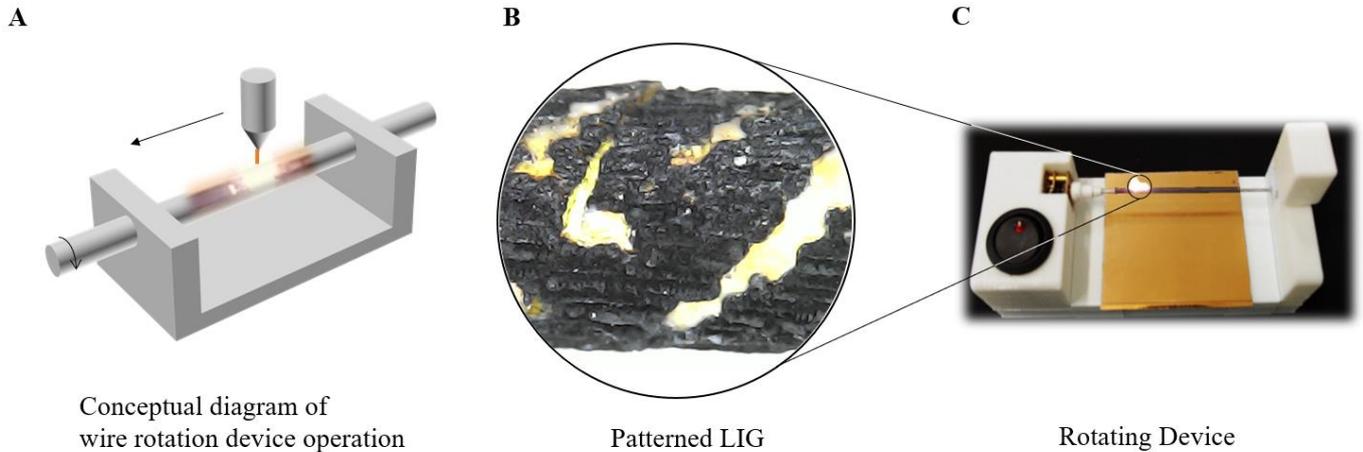
<sup>2</sup>Department of Mechanical Engineering, Northwestern University, Evanston, Illinois 60208, USA

**\*Corresponding author:** C. J. Arnusch, [arnusch@bgu.ac.il](mailto:arnusch@bgu.ac.il);

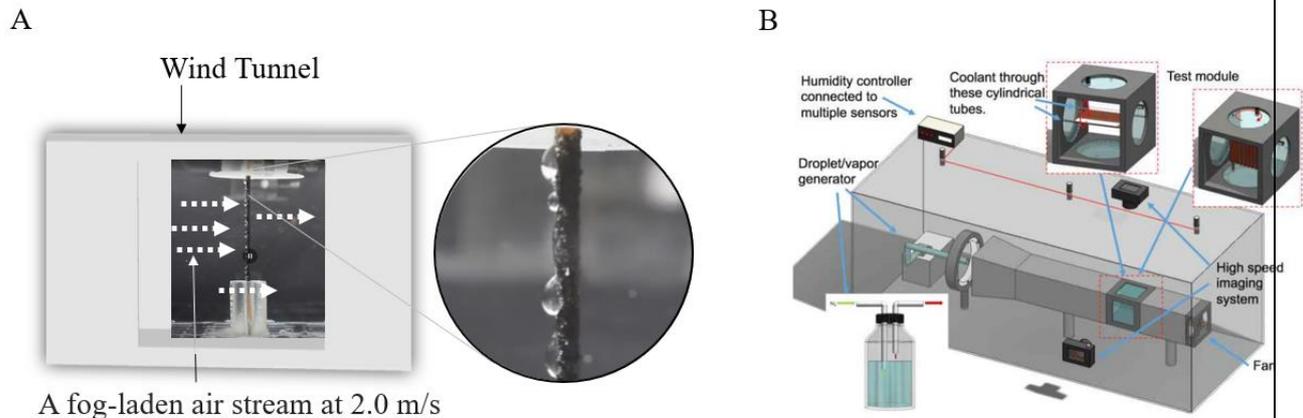
Water scarcity is a crucial global problem, affecting not only drinking water for humans and livestock, but also for energy generation such as cooling water for thermal power plants. For example, cooling water for thermoelectric power plants is the largest water consuming sector in the US and, much of the cooling water used is lost due to evaporation. Most technological solutions to alleviate water scarcity aim at conventional water sources, including river, lake, or sea water, but has yet to fully address the problem; water scarcity still exists. Thus, a new approach focusing on non-conventional sources such as atmospheric water (e.g., fog, dew) is required. Fog collection (from nature or industrial practices) can be a sustainable solution to water scarcity in many regions around the world. In addition, atmospheric water vapor is the most potent greenhouse gas causing a positive feedback loop of global warming. Reducing atmospheric water vapor can contribute to global warming and prevention of climate change.

Laser-induced graphene (LIG) is a three-dimensional porous carbon material prepared by direct laser writing with a CO<sub>2</sub> laser, for surface patterning on various polymers. Therefore, we can freely design a three-dimensional biomimetic pattern for effective water harvesting and implement it on polymer surfaces. We experimentally measure and propose a method for quantifying fog water collection efficiency for a single wire with a curved surface, 3D biomimetic pattern. As a part of such, we identified optimal collection patterns and provide insight into designing effective fog harvesting wire surfaces. Laser Induced 3D patterns increased fog harvesting by 27.7% and reduced fog yield by 83.1% as compared to the controls. Herein, we demonstrate the effectiveness

of our patented method that can apply a Laser Induced 3D pattern to a curved surface of a wire with a diameter of less than 2 mm for fog harvesting applications.



*Fig 1: How to make a pattern with a constant focal length on a PI curved surface utilizing a wire rotator. A) The axis rotation value is the Y-axis value, the laser beam head movement value is the X-axis value, and the Z value is determined by the focal length. C) PI coated wire rotation device made using low speed gear and 3D printer B) 3D pattern LIG applied to PI curved surface wire.*



*Fig 2: This study was conducted in collaboration with the Department of Mechanical Engineering and Northwestern University, and the fog collection experiment measured the fog yield of 24 samples through the B) wind tunnel designed by the Department of Mechanical Engineering. A) The formation process of droplets made by the difference in the surface was observed through a high-speed camera during the fog fabrication experiment.*

## Fabrication of Fluorescent Thin films Using Nanobead Emitters

I.Olevsko-Arad, S. White, A.solomon<sup>1</sup>, and G.Byk<sup>1</sup>

<sup>1</sup>Department of chemistry, Bar Ilan University, Israel

Fluorescent molecules fall into two distinct groups; the first is comprised of molecules that fluoresce intensely in dilute solution but that lack emission in the solid-state. The second group shows strong emission when forming aggregates or in crystalline (amorphous) form, making them suitable for solid-state devices and opto-electronic applications. The second group is relatively small. In order to develop solid state devices, new materials that act like the second group need to be researched.

A promising candidate is a large group of conventional dyes, that fluoresce when deposited in thin films. Major challenges remain in fabrication of such fluorescent thin films; (i) insufficient brightness (ii) aggregation (iii) isotropic emission, resulting in signal loss within a given collection aperture.

Our present research brings to the table a new platform of thin film fabrication. This platform involves nanobead emitters (NBEs)<sup>[1]</sup>, that allow for the creation of fluorescent thin films with different colors as well as a facile process (click chemistry) for the preparation thereof. Furthermore, using LBL technique, deposition of NBEs on different surfaces showed a homogeneous, bright fluorescent thin films with a depth of a few nanometers.

[1] [\*Journal of Nanoparticle Research\*](#) volume 16, Article number: 2796 (2014)

## Self-Assembly Based Fabrication of Optical Sub-Wavelength Structures

<sup>1,2</sup>Sivan Tzadka, <sup>1,2</sup> Lotem Kitaroo, <sup>1,2</sup> Mark Schwartzman

1 Department of Materials Engineering and 2 Ilse Katz Institute for Nanoscale Science

& Technology, Ben-Gurion University of the Negev, P.O. Box 653, Beer-Sheva

84105, Israel

Any optical surface reflects light, and this reflection reduces the quality of the image passed through eyeglasses, telescopes, or optics for autonomous driving. This reflection also produces ghosting and glare in the camera and displays. Traditionally, the reflection is addressed by thin antireflective films, which are, however, effective only for a limited range of the spectrum. Furthermore, these films are quickly damaged due to scratching, cracking, and detachment, especially when exposed to harsh environments or sudden temperature changes. The solution comes from nature: It was discovered that the cornea of some insects, such as moths, are covered with nanometric conical bumps. While smaller than the wavelength of light, these bumps produce an optical effect that prevents light reflection for a broad range of light colors and angles, which is unachievable by thin films. The idea of using artificial biomimetic moth-eye structures to reduce reflection from optical surfaces has been extensively discussed over the last two decades. Yet, the realization of this idea was challenged by the lack of scalable methods to produce biomimetic objects sized a few times smaller than the wavelength of light, i.e. down to one hundred nanometers.

In this work, we examine two novel approaches to fabricating moth-eye nanostructures using nanopatterning from the bottom up. In the first approach, polystyrene nanoparticles are assembled on the optical surface using Langmuir-Blodgett technique, following the controlled reduction of the nanoparticle diameter by Oxygen plasma, deposition of a metallic mask, plasma etching of the substrate, and removal of the remained mask by wet etching. In the second approach, the assembly of nanoparticles is done by a novel approach based on the mechanical assembly of nanoparticles onto a surface of elastomer to get a packed particle monolayer and transfer of these nanoparticles onto the optical surface. We first compared between the two approaches in terms of the quality of the particle assembly, using home-made algorithm for image processing of the SEM of the resulting monolayers. We then used both approaches to fabricate broadband antireflective nanostructures on Sapphire, and characterized their optical performance by surface reflection. The experimentally obtained reflection spectra also showed good agreement with those obtained by simulations using Effective Medium Theory. Overall, our work provides a new route for facile and high-throughput nanostructuring of optical surfaces, and paves the way for numerous optical applications.

## **Combined nanofiltration and advanced oxidation processes with bifunctional carbon nanomembranesI.**

**Barak Shapira<sup>1,2</sup>, Tirupathi Rao Penki<sup>1,2</sup>, Izaak Cohen<sup>1,2</sup>, Raphael Dalpke<sup>3</sup>, André Beyer<sup>3</sup>, Armin Götzhäuser<sup>3</sup>, Eran Avraham<sup>1,2</sup> and Doron Aurbach<sup>1,2</sup>**

*1-Chemistry Department, Bar Ilan University, Ramat Gan 592002, Israel*

*2-Institute of Nanotechnology & Advanced Materials, Bar Ilan University, Ramat Gan 592002, Israel*

*3-Fakultät für Physik, Bielefeld University, Universitätsstraße 25, Bielefeld D-33615, Germany*

Wastewater reclamation is becoming a top global interest as population growth and rapid industrialization pose a major challenge that requires development of sustainable cost-effective technologies and strategies for wastewater treatment. Carbon nanomembranes (CNMs)—synthetic 2D carbon sheets—can be tailored chemically with specific surface functions and/or physically with nanopores of well-defined size as a strategy for multifunctional membrane design. Here, we explore a bifunctional design for combined secondary wastewater effluent treatment with dual action of membrane separation and advanced oxidation processes (AOP), exploiting dissolved oxygen. The bifunctional membrane consists of a CNM layer on top of a commercial ultrafiltration membrane (Microlon™) and a spray-coated reduced graphene oxide (rGO) thin film as the bottom layer. The CNM/support/rGO membrane was characterized by helium ion and atomic force microscopy, FTIR, XPS with a four-point conductivity probe, cyclic voltammetry, galvanostatic measurements, and impedance spectroscopy. Combined treatment of water by nanofiltration and AOP was demonstrated, employing a unique three electrode-dead end filtration setup that enables concurrent application of potential and pressure on the integrated membrane. For the model organic compound methylene blue, oxidation (by the Fenton reaction) was evaluated using UV-vis (610 nm). The rejection rate and permeability provided by the CNM layer were evaluated by dissolving polyethylene glycol (400 and 1000 Da) in the feed solution and applying pressure up to 1.5 bar. This demonstration of combined membrane separation and AOP using an integrated membrane opens up a new strategy for wastewater treatment.

## **Laser-induced graphene-Titanium (IV) oxide composite for adsorption enhanced photodegradation of methyl orange**

Brhane A. Tesfahunegn, Maurício Nunes Kleinberg, Camilah D. Powell, Christopher J.

Arnusch\*

Department of Desalination and Water Treatment, Zuckerberg Institute for Water Research,  
The Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede-Boqer Campus,  
Midreshet Ben-Gurion, 8499000, Israel

Organic micropollutants, such as pharmaceuticals or dyes, can be challenging to remove by conventional methods. Despite their low concentrations, their persistence in aquatic systems can be harmful to humankind and the environment. Numerous treatment methods such as biological digestion, chemical oxidation, and coagulation have been used to remedy this problem. However, such wastewater treatment methods can be either inefficient, expensive, or environmentally unsound. Here we embedded TiO<sub>2</sub> nanoparticles in laser-induced graphene (LIG) and obtained a highly efficient photocatalyst composite with pollutant adsorption properties. TiO<sub>2</sub> was added on LIG and lased to form a mixture of rutile and anatase TiO<sub>2</sub> with a decreased band gap ( $2.90 \pm 0.06$  eV). The LIG/TiO<sub>2</sub> composite adsorption and photodegradation properties were tested in solutions of a model pollutant, methyl orange (MO) and compared to the individual and mixed components. The adsorption capacity of the LIG/TiO<sub>2</sub> composite was 92 mg/g using 80 mg/L MO, and together the adsorption and photocatalytic degradation resulted in 92.8% MO removal in 10 min. Adsorption enhanced photodegradation, and a synergy factor of 2.57 was seen. Understanding how LIG can modify metal oxide catalysts and how adsorption can enhance photocatalysis might lead to more effective pollutant removal and offer alternative treatment methods for polluted water.

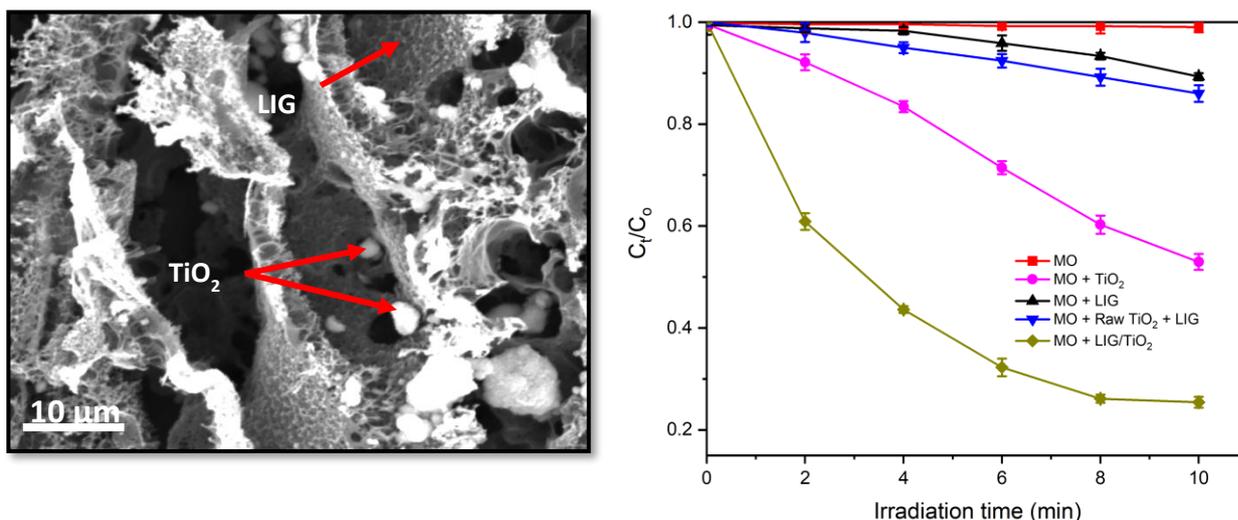


Fig. 1: (a) SEM image showing surface morphology of LIG/TiO<sub>2</sub>; (a) MO Removal efficiency using different catalysts (photocatalysis contribution only) at  $T=298\text{ K}$ ,  $P = 1\text{ atm}$ .

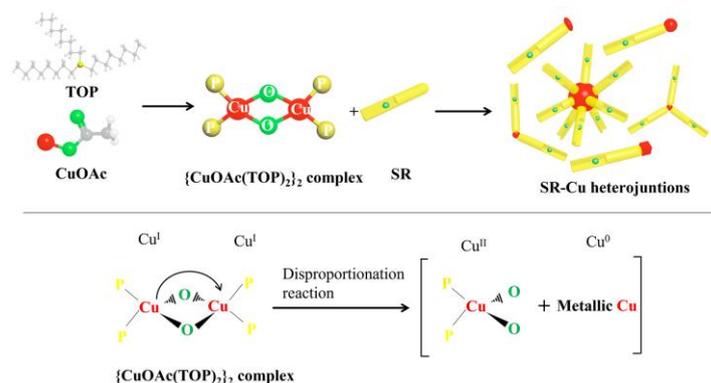
## Tunable Copper Nanocrystals Deposited on Seeded Nanorods

Yuexing Chen and Lilac Amirav

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

The direct manipulation and optimization of each component in semiconductor-metal heterojunction are suggested as essential parameters for their unique functionality and properties [1]. Employing low-cost non-noble metals to build novel semiconductor-metal composites is vital and meaningful for their large-scale applications. Copper as the cheapest plasmonic metal has been rarely manipulated and deserves to investigate, however, the exploration of “on-off” control for cation exchange when Cu is expected to deposit on cadmium chalcogenides is still a practical matter of supreme importance [2]. We present a synthetic strategy that can prevent cation exchange and control the size, morphology, and structure of CdSe@CdS (SR)-Cu heterojunctions by the adjustment of a few reaction parameters. The SR-Cu heterojunctions with different interesting morphologies including elliptic, spherical, cubic Cu tips on one side of SR and the Cu domain with SR branches have been synthesized by a sequential seeded-growth protocol that enables the nucleation and growth of metallic Cu on SR seeds. Our work not only opens an economical pathway to synthesis high-quality morphology-controlled SR-Cu heterojunctions for numerous potential applications (e.g., as solar to fuel conversion, dye photodegradation, surface-enhanced Raman scattering (SERS),

electronic devices, et al) but also provides new opportunities in designing ternary semiconductor-non-noble metal heterojunctions with multifunctionalities.



*Fig. 1: Illustration of possible growth mechanism for the formation of SR-Cu heterojunctions and the disproportionation pathways of  $\{CuOAc(TOP)_2\}_2$  complex, where TOP and OAc are represented by their donor atoms P and O, respectively.*

[1] K. Wu and T. Lian, Chem. Soc. Rev. 45(14), 3781-3810 (2016).

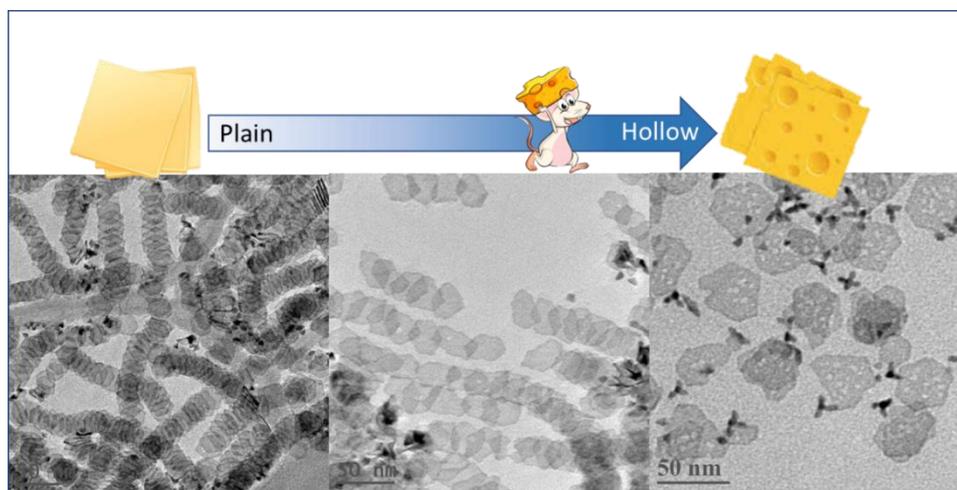
[2] D.H. Son, S.M. Hughes, Y. Yin, A.P. Alivisatos, Science 306(5698), 1009-1012 (2004).

## Hollow Palladium Nanosheets: a Synthetic Study

**Melina Zysler, Mike Rozenberg and David Zitoun**

Department of Chemistry and Bar-Ilan Institute for Technology and Advanced Materials  
(BINA) Bar-Ilan University Ramat Gan 5290002, Israel.

Two-dimensional (2D) palladium nanosheets (PdNS) are of particular importance for a broad variety of applications because of their large surface area and high reactivity, such as gas sensing<sup>[1]</sup> (especially H<sub>2</sub> and CO), a contrast agent for in vivo photoacoustic molecular imaging<sup>[2]</sup>, phototherapy of tumors<sup>[3]</sup>, plasmonic and catalytic properties<sup>[4]</sup>, among others. Several synthetic methodologies were reported in the last few years for this interesting material, either continuous<sup>[5]</sup> or batch process. However, the understanding of the nanoplate formation mechanism is not completely understood. Many experimental parameters like the oxygen pressure, batch size, and order of the addition of the reagent, can modify the properties of the material. Here, we show the synthesis of hollow PdNS, that grow in a (111) plane. We propose a kinetic of the reaction and the influence of the experimental parameters in its properties, specifically the use of CO (gas and W(CO)<sub>6</sub> source). In this work, we adjust the synthesis conditions to obtain different PdNS size distributions, tune the hollows and more (from few holes to highly-hollowed sheets), and achieve the (100) and (111) crystallographic planes. The structural characterization of the particles was done by TEM and HR-TEM (imaging, composition, and electron diffraction) techniques.



*Fig. 1: TEM bright-field image of PdNS. On the left are plain hexagons and the right are hollow nanoplates. Synthesized via a CO-assisted method*

- [1] A. Kumar, Y. Zhao, M. M. Mohammadi, J. Liu, T. Thundat, M. T. Swihart, **2022**, DOI 10.1021/acssensors.1c02015.
- [2] L. Nie, M. Chen, X. Sun, P. Rong, **2014**, 1271.
- [3] S. Li, K. Gu, H. Wang, B. Xu, H. Li, X. Shi, Z. Huang, H. Liu, **2020**, DOI 10.1021/jacs.9b12929.
- [4] X. Huang, S. Tang, X. Mu, Y. Dai, G. Chen, Z. Zhou, F. Ruan, Z. Yang, N. Zheng, *Nat. Nanotechnol.* **2011**, 6, 28.
- [5] V. Sebastian, C. D. Smith, K. F. Jensen, *Nanoscale* **2016**, 8, 7534.

**Smart and Multifunctional Materials and Devices: Transducers,  
Sensors and Actuators  
(SM)**

## Enantioselective Photocatalysis: A Novel Method for Enantiomeric Enrichment Via Chiral Imprinting and Activity Dampening

N. Arbell<sup>1,2</sup>, Y. Paz<sup>1,2</sup>

<sup>1</sup>The Russell Berrie Nanotechnology Institute, Technion, Haifa, Israel

<sup>2</sup>The Wolfson Department of Chemical Engineering, Technion, Haifa, Israel

Despite the increasing demand for enantiopure compounds in industries such as pharmaceuticals and agriculture, currently available chiral purification technologies are still unable to fully meet market needs, due to throughput, complexity or operability considerations. We have developed a novel approach for the kinetic resolution of enantiomers, based on the selective adsorption of a target enantiomer onto a chirally imprinted surface of a photocatalyst, followed by its degradation via a photocatalytic mechanism. The approach is based on a Photocatalytic Enantioenriching Device (PED) composed of a photocatalytic layer, on which the target enantiomer is adsorbed. A suppression layer of a photo-inert material is then grown around the adsorbed target molecules by Atomic Layer Deposition. After removal of the templating molecules, molecularly imprinted cavities with the same chirality as the adsorbed specie are obtained. These stereospecific pores allow for the enantioselective degradation of the templated enantiomer through its enhanced adsorption on the photocatalyst surface in the chiral cavities, while dampening the non-selective degradation on the inert layer around the imprinted sites.

We demonstrated the capabilities of this approach using the dipeptide Leucylglycine as a model degradant, TiO<sub>2</sub> as the photocatalytic material, and Al<sub>2</sub>O<sub>3</sub> as the inert overcoating layer, achieving a selectivity factor towards the degradation of the target enantiomer of up to seven, and an enrichment of a single enantiomer up to 85% from an initially racemic mixture [1]. The wide range of tweakable parameters in the system (photocatalyst, target molecule, concentration of imprinted sites, type of passivating layer, etc.), shows promise as a new possible industrial method for purifying racemic mixtures into enantiomerically pure compounds.

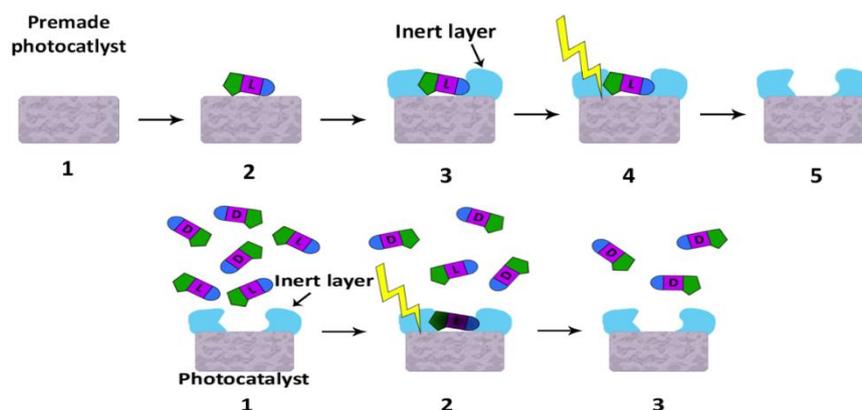


Figure 1. Schematic representations of (A) the preparation process of a PED and (B) its use for the enantiomeric enrichment of a racemic solution.

[1] – N. Arbell, K. Bauer and Y. Paz, ACS Appl. Mater. Interfaces, **33**, 39781–39790 (2021).

# Lactate Analysis using Flexible non-Enzymatic Electrochemical Sensor

**Dayananda Desagani<sup>1</sup>, Ariel Furer<sup>2,3</sup>, and Hadar Ben-Yoav<sup>1,\*</sup>**

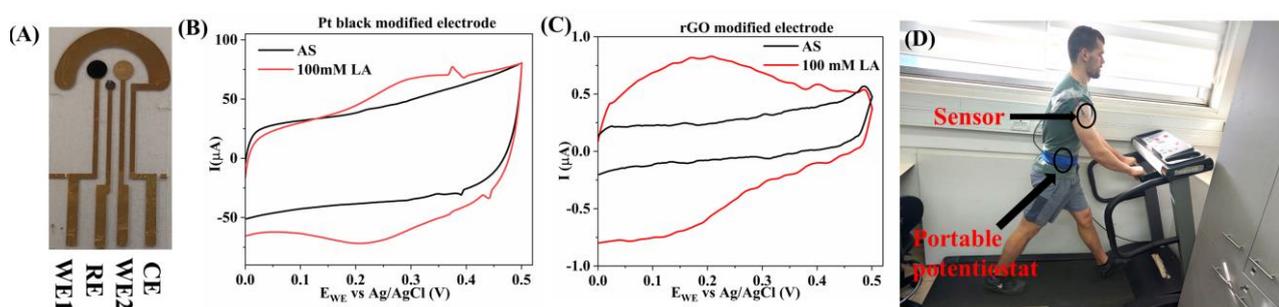
<sup>1</sup> Nanobioelectronics Laboratory, Ben-Gurion University of the Negev, Beer Sheva, Israel

<sup>2</sup> Medical Corps, Israel Defence Forces, Ramat Gan, Israel

<sup>3</sup> Hebrew University of Jerusalem, Jerusalem, Israel

\*Email: [benyoav@bgu.ac.il](mailto:benyoav@bgu.ac.il)

Lactate is a diagnostic biomarker for various physiological conditions; lactate is produced in various tissues such as the brain, red blood cells, and muscles, and is present in various body fluids such as blood, cerebrospinal fluid, and sweat. Monitoring lactate levels at the point of care is crucial for personalized health monitoring, however, commercially available lactate sensors are based on enzymes as the biorecognition elements and exhibit limited stability. Here, we present a novel flexible electrochemical sensor for lactate detection in sweat. The sensor was fabricated on a polyethylene terephthalate (PET) substrate and consisted of two gold disks working electrodes ('WE1' & 'WE2'; 2 mm in diameter), an Ag/AgCl pseudo-reference electrode ('RE'; 1 mm diameter), and a gold arc-shaped counter electrode ('CE') to maximize the symmetry around the WEs (Fig. 1A). The two WEs were modified with reduced graphene oxide (rGO) and platinum black by using electrodeposition method. The modified electrodes were used to record electrochemical signals in lactate-spiked artificial sweat and demonstrated significantly different cyclic voltammograms in comparison to artificial sweat alone (Figs. 1B&1C). The developed sensor was placed onto the skin of a human volunteer and was used to successfully record electrochemical signals during physical activity for 30 min (Fig. 1D). By providing an enzyme-free sensor for lactate sweat levels detection, we aim to improve the sensor's stability under field conditions and to test its ability to monitor a variety of physiological conditions, such as stress.



**sensor.** (A) sensor design. Cyclic voltammograms of lactate (LA)-spiked artificial sweat (AS) using either (B) the Pt black- or the (C) rGO- modified electrodes. (D) The sensor was placed on the skin of a human volunteer and was used to continuously record electrochemical signals.

## Fabrication and characterization of Ni/Si Schottky diodes

Aya Mrar<sup>1</sup>, Yonatan Calahorra<sup>1</sup>

<sup>1</sup>Department of Material science and Engineering, Technion-Israel Institute of Technology, Israel

The electric field at heterostructure interfaces (e.g., PN or Schottky junctions) can break the inversion symmetry and induce a polarization[1], which is mechanically sensitive. Thus, a linear relation between the potential in the depletion layer and the stress-strain on it can be found – a “pseudo” piezoelectric effect. From literature survey and calculations, we conclude that although measurable, the effective piezoelectric response of a silicon Schottky diode is rather small ( $<1$  pm/V), and thus the best characterization method is to fabricate resonant structures in MEMS technology.

Schottky diodes were fabricated on n-type Silicon wafer evaporated with Ni/Au resulting in Schottky contact in different diameters range from (1-50) nm, the back side was evaporated with Aluminum producing an ohmic contact. Current-Voltage (I-V) and electrical impedance measurements were performed in order to evaluate the quality of the contacts, study and determine the devices parameters like the doping profile, the height of the barrier and the built-in voltage. The I-V profile of the fabricated diodes shows a rectifying behavior indicates Schottky contact obtaining current of  $\mu$ As at the forward bias. The depletion layer capacitance was obtained using Electrical Impedance Microscopy (EIS). This technique determines the impedance  $Z$  as a function of the AC frequency at different DC bias voltages, the resulting spectra of the Resistance  $R(\omega)$  and the Reactance  $X(\omega)$  displayed and analyzed to get the C-V curve of the devices obtaining a capacitance of  $\sim$ pFarads. The resonance frequency showed in the reactance spectra is a tool to conceive the electromechanical response of the diodes and proposed resonant structures.

These results lead to the next steps which are demonstrating Schottky diode in resonant structure based on the fabricated devices and characterize their electromechanical response. These structures can be a cantilever or a membrane structure that will enhance the electromechanical response of the depletion layer at the Si-Ni interface.

- [1] M. M. Yang, Z. D. Luo, Z. Mi, J. Zhao, S. P. E, and M. Alexe, “Piezoelectric and pyroelectric effects induced by interface polar symmetry,” *Nature*, vol. 584, no. 7821, pp. 377–381, 2020.

## Plasmonic based Sensor for Quantification of Chemical Pollutants in Water and its Improvement By Machine Learning

Mohamed Hamode, Bruria Rubin, Omer Kaspi, Bruria Rubin, David Zitoun and Adi Salomon\*

Department of Chemistry, BINA Institute of Nanotechnology and Advanced Materials, Bar-Ilan University

Chemical pollutants in drinking water can have many sources among them pharmaceutical waste, agricultural runoff, and industrial discharges<sup>1,2,3</sup>. The development of reliable, sensitive, and handheld sensor for detection of mix of contaminations is important both for human health and the environment. My aim is to develop plasmonic sensor for Surface-enhanced Raman spectroscopy (SERS) and colorimetry measurements. Two types of plasmonic surfaces which enhance the electromagnetic field are presented here; (i) well-defined cavities milled in silver substrates which are covered with 5 nm of SiO<sub>2</sub> for stability. Those structures have also unique physical colors which may change under physical adsorption of small molecules. (ii) scalable 3D disorder metallic network, with large surface area, for increasing the sensitivity of our measurements. In order to improve the sensitivity and selectivity of SERS and Colorimetric measurements and analysis, machine learning algorithms will be applying in collaboration with Prof. Hanoch Senderowitz.

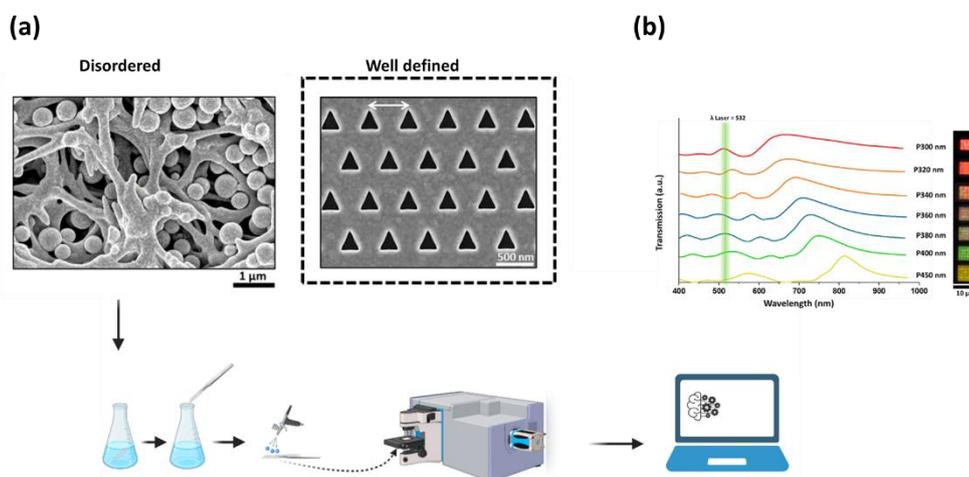


Fig. 1: (a) Schematic illustration of the plasmonic sensing device and the steps of performing the measurement, (b) Transmission spectra/images of hexagonal arrays of triangular holes of Ag200nm in different periodicity.

### REFERENCES:

1. Europe, W. R. O. for. Health risks of heavy metals from long-range transboundary air pollution. 148, 148–162.

2.Kirkman, M. S., Mahmud, H. & Korytkowski, M. T. Intensive Blood Glucose Control and Vascular Outcomes in Patients with Type 2 Diabetes Mellitus. *Endocrinol Metab Clin North Am* 47, 81–96 (2018).

3.Sharma, H. & Mutharasan, R. Review of biosensors for foodborne pathogens and toxins. *Sens Actuators B Chem* 183, 535–549 (2013).

## Optimization of highly magnetostrictive layer for efficient magnetoelectric heterostructures

Nivedita Lalitha Raveendran<sup>1</sup>, and Yonatan Calahorra<sup>1</sup>

<sup>1</sup>MEMSM, Department of Materials Science and Engineering, Technion- Israel Institute of Technology, Haifa, Israel

The notion of using magnetostrictive nanomagnets as the primitive units of the hardware platforms and their magnetization manipulation with electrically generated static or time-varying mechanical strain is the most notable amongst them since it elicits myriad functionalities. Galfenol, an alloy of Gallium and Iron, is one such emerging smart material capable of the above applications with better mechanical and physical properties rather than the materials that are commercially used today. They are preferred over Terfenol-D and PZT due to their rare earth-free composition, lower production cost, higher operating range, lower saturation field and coercivity. Galfenol thin films were sputtered onto Glass/Si substrates using DC magnetron sputtering. The structural and morphological analysis of the samples was carried out using X-Ray diffraction (XRD) and Field emission scanning electron microscope (FESEM). Vibration sample Magnetometry (VSM) measurements were carried out in in-plane and out-plane modes to study the anisotropy in the sample. It was observed that the FeGa thin films had superior magnetic properties with a coercivity of ~200 Oe and significant magnetic anisotropy. The XRD pattern shows the FeGa thin films are single-phased (A2) with ~20 nm crystallite size and SEM micrographs show uniform grain growth with columnar structure. Motivated by the concept of magnetoelectric property coupling by piezoelectric and ferromagnetic material composites, these thin films will be used to investigate the electric-field control of magnetic anisotropy in magnetostrictive/piezo(ferro)electric heterostructure films.

[1] A. Javed, T. Szumiata, N. A. Morley, and M. R. J. Gibbs, *Acta Materialia* **58** (11), 4003 (2011)

[2] N. Song, Boyao Lv, Jing Meng, Zizhao Gong, Xudong Zhang, and Qingfeng Zhan *Journal of Magnetism and Magnetic Materials* **519** 167510 (2021).

## Elastin Like Peptides-Modified Electrodes for Per-and Polyfluoroalkyl substances (PFAS) Detection

Meghna Khadka<sup>1</sup>, Avner Ronen<sup>2</sup>, Miriam Amiram<sup>3</sup>, and Hadar Ben-Yoav<sup>1\*</sup>

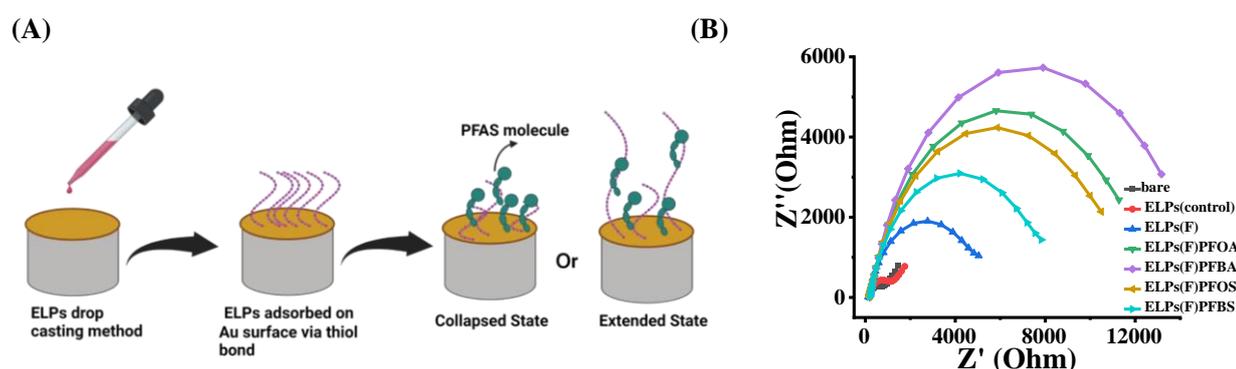
<sup>1</sup>Nanobioelectronics Laboratory (NBEL), Department of Biomedical Engineering,

<sup>2</sup>Zuckerberg Institute of Water Research,

<sup>3</sup>Department of Biotechnology Engineering, Ben-Gurion University of the Negev,  
Beer Sheva, Israel.

\*email: [benyoav@bgu.ac.il](mailto:benyoav@bgu.ac.il)

Per-and Polyfluoroalkyl substances (PFAS) are currently in wide use in the manufacturing of many industrial products, such as non-stick cookware, paints, and firefighting foams. Furthermore, PFAS pose a serious concern as it is bio-accumulative, toxic and persistent to the environment with harmful impact on human health. Current methods to detect PFAS are based on LC-MS or GC-MS, yet these methods are time consuming and require centralized instrumentation techniques, hence cannot be done rapidly in the field. The goal of the presented work is to develop a portable electrochemical sensor for in-field PFAS detection. The sensor's selectivity is based on hydrophobic interactions between PFAS and the electrode's surface modified with hydrophobic/fluorophilic Elastin like peptides (ELPs) films. We used photolithography and thin film deposition techniques to fabricate gold single electrode (2 mm in diameter) on a glass wafer followed by the modification of electrodes with ELPs via drop casting method (**Fig. 1A**), as the ELPs possess stimuli responsive behavior that enables reversible extended and collapsed structural state. Electrochemical impedance spectroscopy (EIS) analysis was performed with different PFAS molecules and showed that the hydrophobic and F-F interactions of the ELPs increased the charge transfer resistance characteristic (**Fig. 1B**). By modifying an array of electrodes with



functionalized hydrophobic and charged materials we plan to detect PFAS having various chain length and functionalities.

**Figure 1.** (A) Scheme of the workflow required to modify and use ELPs as selective layers for electrochemical sensors. (B) Electrochemical impedance spectra generated in the presence of the redox mediator ferrocyanide/ferricyanide (5 mM) by either the bare gold (black; without PFAS), non-fluorinated ELPs (red; without PFAS), fluorinated ELPs(F)- (blue; without PFAS), fluorinated ELPs(F)- (cyan; with PFOA); fluorinated ELPs(F)- (beige; with PFOS), fluorinated ELPs(F)- (green; with PFBS), and fluorinated ELPs(F)- (lilac; with PFBA) modified electrodes.

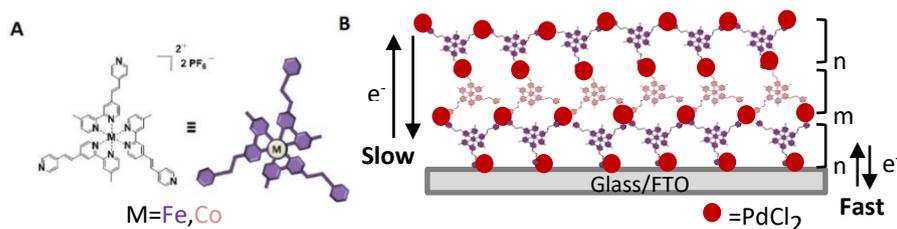
## Diverting Electron Flow in Electrochromic Metal-Organic Assemblies

**Noga Levinson<sup>1</sup>, Yonatan Hamo<sup>1</sup>, Olga Brontvein<sup>2</sup>, Katya Rechav<sup>2</sup>, Michal Lahav<sup>1</sup>,  
Milko E. van der Boom<sup>1</sup>**

<sup>1</sup>Department of Molecular Chemistry and Materials Science, The Weizmann Institute of Science, Rehovot 7610001, Israel

<sup>2</sup>Department of Chemical Research Support, Weizmann Institute of Science, Rehovot 7610001, Israel

Directional electron transfer and charge trapping events are the basis of many biological processes and technologically important systems.<sup>1,2</sup> The molecular basis for directional electron transfer has been studied for decades.<sup>3</sup> The design of large assemblies consisting of individual molecules bound by weak interactions that exhibit directional electron flow accompanied by charge trapping is a large challenge.<sup>4</sup> Our lab has demonstrated a versatile approach for the formation of electrochromic nanoscale assemblies on transparent conductive oxides.<sup>5</sup> Alternating spin-coated layers of well-defined metal polypyridyl complexes and a palladium(II) salt result in electrochemically addressable films with a high chromophore density. By varying the central metal ion of the polypyridyl complexes (Os, Ru, and Fe) and by mixing these complexes, coatings with a wide range of colors and properties have been achieved.<sup>6</sup> These coatings also have properties that can be utilized for the fabrication of energy storage and memory components that have distinct optical states.<sup>6</sup> There is an ongoing debate in the literature regarding the possible electron-transfer pathways in metal-organic films. In order to further study this phenomenon, I have prepared unique coatings that consist of two electrochromic layers made from iron polypyridyl complexes separated by a redox-silent, nanoscale layer consisting of cobalt polypyridyl complexes. In this assembly, we have observed two separate electron transfer processes. The bottom layer is in direct contact with the electrode, resulting in fast and reversible electron transfer with little effect of the inactive top layers. In contrast, the top layer's electron transfer is hampered by the inactive layer consisting of cobalt polypyridyl complexes, resulting in a much slower redox process. The film presents two separate states: initially there is communication only with the bottom layer whereas the top layer is completely inactive. In time, the top layer becomes addressable and



we achieve fully reversible redox-chemistry of the iron polypyridyl complexes.

*Fig. 1: (A) Molecular structures of the iron and cobalt polypyridyl complexes. (B) Schematic of the molecular assembly consisting of two layers of iron polypyridyl complexes made by  $n$  deposition steps, separated by an inactive layer of cobalt polypyridyl complex made by  $m$  deposition steps. The electron transfer process to the bottom layer is relatively fast, while to the top layer a slower process occurs.*

### References:

- [1] Moser, C. C., Page, C. C., Farid, R. & Dutton, P. L. Biological Electron Transfer. *J Bioenerg Biomembr* **27**, (1995).
- [2] Tuccitto, N. *et al.* Highly conductive ~40-nm-long molecular wires assembled by stepwise incorporation of metal centres. *Nature Materials* 2009 **8**:1 **8**, 41–46 (2008).

- [3] Beratan, D. N. & Skourtis, S. S. Electron transfer mechanisms. *Curr Opin Chem Biol* **2**, 235–243 (1998).
- [4] Erbas-Cakmak, S. *et al.* Molecular logic gates: the past, present and future. *Chem Soc Rev* **47**, 2228–2248 (2018).
- [5] Eloul Dov, N. *et al.* Electrochromic Metallo-Organic Nanoscale Films: Fabrication, Color Range, and Devices. *J Am Chem Soc* **139**, 11471–11481 (2017).
- [6] Hamo, Y., Lahav, M. & van der Boom, M. E. Bifunctional Nanoscale Assemblies: Multistate Electrochromics Coupled with Charge Trapping and Release. *Angewandte Chemie - International Edition* **59**, 2612–2617 (2020).

**Computational Modeling and Data Science for New Materials**  
**(CM)**

**Accurate band gaps and optical spectra of halides and oxides  
from a non-empirical, localization based optimal tuning  
of a screened range-separated hybrid functional**

**G. Ohad<sup>1</sup>, S. E. Gant<sup>2,3</sup>, D. Wing<sup>1</sup>, J. B. Haber<sup>2,3</sup>, M. Camarasa-Gomez<sup>1</sup>, A. V. Cohen<sup>1</sup>, F. Sagredo<sup>2,3</sup>, A. Ramasubramaniam<sup>4</sup>, M. R. Filip<sup>5</sup>, J. B. Neaton<sup>2,3,6</sup> and L. Kronik<sup>1</sup>**

<sup>1</sup>Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovoth, Israel.

<sup>2</sup>Department of Physics, University of California, Berkeley, CA, United States.

<sup>3</sup>Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States.

<sup>4</sup>Department of Mechanical and Industrial Engineering, University of Massachusetts, Amherst, MA, United States.

<sup>5</sup>Department of Physics, University of Oxford, Oxford, United Kingdom.

<sup>6</sup>Kavli Energy NanoSciences Institute at Berkeley, University of California, Berkeley, CA, United States.

Accurate prediction of fundamental band gaps of crystalline solid-state systems, entirely within density functional theory, has been a long-standing challenge. Previously, we developed a simple and inexpensive method that achieves this by means of nonempirical optimal tuning of the parameters of a screened range-separated hybrid functional [1]. The tuning involves the enforcement of an ansatz that generalizes the ionization potential theorem to the removal of an electron from an occupied state described by a localized Wannier function in a modestly sized supercell calculation. Here we present applications of the method to more complex systems, notably halide perovskites and metal oxides. We demonstrate quantitative accuracy in band gaps and optical absorption spectra with respect to experiment and a comparable level of accuracy to many-body perturbation theory calculations. We further demonstrate the merit of using the optimally tuned eigensystem as a starting point in combined *GW* plus Bethe-Salpeter calculations.

[1] D. Wing et al., PNAS 118, e2104556118 (2021).

## **Polymorphism, Structure, and Nucleation of Cholesterol·H<sub>2</sub>O at Aqueous Interfaces and in Pathological Media: Revisited from a Computational Perspective**

**Margarita Shepelenko,<sup>1</sup> Anna Hirsch,<sup>1</sup> Neta Varsano,<sup>2</sup> Fabio Beghi,<sup>3</sup>  
Lia Addadi,<sup>2</sup> Leeor Kronik,<sup>\*1</sup> and Leslie Leiserowitz<sup>\*1</sup>**

<sup>1</sup>Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovoth, Israel

<sup>2</sup>Department of Chemical and Structural Biology, Weizmann Institute of Science, Rehovoth, Israel

<sup>3</sup>Università degli Studi di Milano, Department of Chemistry, I-20122 Milano, Italy

We revisit the important issues of polymorphism, structure, and nucleation of cholesterol·H<sub>2</sub>O using calculations based on dispersion-augmented density functional theory. For the lesser known monoclinic polymorph, we obtain a fully extended H-bonded network in a structure akin to that of hexagonal ice. We show that the energy of the monoclinic and triclinic polymorphs is similar, strongly suggesting that kinetic and environmental effects play a significant role in determining polymorph nucleation. Furthermore, we find evidence in support of various O-H···O bonding motifs, in both polymorphs, that may result in hydrogen disorder. We have been able to explain, via computation, why a single cholesterol bilayer in hydrated membranes always crystallizes in the monoclinic polymorph. We rationalize what we believe is a single-crystal to single-crystal transformation of the monoclinic form on increased interlayer growth beyond that of a single cholesterol bilayer, interleaved by a water bilayer, and show that the ice-like structure is also relevant to the related cholestanol·2H<sub>2</sub>O crystal. Finally, we posit a possible role for one of the sterol esters in the crystallization of cholesterol·H<sub>2</sub>O in pathological environments, with a composite of a crystalline bilayer of cholesteryl palmitate bound epitaxially as a nucleating agent to the monoclinic cholesterol·H<sub>2</sub>O form.

## Band Gap Engineering of Lead Titanate Perovskite Oxide

O. Rudich<sup>1</sup>, O. Shafir<sup>1</sup> and I. Grinberg<sup>1</sup>

<sup>1</sup>Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

The use of photovoltaics for electricity generation is a promising approach for renewable power generation due to the essentially unlimited supply of solar energy and lack of harmful CO<sub>2</sub> emissions and other byproducts. This type of photovoltaics has several drawbacks, the major one is that it is limited by the Shockley-Queiser (SQ) limit that predicts the maximum conversion efficiency (PCE) of a single p-n junction solar cell to be approximately 33.7% for a single p-n junction solar cell. In order to tackle this problem ferroelectric perovskite oxides are promising candidates due to the bulk photovoltaic effect (BPVE), which in theory can be exploited to allow greater PCE. However, the use of oxide FE materials for PV application has been limited by the high gaps of these materials that prevent absorption and conversion of the energy of the vast majority of the solar spectrum. Recent studies[1] have demonstrated that the substitution of the d<sup>0</sup> Mo<sup>+6</sup> cation into the classic BaTiO<sub>3</sub> and KNbO<sub>3</sub> perovskites can be used to lower the gap to ~2.0 eV.

In this study, the parent PbTiO<sub>3</sub> (PTO) perovskite oxide was modified to form a solid solution containing Mo to substitute the Ti in the *B*-sites and Na to substitute the Pb in the *A*-sites for charge balance, in order to achieve a stable tetragonal phase and a band gap lower than 2 eV and the PTO-NTM solid solution was investigated theoretically with DFT calculations.

Specifically, the [PbTiO<sub>3</sub>]<sub>x</sub> - [Na(Ti<sub>0.5</sub>Mo<sub>0.5</sub>)O<sub>3</sub>]<sub>1-x</sub> solid solution was studied at compositions of 25% NTM (0.75[PbTiO<sub>3</sub>]-0.25[Na(Ti<sub>0.5</sub>Mo<sub>0.5</sub>)O<sub>3</sub>]) and 12.5% NTM (0.875[PbTiO<sub>3</sub>]-0.125[Na(Ti<sub>0.5</sub>Mo<sub>0.5</sub>)O<sub>3</sub>]). It was found that the band gap was successfully decreased by ~1 eV while maintaining high polarization. In addition, linear correlations were found to exist between the O-Me-O angles ( $\alpha$ ) and the band gap energy, and between the bond valence of the oxygen atoms and the total energy.

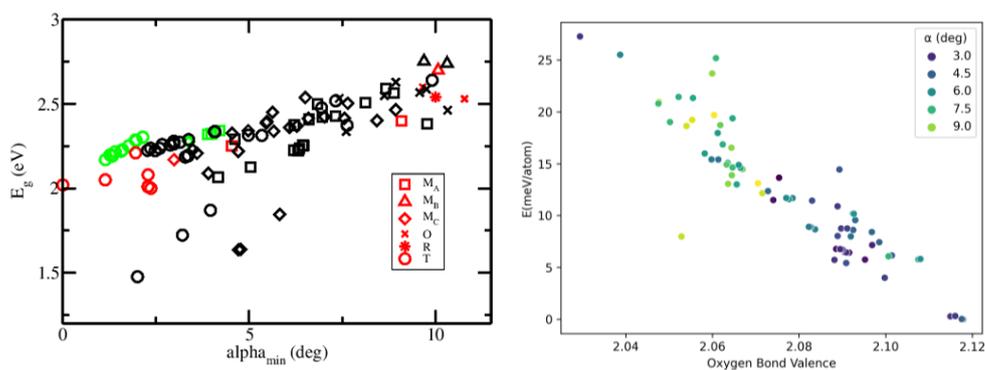


Fig. 1: left: linear correlation between  $E_g$  and  $\alpha$ , right: linear correlation between  $E_{tot}$  and the bond valence of the oxygen atoms.

[1] O. Shafir, Y. Bai, J. Juuti and I. Grinberg, Phys. Rev. Appl., **14**, 44052 (2020).

# Physics-aware Deep Learning Networks for High Accuracy Electronic Properties and Forces Prediction

O. Shafir<sup>1</sup> and I. Grinberg<sup>1</sup>

<sup>1</sup>Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

The electronic properties of materials, such as the density of states (DOS), can provide fundamental understanding and insights toward their application, with first-principles methods being the basic methods for studying these properties. While proved to be reliable, these methods are limited due to their high computational cost. To address this problem, machine learning (ML) methods can be used. In this work, we use such an ML-based approach, developing deep learning (DL) models which allow large-scale materials investigation.

Focusing on the electronic properties of the materials, we developed physics-based features for an efficient structure-based description of crystalline materials based on self-returning paths (i.e., cycles of bonds) for each atom in the crystal structure. These paths are related to the shape of the projected DOS (PDOS) according to the moments' theorem, and therefore are a set of features that can be used for a physics-aware ML model. Using the paths, we construct DL models to predict the PDOS, Mulliken charge, and forces for the  $\text{MoO}_3$ ,  $\text{BaTiO}_3$ , and  $\text{TiO}_2$  crystalline materials (Fig. 1). In addition to showing high accuracy, we find that they allow the application of DL in its simplest form, a shallow dense network, due to the awareness of the physics of the system. This is in contrast to the SOAP or LMBTR-based DL models, which require more sophisticated network architectures for such a task. The ability to use dense shallow networks translates into a quick prediction, which alongside the highly accurate prediction of the forces allows implementation in molecular dynamics simulations.

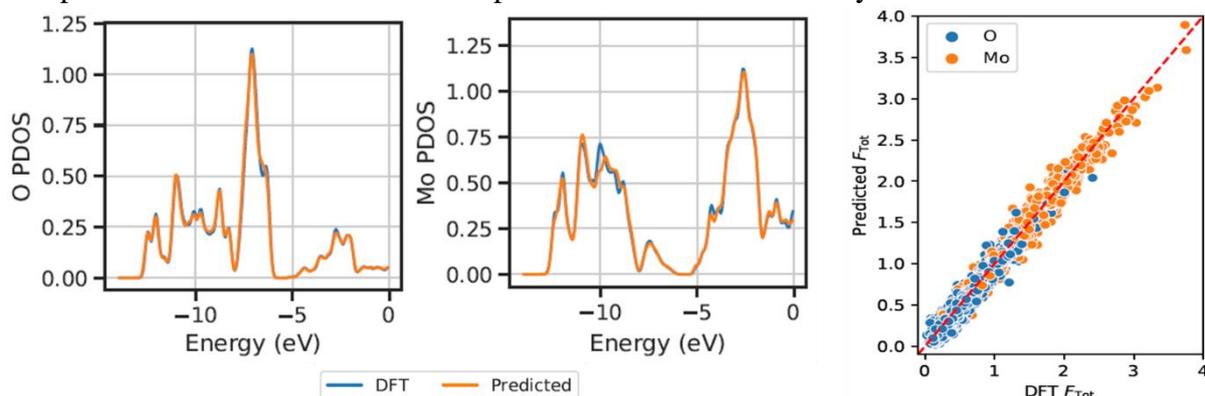


Fig. 1: Projected and DFT density of states for O and Mo atoms in  $\text{MoO}_3$ , alongside the predicted and DFT forces for all  $\text{MoO}_3$  structures. The Mo and O atoms presented are those which exhibit the error closest to the average error of the PDOS prediction model.

**Nanoscience for future quantum technologies: novel materials,  
devices, and characterizations**

**(NS)**

## Novel split-well resonant-phonon terahertz quantum cascade laser structure

Shiran Levy<sup>1</sup>, Nathalie Lander Gower<sup>1</sup>, Silvia Piperno<sup>1</sup>, Sadhvikas J. Addamane<sup>2</sup>, John L. Reno<sup>2</sup>, Asaf Albo<sup>1, a)</sup>

<sup>1</sup> Faculty of Engineering, Bar-Ilan University, Ramat Gan 5290002, Israel.

<sup>2</sup> Center for Integrated Nanotechnologies, Sandia National Laboratories, MS 1303, Albuquerque, New Mexico 87185-1303, USA

a) [asafalbo@gmail.com](mailto:asafalbo@gmail.com)

Right after the invention of the quantum cascade lasers [1] (QCLs) it was claimed that these structures could operate at terahertz (THz) frequencies. THz radiation has many applications and it has a huge impact on the international industrial market. The THz frequency is non-ionizing but yet it can penetrate paper, fabric, ceramic, and plastic in a non-invasive way. In addition, THz radiation has different absorption across the THz spectrum, and it provides a good contrast for imaging applications in a variety of fields [2] [3] [4] [5] [6]. In order to be able to use all of these applications, a coherent and compact source is required.

The electromagnetic spectrum has been divided for years between the wavelengths accessible with electronic sources and the ones with photonic devices. But in between both these regions we can find the so called “Terahertz (THz) gap”. THz-QCLs are the most promising THz source to bridge this gap.

Despite all of the THz-QCLs advantages, there are still no leads to a commercial THz source. The cooling requirements confine the THz-QCLs to a laboratory environment, thus, preventing the achievement of a compact portable THz source. Therefore, raising the maximum operating temperature is the main goal in the field.

We present a novel highly diagonal “split-well resonant-phonon” (SWRP) active region design for THz QCLs with the potential to work at room temperature. The design includes a thin intrawell barrier, that pushes the excited states to higher energies. By adjusting the barrier thickness the energy separation between LLL and the ground state can be tuned to match the exact LO-phonon scattering energy (36 meV). Negative differential resistance is observed at room temperature, which indicates the suppression of thermally activated leakage channels. We believe that this design should serve an excellent platform to study the temperature performance of the THz-QCLs lasers.

### References:

1. J. Faist, F. Capasso, D. L. Sivco, C. Sirtori, A. L. Hutchinson, and A. Y. Cho, *Science.*, **553–556**, 264.5158 (1994).
2. S. M. Kim *et al.*, *Appl. Phys. Lett.*, **153903**, 88.15 (2006).
3. J. F. Federici *et al.*, *Semicond. Sci. Technol.*, **S266**, 20.7 (2005).
4. C. Walker *et al* Millimeter, Submillimeter, and Far-Infrared Detectors and Instrumentation for Astronomy XI. **12190** (2022).
5. T. M. Korter and D. F. Plusquellic, *Chem. Phys. Lett.*, **45–51**, 385.1-2 (2004).
6. H.-W. Hübers *et al.*, *Appl. Phys. Lett.*, **061115**, 89.6 (2006).

## Investigating the effect of doping concentration on the performance of Terahertz Quantum Cascade Lasers

**N. Lander Gower<sup>1</sup>, S. Piperno<sup>1</sup>, A. Albo<sup>1\*</sup>**

<sup>1</sup>Faculty of Engineering, Bar-Ilan University, Ramat Gan 5290002, Israel  
\*[asaf.albo@biu.ac.il](mailto:asaf.albo@biu.ac.il).

Terahertz (THz) quantum-cascade laser (QCL) are noteworthy because of their range of potential applications. Although a maximum operating temperature ( $T_{max}$ ) of 250 K was achieved and demonstrated [1] in 2020, room temperature performance has not been achieved yet.

Our goal was to improve the temperature performance. Achieving a system that is as close as possible to a clean n-level system proved to be the strategy that led to the best temperature performance in THz-QCLs [1,2]. We have studied the effect of doping on the temperature performance of a split-well (SW) direct-phonon (DP) THz QCL scheme (Fig. 1) supporting a clean three-level system [3-5]. We expected to obtain a similar improvement to that observed in resonant-phonon (RP) schemes after increasing the carrier concentration from  $3 \times 10^{10} \text{ cm}^{-2}$  to  $6 \times 10^{10} \text{ cm}^{-2}$ [6]. By increasing the doping, ideally the results should have improved. But, to our surprise, the results show the contrary.

Our unique designs have allowed us to observe experimentally the effect of doping on dephasing times and line broadening. We observed a significant increase in line broadening as the doping and temperature increased and attribute this effect to enhanced ionized-impurity scattering (IIS). These insights into the role of doping suggest an approach to improving THz QCLs by engineering the doping profile and its spatial location. Our approach should serve as an excellent platform for eventually achieving terahertz frequency lasing at room temperature.

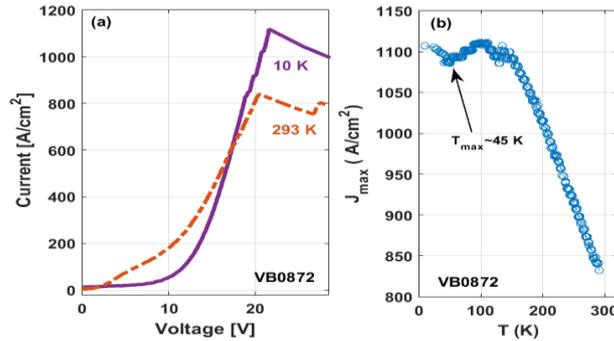


Figure 1. (a) Current-voltage curves at low and room temperatures and (b)  $J_{max}$  versus temperature, of a novel split-well direct-phonon (SW-DP) THz-QCL structure with doping  $6 \times 10^{10} \text{ cm}^{-2}$ .

### References

- [1] A. Khalatpour, A. K. Paulsen, C. Deimert, Z. R. Wasilewski and Q. Hu, Nat. Photonics **15**, 16-20 (2021).
- [2] A. Albo, Q. Hu and J. L. Reno, Appl. Phys. Lett. **109**, 081102 (2016).
- [3] A. Albo, Y. V. Flores, Q. Hu and J. L. Reno, Appl. Phys. Lett. **114**, 191102 (2019).
- [4] N. Lander Gower, S. Piperno and A. Albo, AIP Adv. **10**, 115319 (2020).

- [5] N. Lander Gower, S. Piperno and A. Albo, *Photonics* **8**, 195 (2021).
- [6] C. W. I. Chan, A. Albo, Q. Hu, and J. L. Reno, *Appl. Phys. Lett.* **109**, 201104 (2016).

**Plasma Science**  
**(PS)**

## Electrical properties of different materials at extreme conditions

**<sup>1</sup>Ron Grikshitas, <sup>1</sup>Nikita Asmedianov, <sup>1</sup>Daniel Maler, <sup>1</sup>Sergey Efimov, and <sup>1</sup>Yakov E. Krasik**

*<sup>1</sup>Physics Department, Technion, Israel Institute of Technology, Haifa 3200003, Israel*

Studies of properties of various materials at extreme conditions is subject which is related to Warm Dense Plasma and High Energy Density Matter. We explored how the resistivity and temperature of wires made of tin, molybdenum, silver, and platinum evolves with time during underwater electrical explosion by ~110 kA in amplitude current pulse with rise-time of ~220 ns [1]. The discharge voltage and current were measured using a Tektronix high voltage divider and Rogowski coils, respectively. Shadow streak images of exploding wire and generated shock in water were obtained by streak camera. Time evolution of the spectrum of the light emitted by exploding wire was obtained using a spectrometer and an array of nine photomultipliers, covering a spectral range of 400 – 700 nm. The data obtained was used to determine the energy deposited at instants of solid-state – liquid – vapor phase transitions and was compared with tabulated values.

[1] S. Gleizer, D. Maler, E. Flyat, A. Rososhek, S. Efimov, J. Leopold, and Ya. E. Krasik, “Compact high-current pulse generator for laboratory studies of high energy density matter”, Rev. Sci. Instrum. **92**, 023510 (2021) <https://doi.org/10.1063/5.0039728>

## Radiation Propagation Analysis of an Advanced Israeli FEL

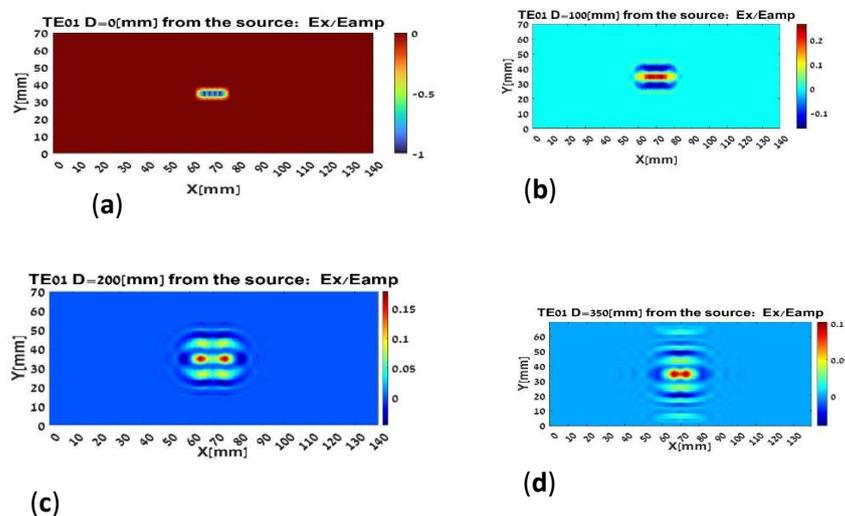
M. Gerasimov<sup>1,3</sup>, E. Dyunin<sup>1,3</sup>, J. Gerasimov<sup>1,2,3</sup> and A. Friedman<sup>1,3</sup>

<sup>1</sup>Department of Electrical and Electronic Engineering, Ariel University, Ariel, Israel

<sup>2</sup>Department of Physics, Ariel University, Ariel, Israel

<sup>3</sup>The Schlesinger Family Center for Compact Accelerators, Radiation Sources, & Applications (FEL) The Ariel City, Israel

We propose here a method for the analysis and characterization of the terahertz (THz) radiation of the advanced free-electron laser (FEL), operating in various operational parameters in superradiance regimes, as spontaneous emission. A visualization contributes to pre-design considerations of the transmission line (TL) for a wide-tunable broad-spectrum radiation source. The simulation of radiation propagation, which represented in terms of optical geometric rays/light field, is carried out through ZEMAX simulation. The final goal is to examine the effect of each mode on the TL and to examine the exact location of the mirrors. A final tool constitutes a unique platform for the diagnostic of the THz ultra-short pulses, which are represented in the frequency domain in terms of cavity eigenmodes.



*Fig. 1:* The TE<sub>01,21,23</sub> mode propagation in term of the rays: (a) at the out of the waveguide; (b) after passing 100 mm, (c) after passing 200 mm, and (d) after passing 350 mm.

[1] M. Gerasimov, E. Dyunin, J. Gerasimov, J. Ciplis, and A. Friedman, “Application of wigner distribution function for THz propagation analysis,” *Sensors*, vol. 22, no. 1, 2022, doi: 10.3390/s22010240.

[2] M. Gerasimov, E. Dyunin, and A. Friedman(2019). Development of an Artificial Intelligence System for the Design of an Optical Mode Converter. In 39th Int. Free-Electron Laser Conf. Hamburg, Germany.

## **Mass-separation by standing waves near the cyclotron frequency**

**A. Fruchtman<sup>1</sup> and G. Makrinich<sup>1</sup>**

<sup>1</sup>Department of Physics, H.I.T. – Holon Institute of Technology, Holon 58102, Israel

The motion of a charged particle, under forces exerted by a steady magnetic field and by two planar waves that propagate parallel to the steady magnetic field, is calculated. When the two waves propagate in opposite directions, a ponderomotive force by the waves pushes the particles along the magnetic field. It has been pointed out that the direction of the force depends on whether the cyclotron frequency of the particle is smaller or larger than the wave frequency. This has been suggested as a mechanism to be explored for mass separation, a much-needed process for various applications. We solve the equations of motion for the case that the particle displacement is much smaller than a quarter wavelength. In that case we present analytical solutions that show the particle pushing along the magnetic field with the mass-dependent direction as well the growth of particle perpendicular velocity. We also compare the cases of travelling and standing waves. We find numerically the particle trajectories when the particle displacement is close to a quarter wavelength and show when the trajectory deviates from the analytical solution.

In the continuing study, we will include a self-consistent description of the waves in a plasma, which should be a variation of shear-Alfven waves. The interesting influence of space-charge fields will also be considered.

## Adhesion improvement of boron carbide coating on aluminum substrates

M. Chachashvili<sup>2</sup>, S. Froim<sup>2</sup>, S. Waichman\*<sup>1,2</sup> and S. Barzilai\*<sup>1</sup>

<sup>1</sup>NRC – Negev, P.O.B 9001, Beer-Sheva, Israel

<sup>2</sup>Rotem Industries Ltd, Mishor Yamin D.N. Arava 86800, Israel

\*Corresponding author. Email: [barzilai.shmuel@gmail.com](mailto:barzilai.shmuel@gmail.com), [sharonw@rotemi.co.il](mailto:sharonw@rotemi.co.il)

Boron carbide is a ceramic material that has a high cross-section for neutron absorption and therefore can be employed as a coating for neutron-based applications. We deposited a thin boron carbide coating layer (1.0-3.5  $\mu\text{m}$ ) on an aluminum substrate using pulsed-DC magnetron sputtering. Aluminum is a typical substrate material for neutron detection applications because it is transparent for neutrons. However, the adhesion between boron carbide and aluminum is challenged because of their thermal expansion coefficient differences and the probable formation of unstable aluminum-carbon bonds that may cause adhesive failure. For efficient attachment of these two materials, we applied an adhesive intermediate titanium layer (0.3-1.5  $\mu\text{m}$ ) and methodically studied the effect of the negative bias applied during deposition, as well as the impact of the titanium interlayer thickness, on the coating. Here, we determined the parameters for long-term adhesion (over 27 months, stored in 2 % RH), by a combination of different and complementary characterization methods including SEM/HRSEM and TEM imaging, XPS analyses, residual stress, and hardness measurements. Qualitative testing of adhesion strength showed that coatings deposited with a bias voltage higher than  $\sim -150$  V presented high residual stress of  $> -1$  GPa and poor adherence to the substrate. Based on the results, we propose two main mechanisms for the adhesion failures: Immediate and delayed failures, where coating delamination occurs. The immediate failure is attributed to the high residual stress evolved during/promptly after deposition. The delayed delamination occurred over time and can be attributed to surface reaction with water vapors from the environment, followed by diffusion of hydrogen atoms towards the  $\text{B}_4\text{C}/\text{Ti}$  interface. This enhances the stress evolution causing the detachment of the boron carbide coating from the Ti interlayer. Based on this work, the optimal bias voltage range is  $\sim -25 \pm 5$  V to  $-60$  V, presenting a continuous and strongly adherent coating layer together with a 1.5  $\mu\text{m}$  thick titanium adhesive layer.

## **Investigation of High-Power Microwave Radiation from an Axial Output Compact S-Band A6 Segmented Magnetron Powered by a Linear Induction Accelerator**

**O. Belozerov<sup>1</sup>, Ya. E. Krasik<sup>1</sup>, J. G. Leopold<sup>1</sup>, S. Pavlov<sup>1</sup>, Y. Hadas<sup>1</sup>, K. Kuchuk<sup>1</sup> and E. Schamiloglu<sup>2</sup>**

<sup>1</sup>Department of Physics, Technion, Haifa, Israel

<sup>2</sup>Department of Electrical and Computer Engineering, University of New Mexico, Albuquerque, USA

A recent publication [1] presented the first demonstration of microwave generation using a segmented A6 S-band axial output relativistic magnetron (RM) that is fed by a split cathode and powered by a small pulsed power generator. In this study, the authors extend this research by incorporating a mode converter and an antenna to the RM and driving it with a modified Linear Induction Accelerator (LIA) ( $\leq 450$  kV,  $\leq 4$  kA,  $\sim 150$  ns).

The study found that the operation of the RM with a split cathode differs significantly from that of a common explosive emission cathode. By optimizing the geometrical parameters, external magnetic field and the LIA's charging voltages, the RM was able to generate  $\sim 160$  ns long microwave pulses of  $\sim 130$  MW, at a frequency of 1.78 GHz, with an electronic efficiency of  $\sim 40\%$ , without pulse shortening. In contrast, the use of a common solid cathode resulted in shortened microwave pulses. The authors also found that when a mode converter is attached to the RM that is fed by a solid cathode, it produced  $\sim 80\%$  efficiency of  $\sim 240$  MW power of high power microwave pulses but only  $\sim 45$  ns long. The authors suggest that further research is needed to increase the efficiency of the split cathode fed RM and to clarify the reduction of the output power by the mode converter when a split cathode is used. The study demonstrates that using a segmented anode allows for a much more compact microsecond-scale magnetic field producing system, enabling repetitive operation of the RM.

[1] Ya. E. Krasik, J.G. Leopold, Y. Hadas, Y. Cao, S. Gleizer, E. Flyat, Y. P. Bliokh, D. Andreev, A. Kuskov, and E. Schamiloglu, *J. Appl. Phys.* **131**, 023301 (2022)