

# **Conference Organizing Team**

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# **Plenary Speaker**

09:30-10:10 Yi Cui

Director, Precourt Institute for Energy Professor of Materials Science and Engineering, Stanford University Photon Science, SLAC National Accelerator Laboratory Session Chair: Doron Aurbach (BIU)



# **Reinventing Batteries Through Materials Design**

#### Abstract

The fast growth of portable power sources for transportation and grid-scale stationary storage presents great opportunities for battery development. The invention of lithium ion batteries has been recognized with Nobel Prize in 2019. How to increase energy density, reduce cost, speed up charging, extend life, enhance safety and reuse/recycle are critical challenges. Here I will present the 156 year research in my lab to reinvent batteries and address many of challenges by understanding the materials and interfaces through new tools and providing guiding principles for design. The topics to be discussed include: 1) A breakthrough tool of cryogenic electron microscopy, leading to atomic scale resolution of fragile battery materials and interfaces. 2) Materials design to enable high capacity materials: Si and Li metal anodes and S cathodes. 3) Interfacial design with polymer and inorganic coating to enhance cycling efficiency of battery electrodes. 4) Materials design for safety enhancement. 6) Lithium extraction from sea water and for battery recycling. 7) New battery chemistry for grid scale storage.

# Plenary Session II IVS-IPSTA Research Excellence Awardees Noam Eliaz (TAU) & Milko van der Boom (WIS) Joint winners of this year's IVS Excellence Award for Research



#### Electrodeposition in the Era of Additive Manufacturing Noam Eliaz Department of Materials Science and Engineering, Tel-Aviv University

#### Abstract

Great interest in electrodeposition has evolved in recent years in the context of additive manufacturing (AM), either for functionalization of powders for AM by common technologies such as directed energy deposition (DED) or powder bed fusion (PBF), as a post-printing finishing stage (e.g., on cellular AM'ed structures), or as a standalone three-dimensional (3D) printing technique. This presentation will review our research activities in two of the aforementioned routes. Meniscus-confined electrodeposition (MCED) of freestanding vertical pillars and overhang copper structures with submicron resolution, using an atomic force microscope and its closed-loop control [1,2], will be presented. Electrodeposition of pure and dense nanocrystalline aluminum from room-temperature ionic liquids (RTILs) on copper and nickel substrates [3] as well as electrodeposition of exceptionally well adhered CoP coatings on copper will be demonstrated. We plan to print in the near future such functional metals and alloys in our lab. Finally, I will present our novel electrochemical processing of functional core/multi-shell ZnAl/Ni/NiP powders [4,5] and core/shell ZnAl/Al<sub>2</sub>O<sub>3</sub> powders [6].

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#### **Crystals and Thin Films Made in Israel**

#### Milko van der Boom

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

#### Abstract

Enabling and understanding new methodologies to fabricate molecular assemblies driven by intermolecular interactions is fundamental in chemistry. Coordination chemistry can be used to control crystal growth and enables surface-confinement of molecular materials, which remains challenging. Coordination-based polymers and metal-organic frameworks (MOFs) have been explored since their discovery at the beginning of the 18<sup>th</sup> century. Such materials are generated by the dozens in a gold-rush-type search for properties mainly related to the storage and release of energy (e.g., hydrocarbons, dihydrogen). How the molecular components, metal salts and experimental conditions control the dimensions, shapes, chirality and homogeneity of these materials is barely known. Using achiral ligands that binds late-transition metals in a defined manner, we address issues related to the mechanism underlying the formation of hollow and chiral structures. In this overview, the formation and properties of our latest materials will be discussed: chiral MOFs[1,2] the electrochromic properties of coordination-based films[3] and a solvent-free on-surface crystal-to-co-crystal conversion process.[4] This stepwise vapor-based approach offers a new strategy for the formation of hybrid supramolecular materials

#### **References:**

1 Unusual Surface Texture, Dimensions and Morphology Variations of Chiral and Single Crystals. Singh, V.; Houben, L.; Shimon, L.; Cohen, S.; Golani, O.; Feldman, Y.; Lahav, M.; van der Boom, M. E. *Angew. Chem., Int. Ed.*, **2021**, *60*, 2-11.

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3 Pathway-Dependent Coordination Networks: Crystals versus Films. Malik, N., Singh, V.; Shimon, L. J. W.; Houben, L.; Lahav, M.; van der Boom, M. E. J. Am. Chem. Soc. **2021**143, 16913-16918

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# **Surface Science Session**

**Chair: Baran Eren (WIS)** 

## 10:20-10:40 Leo Gross (IBM Zurich) Keynote Speaker

### Title: Molecular reactions, charge transitions and excited states investigated by AFM

#### **Abstract**:

Atomic force microscopy (AFM) with functionalized tips achieves atomic and bond-resolved resolution providing insights into the structure, aromaticity, charge states and bond-order relations of individual molecules [1]. Importantly for on-surface synthesis, the products and intermediates of chemical reactions can be identified and characterized. Recently, we generated by atom manipulation the elusive carbon allotrope cyclo[18]carbon and resolved its debated structure [2].

On insulating substrates, we can control the charge states of molecules. With ultra-high-resolution imaging we resolve how the charge state of molecules affects their structure [3]. By alternatively attaching and detaching single charges from a molecule on an insulator, we probe transitions between different charge states including neutral excited states and quantify the reorganization energy [4] and singlet and triplet excitation energies [5]. Accessing excited states this way, triplet lifetimes and their quenching by molecular oxygen have been measured recently by J. Peng et al. [6].

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   S. Fatayer et al. Nat. Nano. 13, 376 (2018)
- [5] S. Fatayer et al. Science 365, 142 (2019)

[4] S. Fatayer et al. Science 365, 142 (2019) [5] S. Fatayer et al. Phys. Rev. Lett. 126, 176801 (2021)

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# 10:40-11:00 Martin Castell (Oxford) Keynote Speaker

#### Title: Multiple frame averaging of scanning tunneling microscope images

#### Abstract:

The resolution of the STM has barely improved since its inception. Only small advances have been achieved through low noise electronics, enhanced vibration damping, and low temperature operation. These incremental gains stand in stark contrast to the advances made with the atomic force microscope (AFM), and it is now possible to take non-contact AFM (nc-AFM) images with intramolecular resolution. The advantage however, that the STM still has over nc-AFM is that the scan speed is typically around two orders of magnitude faster. In effect this means that for the time taken to acquire one nc-AFM image it is possible to acquire around a hundred STM images. This has not been viewed as a particularly significant advantage because operator practice is such that only the best one of these hundred images will be used and the others discarded. However, if all the hundred images are averaged then we would expect a ten-fold improvement in the signal to noise ratio (SNR) as the random noise diminishes with the square root of the number of averaged images. This improved SNR leads to a commensurate increase in the resolving power of the STM. The reason that this kind of multiple frame averaging (MFA) is not performed routinely is that unique and locally varying distortions in each of the images prevent them from being aligned in perfect registry with each other. However, software packages now exist to circumvent these issues [1]. In this presentation I will show how a step change in the resolving power of the STM can be achieved through automated distortion correction and MFA [2]. I will demonstrate the broad utility of this approach with examples from a variety of surfaces. I will show a 6-fold enhancement of the SNR of the Si(111)-(7 × 7) reconstruction, and will demonstrate that images with sub-picometre height precision can be routinely obtained as demonstrated for a monolayer of Ti<sub>2</sub>O<sub>3</sub> on Au(111). I will show automated classification of the two chiral variants of the (4 × 4) reconstructed SrTiO<sub>3</sub>(111) surface. I wil

show how dynamic effects in STM movies can easily be identified using this technique. Our new approach to STM imaging allows a wealth of structural and electronic information from surfaces to be extracted that was previously buried in noise.

- [1] L. Jones, H. Yang, T.J. Pennycook, M.S.J. Marshall, S.V. Aert, N.D. Browning, M.R. Castell and P.D. Nellist, Advanced Structural and Chemical Imaging, 1, 8 (2015).
- [2] L. Jones, S. Wang, X. Hu, S.U. Rahman and M.R. Castell, Advanced Structural and Chemical Imaging, 4, 7 (2018).

## 11:00-11:15 Nurit Avraham (WIS) **Invited Speaker**

#### Title:

Visualization of Topological Boundary Modes Manifesting Topological Nodal-Point **Superconductivity** 

#### Abstract:

Topological superconductors are an essential component for topologically protected quantum computation and information processing. Although signatures of topological superconductivity have been reported in heterostructures, material realizations of intrinsic topological superconductors are rather rare. In my talk I will present scanning tunneling spectroscopy measurements of the transition metal dichalcogenide 4Hb-TaS<sub>2</sub>, that interleaves superconducting 1H-TaS<sub>2</sub> layers with strongly correlated 1T-TaS<sub>2</sub> layers, showing spectroscopic evidence for the existence of topological surface superconductivity [1]. These include edge modes running both along 1H layer terminations and under 1T layer terminations, where they separate between superconducting regions of distinct topological nature. We also observe signatures of zero-bias states in vortex cores. All boundary modes exhibit crystallographic anisotropy, which together with a finite in-gap density of states throughout the 1H layers allude to the presence of a topological nodal-point superconducting state. Our theoretical model attributes this phenomenology to an inter-orbital pairing channel that necessitates the combination of surface mirror symmetry breaking and strong interactions.

[1] A. Nayak et. al. Nature physics, November (2021)

## 11:15-11:30 **Oded Millo (HUJI) Invited Speaker**

#### Title:

# Magnetic-like states and triplet superconductivity induced in a conventional superconductor upon chiral molecules adsorption

#### **Abstract:**

Motivated by our previous scanning tunnelling spectroscopy (STS) works that provide evidence for the emergence of triplet superconductivity at superconductor-ferromagnet interfaces, which will be briefly reviewed, we demonstrate that similar phenomena can be induced on a surface of a conventional superconductor upon chemisorbing non-magnetic chiral molecules. By applying scanning tunneling spectroscopy, we show that the singlet-pairing s-wave order parameter of Nb, NbN and NbSe<sub>2</sub> is significantly altered upon the adsorption of chiral polyalanine alpha-helix molecules on the surface. The tunneling spectra exhibit zero-bias conductance peaks embedded inside gaps or gap-like features, suggesting the emergence of a triplet-pairing component, corroborated by fits to theoretical spectra. Conductance spectra measured on devices comprising exfoliated NbSe<sub>2</sub> flakes over which these chiral molecules were adsorbed, exhibit, in some cases, in-gap states nearly symmetrically positioned around zero bias. These states shift apart with magnetic field, akin to magneticimpurity induced Shiba states, as corroborated by theoretical simulations. Other samples show evidence for a collective phenomenon of hybridized Shiba-like states giving rise to unconventional, possibly triplet superconductivity, manifested in the conductance spectra by the appearance of a zero bias conductance peak that diminishes, but does not split, with magnetic field. The transition between these two scenarios appears to be governed by the density of adsorbed molecules. Recent muon spin rotation data indicate the appearance of unconventional Meissner screening and a broken time-reversal state upon the adsorption of these chiral molecules on Nb films, providing further evidence for chiral-induced triplet superconductivity.

# 11:30-11:40 Sidney Cohen (WIS) Contributed Speaker

#### Title:

# In-situ measurement of the influence of ice-binding proteins on ice growth by atomic force microscopy in aqueous solutions

#### **Abstract**:

Besides enabling organisms to thrive in cold environments, ice-binding proteins (IBPs) hold great promise in tissue preservation and food processing. These proteins lower the freezing point by binding to ice surfaces thus inhibiting crystal growth. Despite their importance, the microscopic action of these proteins is largely unknown due to until-now unresolved difficulties of achieving high-resolution, in-situ imaging. We present here a novel system design which enables dynamic atomic force microscopy (AFM) imaging of the ice-IBP system. Two different types of protein systems were studied, one exhibiting moderate ice-growth inhibition, and the other hyperactive inhibition. These proteins bind to different faces of the growing ice crystals, leading to characteristic structures which can be rationalized by the selective inhibition. AFM images reveal such structures at the tens of nm scale for the first time, and will be discussed in relation to previous, lower resolution optical images. Besides revealing the nascent crystal growth, the AFM was used to create mappings of local adhesion which gave insights on the location of protein binding.

In order to achieve these results, several challenges had to be overcome including moderating and controlling heating from the AFM head and detection laser, preventing cantilever freezing, and isolating and monitoring the boundary between liquid and solid as observed at the growing ice front. Using the new set-up enabled control of growth in both slow and fast regimes, and even demonstrated the feasibility of measuring less-controlled ice growth in absence of the IBPs. Small pits were observed near the apex of growing tapered structures, which can be understood in light of the attachment of the IBP to specific planes. Although there exist several studies on crystals growing in thin films, this is the first demonstrated imaging of a growing bulk crystal immersed in its own melt with AFM.

# 11:40-11:50 Elad Gross (HUJI) Contributed Speaker

#### Title:

# What makes a catalyst active? Insights from IR nanospectroscopy measurements on single nanoparticles

#### Abstract:

The development of optimized catalysts that can address the grand energy challenges of the 21st century requires in depth understanding of the basic elements that direct the reactivity and selectivity of catalytic nanoparticles. In this talk I will demonstrate that structure-reactivity correlations within single catalytic nanoparticles can be identified by conducting Infrared nanospectroscopy measurements, while using N-heterocyclic carbene molecules as probes for surface-induced reactivity. Using this approach, we probed the influence of different surface sites on the catalytic reactivity of Au and Pt particles and the ways by which site-dependent reactivity varies in response to reaction conditions. In addition, by conducting single particle measurements we uncovered the influence of communication between highly-reactive and less-reactive surface sites on the nanoscale and globular reactivity pattern. These findings demonstrated the crucial impact of nanoscale properties on the catalytic reactivity to provide guidelines for the design of optimized catalysts.

## 11:50-12:10 Roundtable Discussion

Moderator: Sidney Cohen (WIS) Panel members:

# Michael Stern (BIU), Andrea Morello (Univ. New S. Wales, Australia)

# Atomic-scale manufacturing, surface science and quantum circuits

Atomically-precise techniques, including but not limited to scanning probes, are now able to construct memories and devices of nm or even single-atom size. At the same time, great strides have been made in quantum computing and the potential for harnessing these tools to push computing into the quantum age is enormous. We will discuss current trends and efforts, and analyze the feasibility of some of the pioneering approaches.

# **Energy & Catalysis Session**

**Chair: Gil Shalev (BGU)** 

# 10:20-10:40 Avner Rothschild (Technion) Keynote Speaker

# Title: Decoupled Water Splitting for Green Hydrogen Production at Scale

#### Abstract:

Green hydrogen produced by splitting water molecules into hydrogen and oxygen using renewable sources is expected to play a major role in the transition to carbon neutral economy, serving as an energy carrier that can facilitate the penetration of an higher share of intermittent renewable energy, the decarburization of hard-to-abate industrial sectors (e.g. industrial processes which require high-grade heating or rely on hydrogen as a feedstock) and the cross-sectorial coupling (linking power, gas and other energy vectors or energy intensive commodities and replacing them in their respective usages). The baseline technology for green hydrogen production is called water electrolysis, where renewable power is applied to break the chemical bonds in water molecules and produce hydrogen and oxygen simultaneously at two electrodes, cathode and anode, in alkaline or acidic solution. The coupled generation of hydrogen and oxygen at the same time in the same cell presents a safety risk, since the mixture of the two is highly flammable. Therefore, a membrane and sealing are used to isolate the electrodes from each other, which complicates cell construction and requires maintenance, both increasing the production cost of green hydrogen. In addition, severe (20-30%) energy losses, mostly due to the difficult reaction that evolves oxygen, increase the cost of energy in this energy intensive technology. These drawback present challenges for wide scale adoption of green hydrogen. In order to overcome these challenges, we develop an alternative technology that decouples the generation of hydrogen and oxygen into two stages, separated by time, or two cells, space separated, avoiding the need for membrane and sealing. In addition, we divide the oxygen evolution reaction, a difficult electrochemical reaction that requires four electrons to generate an oxygen molecule on an atomic reaction

evolution reaction, a difficult electrochemical reaction that requires four electrons to generate an oxygen molecule on an atomic reaction site, into two sub-reactions that occur on four sites instead of one, thereby enabling easier reactions and saving most of the losses in water electrolysis. An ultrahigh efficiency of nearly 99% was demonstrated at lab scale, and we expect reaching 95% at system scale. To bring this transformative concept to reality we established H<sub>2</sub>Pro, and Israeli company that aims to provide green hydrogen at scale based on our innovation.

10:40-11:00 Nir Tessler (Technion) Keynote Speaker

### Title: Device Synthesis applied to Organic Solar Cells

#### **Abstract:**

In the past 15 years, our group developed the methodology which we name "Device Synthesis." The approach is based on the notion that it does not make sense to develop 3<sup>rd</sup> generation devices while forcing the materials to match the structure of the 1<sup>st</sup> generation devices. I will introduce the methodology in the context of device chemical-physics of organic solar cells. An example of the new approach is the realization that since organic molecules are not silicon, optimizing the maximum power point of a solar cell is not replaced by optimizing the short-circuit current and the open-circuit voltage. I will present two device structures designed with the above in mind.

11:00-11:15 Rafi Shikler (BGU) Invited Speaker

#### Title:

# On the effect of the finite conductivity and dielectric nature of ITO on the performance of organic based optoelectronic devices

#### **Abstract**:

Indium-Tin-Oxide (ITO) is one of the most commonly used materials for the fabrication of transparent electrodes for organic based optoelectronic devices. It is well known that its finite conductivity affects the scaling up of the area of organic solar cells. I will present a model that show how we use a 2D simulation to efficiently design a metal grid to overcome this issue. Another, rarely refer to, property of ITO is its relatively low dielectric constant. I will show that why it is important in the context of charge injection and collection into organic devices and present a modification to the commonly used Scott Malliaras model for contacts to organic materials.

### 11:15-11:30 Gideon Segev (TAU) Invited Speaker

#### Title:

# Operando characterization of charge extraction and recombination profiles in solar cells with nanoscale resolution

#### **Abstract**:

The next generation of solar energy conversion systems requires design and integration of new semiconductor materials. Detailed understanding of the opto-electronic properties of these materials, their driving forces and the loss mechanisms that limit device performance is essential to the development of high efficiency systems. However, these materials and systems are difficult to model and only few experimental methods are available for direct characterization of dominant loss processes under relevant operating conditions. To this end, empirical extraction of the spatial collection efficiency (SCE) and the spatial external luminescence efficiency (SELE) are operando, analytical tools that provide functional depth profiles of the active regions in the device.

By coupling external quantum efficiency (EQE) measurements and optical modeling, SCE extraction allows quantifying charge transport properties and loss mechanisms across the device depth profile under real operating conditions with very few assumptions. Similar to SCE, combining optical modeling with wavelength dependent photoluminescence quantum yield (PLQY) measurements enables extracting the SELE - the probability that an electron hole pair photogenerated at a specific point will contribute to photoluminescence from the device. In this contribution we will introduce the SELE concept and will show a first demonstration of the SELE extraction method applied to InP samples. Extracting the SELE enables simple distinction between different losses such as surface recombination and self-absorption. The quantification of surface recombination losses makes this an excellent tool for characterizing the effect of surface passivation layers. Furthermore, since the PLQY is directly related to the obtainable photovoltage from the device, the SELE also maps the contribution of different regions in the device to the photovoltage. As a result, combining the SELE and SCE profiles at specific operating points provides detailed spatial information on charge extraction, contribution to the photovoltage, and discrimination between radiative and non-radiative recombination processes at the surface and in the bulk of the device.

# 11:30-11:40 Igor Rahinov (OUI)

**Contributed Speaker** 

#### Title:

The Kinetics of NH<sub>3</sub> Desorption and Diffusion on Pt: Implications for the Ostwald Process

#### Abstract:

The Ostwald process is a critically important stepping-stone for industrial production of artificial fertilizers, converting ammonia (NH<sub>3</sub>) to nitric acid (HNO<sub>3</sub>) in the presence of oxygen and water. The key to its success is the efficient oxidation of NH<sub>3</sub> to nitric oxide (NO) on a Pt catalyst. In industry the Ostwald process is conducted at temperatures of 1050-1250 K and total pressures between 1 and 12 bar with an ammonia to air ratio of 1:10<sub>1</sub>. To initiate the oxidation, NH<sub>3</sub> adsorbs with high probability to the majority terrace site and must then diffuse to low-coordination step-sites, where it is able to react with oxygen. Thus, the competition between desorption and diffusion and the equilibrium between adsorption at step and terrace-sites are critical factors in determining reaction probability; yet the competition between NH<sub>3</sub> desorption and diffusion on Pt has never been investigated. There is not even an experimental consensus concerning such a basic parameter as the binding energy of NH<sub>3</sub> at Pt(111). The lack of reliable quantitative information concerning NH<sub>3</sub>/Pt interactions led to surrogate empirically optimized models, which unfortunately lack universality and transferability.

In this work [1] we report accurate time-resolved measurements of NH<sub>3</sub> desorption from Pt(111) and Pt(332) and use these results to determine elementary rate constants for desorption from steps, from (111) terrace sites and for diffusion on (111) terraces. Modeling the extracted rate constants with Transition State Theory (TST), we find that conventional models for partition functions, which rely on uncoupled degrees of freedom (DOFs), are not able to reproduce the experimental observations. The results can be reproduced by using a more sophisticated partition function, which couples DOFs that are most sensitive to NH3 translation parallel to the surface; this approach yields accurate values for the NH<sub>3</sub> binding energy to Pt(111) ( $1.13\pm0.02$  eV) and the diffusion barrier ( $0.71\pm0.04$  eV). In addition we determine NH3's binding energy preference for steps over terraces on Pt ( $1.23\pm0.03$  eV). The ratio of the diffusion barrier to desorption energy is ~0.65, in violation of the so-called 12%-rule. Using our derived diffusion/desorption rates, we explain why established rate models of the Ostwald process incorrectly predict low selectivity and yields of NO under typical reactor operating conditions. Our results suggest that mean-field kinetics models have limited applicability for modelling the Ostwald process.

#### References

[1] J. Am. Chem. Soc. 2021, Published Online Ahead of Print, October 21, 2021; https://doi.org/10.1021/jacs.1c09269

# 11:40-11:50 Isaac Buchine (BIU) Contributed Speaker

#### Title: How does Humidity Affect Halide Perovskites' Mechanical Properties?

#### **Abstract**:

ABX<sub>3</sub> Halide Perovskites, HaPs, where A= Methylammonium (MA), Formamidinium (FA), or Cesium (Cs), B= Pb or Sn, X=Chloride (Cl), Bromide (Br), or Iodide (I), are promising materials for optoelectronics. Their intriguing optical and electronic properties, paired with their straightforward fabrication, make them outstanding candidates for incorporation into a variety of next generation technologies, as well as for exploring new material behavior.

The effect of humidity on HaP *optoelectronic properties* and degradation mechanisms has been thoroughly investigated, yet no studies exist on how it influences their *structural and mechanical integrity*, which is critical for their successful integration into future technologies. The humidity-dependent performance can also cast doubt on the generality of fundamental behavior, measured under uncontrolled humidity conditions.

Five different HaP single crystals, MAPbX<sub>3</sub> (X = Cl, Br, and I) and APbBr<sub>3</sub> (A = Cs and FA) were selected and grown to investigate the role that different A cations and X anions play for humidity-dependence of mechanical properties. A two-pronged approach employing both instrumented nanoindentation, and atomic force microscopy (AFM)-based nanomechanical measurements, was used to measure *in situ* changes in elastic and plastic deformation under different humidity conditions. AFM measurements included both elastic modulus determination using a contact resonance technique and hardness measurements using a diamond AFM tip to indent the sample and measure the profile *in situ* using the same tip. Hardness and modulus values were also measured by continuous stiffness measurements via instrumented nanoindentation, using the Oliver & Pharr approach.

We find that for MAPbCl<sub>3</sub>, MAPbBr<sub>3</sub>, MAPbI<sub>3</sub> and FAPbBr<sub>3</sub> the elastic modulus (E) increases 3-10% while the hardness (H) decreases by as much as ~25%, when RH (relative humidity) increases from 10% to 60% and that these changes are reversible. the A-site cation is found to play a critical role in determining the mode of deformation. The hardness values measured for FAPbBr<sub>3</sub> and MAPbI<sub>3</sub> were humidity dependent in the AFM measurements but not in the NI measurements, which is explained by the somewhat different properties obtained from these two techniques. CsPbBr<sub>3</sub> shows negligible humidity dependence within experimental uncertainty.

We will discuss how the interplay between HaP composition and structure (how densely is the unit cell volume "filled" by the HaP constituents), and absorbed H2<sub>0</sub> can explain these observations.

11:50-12:10 Roundtable Discussions

# Energy challenges that we face today, the Israeli corner

Moderator: Doron Aurbach (BIU) Panel members: Emanuel Peled (TAU)

# Nanoelectronics & Spintronics Session Chair: Ilan Shalish (BGU)

10:20-10:40 Andras Kis (EPFL) Keynote Speaker

# Title: Logic-in-Memory Based on an Atomically Thin Semiconductor

#### **Abstract**:

The growing importance of applications based on machine learning is driving the need to develop dedicated, energy-efficient electronic hardware. Compared with von-Neumann architectures, brain-inspired in-memory computing uses the same basic device structure for logic operations and data storage, thus promising to reduce the energy cost of data-centric computing significantly. Two-dimensional materials such as semiconducting MoS<sub>2</sub> could stand out as a promising candidate to face this obstacle thanks to their exceptional electrical and mechanical properties. Here, we show that wafer-scale grown MoS<sub>2</sub> can be used as an active channel material for developing logic-in-memory devices and circuits based on floating-gate field-effect transistors (FGFET). The conductance of our FGFETs can be precisely and continuously tuned, allowing us to use them as building blocks for reconfigurable logic circuits where logic operations can be directly performed using the memory elements. We show that this design can be simply extended to implement more complex programmable logic and functionally complete sets of functions. Our findings highlight the potential of atomically thin semiconductors for the development of next-generation low-power electronics.

10:40-11:00 Zeev Zalevsky (BIU) Keynote Speaker

#### Title:

# Silicon-integratable tunable photonic nano-circuitry involving energetically efficient and hardware security architecture

#### **Abstract**:

In this presentation I will discuss optical cascadable Boolean data processing modules based upon linear optics i.e. functioning in regular silicon wafer without the need of integrating additional materials to enhance various nonlinear optical effects. This capability for cascading logic gates is obtained via intra-bit encoding. Such photonic Boolean logic gates that are based upon multi modal interference, are the building blocks of any higher order processor and the fact that they can be integrated as devices in conventional silicon wafers is highly important to the field of silicon photonics.

In addition, I will present technology allowing enhancing the energetic efficiency of the silicon processing circuit and reducing its power dissipation. The energetic efficiency enhancement will be obtained due to two novel building architectures: (1) Connecting electronic and photonic processing units via wireless interconnects. That way hybrid photonic and electronic processing units could work together side by side while the connectivity between them will be losses reduced due to the proposed wireless connectors. The connectors are based upon nano antennas converting surface plasmonic currents to photonic free space radiation and vice versa. (2) Encoding the transmitted information via time and frequency domains in such a way that information transmission is to be performed at lower SNR. The information could be transmitted much below the noise level and yet being detectable by the receiver unit. The concept is based upon physical level encryption or cyber photonic configuration that could also enhance the hardware security of the silicon circuitry in which the proposed configuration is being deployed.

# Ron Folman (BGU)

**Invited Speaker** 

#### Title:

# Quantum optics on the atom chip

#### Abstract:

Atom chips provide an excellent tool for fundamental studies as well as technological applications. In our group, several interferometry experiments have been done with a BEC on an atom chip [1] examining different effects. For example, we studied fluctuations in the nearby environment by an interference of atoms trapped in a magnetic lattice very close (5µm) to a room temperature surface [2,3]. We realized a new interferometry scheme of self-interfering clocks and showed, in a proof-of-principle experiment, how this could probe the interplay of QM and GR [4]. We also described a rule for "clock complementarity", which we deduce theoretically and verify experimentally [5]. In the clock interferometer, we have observed phase jumps due to the existence of a geometric phase [6]. Furthermore, we realized Stern-Gerlach interferometry [7-10] despite several theoretical works which have shown over the years that fundamental barriers exist. I will give a brief description of atom chip technology, and will then describe several fundamental and industrial applications. I will conclude with an outlook concerning ideas for possible tests of exotic physics such as quantum gravity [11].

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# 11:15-11:30 Leeor Kronik (WIS) Invited Speaker

### Title: Understanding collective effects that drive molecular spintronic devices

#### **Abstract**:

Molecular spintronic devices often involve collective effects, i.e., phenomena that the individual molecule or leads comprising the device do not exhibit. Understanding such effects often forces us to bridge two different "world views" – that of molecular orbital theory, which underlies much of chemistry, and that of delocalized electron waves, which underlies much of solid-state physics. Here, I will review our recent progress in understanding some novel classes of collective spintronic effects from first principles. I will focus on analysis and/or prediction of specific experiments, with an emphasis on the "fingerprints" that collective effects leave in experimental data.

11:30-11:40 Yaakov Tischler (BIU) Contributed Speaker

## Title: Low-Frequency Raman to Characterize Layered Materials

#### Abstract:

Raman spectroscopy is a powerful technique for identifying chemicals and characterizing materials. Raman spectra can provide insight into numerous properties, including morphology, stress/strain, crystallinity, doping level, conductivity, local temperature, and polarizability, whether in bulk, thin film, monolayer or nanostructure form. Raman spectroscopy finds applications in physical sciences, life sciences, medicine, drug discovery, and semiconductor metrology. Due to instrumental limitations associated with filtering out the incident laser from being detected by the spectrometer, the Raman spectrum is typically obtained for Raman shifts of 100 cm<sup>-1</sup> away from the laser up to 3500 cm<sup>-1</sup>, which is more than sufficient range to capture the whole "chemical fingerprint region". Modern laser filters, based on volume holographic gratings amongst other approaches now make it relatively straightforward to obtain Raman spectra from 100 cm<sup>-1</sup> down to 5 cm<sup>-1</sup>. In this low-frequency spectral range, the Raman scattering is sensitive to the phonon dispersion relation and vibrational modes associated with the nanostructure of the material. Here we present applications of Low Frequency Raman Spectroscopy (LFR) to characterize nanoscale layered materials, chiral purity of organic crystals and formulations, biomolecular assemblies, hybrid organo-metallic perovskites, and metal-organic frameworks. We show how the LF-Raman spectrum can be related to the mechanical vibrational modes that are present at the molecular level, and discuss our recent efforts to link LF-Raman to topographic features characterized by AFM.

# 11:40-11:50 Subhrajit Mukherjee (Technion) Contributed Speaker

#### Title:

# **Opto-Electronic Modulation of the Monolithically Integrated Ferroelectric-Semiconductor Heterojunction for Multibit Memory devices**

#### **Abstract:**

In recent years, ferroelectric-semiconductor (FS) heterojunctions are drawn massive interest in the field of multifunctional nanoelectronics, such as phototransistor, memory, data processing, neuromorphic computing etc.[1,2] Furthermore, the stable remnant polarization with unique in-plane (IP) and out-of-plane (OOP) dipole coupling down to the monolayer limit (~1.2 nm) in In<sub>2</sub>Se<sub>3</sub> becomes the central attention of ferroelectric research interest. The strong light-sensitivity towards visible-to-near-infrared illumination also making it attractive for photoactive applications. Herein, we demonstrated a scalable and site-specific direct writing approach on few-layers of indium selenide (In<sub>2</sub>Se<sub>3</sub>) to creat the In<sub>2</sub>Se<sub>3</sub>-In<sub>2</sub>O<sub>3</sub> coplanar heterojunction using scanning visible-laser probe. The locally converted region was thoroughly characterized by in-depth microscopic (HRTEM, AFM and KPFM) and spectroscopic (Raman, PL and ToF-SIMS) means to understand the conversion dynamics.[3] Furthermore, the fabricated planar heterojunction has been utilized as self-powered broadband photodetector by using the built-in interfacial potential along with the ferroelectric polarization states in  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> are utilized to control the device characteristics and thereby used to realize non-volatile memory (NVM). The state-of-art multibit logic device was demonstrated by utilizing the polarization directions dependent opto(electronic) output currents. The presented process enables a promising technological prospect to make all 2D lateral heterojunctions construction and could provide a platform for realizing wafer-scale integration of nanoscale devices with multiple advanced functionalities.

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# 11:50-12:10 Roundtable Discussion

# **Future of Electronics**

Moderator: Yossi Paltiel (HUJI) Panel members: Uriel Levi (HUJI)

# Plasma I

# **Chair: Reuven Boxman (TAU)**

## 10:20-11:00 Otto Landen (LLNL) Keynote Speaker

## Title: Breakthrough in Inertial Confinement Fusion (ICF) on the NIF

#### **Abstract**:

In August, the 192 laser beam 0.5 Petawatt (PW), 1.9 Megajoule (MJ) National Ignition Facility (NIF) [1] sufficiently compressed, heated and confined a deuterium-tritium (DT) plasma [2] such that it liberated enough exothermic fusion energy in a runaway "burn propagating" mode to double its temperature to 100 million degrees, producing ~10x more peak fusion power (10 PW) and energy (1.3 MJ) than any prior attempt. This is the same form of energy that powers the Sun and the stars through gravitational confinement, and that potentially could be an enduring source of clean energy on Earth. The accomplishment was built on decades of hard work and dedication by many theoretical, computational and experimental plasma physicists, laser physicists, material scientists, chemists, precision engineers and technical staff at LLNL, in partnership with the inertial fusion, plasma, and the high energy density science community. In terms of fusion energy gain, 1.3 MJ represents 5x the energy deposited in the capsule that confines the DT and 0.7x of the incident laser energy. In context, a future inertial fusion energy power plant would require 100x more gain delivered several times a second. This talk will review the basic physics of indirect-drive ICF [3], the scientific and technical challenges that led up to creating this new regime in the laboratory, and present the unique time and space dependent conditions extracted from an array of x-ray and nuclear bolometers, cameras and spectrometers. The talk will conclude by discussing strategies based on extrapolations using a combination of simulations, theory and current results for increasing the system efficiency and hence fusion gain a further 10x in the next few years at NIF.

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## 11:00-11:10 Hank Strauss (HRS Fusion) Contributed Speaker

# Title: Solution of the Disruption Problem in ITER

#### **Abstract:**

Disruptions in ITER will be much milder in ITER than in present experiments. They will be self mitigating: disruption precursors rather than disruptions.

ITER is a large tokamak under construction in France, which is supposed to achieve magnetic fusion. It has a high strength magnetic field produced by superconducting magnets.

Like all tokamaks, it is expected to experience disruptions, caused by magnetohydrodynamic (MHD) instabilities. Because of the large size, stored energy, and magnetic field, the disruptions could damage the machine. A great deal of effort has been made to develop a disruption mitigation system, which has its own problems.

A new analysis [1,2] has shown that ITER should be much more MHD stable than previously thought. The reason is the highly conducting shell surrounding ITER, which stabilizes or slows down resistive wall modes. The new analysis shows that most disruptions in the JET tokamak are caused by resistive wall tearing modes, which are also stabilized. Simulations of ITER show that the expected disruptions will also be resistive wall tearing modes.

A key metric of ITER is the thermal quench time. This determines the thermal wall load of a disruption. Until now it has been estimated to be a few ms. This would cause severe damage unless mitigated by injection of radiative material, which can cause further problems. The new theory shows that the thermal quench time is 10 - 100 times longer than previous estimates, greatly reducing the possibility of damage. Analysis of data, theory, and MHD simulations will be presented.

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## 11:10-11:20 Nir Druker (Technion) Contributed Speaker

#### Title:

# **Enhancement of Plasma Assisted Ignition by Multi-Voltage Pulse Discharges**

#### Abstract:

The use of cold plasma for ignition improvement in internal combustion engines has been widely investigated in the past two decades. Usually, high voltage nanosecond pulses are repeatedly applied to facilitate such a process. Compared to traditional ignition, nanosecond repetitive pulse ignition systems demonstrate improvement in heat release rate during combustion, ignition delay time reduction and enhanced ignition process in flowing and lean reactive gas mixtures.

In this research, we conducted a preliminary, theoretical/numerical investigation into the possibility of use of on-board control of electrically-based cold plasma-assisted ignition and combustion. The focus was on diagnostics and enhancement of energy deposition in specific modes, by application of bi-polar short duration voltage pulses in low-pressure air. The physical model couples the electric field, potential and current, with the relevant conservation equations for 24 species via 168 kinetic reactions, including molecules' rotation, vibration, electronic excitation, dissociation, and ionization inside the electrodes gap. Evaluation using various pulse repetition frequencies and different pulse shapes was conducted. Special attention was given to the overall coupled energy deposited during the discharge, and to energy channeled to known ignition supportive modes such as nitrogen electronic excitation and oxygen radicals' generation. The results of the analysis show that for the considered conditions, energy deposition can be divided into two main stages, characterized by high and low voltage magnitudes, respectively. It was found for the first time, that the (low voltage) second stage's energy deposition can be higher than that of the first (high voltage) stage. At the second stage, the deposition of energy into specific modes can be tuned by setting appropriate voltage magnitudes. In addition, the energy deposited in modes important for ignition exhibits a simple linear relation to the overall energy deposition. Furthermore, based on these findings, we demonstrate how a new sequence of voltage pulses can further increase enhancement of ignition and combustion supportive processes.

## 11:20-11:30 Yang Cao (Technion) Contributed Speaker

#### Title:

# The Non-Linear High-Power Microwave Complete Absorption Phenomenon in a Plasma Filled Waveguide

#### **Abstract**:

We present the first experimental observation of a fully-absorption of a K-band high-power microwave (HPM) pulse (1.2 GW, 0.5 ns, 25.6 GHz)(1) in a plasma-filled waveguide.(2) The plasma density dependent waveguide cut-off frequency is near to the pulse frequency. In the plasma-filled waveguide, due to the ponderomotive force caused by HPM pulse, plasma electrons being kicked towards the waveguide wall, generating a potential well in the waveguide where the remaining electrons keeps oscillate in the HPM pulse field. At this near critical plasma density, the group velocity of the pulse decreases, which provides sufficient time for these trapped electrons to collide with ions while their regular field-induced oscillation motion becomes chaotic and thermal. This results in all the energy of the pulse being transferred to the kinetic energy of electrons. This nonlinear full-absorption phenomenon of HPM pulse is absent when pulse power is low and the potential well does not form in the waveguide. The experimental result is confirmed by 3D particle-in-cell (PIC) simulations. 1.) Y. Cao, Y. Bliokh, J.G. Leopold, V. Rostov, Y. Slutsker, and Y.E. Krasik, Phys. Plasmas 26, 023102 (2019). 2). Y. Cao, J.G. Leopold, Y.P. Bliokh, G. Leibovitch, and Y.E. Krasik, Phys. Plasmas 28, 062307 (2021).

# Marko Cvejic (WIS)

**Contributed Speaker** 

#### Title:

# Spectroscopic measurements of the magnetic field curvature and self-rotating plasma

#### Abstract:

Z-pinches with preembedded axial magnetic field  $B_{z0}$  undergo a radial implosion while compressing the plasma and the embedded magnetic flux. While the  $B_z$  flux is compressed, the  $B_z$ -lines in the metal electrode continue to be frozen at their initial radius. Thus, a transition region where the field lines are bent radially is formed. We developed novel polarization-based spectroscopic technique, that utilizes the combined effect of the Zeeman splitting and Doppler shift due to the implosion velocity, to directly measure the  $B_z$  and  $B_r$ , namely the curvature. The measurements of  $B_r$  allow for study the self-rotation seen for the first time, to develop in the plasma, and for correlating the rotation and the implosion with the effect of the  $j_z \times B_r$  forces.  $B_r$  measurements are essential because  $B_r$  determines the rotation  $j_z \times Br$  and the implosion of the plasmas near the electrodes.

# 11:40-11:50 Sharon Waichman (NRCN, Rotem Industries) Contributed Speaker

#### Title: Enhanced adhesion of boron carbide coatings on aluminum substrates

#### Abstract:

Boron carbide is a ceramic material having superior properties, in particular big cross section for neutron absorption, which makes it suitable for nuclear applications including homeland security and accelerators. We deposited 2.0-3.5  $\mu$ m boron carbide coating on an aluminum substrate using pulsed-DC magnetron sputtering. The adhesion between these two materials is challenged because of the formation of an unstable aluminum-carbon bond and the difference between their thermal expansion coefficients that may cause stress and subsequent adhesive failure. Hence, we applied an adhesive intermediate titanium layer (0.5-1.5  $\mu$ m) and systematically studied the coating process parameters that affect the deposited film, mainly the impact of the titanium interlayer thickness on the adhesion, and the effect of the bias voltage applied during deposition on the growing film. We discovered that increasing the deposition and surface morphology were studied by SEM. XRD and XPS, respectively, confirmed the predicted amorphous structure and B<sub>4</sub>C composition. XPS also revealed oxidized and carbonaceous species on the substrate. Boron carbide coatings with thickness of at least 3.5  $\mu$ m, deposited over a 1.5  $\mu$ m thick titanium layer, adhered for several months (until today), in a 2% RH environment. We determined that the optimal bias voltage applied to the substrate if an intermediate titanium layer is first deposited, and optimal coating parameters are used when depositing the boron carbide layer.

11:50-12:10 Roundtable Discussion

Moderator: Reuven Boxman (TAU) Panel members: Otto Landen (LLNL-NIF), Sharon Waichman (NRCN/Rotem Industries), Michael Keidar (GWU), Hank Strauss (HRS Fusion), Asher Yahalom (Ariel U.), Amnon Fisher (RAFAEL), Joe Lefkowitz (Technion) *Plasma for a Greener Earth*  Humankind is facing an extreme challenge this century: providing for the health, welfare, and prosperity of a burgeoning human population on planet Earth, which is experiencing human induced climate change, fresh water insufficiency, rapidly spread disease, and pollution. This panel will address how plasma can help face this challenge. The much-sought "killer" plasma application is controlled nuclear fusion, which has the potential to supply power without burning fossil fuel or producing copious radioactive waste. When, if at all, can it be realized? In the shorter term, plasma can be used to depollute effluent gases and waste water from industry and agriculture. Plasma is used to produce wear resistant low friction coatings for mechanical components, which reduce energy use for the manufacture, maintenance and operation of vehicles and other machines. What else can plasma do?

# **Sensors & Printing Session**

**Chair: Hila Elimelech (Plantish)** 

# 13:30-13:50 Oded Shoseyov (HUJI) Keynote Speaker

## Title: 3D Printing; from tissues and organs to food and wood

#### Abstract:

Bringing together the toughness of cellulose nano-fibers from the plant kingdom, the remarkable elasticity and resilience of resilin that enables flees to jump as high as 100 times their height from the insect kingdom combined with Human Recombinant Type I collagen produced in tobacco plants; These are the materials of future 3D Printing. Resilin is a polymeric rubber-like protein secreted by insects to specialized cuticle regions, in areas where high resilience and low stiffness are required. Plant cell walls also present durable composite structures made of cellulose, other polysaccharides, and structural proteins. Plant cell wall composite exhibit extraordinary strength exemplified by their ability to carry the huge mass of some forest trees. Inspired by the remarkable mechanical properties of insect cuticle and plant cell walls we have developed novel composite materials of resilin and Crystalline Nano-Cellulose (resiline-CNC) that display remarkable mechanical properties combining strength and elasticity. As a central element of the extracellular matrix, collagen was always extracted from animal and human cadaver sources, which pose risk of human pathogens. A tobacco plant expression platform has been recruited to effectively express human collagen, along with three modifying enzymes, critical to collagen maturation. The plant extracted recombinant human collagen type I forms thermally stable helical structures, fibrillates, and demonstrates bioactivity resembling that of native collagen. Today in greenhouses all over Israel farmers grow transgenic tobacco plants producing human recombinant collagen that is used for the production of medical implants that have already in clinical use. We will demonstrate utility of hrCollagen, Cellulose Nano Crystals and resilin using Additive Manufacturing technologies in tissue and organ printing, food and wood products manufacturing.

13:50-14:10 Yossi Rosenwaks (TAU) Keynote Speaker

### Title: Ultra-Sensitive and Selective Sensing using CMOS Compatible Nanowire Transistors

#### Abstract:

For the past several decades, there is a growing demand for the development of low-power gas sensing technology for the selective detection of volatile organic compounds (VOCs), important for monitoring safety, pollution and healthcare. Inspired by the sensitive Si nanowire sensors we have developed the Si Electrostatic-Formed Nanowire (EFN), as a new paradigm that combines a highly sensitive and selective platform for detection of various target molecules with standard VLSI compatible fabrication. Recently, a Pd modified Si-EFN have demonstrated world record response of  $\sim 1x10^9$ % for 0.8% H2 and a sensitivity of 398%/ppm at room temperature. This is most probably due to the EFN ability to control the size, shape and the location of its channel post fabrication, which allows to tune and optimize the EFN sensitivity for different analytes. We expect that this novel paradigm will pave the way to a robust sensing platform for real world applications.

14:10-14:25 Vladimir Popov (Technion) Invited Speaker

## Title: New modalities and facilities by Metal Additive Manufacturing Center

#### **Abstract:**

Metal Additive Manufacturing Center (MAMC) works on the development and characterization of new and existing metals and alloys. The research uses Powder Bed Fusion machines for Selective Laser Melting (SLM) and Electron Beam Melting (EBM). We will present our current activities in aerospace, medical, and advanced materials applications. For the last application, we have developed a customized system for small amounts of powders. Even mixed powders could be manufactured by this approach performing in-situ alloying. We will present the gas atomizer and first experimental findings in gas atomization powders production for the development of new metal alloys for additive manufacturing and powder metallurgy. Among the newest facilities of the MAMC, the nondestructive testing (NDT) system by VibrantNDT will be shown and explained. The revolutionary Process Compensated Resonance Testing (PCRT) measures resonance frequencies through whole parts, allowing customers to test every part and significantly increase final product quality by detecting process variation and structural defects.

14:25-14:40 Nurit Atar (SNRC) Invited Speaker

# Title: 3D Printing of Bismaleimide-Based Dielectric Materials

#### Abstract:

Additive manufacturing is a novel paradigm which has numerous potential applications in industry and research. 3D printing technologies allow formation of extremely complex geometrical structures with high precision and smooth surface. New engineering polymers with diverse characteristics should be developed to expand 3D printing into new applications. Additive manufacturing is of growing interest in particular to the electronics industry as it offers great potential to rapidly build complex objects of embedded electronics, reduce weight, simplify manufacturing processes, and produce flexible circuits. Metals are being widely used as conductive materials for 3D printing in various printing techniques such as inkjet, aerosol jet printing, and laser induced forward transfer (LIFT). High performance dielectrics, on the other hand, are currently not commercially available. Therefore, the development of highly insulating polymers, possessing high breakdown voltage and high thermal and chemical stability, attains significant research efforts. Bismaleimides (BMIs), a class of polyimides, are very attractive polymers for 3D printing due to their excellent thermal, mechanical, and chemical stability, and their superior dielectric properties. This work presents a novel UV-curable BMI-based dielectric ink for hybrid 3D printing. The UV reactivity and ink viscosity are optimized by addition of a mixture of photoinitiators and environmentally friendly diluents. Optimization of the jetting and printing conditions allows for the first ever production of 3D thermosetting BMI objects by 3D printing. Thermal post curing is used to enhance mechanical properties and thermal stability of the printed material. The printed BMI demonstrates high dielectric strength, high chemical and thermal stability, low moisture absorption, and low outgassing in high vacuum environment. Free-form 3D functional electronic devices were designed and manufactured using a hybrid approach which combines multimaterial printing of metal interconnects within dielectric BMI matrix, including embedded electronic elements. The resulting properties of the printed BMI material open a wide range of potential applications in robotics, electronics, automotive, aerospace, and space technologies.

14:40-14:50 **Rajashree Konar (BIU)** Contributed Speaker

#### Title:

Robust Room-Temperature NO2 Sensors from Exfoliated 2D Few-Layered CVD-Grown Bulk Tungsten Di-selenide (2H-WSe<sub>2</sub>)

#### Abstract:

Fossil fuel combustion and automotive emissions always result in highly toxic emissions. Some of the most commonly known pollutants are nitrogen dioxide (NO<sub>2</sub>), hydrogen disulfide (H<sub>2</sub>S), ammonia (NH<sub>3</sub>), and acetone, to name a few. Among the various gas sensors, resistance-type gas sensors are the most attractive and practical for use in sensing toxic analytes and explosive gases due to their facile fabrication, ease of operation, low cost, and miniaturization. In this regard, 2D materials (2DMs) and especially transition-metal chalcogenides (TMCs) or transition-metal di-chalcogenides (TMDCs) specify a massive range of unique properties that prove their usefulness in applications toward

gas sensing. Semiconducting two-dimensional (2D) TMDCs of the type MX<sub>2</sub>, where M = Mo, W and X = S, Se, are encouraging materials to be explored in areas of gas-sensing because they are exceptionally sensitive to the ambient conditions. We report a facile and robust roomtemperature NO<sub>2</sub> sensor fabricated using bi- and multi-layered 2H variant of tungsten di-selenide (2H-WSe2) nanosheets, exhibiting high sensing characteristics. A simple liquid-assisted exfoliation of 2H-WSe2, prepared using ambient pressure chemical vapor deposition, allows smooth integration of these nanosheets on transducers. Three sensor batches are fabricated by modulating the total number of layers (L) obtained from the total number of droplets from a homogeneous 2H-WSe2 dispersion, such as ~2L, ~5–6L, and ~13–17L, respectively. Room temperature (RT) experiments show that these devices are specifically tailored for NO2 detection. 2L WSe2 nanosheets deliver the best rapid response compared to ~5–6L or ~13–17L. The response of 2L WSe2 at RT is 250, 328, and 361% to 2, 4, and 6 ppm NO2, respectively. The sensor showed nearly the same response toward low NO<sub>2</sub> concentration even after 9 months of testing, confirming its remarkable long-term stability. A selectivity study, performed at three working temperatures (RT, 100, and 150 °C), shows high selectivity at 150 and 100 °C. Full selectivity toward NO<sub>2</sub> at RT confirms that 2H-WSe2 nanosheet-based sensors are ideal candidates for NO<sub>2</sub> gas

15:00-15:20 Roundtable Discussion

# 3D printing for Defence applications

Moderator: Ehud Galun (MAFAT) Panelists from Rafael, Elbit and IAI

# **Soft & Biological Matter Session**

**Chair: Nadav Amdursky (Technion)** 

13:30-13:50 Uri Raviv (HUJI) Keynote Speaker

## Title: Mechanism of Virus Capsid Assembly

#### **Abstract:**

There is a huge number of possible intermediates on the assembly path from hepatitis B capsid protein dimers to 120-dimer capsid. If every intermediate were tested, assembly would often get stuck for entropic reasons and essentially every capsid would follow a unique assembly path. Yet, capsids assemble rapidly with minimal trapped intermediates. To understand the fundamental mechanisms of capsid assembly it is critical to resolve the early stages of the reaction. To observe assembly, we used time-resolved Small Angle X-ray Scattering, which is sensitive to solute size and shape and has millisecond temporal resolution. Scattering curves were fit to a thermodynamically curated library of assembly intermediates, using a maximum information entropy approach to provide a physical rationale for the selection of intermediates. We found that capsid assembly was controlled by the supersaturation state of the system at the onset of assembly, dictating the intermediate structures during the early stages of the reaction. With the mildest conditions tested, we observed a nearly two-state reaction from dimer to capsid with a small number of dimers-of-dimers and trimers-of-dimers. In slightly more aggressive conditions, we observed a decamer-of-dimers and a 90-dimer species. In conditions where there is measurable kinetic trapping, we found a greater diversity of early intermediates >30 and <90 subunits did not accumulate. These results indicate the presence of low barrier paths that connect intermediates that can direct the ultimate assembly path to late intermediates where assembly can be paused.

# 13:50-14:05 Boaz Mizrahi (Technion)

**Invited Speaker** 

#### Title:

# Multi-Armed Polymers as Tissue Adhesives: Fundamentals to Applications

#### **Abstract**:

Multi-armed polymers, often termed star polymers, are highly branched macromolecules with three-dimensional architectures. Each molecule is composed of a central core from which linear arms emanate. Star polymers have a number of chemical and physical properties (e.g. their solubility and low melting point) that make them useful in several biomedical fields, from drug-delivery, tissue adhesives to tissue engineering and coatings. While solid polymers with high molecular weights (>5000 Da) are receiving significant attention in polymer science, the development of liquid star polymers remains relatively unexplored. I will discuss new concepts and strategies and present some bio-adhesion applications based on the unique structure of soft- star polymers.

# 14:05-14:15 Irit Rosenhek-Goldian (WIS) Contributed Speaker

Title:

AFM for biophysical characterization of soft matter: from extracellular vesicles to cells and tissues

#### Abstract:

In atomic force microscopy (AFM) the surface is probed by a tip attached to a cantilever (spring) that can measure the surface topography

along with biophysical properties like stiffness, adhesion and viscoelasticity. AFM enables gentle scanning of soft biological samples, under physiological buffer solutions to mimic the natural environment. It is applicable to a large variety of samples at various length scales, from tiny extracellular vesicles (EVs), through cells to whole tissue. However, each study represents a new set of considerations, requiring custom-tuned experimental design to ensure meaningful results. For example, the sample preparation step is critical in terms of purity and robust attachment of the object of interest to the surface. The choice of cantilever, scanning conditions, and measurement procedure are important to enable proper, stable and gentle measurement.

In this presentation these issues will be discussed, based on our hands-on experience with 3 different projects applying AFM to study of soft biological samples: imaging of malaria-derived EVs, imaging and stiffness measurements on red blood cells, and viscoelasticity measurements on colon tissue. Each measurement will be presented along with the strategic approach employed and how the complications encountered were overcome.

## 14:15-14:25 Esti Toledo (BGU) Contributed Speaker

#### Title:

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

#### **Abstract**:

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 that control spatial organization of receptors within the cell membrane have been extensively used to study how the receptor spatial order regulates cell function, including that of immune lymphocytes. These 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 ignads, which was applied to elucidate KIR2DL1-mediated inhibitor of NKG2D signalling receptors of natural killer cells. This platform was conceived by bimetallic nanodot patterning with molecular-scale registry, followed by a ternary functionalization with distinct modelling, we interpret these findings because of the size mismatch and conformational flexibility of ligands in their spatial interaction. 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.

# 14:25-14:40 Alireza Dolatshahi-Pirouz (DTU, Denmark) Invited Speaker

#### Title:

# Human-adaptable cyborg-like biomaterial sensors for healthcare monitoring

#### **Abstract**:

Historically the field of biomaterials science has primarily focused on assuring biocompatibility between materials and humans. Less effort has been directed towards transforming biomaterials into life-like entities with the capacity for continuously adapting to our dynamic body and tissues. Most conventional medical devices, are actually still in disharmony with biological systems, which are in a never-ending progress of **adaption** and **evolution**. The central theme behind our research is mitigating a new avenue into this hitherto uncharted territory by developing an innovative class of materials that can become 3D printed into custom-adaptable medical devices capable of reconfiguring in response to dynamic environments, while simultaneously enabling real-time monitoring of important biological events. Notably, our proposed monitoring platform is multifunctional and based on a simple, cheap and scalable approach. Biomaterials that can reconfigure and adapt in response to dynamic stimuli is indeed an emerging concept that ultimately could change medical devices from being a foreign foe to a fully integrated part of us.

# Molly Stevens (ICL, London)

**Keynote Speaker** 

#### Title:

# Designing the bio-material interface for biomedical applications

#### Abstract:

This talk will provide an overview of our recent developments in bio-instructive, self-assembling and gradient materials for applications in regenerative medicine with focus on establishing translational pipelines to bring our innovations to the clinic [1]. I will discuss recent developments in our tunable nanoneedle arrays for multiplexed intracellular biosensing at sub-cellular resolution and modulation of biological processes [2] and will talk about our portfolio of nanoparticle-based sensing probes for disease monitoring in vivo such as renal clearable gold nanoclusters for cancer detection [3]. We integrate our nanomaterial-based assays into smartphone enabled tests for point-of-care cancer diagnostics and monitoring of disease progression and response to treatment [4]. Finally, I will present our advances in Raman spectroscopy characterisation techniques for high-throughput label-free characterization of single nanoparticles (SPARTA®) which is becoming an integral tool for the design of advanced nanotherapeutics [5]. I will explore how these versatile technologies can be applied to transformative biomedical innovations.

[1] J. P. K. Armstrong... M. M. Stevens. "A blueprint for translational regenerative medicine." Science Translational Medicine. 2020. 12(572): eaaz2253.

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[3] C. N. Loynachan... M. M. Stevens. "Renal clearable catalytic gold nanoclusters for in vivo disease monitoring." Nature Nanotechnology. 2019. 14: 883–890.

[4] C. S. Wood, ... M. M. Stevens. "Taking connected mobile-health diagnostics of infectious diseases to the field." Nature. 2019. 566: 467-474.

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15:00-15:20 Roundtable Discussions

Bioderived Materials for Health Applications: Current challenges and opportunities

**Moderator: Nadav Amdursky** 

# Nanomaterials & Nanotechnology Session

**Chair: Hagay Shpaisman (BIU)** 

13:30-13:50 **Reshef Tenne (WIS)** Keynote Speaker

#### Title:

# Inorganic nanotubes and fullerene-like nanoparticles at the crossroad between materials science and nanotechnology and their applications

#### Abstract:

Update on the synthesis of new inorganic nanotubes from 2D compounds, like WSe<sub>2</sub> and from the asymmetric "misfit" layer compounds (MLC), RES-TaSe<sub>2</sub> and RE-(TaSe<sub>2</sub>)<sub>2</sub> (with RE=La, Sm) will be given.[1] Major progress has been achieved in elucidating the structure of INT and IF and their mechanical, electrical and optical properties.[2] These analyses revealed their for reinforcing variety of polymers was demonstrated leading to numerous potential commercial products.[3-5]

1. M.B. Sreedhara et al., PNAS 118, 35 e2109945118 (2021);

https://doi.org/10.1073/pnas.2109945118

2. J. Musfeldt, Y. Iwasa and R. Tenne, Physics Today 8, 42-48, August (2020).

3. H. Shalom, S. Kapishnikov, V. Brumfeld, N. Naveh, R. Tenne and N. Lachman, Scientific Reports, 10:8892 |

https://doi.org/10.1038/s41598-020-65861-w (2020).

4. H.-T. Kim and co-workers, ACS Appl. Energy Mater. 3, 4619-4628 (2020).

5. D.M. Simic et al., Composite- Part B 176, 107222 (2019).

# 13:50-14:05 Gil Markovich (TAU) Invited Speaker

## Title: Symmetry breaking in the formation of chiral nanocrystals

#### Abstract:

We are interested in symmetry breaking in inorganic compounds. Many inorganic compounds crystallize in chiral space group, such as quartz, for example. Our group has been studying the breaking of left-right symmetry in the formation of nanocrystals of such compounds. We have shown, that using small chiral bio-molecules which interact with the crystals' building blocks, it is possible to achieve such symmetry break. In particular, we have been working with the chiral TbPO<sub>4</sub>×H<sub>2</sub>O nanocrystals, and have shown that their handedness can be controlled by preparing the nanocrystals in the presence of certain natural chiral molecules, such as tartaric acid. We use circularly polarized luminescence measurements of Eu<sup>3+</sup> dopant ions in the nanocrystals to follow the handedness and enantiomeric purity of the produced nanocrystals and confirmed that we obtain a single mirror image (enantiomer) of the terbium phosphate nanocrystals when prepared with tartaric acid molecules.[2]

References

1. U. Hananel, A. Ben-Moshe, H. Diamant, G. Markovich, Proc. Natl. Acad. Sci. USA 116, 11159-

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2. E. Vinegrad, U. Hananel, G. Markovich, O. Cheshnovsky, ACS Nano 13, 601–608 (2019).

# Tamar Segal-Peretz (Technion)

**Invited Speaker** 

#### Title:

# Atomic layer deposition onto and within polymers for controlling interfaces and nano-structuring water filtration membranes

#### **Abstract:**

Atomic layer deposition (ALD) is a powerful technique for thin layer deposition of inorganic materials on tortures, high aspect ratio, substrates. By using ALD, a wide variety of inorganic compositions can be deposited on organic and inorganic substrates with sub-nm accuracy. Here, I will present our work on ALD onto and within polymers. We show, using high-resolution electron microscopy, that controlling the diffusion time of ALD precursors dictates the metal oxide deposition through the depth of the polymeric, phase inverted, ultrafiltration membranes. With just several cycles of Al<sub>2</sub>O<sub>3</sub> ALD, we were able to modify the polymer membranes' interface, enhancing the membrane hydrophilicity, and oil anti-fouling behavior. We further explore ALD within polymers, also known as sequential infiltration synthesis (SIS). In SIS, long diffusion times and precursor-polymer reactivity enables metal oxide growth within the polymers' volume, creating organic-inorganic composite materials. We performed SIS on self-assembled block copolymer (BCP) layers, where the polymer block chemistry yields selective SIS metal oxide growth in only one block. Following the growth, we removed the BCP template to obtain isoporous metal oxide membranes with enhanced pollutant selectivity. Finally, we combine both approaches to tune the pore size and surface properties of anisotropic BCP membranes where we selectively grow metal oxides in the polymer block surrounding the pore with SIS and further perform ALD cycles to tune pore size from ultrafiltration to nanofiltration. The metal oxide pore interface allows us to control the filtration selectivity as well as be the basis for new functional moieties addition.

# 14:20-14:30 Sujit Kumar (WIS, BIU) Contributed Speaker

#### Title:

# Evidence for Atomic Scale Structural Dynamics of the 2D-on-3D Halide Perovskite Interfaces

#### Abstract:

An ultra-thin layer of 2D-on-3D Halide Perovskites (HaPs) is often reported to be beneficial in order to prevent the surface reactivity, defects and possibility of water and O2 absorption of/by 3D HaPs. However, the stability of 2D-on-3D HaP composites have often been questioned based on the results from GI-XRD and PL studies. The question of what is happening at such 2D/3D interfaces is a vexing, yet fascinating one considering that the ultimate objective of using such configurations is to gain stability while the dynamic nature of the HaPs lattices is often being reported lately. In this work, we studied FIB-(optimally) prepared cross-sections of 2D-on-3D HaP composite films by TEM-based methods. A new controlled gas-phase surface cation exchange process of the spin-coated 3D MAPbI<sub>3</sub> film was employed to synthesize the 2D Ruddlesden-Popper FPEA<sub>2</sub>PbI<sub>4</sub> HaP layers, where FPEA = monofluorinated derivative of phenyl-ethylamine. All through the study we strove to minimize the electron and ion fluences to lessen the effects of the beam damage on our samples. We used 4D-STEM and scanning nanobeam electron diffraction (NBED) measurements on fresh and aged (all in inert atmosphere) samples. We find evidence for the 2D n=1 phase appearing inside the 3D matrix and also for the formation of quasi 2D phases near the interface with the carbon coat. The results suggest 2D/3D perovskite heterointerface lattice rearrangements involving migration of not only (the smaller) MA<sup>+</sup>, but also of (the larger) FPEA<sup>+</sup> cation. The structural evolution under the beam shows the loss of long-range periodicity as well structural rearrangements, leading to quasi 2D phase formation. These results thus, complement the extensive empirical and semi-empirical data to engineer stable 2D-on-3D composites and also define conditions for atomic resolution studies of 2D/3D samples in device-relevant configurations.

14:30-14:40 Sivan Tzadka (BGU) Contributed Speaker

Title: Directly moldable functional nanostructures on plastic optical flat/curve components

#### **Abstract**:

Silica glass is a traditional material for optics in the visible range. However, there has recently been an emerging interest in the optical polymer as an alternative to glass, due to the low price of raw materials, excellent optical properties, low weight, and the ability to produce freeform optical components by precision molding. However, the main obstacle toward the optical applications of polymers is the need for antireflective coatings.

Traditional antireflective coatings based on vacuum-deposited films are broadly used for glass, yet they are non-applicable for polymers, because of pure adhesion and thermal stresses they generate. An alternative to films is moth-eye subwavelength nanostructures, which produce broadband and omnidirectional antireflective effect. However, moth-eye nanostructures have not been yet implemented on polymeric optics. In this research, the application of moth-eye antireflective nanostructures on polymeric optics will be explored, by several routes.

First, the direct soft imprint of the polymer surface, covered with film which made of its own monomer mixed with UV sensitive powder, will be studied.

An additional route will be based on the precision molding of polymeric optical components with built-in antireflective structures patterned on the inner surface of the mold cavity. The study will also include optical characterization of the imprinted polymers and a demonstration of their optical function. This research will establish novel nanotechnological approaches for material nano-structuring and will pave the way to numerous applications of polymers in optics.

14:40-15:00 **Oleg Gang (Columbia University)** Keynote Speaker

#### Title: Programmable Assembly of Nanoscale Architectures

#### Abstract:

The ability to organize functional nanoscale components into the targeted architectures promises to enable a broad range of nanotechnological applications, from new classes of engineered biomaterials to photonic devices and chemically active media. However, we are currently lacking a broadly applicable methodology for the 3D bottom-up formation of nanostructures with ability to prescribe their architecture, to integrate different types of nanocomponents and to control their organization on different scales. The talk will present our progress in establishing a versatile self-assembly platform for the fabrication of designed large-scale and finite-size nano-architectures from diverse inorganic and biomolecular nanocomponents through the DNA-programmable assembly. The recent advances in creating periodic and hierarchical organizations from inorganic nanoparticles and proteins will be discussed. The formed 3D nanostructures can be farther transformed into fully inorganic replica via nano-templating. The use of the developed assembly approaches for generating functional nanomaterials with nano-optical, electrical, mechanical, and biochemical functions will be demonstrated.

## 15:00-15:20 Roundtable Discussion

# Nanomaterials & Nanotechnology: the next 20 years

Moderator: Reshef Tenne (WIS) Panel members: Gil Markovich (TAU), Tamar Segal-Peretz (Technion), Oleg Gang (Columbia Univ.)

# **Plasma Session II**

# **Chair: Joseph Lefkowitz (Technion)**

13:30-13:50 Michael Keidar (GWU) Keynote Speaker

### Title: Adaptive Plasmas for Medical Applications

#### **Abstract**:

The uniqueness of plasma is in its ability to change composition in situ [1,2,3]. Plasma self-organization could lead to formation of coherent plasma structures. These coherent structures tend to modulate plasma chemistry and composition, including reactive species, the electric field and charged particles. Formation of coherent plasma structures allows the plasma to adapt to external boundary conditions, such as different cells types and their contextual tissues. In this talk we will explore possibilities and opportunities that the adaptive plasma therapeutic system might offer. We shall define such an adaptive system as a plasma device that is able to adjust the plasma composition to obtain optimal desirable outcomes through its interaction with cells and tissues.

We propose various approaches for plasma therapy based on plasma adaptation to target conditions. This approach is based on the ability of measuring the cellular response to plasma immediately after treatment and modifying the composition and power of plasma via a feedback mechanism. Plasma self-adaptation might be feasible due to self-organization and pattern formation when plasma interacts with targets. Plasma effect on cancer cells is influenced by various factors including the plasma jet discharge voltage, gas composition, humidity and cancer cell type [4]. To address this, we present an optimal feedback control scheme to adjust treatment conditions responsive to the actual cancer cell response [5].

References

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 L. Lin, Z. Hou, X. Yao, Y. Liu, J. R. Sirigiri, T. Lee, and M. Keidar, Physics of Plasmas, 27, 063501, 2020. [3] D. Yan, W. Hu, L. Lin, X. Yao, J. Sherman and M. Keidar, Scientific Reports, 2018, 8(1) 15418
 L. Lin, Y. Lyu, B. Trink, J. Canady, and M. Keidar, J. Applied Physics, 125, 153301, 2019.
 Y. Lyu, L. Lin, E. Gjika, T. Lee, M. Keidar, J. Phys. D: Appl. Phys., 2019, 52, 18520

13:50-13:10 Eduardo Ahedo (UC3M) Keynote Speaker

## Title: Modeling propulsion plasma physics

#### **Abstract**:

Plasma-based thrusters have become the dominant technology for in-space propulsion in near-Earth and inner Solar system missions, ranging from internet-services constellations to geostationary satellites and the planned Lunar orbit station Gateway. Different technologies compete fiercely for this in-expansion market and applications.

This talk will comment some of the main aspects framing that competition, such as the level of complexity of the thruster, the propulsionrelated figures and operation envelope, and the technology qualification process for space flight.

Second, we will discuss how the technology competitiveness can be improved through thruster design, experimental characterization, understanding and mastering of discharge physics, and development of predictive simulation tools.

Third, and to illustrate the modeling challenges, we will first discuss the main physical phenomena on Hall-effect thrusters, focusing on turbulent transport and non-Maxwellian features electron velocity distribution function (eVDF). We will present recent eVDF results on a 1D kinetic model, and how they lead to anisotropy and gyroviscosity in the pressure tensor, an unconventional parallel heat flux, and reduced wall losses, three aspects precluding a standard macroscopic characterization.

Finally, the unconventional heat flux will be found to also appear, together with collisionless cooling, in the kinetic description of a magnetically channeled plasma plume.

## 14:10-14:20 Dan Lev (Technion) Contributed Speaker

#### Title:

# Heaterless Cathode Technology for Plasma Propulsion Applications

#### Abstract:

Hollow cathodes are electron generating devices used to supply a stream of electron necessary for the operation of electric propulsion devices, specifically Hall thrusters or gridded ion engines. The electrons provided by the hollow cathode are used to initiate the thruster discharge, sustain thruster operation and neutralize the ion beam ejected out of the thruster to open space.

Heaterless Hollow Cathodes (HHCs) are a subclass of hollow cathodes that do not require external heating to bring the electron emitter to its operation temperature[1]. Instead of using external heating, as with conventional cathodes [2], HHCs are heated via plasma heating. The plasma, which is generated inside the cathode cavity, exerts the required heat fluxes to heat up the electron emitter. When the electron emitter is sufficiently hot, the HHC may function as any other conventional hollow cathode, under steady state conditions.

The ignition process of HHCs can be divided into three phases[1][3]. In the first phase, gas breakdown is initiated inside the cathode cavity, and between two ignition electrodes – the emitter tube and the keeper. The purpose of this stage is to generate plasma to heat up the electron emitter, or alternatively, to create a burst of electrons able to reach the thruster and initiate the main discharge, a.k.a the anode discharge. In the second phase, the plasma discharge is sustained inside the cathode cavity. During this phase the emitter is heated up gradually until it obtains sufficiently high temperature to emit electrons. In the last stage the main anode discharge is initiated, and the cathode transitions to steady state operation.

Since HHCs do not use external heating for ignition they possess several advantages over heater-utilizing cathodes such as higher reliability, lower design complexity, reduced size and mass and energy-efficient operation.

Despite their advantages HHCs have some drawbacks that make their design challenging such as the requirement to start the cathode under high voltages (>300V), adequate thermal design to allow for efficient plasma heating during the first phases of ignition and the need to develop methods for outgassing the electron emitter before the initial use.

In this presentation we review the operation scheme of conventional hollow cathodes for space propulsion with an emphasis on heaterless hollow cathodes. We also present recent progress in the research and development of HHCs. The presentation will focus on the engineering aspects of HHC design and operation, as well as on the proved performance of these cathodes. We start by introducing the common HHC configurations used today. We then present recent findings regarding the plasma breakdown, heating transient and steady state phases of HHC ignition and operation. Subsequently, we address the destruction mechanisms reported in recent studies. Lastly, we identify some of the current challenges to be solved for further progress of HHC technology.

#### References

[1]. D. Lev and L. Appel. "Heaterless Hollow Cathode Technology - A Critical Review". The 5th Space Propulsion Conference (SPC), 2-6 May, 2016, Rome, Italy, SP2016\_3125366.

[2]. D.M. Goebel and I. Katz, Fundamentals of Electric Propulsion: Ion and Hall Thrusters, John Wiley & Sons, NJ, USA 2008.

[3]. Vekselman, V., et al. "Characterization of a Heaterless Hollow Cathode." Journal of Propulsion and Power, vol. 29, no. 2, 2013, pp. 475–486., doi:10.2514/1.b34628.

### 14:20-14:30 **Omri Hamo (Technion)** Contributed Speaker

#### Title:

# **Optical Emission Spectroscopy Measurements of the Narrow Channel Hall Thruster Plume**

#### Abstract:

A non-intrusive optical emission spectroscopy technique for studying Xenon plasma was used for studying a low power Hall effect thruster, known as the Narrow Channel Hall Thruster (NCHT). The relevant optical setup was assembled and calibrated. A Xenon collisional radiative model, crucial for extracting the plasma properties from the measurements, was implemented. Electron temperature measurements were obtained in the plume region of the NCHT. The preliminary results show similar qualitative behaviour to conventional measurements techniques and simulation results.

## 14:30-14:40 Amnon Fruchtman (H.I.T) Contributed Speaker

#### Title:

## Plasma-based mass separation by waves and space-charge fields

#### **Abstract**:

Standing or evanescent electromagnetic waves can accelerate charged particles by the ponderomotive force. The direction of acceleration is mass dependent, depending on whether the cyclotron frequency of the particle in the steady magnetic field is larger or smaller than the wave frequency. Schemes for mass separation can be proposed based on the different dynamics of particles of different mass. For a significant yield, the space-charge fields of the plasma have to be considered. A configuration for mass separation for industrial needs is considered, where one particle is resonant and other particles are pushed by space-charge electric fields.

# 14:40-14:50 Asher Yahalom (Ariel U.)

**Contributed Speaker** 

#### Title:

### A Three Function Variational Principle for Stationary Non-Barotropic Magnetohydrodynamics

#### **Abstract**:

Variational principles for magnetohydrodynamics were introduced by previous authors both in Lagrangian and Eulerian form. In this paper we introduce simpler Eulerian variational principles from which all the relevant equations of non-barotropic stationary magnetohydrodynamics can be derived for surface covering field topologies. This is thus a generalization of a similar variational principle for stationary barotropic magnetohydrodynamics which was previously introduced. The variational principle is given in terms of only three independent functions for stationary non-barotropic flows. This is a smaller number of variables than the eight variables which appear in the standard equations of non-barotropic magnetohydrodynamics which are the magnetic field B the velocity field v, the specific entropy s and the density  $\rho$ . The three functions are two surfaces  $\chi$  and  $\eta$  the intersection of which are the magnetic field lines. And an additional function which varies along the magnetic field lines the magnetohydrodynamic metage  $\mu$  (however, its surfaces are generally not orthogonal to the field lines). We further investigate the case in which the flow along magnetic lines is not ideal, and we transport phenomena along the temperature gradients.

# 14:50-15:00 Amir Weinberg (Ariel U.)

**Contributed Speaker** 

#### Title:

Dogleg design for an MeV Ultra-fast electron Diffraction beamline for the hybrid Photo-emitted RF GUN at Ariel University

#### Abstract:

A secondary parallel beamline is proposed for the construction of a Mega electron Volt Ultrafast electron Diffraction (Mev UED) facility, based on the novel hybrid 6 MeV RF-GUN in the Schlesinger center for compact accelerators in Ariel University. The Addition of a second beamline requires kicking the beam sideways and back, using a dogleg section. In order to change the trajectory of the beam, while preserving as much as possible the quality of the relativistic electron beam, requires a careful design and simulation process. Start-to-end comprehensive simulations of the dogleg design were performed using GPT (General Particle Tracer) software followed by analysis and optimization for the simulations in order to achieve optimal beam parameters in the second beamline. We present the results of the dogleg

# 15:00-15:20 Roundtable Discussion

Moderator: Igal Kronhaus Panel members: Aduardo Ahedo, Michael Keidar, Amnon Fruchtman, Dav Lev

# Space Plasma Propulsion

One of the most successful examples of industrial application of plasma technology is in space propulsion. More than one thousand plasma thrusters are currently in space aboard various spacecraft: from miniature satellites, no larger than a shoebox, to large multi-ton communication satellites, up to manned orbital stations. In this panel we will discuss current and near-future developments in plasma thruster science and technology. The panel will host top scientists in the field of electric propulsion.

# Posters

# Enhancing ammonia combustion with plasma-created species: plasma assisted reforming, ignition and flames

Galia Faingold<sup>1</sup> and Joseph K. Lefkowitz<sup>1</sup>

<sup>1</sup>Faculty of Aerospace Engineering, Technion I.I.T, Haifa, Israel

Mitigating the ongoing climate crisis requires a sharp reduction in greenhouse gas emissions. The search for alternatives to fossil fuel combustion, and the need to find scalable energy storage methods for renewable electrical generation, has driven the scientific community to search for alternative chemical energy carriers. The emerging consensus is that ammonia (NH<sub>3</sub>) will be the most scalable renewable fuel in the long term, as well as potentially being zero emissions. However, poor combustion qualities prevent NH<sub>3</sub> from being a replacement drop-in fuel in conventional combustion systems. Ammonia is resistant to both auto- and forced ignition, has a low flame speed, high NOx emissions and narrow flammability limits. Mixing ammonia with hydrogen (H<sub>2</sub>) can improve its performance as a fuel, and mixtures can be attained by partially dissociating NH<sub>3</sub> in situ. To match the qualities of conventional fuels, a high level of dissociation is required, which involve large levels energy input and complex systems.

Non-equilibrium plasma discharges can also be used to partially dissociate  $NH_3$ , and can create a variety of reactive species. A pulsed, non-equilibrium discharge in a cold mixture can create species that support and promote ignition and increase flame speed. While the operating conditions of non-equilibrium plasma are often not compatible within combustion chambers (high pressure, large volume), an alternative is to apply a discharge to the mixture before injection, providing long-lived plasma species into the combustion chamber.  $H_2$  and ozone ( $O_3$ ) are two such species, the latter being a strong oxidizer that accelerates ignition, enhances flame propagation and stabilization and modifies fuel characteristics.

This study combines a plasma model with an extended nitrogen dilution mechanism as well as a  $NH_3/H_2$  combustion model with an  $O_3$  sub-mechanism. The models are applied to explore the production of long-lived plasma reforming products, and the effect of different mixtures of  $H_2/O_3$  on the combustion qualities of  $NH_3$  under engine conditions. The production of species in a discharge is explored for mixtures of ammonia with air and for pure ammonia. With air present, the discharge yields very little  $H_2$ , but produces substantial amounts of  $O_3$ . For pure ammonia reforming, hydrogen yields improve under higher discharge energies. Under higher energies, there is an additional effect of mixture heating which further enhances conversion to hydrogen. For higher initial mixture temperatures, ammonia yields improve exponentially.

The addition of both  $H_2$  and  $O_3$  results in faster ignition and faster laminar flame velocities than would be achieved by either one of them separately. These results imply that reforming a mixture of air and ammonia can yield comparable results with less energy input than reforming either alone. The mixture conditions and degree of energy addition are discussed, as well the resultant effects on ignition timing and laminar flame speed.

# Zr Thin Film Deposition by a Hot Refractory Anode Vacuum Arc

## I.I. Beilis, D. Arbilly Y. Yankelevich and R.L. Boxman

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#### Abstract

Zr films were deposited using plasma generated in a Hot Refractory Anode Vacuum Arc. (HRAVA). The cathode and anode were fabricated from Zr and graphite respectively. The arc was sustained between a water cooled Zr cathode and a graphite anode. Both electrodes had 32 mm diameter and 30 mm length, with a gap of 10 mm between them. The radial distance from the arc axis to the substrate was 110 mm. The arc was operated for either 40 or 60 s before a glass substrate was exposed to the plasma for 15 s. The film thickness was measured by profilometry. The deposition rate was obtained using the film thickness and exposure time. The visual radiation emitted by the plasma plume was photographed with a digital camera.

The HRAVA started as a cathodic arc, which heated and deposited cathodic material on the anode. When the anode was sufficiently hot, all the deposited cathodic material was re-evaporated from it, and a steady state was established in which all cathodic material reaching the anode was evaporated from it. The arc emitted a radially expanding highly ionized plasma with significantly reduced macroparticle contamination. The rate of film deposition increased from 0.44 to 0.64  $\mu$ m/min and 0.47 to 0.71  $\mu$ m/min when the arc current was increased from 150 to 225 A for times before exposure of 40 and 60 s, respectively.

### On Energy Distribution in Nanosecond-Pulsed High-Frequency Discharge Ignition

#### Si Shen, Iker Laso Miqueo, Natali Rozin, Joseph Lefkowitz

Nanosecond-Pulsed High-Frequency Discharge (NPHFD) ignition has great potential as being a better alternative to conventional spark ignition. Previous studies present its ability to extend ignition limits (Xu, Lacoste, & Laux, 2016); to reduce ignition delay times (Pancheshnyi, Lacoste, Bourdon, & Laux, 2006) in combustion applications such as scramjet (Do, Cappelli, & Mungal, 2010; Lefkowitz & Ombrello, 2017b, 2017a); to generate a good level of electronic number density (Nagulapally et al., 2000) and fast flame kernel growth (Opacich et al., 2021) with less power; and to allow more accurate control over discharge duration and energy deposition for discharge optimization (Ballal & Lefebvre, 1975a, 1975b). Special to NPHFD, three inter-pulse coupling regime were observed: (1) fully-coupled regime – at short inter-pulse time (IPT), ignition probability (P<sub>1</sub>) is high, (2) partially-coupled regime – At intermediate IPT, P<sub>1</sub> drops to near zero possibly due to destructive interaction between flame kernels of each discharge pulse, (3) decoupled regime – at long IPT, P<sub>1</sub> becomes a function of the number of pulses and the single pulse discharge probability.

This study focuses on understanding the effect of energy distribution on  $P_I$ , global flame kernel growth and inter-pulse coupling for NPHFD in 4m/s CH4-air flow. For levels of energy per pulse ( $E_{pp}$ ) are studied for a wide range of IPT and different numbers of pulses (N). It is found that for low  $E_{pp}$  (1.5mJ), there is no successful ignition outside of the fully-coupled regime; while for high  $E_{pp}$  (6.7mJ) all cases ignite crossed the whole range of IPT. With intermediate  $E_{pp}$  (3mJ & 4.5mJ), all 3 inter-coupling regimes are observed, but higher  $E_{pp}$  results in a narrower partially-coupled regime. In addition, for a fixed total energy or total discharge duration of a NPHFD sequence, IPT appear to be the dominate factor affecting  $P_I$ , and inter-coupling regimes.

In the fully-coupled regime, the global flame kernel growth, measured using high-speed schlieren imaging and a costume built ellipse fitting code, is shown to be independent from  $E_{pp}$ , IPT and N, which is in line with previous study showing little variation in kernel growth for flow slower than 5m/s. However, in the decoupled regime, the kernel size and growth of an individual pulse is correlated with  $E_{pp}$ . High  $E_{pp}$  generates large initial flame kernel, which can increase destructive interactions between sequential kernels in the partially-coupled regime, and decrease P<sub>I</sub>. Therefore, low  $E_{pp}$  is more efficient in generate successful ignition. In conclusion, low  $E_{pp}$  with short IPT (fully-coupled regime) should be an optimal method for successful ignitions in a NPHFD system.

## Laser Wakefield Acceleration from Nebular-Shaped Plasmas

### Itamar Cohen (TAU)

Intense lasers made available for the first-time high-energy electron sources at university scale laboratories. For the past two decades, the community focused on optimizing the accelerated beam quality in terms of higher energy, sharper energy spectrum, and improved repeatability.

Early works observed ultra-collimated, multi-MeV beams of electrons, that were generated following multi-TW irradiation of thin solid foils pre-exploded by uncontrollable precursor light. In these experiments, the unprecedented conversion efficiency of laser light to electrons was hypothesized to relate to the nearly critical density of the plasma plume.

I will present a first controlled investigation of this method, conducted on the high-contrast 20 TW laser system at Tel-Aviv U. In these experiments, we pre-exploded thin foil targets with a controlled pre-pulse, nanoseconds prior to the interaction with the main beam. We tailored the pre-plasma plume profile by varying the pre-pulse energy, and the time delay between the pre- and main-pulses.

I will show preliminary results, along with an analytical model for the expansion of a sub-µm foil into a nebular-shaped plasma, and insights of the underlaying dynamics gained from particle-in-cell simulations. I will conclude with the prospects of scaling this method to PW-level lasers, and using the accelerated electrons for photo-nuclear reactions studies.

### Generation of supersonic water jets by underwater electrical explosion of wire arrays

<sup>1</sup>D. Maler, <sup>1</sup>S. Efimov, <sup>1</sup>A. Rososhek, <sup>2</sup>M. Kozlov, <sup>3</sup>S.N. Bland and <sup>1</sup>Ya. E. Krasik <sup>1</sup>Physics Department, Technion, Israel Institute of Technology, Haifa 32000, Israel <sup>2</sup>Nazarbayev University, Nur-Sultan 010000, Kazakhstan <sup>3</sup>Plasma Physics Group, Imperial College London,

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Studies of matter at extreme pressures and densities is the subject of High Energy Density Physics (HEDP) which is of great importance for basic physics, including physics of astrophysical objects and various applications. To conduct such studies in a laboratory environment, different systems with stored energy of  $>10^5$  J are used, namely Z-pinch, plasma focus, powerful pulsed laser system, multistage gas guns, high energy heavy ion beams and chemical explosives.

In our presentation we will describe and compare the results of supersonic water jets, generated by underwater electrical explosion of wire arrays. These explosions are realized using two pulse generators with different energy deposition rates. We will show that the underwater electrical explosion of a cylindrical or conical wire array is accompanied by the generation of extremely fast (up to  $\sim 4$  km/s) water jet and shock in air. In experiments, ns and  $\mu$ s time-scale pulse generators, with stored energy of up to  $\sim 6$  kJ, current amplitudes of up to  $\sim 400$  kA, and rise time of  $\sim 400$  ns and  $\sim 1000$  ns, respectively, were used for the underwater electrical explosion of a copper wire array. Streak and fast framing shadow imaging were applied to study time–space resolved velocity of the jet, ejected from the array and propagating in air. The jet generation occurs due to extremely high pressure and density of water formed in the vicinity of the axis by imploding shockwave. It was shown that the velocity of the jet ejected from the array side depends on the array geometry and the thickness of the water layer above the array. The results obtained showed that a major part of the energy deposited into the array is transferred to the kinetic energy of this jet and to the axial flow of water generated by relatively slow radial expansion of wires. This approach of generating supersonic water jets and strong shocks in air can be considered a promising method for HEDP research. Furthermore, by modifying the experimental configuration such as to collide two water jets, generated by opposing wire arrays explosion, the study of shocks interaction and high energy density jets can be performed, which is a subject of astrophysical intriguing phenomenon.

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# **Quantum Electron-Optics**

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We review recent research directions in "Quantum Electron Optics", an emerging area owing its parentage to the fields of electron optics and quantum optics. This field emerged in great part from the development of ultrafast femtosecond lasers and photocathode guns, that led to development of Dielectric Laser Accelerators (DLA) [1,2], and on the other hand of Photon-Induced Near Field Electron Microscopy (PINEM) [3,4]. It has been demonstrated that the shape of single Quantum Electron Wavepackets (QEWs) [5] can be controlled and also density modulated at optical frequencies [4]. Some of the more significant conceptual and technological developments in this field include transverse shaping of the electron wavefunction [6], attosecond electron bunches generation and control [4,5], the quantum klystron [7], laser phase-plate for transmission electron microscope [8], measurement of quantum state of light by electrons [8,9] and integrated photonic microscopy [16].

Our main contribution to the evolution of this research field is by modeling the electron in terms of a Quantum Electron Wavepacket (QEW) and solving a relativistic version of Schrodinger equation in interactions with light [11,12] and in interaction with bound electrons in matter<sup>5</sup>. In this model, the reality of the technically demonstrated spatio-temporal shaping of the quantum electron wavefunction is demonstrated both in interaction with light and with quantized matter. In these interactions, the fundamental principles of wave-particle duality are manifested in the two limits of near point-particle acceleration/deceleration regime of DLA and FEL (1), and of wave-like (or quantum recoil) PINEM regime (2). For the case of stimulated interaction with coherent light, these conditions are:

Wavepacket size bigger than light optical period (1)

Photon energy bigger than wavepacket energy spread (2)

where the wavepacket size is the "history-dependent" standard deviation temporal breadth of the QEW at the entrance to the interaction region, and the energy spread is the standard deviation of a Gaussian (Heisenberg uncertainty limited) quantum electron wavepacket. This distinction marks the classical to quantum transition from the point-particle operating schemes of FEL and DLA [1,2] to the quantum electron microscopy PINEM [4].

Similar physics is observed also in the interaction of finite size QEW with a Two-Level System (TLS). The conditions (1) (2) apply as well with the energy gap of the TLS replacing the photon energy in condition (2) and the period corresponding to the TLS transition frequency replacing the optical period in condition (1) [13,14].

We further examine the case when an ensemble of QEWs is density modulated by the same laser by a process of PINEM, followed by dispersive drift, and then interacting with light in the near field of a nanoscale structure (e.g. Smith-Purcell grating). In this case, the modulation-correlated electrons can interact coherently with light at harmonic frequencies of the modulating laser, and also emit spontaneous superradiant radiation proportional to N<sup>2</sup>. This emission is analogous to Dicke's superradiance [15] and to FEL superradiance by a bunched electron beam [16]. Similar N<sup>2</sup> scaling of transition probability of the TLS from ground to upper level is predicted in the FEBERI process when a harmonic (n) of the modulation correlated QEWs is resonant with the TLS transition [13]. This scaling is merely a reflection of the quadratic start of electron beam indued Rabi oscillation.

The limitations as well of the prospective future developments of these schemes will be presented in the context of the emerging new field of quantum-electron optics.

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# Consequence of Pb doping mediated surface morphology on conductivity of CdS thin films – A stereometric and fractal based study

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In this work, we have analyzed the dynamics of surface morphology and conductivity of pulsed laser deposited cadmium sulfide (CdS) thin films doped with varying lead (Pb) concentration. Stereometric and fractal analysis were carried out using image processing and power spectral density (PSD) study of obtained Atomic Force Microscopy (AFM) data. An influence on CdS surface roughness with doping is observed from height parameters. Further, stereometric analysis revealed an influence on the surface microtexture porosity, elastic deformation and dominance of lower spatial frequencies with Pb doping. Local slope validates the observed trend in roughness while the fragility and sensitivity of as-deposited film surfaces to external environment is probed using RMS slope. Interdependence between self-affinity of the CdS film surfaces and Pb concentration is revealed from Hurst coefficient while a semi-regular behavior is observed for the fractal dimension of the film surfaces. In addition, increase in topographic uniformity and non-linear behavior of surface percolation is attributed to surface entropy and succolarity values. Moreover, the trend in conductivity of CdS thin films due to Pb doping in the context of fractal parameters. This study presents the significance of fractal parameters for tuning the surface morphology and conductivity of Pb doped CdS thin films for practical applications.

Keywords: CdS; conductivity; fractal; Pb; roughness

### Charging Amorphous Solid Water Films by Ne+ Ions Characterized by Contact Potential Difference Measurements

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ASW is the most abundant form of water found in the universe. The study of amorphous solid water (ASW) films on metal substrates has been instrumental in understanding the structure and morphology of water-ices. Additionally, they have the potential to help researchers understand how complex molecules are formed in the interstellar medium (ISM), where dust grains are coated with ASW. The icy dust grains also contain small molecules such as CH<sub>3</sub>OH, CO, CO<sub>2</sub>, NH<sub>3</sub>, and CH<sub>3</sub> in varying (smaller) abundances with respect to water. These layers of water are subject to bombardment by charged particles and UV photons, which could lead to some interesting chemistry, including the formation of complex molecules. When ASW films on top of a metallic substrate are charged with ions or electrons, strong electric fields are generated within the films [1-4]. The photochemistry of molecules caged (frozen) in positively charged ASW films has not yet been explored and could lead to the discovery of new photochemical pathways and products.

This research focuses on the positive charging of ASW films grown on a single crystal ruthenium (0001) substrate under ultrahigh vacuum (UHV) conditions. Low energy neon ions (Ne<sup>+</sup>) are used to positively charge ASW films through a charge-transfer mechanism in which the impinging neon ion oxidizes a near-surface water molecule and scatters back to the vacuum as a neutral neon atom. The effects of the ASW layer thickness, ion beam energy, irradiation time, film growth temperature and irradiation temperature on the resulting film voltage, charge stability, and thermal binding energy were investigated. A Kelvin probe, which measures the contact potential difference (CPD) between the Kelvin probe electrode and the ASW film, is used to measure the film voltage that results from the charging process. Additionally, temperature-programmed- $\Delta$ CPD (TP- $\Delta$ CPD) experiments, measure the  $\Delta$ CPD of the surface as the temperature is gradually increased. Positive charging of ASW films by low energy Ne<sup>+</sup> ions leads to the formation of a stable nanocapacitor that follows parallel plate capacitor physics. The charges are trapped in under-coordinated water molecule defect sites and L-defect sites, whose distribution is dependent on the film growth temperature. The charge level, charge stability, and thermal binding energy of the charges to the ASW film are highly dependent on the film morphology (growth temperature) and Ne<sup>+</sup> ion bombardment temperature. Electric fields as strong as 2 x 10<sup>8</sup> V/m are generated within the ASW films.

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

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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<sup>...</sup>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.

# A protein-based free-standing proton-conducting transparent elastomer for large-scale sensing applications

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Human machine interfacing is a long challenge for researcher, in last few decades we have witnessed emerging of different materials and electrodes for the purpose. Successful interfacing of human body with machine involves coupling of ionic and electronic signal at the interface. In addition to the successful interfacing of the ionic and electronic signals, any conductive material for biological interfacing should be stretchable, flexible, stable in aqueous or humid environment, biocompatible and bio-degradable. Developing a single material having all these property is a challenge by itself. However, conductive polymers are one of the promising materials for this purpose due to their organic carbon-based nature. Over the years, many different types of conducting organic polymers have been emerged using different synthetic organic analogues, however, the development of a synthetic polymer which fits all the above-mentioned criteria is still consider a challenge for researchers. Inspired by natural electron and ion transfer processes mediated mainly by proteins, here we present a novel conductive polymer made out of 100% natural Bovine Serum Albumin (BSA) protein, which is a side product of bovine industry, cheap and available in large scale. The polymer film is free standing, transparent, stretchable, and highly stable in aqueous environment. Moreover, it is bio-compatible and biodegradable due to its biological nature, the synthesis method is within one pot and energy efficient process and there is no need of any post synthetic purification. This polymer film can efficiently record brain (electroencephalogram) and heart signal (electroencephalogram) from the human body in a non-invasive way with several other potential applications. While considering its novelty, our polymer can be considered a new class of materials in the field of bioelectronics.

Keywords: Biological Interfacing, Conductive Polymers, Polymer Film, electroencephalogram, electroencephalogram.

## Ar-annealing: Tailoring the Interface of Vertically Aligned Carbon Nanotubes for Enhancement of Nanocomposite Homogeneity

#### Lev Rovinsky (TAU)

Vertically-aligned carbon nanotube (VACNT) arrays are architectures which conserve the exceptional anisotropic properties of CNT and bypass the dispersion challenge of randomly aligned CNT. As a result, VACNT arrays have many potential applications, including field emitters for displays, biological sensors, energy storage devices and thermal interface materials. These applications sometimes require assembly of the VACNT arrays in a complimentary matrix. Due to their structure, CNT are inherently inert. Thus, surface treatments are required in order to enhance adhesion and property transfer between CNT and the matrix. In order to protect the VACNT architecture, the list of post-processing surface treatment methods narrows, as capillary forces make most wet methods detrimental to the alignment. Dry methods, such as gaseous, vapor and plasma methods are the most commonly applied. The high aspect ratio of VACNT architecture results in different accessibility to the surface treatment throughout the sample, manifested as process inhomogeneity. In the coating step, this inhomogeneity is a sharp transition in coating quality, occurring upon reaching a certain depth from the outermost surface of the sample.

In this work we test the feasibility of Ar-annealing as a possible method for tailoring the morphology of VACNT, which may result in enhancement of the accessible volume, and pave the way towards fabrication of homogeneous composite materials. Macro-morphological, micro-structural and chemical analyses will be presented, of samples annealed at different temperatures, between 430 and 500 °C, for different durations, between 30 and 90 minutes.

#### Synthesis of reduced graphene oxide using ascorbic acid for supercapacitor applications: A simple and

#### green approach

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**Abstract:** The present work reports a simple and green approach to produce reduced graphene oxide (rGO) nanomaterial from graphene oxide (GO) using ascorbic acid as a reduction agent. UV-Vis spectroscopy and Fourier transform infrared spectroscopy (FTIR) result endorsed the formation of high quality rGO nanomaterial. The electrochemical properties of the rGO were investigated for the supercapacitor applications. The cyclic voltammetry (CV) of the rGO of GO showed that in general, specific capacitance reduces with increasing scan rate within the range (10-100mV/s). It was observed that the synthesized rGO nanomaterial exhibits high specific capacitance ( $C_{sp, rGO} = 9.8$  F/g at 10 mV/s) as compared to GO ( $C_{sp, GO} = 5.6$  F/g at 10 mV/s). Thus, this uniquely synthesized rGO nanomaterial using ascorbic acid as a reduction agent, is a simple and green approach, which could be an ideal substitute for hydrazine in the reduction process of GO, and highly desirable for the development of high performance supercapacitors.

Keywords: Graphene oxide; Reduced graphene oxide; Ascorbic acid; Supercapacitors.

# Synthetic Route Towards Scalable Production in Pure Phase of WS<sub>2</sub> & MoS<sub>2</sub> Inorganic Nanotubes and their Unusual Properties

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Solid-gas reaction of tungsten oxide with  $H_2/H_2S$  gases applied for the synthesis of  $WS_2$  inorganic nanotubes (INTs) resulted in pure phases and scalable process. However, due to the instability of the intermediate products, similar reaction to obtain INTs of  $MoS_2$ , was found to be highly challenging, resulting in miserable yield, difficult control and poor reproducibility. Recent study succeeded to overcome these obstacles without the assistance of a catalyst and reported on sustainable highyield synthesis of  $MoS_2$  nanotubes 20-100nm in diameter and up to  $10\mu$ m in length [1]. Individual  $MoS_2$  nanotubes were characterized by TEM, EDS, selected area electron diffraction and Raman. INTs of  $MoS_2$  are both 40% lighter and 40% stronger compared to their  $WS_2$  analogous and hence more beneficial for tribological and composite applications. Being semiconductors, both  $MoS_2$  and  $WS_2$  nanotubes are good candidates for photovoltaics and optoelectronics.

INTs of WS<sub>2</sub>/MoS<sub>2</sub> demonstrate unique properties due to their nanosize, closed-cage arrangement of the layers into chiral tubes and mechanical strength: 1) The bulk photovoltaic effect (BPVE) was recently discovered in INT-WS<sub>2</sub> [2]. The photocurrent in the nanotube-based devices was orders of magnitude larger than in other BPVE materials. The BPVE does not require p–n junction of traditional PVE for generation of electric current, and occurs due to the intrinsic properties of INT-WS<sub>2</sub>: small band gap (1.4-2.1eV), broken inversion symmetry and polar structure. This progress is particularly important for environmentally benign energy harvesting whereas the efficiency of PVE has been almost reached the theoretical limit. 2) An exponential increase of the resistivity with tensile strain was demonstrated up to a recorded elongation of 16%, thereby making INT-WS<sub>2</sub> suitable for piezoresistive sensor applications [3]. 3) Low temperature CL of single-wall few nm diameter WS<sub>2</sub> nanotubes, produced by high-power plasma irradiation of multiwall INT-WS<sub>2</sub> nanotubes they were used for reinforcement of poly (methyl methacrylate) polymer towards antiballistic applications [5]. The addition of a small amount of WS<sub>2</sub> nanotubes (1.5 wt%) is shown to increase the energy absorption capacity (structure toughness) and impact resistance of such composites quite dramatically, which offers numerous applications in the defence, as well as, sport and automotive industries.

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# Asymmetric "misfit" nanotubes: Chemical affinity outwits the entropy at high-temperature solid-state reactions

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#### Abstract

Asymmetric two-dimensional structures and nanotubes have tremendous scope in material chemistry due to a lack of inversion symmetry and time-reversal symmetry. But the synthesis of these structures is fundamentally difficult due to the entropy-driven randomized distribution of chalcogens. Serendipitously, a family of misfit superstructures such as LaX-TaX<sub>2</sub> (where X= S/Se) were found to form asymmetric structures at high-temperature chemical vapor transport reaction. The Se exclusively bind to Ta atoms and La binds to S atoms, rather than the anticipated random distribution. With increasing Se concentration, the well-known (O-T) superstructure of LaS-TaX<sub>2</sub> gradually transforms into (O-T-T) superstructure (LaS-TaSe<sub>2</sub>-TaSe<sub>2</sub>). Beyond x<sub>Se</sub>>0.8, the MLC became unstable due to sulfur starvation and decomposed into binary compounds. These counterintuitive results shed new light on the chemical selectivity and stability of MLC. The lack of inversion symmetry in these asymmetric compounds and time-reversal symmetry in the chiral nanotubes offers intriguing physical observations and applications as thermoelectric nanomaterials.

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#### Cross-field optoelectronic modulation via inter-coupled ferroelectricity in 2D In2Se3

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#### Abstract -

Ferroelectricity in two-dimensional (2D) materials has been at the forefront of recent research owing to its potential application in low powered non-volatile phase change memory, energy harvesting, strain tuned electronics, artificial brain, neuromorphic sensors. Among the 2D materials exhibiting ferroelectricity in room temperature, α-In<sub>2</sub>Se<sub>3</sub> stands out owing to the presence of both in- (IP) and out-of-plane (OOP) dipole polarizations. In addition, the ability to modulate IP by switching OOP and vice versa owing to their intercoupled nature makes it a promising material for multimodal memory and optoelectronic applications. Herein, we experimentally demonstrate the cross-field modulation of opto- and electronic properties in α-In<sub>2</sub>Se<sub>3</sub> based field effect devices. Gate dependent surface potential measurements using Kelvin Probe Force Microscopy (KPFM) were extensively used in In<sub>2</sub>Se<sub>3</sub> based devices to directly reveal the bi-directional dipole modulation. Electric field calculations obtained from the surface potential studies also show hysteretic behavior of the dipoles following high gate voltage pulses. Also, to explore the consequence of the hysteretic change in the in-plane electrical field, photoresponse measurements following high gate pulses were performed exhibiting its functionality as a non-volatile memory switch. The multi-level photoresponse characteristics for different gate polarities in the fabricated photodetectors show a potential for their implementation and integration into non-volatile memory and electro-optical applications.

# Solvent-free, Smooth and Oriented Pb Halide Perovskite Films by CW Laser Deposition

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To develop a scalable, solvent-free production technology for Halide thin-film fabrication, we designed and got built a mini-Pulser Laser Deposition (PLD) system. By employing the mini-PLD system and a continuous laser, we developed a novel process to deposit methylammonium lead- iodide (MAPbI<sub>3</sub>) thin films at room temperature and at roughing vacuum levels. The deposition yields highly oriented films of MAPbI<sub>3</sub> thin films on a glass substrate and with (110) as preferred orientation. The thin films are relatively smooth with 3.1 nm rms roughness for ones deposited on a polished Si substrate. There have been reports of the pulsed laser-based deposition methods, but our finding that a *low power continuous* laser (orders of magnitude less than the equivalent power used in pulsed laser) adds to the distinctive behavior of Halide Perovskites. This opens a simpler, safer, and versatile solvent-free thin-film deposition process.

# Band gaps of crystalline solids from Wannier-localization-based optimal tuning of a screened range-separated hybrid functional

# Guy Ohad (WIS)

Accurate prediction of fundamental band gaps of crystalline solid-state systems entirely within density functional theory is a long-standing challenge. Here, we present a simple and inexpensive method that achieves this by means of nonempirical optimal tuning of the parameters of a screened range-separated hybrid functional. 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. The method is benchmarked against experiment for a set of systems ranging from narrow band-gap semiconductors to large band-gap insulators, spanning a range of fundamental band gaps from 0.2 to 14.2 electronvolts (eV), and is found to yield quantitative accuracy across the board, with a mean absolute error of  $\sim 0.1 \text{ eV}$  and a maximal error of  $\sim 0.2 \text{ eV}$ .

# CdTe-functionalized ZnO filled porous Si hybrid hierarchical nanostructured thin films for

# low-temperature operable highly-selective/sensitive NO2 sensors

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### Abstract

In this report, we present improved NO<sub>2</sub> gas sensing properties based on CdTe-functionalized ZnO filled porous Si (PSi) hybrid hierarchical nanostructured thin films (CdTe/ZnO@PSi). The CdTe and ZnO nanostructured thin films were grown on the PSi substrate by scalable magnetron sputtering technique. The PSi substrate was prepared using the electrochemical anodization method. The proposed CdTe/ZnO@PSi sensor was characterized in terms of structural, morphological, and compositional properties. The sensing performance and corresponding mechanism of NO<sub>2</sub> gas sensor based on CdTe/ZnO@PSi were described comprehensively. The CdTe/ZnO@PSi sensor displays enhanced NO<sub>2</sub> sensing (~3.5-fold greater sensor response ~19.82%, fast response/recovery time ~13 s/54 s) at the relatively low working temperature of 90 °C towards 1 ppm NO<sub>2</sub> gas in comparison to the pristine ZnO@PSi sensor (sensor response ~5.72% and response/recovery time ~41 s/124 s at an operating temperature of 150 °C).

Keywords: CdTe/ZnO heterostructure; Porous silicon; Nanostructured thin film; Sputtering; NO<sub>2</sub> sensor.

# Measuring the role of energetic ions at the substrate in Thin Film plasma processing

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#### Abstract

This work demonstrates the role of energetic ions in plasmas and how they affect the properties of materials deposited in thin-film plasma processing. The scope of this contribution is limited to discuss the ability to quantify the flux, energy of ions and ion-neutral fraction to optimize industrial plasma-assisted processes. For this purpose, ion energy and ion flux measurements were carried out using fully automated advanced Retarding Field Energy Analyzers (RFEA's) by Impedans Ltd [1, 2]. The *Semion Multi Sensor RFEA* measures the uniformity of ion energies hitting a surface, the uniformity of ion flux, negative ions, temperature, and bias voltage at any position inside a plasma chamber using an array of integrated sensors. On the other hand, the *Quantum RFEA* is an energy resolving gridded quartz crystal microbalance (QCM), used to measure the ion-neutral fraction hitting a surface inside a plasma reactor. This instrument also measures the deposition rate, ion energy, ion flux and bias voltage.

A review of thin-film applications, particularly focusing on plasma-assisted Atomic Layer Deposition (ALD) and Atomic Layer Etching (ALE) processes is presented in detail [3-5]. Some of the major contributions include discussion on the impact of substrate biasing on the ion energy distribution (IED), impact of ion impingement on the chemical and microstructural properties of thin-films, tailored voltage waveforms as a technique to control the ion bombardment energy as well as for precise ion energy control. Further reported are the excellent agreements between the simulated and experimentally observed IEDs at an rf-biased electrode in a helicon plasma system, which surely gains the confidence of thin-film industries in these plasma diagnostic tools [6].

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#### Electron paramagnetic resonance measurements of micro-crystals and subnanoliter liquids

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Electron spin resonance (ESR) spectroscopy of paramagnetic species in single crystals and liquids is a powerful tool for sample characterization. Unfortunately, conventional ESR systems have limited sensitivity and are optimized for millimeter-size solid samples and ~1 ml liquid volume. Therefore, conventional ESR cannot measure many interesting materials in single-crystal form such as enzymes and inorganic catalytic materials (e.g., zeolites), which only form micron-scale crystals (1-200 µm). Furthermore, conventional ESR is not compatible with microfluidics methods, which typically involve the use of liquids with small volume (microliters to picoliters).

Here, we present a unique family of miniature surface resonators optimized for micron-scale single crystals and picoliter liquid samples. The devices' resonant mode(s) were characterized by ESR micro-imaging and compared to the theoretical calculations. Moreover, experimental ESR spectra of single microcrystals with typical sizes of ~25-50 µm and subnanoliter liquid samples are presented. Additionally, we show that microfluidic ESR makes it possible to apply huge (~1000 T/m) and fast (~1 µs) pulsed magnetic field gradients to the sample. This is a key capability to measuring unique properties such as nanoscale real-space diffusion and quantum spin diffusion. Microfluidics experiments were performed at room temperature, making our technique compatible with future microfluidics applications that might employ a full system of compact resonators, microfluidic chips, miniature magnets, and a compact ESR-on-a-chip spectrometer. This could result in a completely new approach to processing and measuring paramagnetic liquid samples for use in a variety of chemical, biological, medical, and environmental applications.