TCESC

Technion Chemical Engineering Student Conference

Speakers list

International:

1. **Dr. Valeri Frumkin -** Massachusetts Institute of Technology.
2. Thomas Little – PhD student, Professor Juliane Nguyen, North Carolina at Chapel Hill.
3. Melissa bodine -PhD student, Professor Jeffry Ealm, Argonne National Laboratory and Professor Andrei Tomakoff, The university of Chicago.
4. Cornelia (Conny) Meissner- PhD student, Professor Alfred J. Crosby and Professor Todd S. Emrick, university of Massachusetts Amherst.
5. Neetu Rani- PhD student, Professor Nini Pryds, Technical University of Denmark.
6. Alexia Simon - PhD student, Professor Karin Oberg, Harvard University.
7. Matthew S. Johnson - PhD student, Professor Judit Zádor, Sandia National Laboratories.
8. Emily Hanhauser - PhD student, Professor Rohit N Karnik, Massachusetts Institute of Technology.

Israel:

1. Rinat Attias – PhD student, Professor Yoed Tsur, Technion.
2. Gal Avioz Cohen – PhD student, Professor Yoed Tsur, Technion and Professor Nini Pryds, Technical University of Denmark (DTU).
3. Gal Chen – PhD student, Professor Avi Schroeder, Technion.
4. Yuejun Yu - PhD student, Professor Yaron Paz, Technion.
5. Michal Levin - PhD student, Professor Noy Cohen, TecPhD studenthnion.
6. Noam Zyser - PhD student, Professor Vogt Charlotte, Technion.
7. Kfir Kaplan - Msc student, Professor Alon Grinberg Dana, Technion.
8. Sapir Willdorf-Cohen – PhD student, Professor Dario R. Dekel and Professor Charles E. Diesendruck, Technion.
9. Or Peleg Evron – PhD student, Professor Havazelet Bianco-Peled, Technion.
10. Yael Hershkovitz Pollak – PhD student, Professor Hossam Haick, Technion.
11. Yaniv Farkash – PhD student, Professor Gideon Grader, Technion.
12. David Attia – PhD student, Professor Rachel Yerushalmi-rosen, Ben Gurion University.
13. Roy Almog, PhD student, Professor Ronen Berkovich, Ben Gurion University.
14. Jonathan Prilusky, Msc student, Professor Lena Yadgarov, Ariel University.
15. Chen Benafsha, PhD student, Professor Joseph Kost, Ben Gurion University.
16. Yaniv Dror, PhD student, Professor Eran Edri, Ben Gurion University.
17. Leo Giloni, PhD student, Professor Oz Gazit, Technion.

Valeri Frumkin, Ph.D.

Massachusetts Institute of Technology

Applications of interfacial phenomena: from space telescopes to quantum simulations

In this talk I will present how interfacial phenomena in fluid mechanics can be applied to the development of innovative technologies across a wide range of scales and disciplines.

In the first part of this talk, I will present the Fluidic Shaping method, which relies on surface energy minimization under neutral buoyancy conditions to shape liquid bodies into optical topographies. This method has enabled rapid fabrication of a wide range of freeform optical components with sub-nanometric surface quality, and was recently used to demonstrate the first fabrication of lenses on board the International Space Station. I will also discuss how the inherent scale invariance of the Fluidic Shaping method, made it the underlying technology behind the Fluidic Telescope Experiment (FLUTE) at NASA – a project aimed at exploring the use of fluids for creation of large space telescopes.

In the second part of my talk, I will introduce the field of Hydrodynamic Quantum Analogs, where small droplets placed on the surface of a vibrating fluid bath may propel themselves through a resonant interaction with their own quasi-monochromatic wave field. These "walking droplets" were shown to exhibit many features previously thought to be limited to the microscopic quantum realm. I will present some of my contributions to this new and exciting field, and will discuss my long-term goal of developing a platform that would allow the implementation of quantum simulations based on pilot-wave hydrodynamics.

Short Bio

Valeri Frumkin is a post-doctoral associate at the Massachusetts Institute of Technology, where he conducts experimental and theoretical research on hydrodynamic quantum analogs. Valeri received his Ph.D. in applied mathematics from Technion, studying nonlinear dynamics of thin liquid films. He continued to a postdoctoral position at the Technion Faculty of Mechanical Engineering, where he focused on experimental research of interfacial phenomena and developed novel technologies with applications in optics and additive manufacturing. He is a recipient of the foundation for excellence in mathematics award, the Gemunder prize for space-defense related technologies, the SPIE Photonics West - 3D printing, Fabrication and Manufacturing Award, and of the Fulbright postdoctoral scholar fellowship.

Kfir Kaplan

Msc student at Dr. Alon Grinberg Dana lab, Technion

Automated rate calculator (ARC): A tool for automated ab-inito kinetics computations

A grand challenge facing the chemical kinetics science is automated generation of predictive kinetic models to affordably and feasibly predict the reactivity of chemical systems. Often, there are orders of magnitude more parameters required for a model than available from experimental data. At the same time, computational chemistry has advanced to the stage where it has a quantitative predictive capability for reaction rate coefficients, making it an indispensable tool for the development of reliable kinetic models. Our group is developing an open-source software tool to facilitate automated computations of species thermodynamic properties and of reaction rate coefficients. The Automated Rate Calculator (ARC) software automates electronic structure calculations (DFT and wavefunction) on high performance/throughput computational servers. ARC is capable of searching for the lowest energy 3D conformer of species, transition states of reactions, and performs geometry optimizations, frequency calculations, n-dimentional torsional scans, molecular orbitals and single-point energy calculations. ARC incorporates automated troubleshooting techniques and returns thermodynamic properties for species and high-pressure limit reaction rate coefficients. It supports a wide variety of electronic structure software (Gaussian, Q-Chem, Molpro, TeraChem, Orca, and more), major cluster scheduling software (Slurm, GSE, PBS, HTCondor) and several transition state search methods (Kinbot, autotst, xtb-gsm). ARC has many advanced features, yet at its core it is simple: It accepts 2D graph representations of chemical species (i.e., SMILES, InChI), and automatically executes, tracks, and processes relevant electronic structure calculation jobs on user-defined server(s). The principal outputs of ARC are thermodynamic properties (H, S, Cp) and high-pressure limit kinetic rate coefficients of species and reactions of interest.
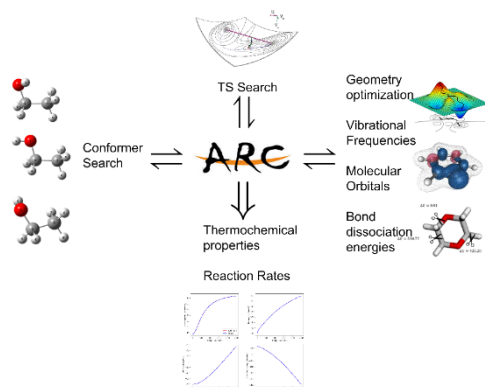
Michal Levin

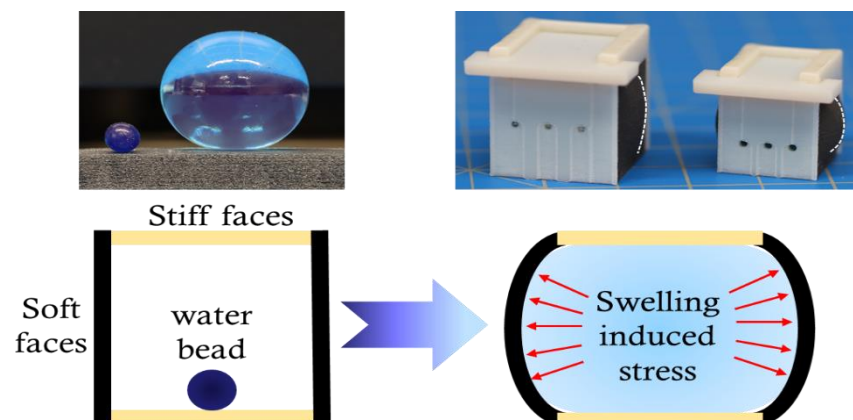**PhD student at Dr. Noy Cohen lab, Technion**

Measuring swelling induced stress of gels under constraints using 3D printing

Stimuli-responsive hydrogels that swell under mechanical constraints as geometrical confinements are widely used to perform work, in applications such as biomedical devices and actuators. During the swelling process hydrogels enlarge, thus applying stress on the environment to which they are bound. Estimation of the developed stress can be useful to optimize the performance of swelling-based systems. To the best of our knowledge, simple methods to measure the swelling-induces stress are lacking. Additionally, due to the complex and heterogeneous deformations that may arise from the constraints, it is hard and computationally expensive to compute the stress.

The aim of this talk is to present an experimental set-up to measure the swelling-induced stress exerted by gels using 3D printing. We designed and printed boxes that are composed of four rigid and two soft walls with varying stiffnesses and sizes. A water bead, superabsorbent hydrogel, is put in the box, and the whole system is immersed in water. The soft walls deform in response to the induced stress. After reaching equilibrium, the swollen configuration of the beads is characterized and investigated. Using the measured deformations and by employing elastic plate theory, we developed a systematic method to quantify the stress that the gel exerted on the soft walls due to swelling.

Our results reveal that the swollen configuration of a gel that swells under mechanical constraints depends on the type of geometric confinement and the stage of swelling. Our findings can be implemented to design, enhance, and even optimize the performance of swelling-based systems in various fields such as drug delivery, actuators, sensors, and soft robotics.

Gal Avioz Cohen

PhD student at Professor Yoed Tsur lab, Technion and

Professor Nini Pryds, DTU

Integration of gadolinia doped ceria as an electrolyte material for low temperature thin-film solid oxide fuel cells

As consumer electronics, such as mobile phones, laptops, tablets, and music players, become an inseparable part of our daily life, their functionalities and energy demand are constantly increasing. To support their performance and assure their autonomy, a power supply and storage system must be integrated within the device. To date, such power supply systems are almost exclusively based on batteries; however, the gap between the portable electronic devices' energy demand and the batteries' energy capacity is constantly increasing. A promising candidate for portable power supply and storage systems is the thin-film solid oxide fuel cell, also known as a micro solid oxide fuel cell.

To be adequately integrated as power supply and storage systems for portable electronic devices, thin-film solid oxide fuel cells must demonstrate high power supply and low-temperature operation capabilities. The key to these capabilities is the function of the electrolyte layer. Ceramic-based electrolytes require high operating temperatures to activate the ionic conductivity within them. The state-of-the-art material for thin film solid oxide fuel cells is the yttrium stabilized zirconia, a material easy to fabricate into dense thin films; however, it does not excel in ionic conductivity compared to other ceramic electrolytes. Another potential electrolyte material is the gadolinia doped ceria, demonstrating high ionic conductivity capabilities. Due to its relatively low activation energy for ionic conduction, its ionic conductivity does not reduce rapidly with decreasing temperature. However, this material has non-negligible electronic conductivity and, as a result, has not been extensively used as an electrolyte material for thin-film solid oxide fuel cells to date.

This research encompasses the integration of gadolinia doped ceria as an electrolyte material for free-standing thin-film solid oxide fuel cells. As a novel deposition technique for gadolinia doped ceria was recently developed, making its electronic conductivity potentially and significantly lower, this material could be used as a promising electrolyte for thin-film solid oxide fuel cells operating at relatively low temperatures.

Rinat Attias

PhD student at Professor Yoed Tsur lab, Technion
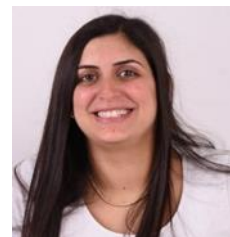
Evaluation of Electro-catalysts Reaction Kinetics for OER by Relaxation Phenomena Analysis

Electrochemical devices can split water into high pure oxygen (O2) and hydrogen (H2) gases by supplying electrical energy from renewable energy sources. The electrochemical water splitting device consists of an anode and a cathode, coated with an electro-catalyst filled with an acidic or alkaline electrolyte solution. In the anode, oxygen gas is evolved via an oxidation reaction, also known as OER. The barrier of the whole process is the OER because of the oxidation of four electrons, which makes the kinetics of the reaction sluggish. Many electro-catalysts have been developed to streamline the OER process. RuO2, which exhibits a superior activity, sets the benchmark for OER catalysts. To learn about the catalyst's behavior and examine where it has failed in its function, it is necessary to characterize it in the most comprehensive way. In this study, we use a very well-known parameter to characterize the reaction kinetics: the Tafel slope. We offer a supportive approach with Electrochemical Impedance Spectroscopy (EIS). EIS is commonly used to identify electrochemical phenomena occurring at the catalyst/electrolyte interface. Instead of using a routine analysis approach of equivalent circuit modelling, we run a MATLAB-based genetic programming software, ISGP, to provide an analytical form of the distribution function of relaxation times (DFRT). The DFRT model allows for separation and identification of three electrochemical phenomena from the EIS. The advantage is that it is straightforward to extract the effective resistance and capacitance of each electrochemical phenomenon involved from the DFRT. Here, through DFRTs, we understood that the improvements in catalytic activity and stability are due to the reduction of effective resistance contributed by various relaxation phenomena. These findings represent a new strategy to optimize catalysts for water Splitting.

Gal Chen

PhD student at Professor Avi Schroeder lab, Technion

Developing Artificial Cell Micro-Factories as Next-Generation Therapeutic Platforms

Recent advances in bottom-up synthetic biology have catalyzed the development of synthetic cells (SCs), autonomous protein-manufacturing particles, as potential biomimetics for replacing diseased natural cells and addressing medical needs. By leveraging the unique properties of cell nature, synthetic cell technologies aim to create well-defined, regulated, and advanced drug delivery systems. In this study, we demonstrate that SCs, genetically engineered to produce proangiogenic factors, induced the physiological process of neovascularization in mice. The SCs were created from giant lipid vesicles and were optimized for enhanced protein production. Upon introducing the appropriate genetic code, the SCs synthesized a recombinant human basic fibroblast growth factor (bFGF), with expression levels reaching up to $9 \cdot 10^6$ protein copies per SC. In cell culture, the SCs stimulated endothelial cell proliferation, migration, tube formation, and intracellular signaling related to angiogenesis, confirming their proangiogenic capabilities. When integrated with bioengineered constructs containing endothelial and mural cells, the SCs promoted the remodeling of stabilized vascular networks, supported by a collagen-IV basement-membrane-like matrix. In vivo, sustained local administration of the SCs in mice activated the infiltration of blood vessels into implanted Matrigel plugs with no detected systemic immunogenicity. These results underscore the potential of SCs as therapeutic platforms that autonomously produce biological drugs inside the body, stimulating physiological processes and treating medical conditions.

Neetu Rani

PhD student, Professor Nini Pryds, Technical University of Denmark (DTU)

Microscale mapping of thermal diffusivity in thermoelectric materials using a micro four-point probe

Thermoelectric materials can convert waste heat into electricity and are an attractive solution for powering Internet Of Things (IOT) devices. Fast and efficient characterization of state-of-the-art thermoelectric materials must be developed to boost their performance; however, comprehensive characterization of thermoelectric properties is a complex and time-consuming task. Here, we demonstrate a new and fast micro four-point probe (M4PP) technique for the direct characterization of a sample's thermal diffusivity, alongside its two other thermoelectric properties (electric resistivity and the Seebeck coefficient). The semiconductor industry routinely employs M4PP to perform electromagnetic characterization of materials (including magnetic tunnel junctions). In recent years, M4PP has been shown also capable of estimating various thermal properties, including the Seebeck coefficient, thermal diffusivity, and the temperature coefficient of resistance.

In contrast to past literature, where thermal diffusivity is usually understood as a spatial average of different grains, our study explores the impact of individual grains and their orientations on thermal diffusivity. We extract thermal diffusivity by passing an alternating current on the μm scale through a test area of the test material, and measuring the phase offset of the second harmonic voltage, arising from a delay in the thermoelectric signal. The methodology allows the construction of spatially resolved maps of thermal diffusivity, demonstrated here for two mainstream thermoelectric materials (Bi_2Te_3 and Sb_2Te_3). The M4PP measurements performed at room temperature were inverted into localized thermal diffusivities with respect to grain orientations; the latter were determined using electron backscattered diffraction (EBSD).

The μm-scale mapping of thermal diffusivity is arguably crucial for deeper understanding of thermal budgets of high-efficiency thermoelectric materials. The M4PP method proposed in this work provides rapid and accurate characterization of thermal diffusivity of such materials on the microscale.
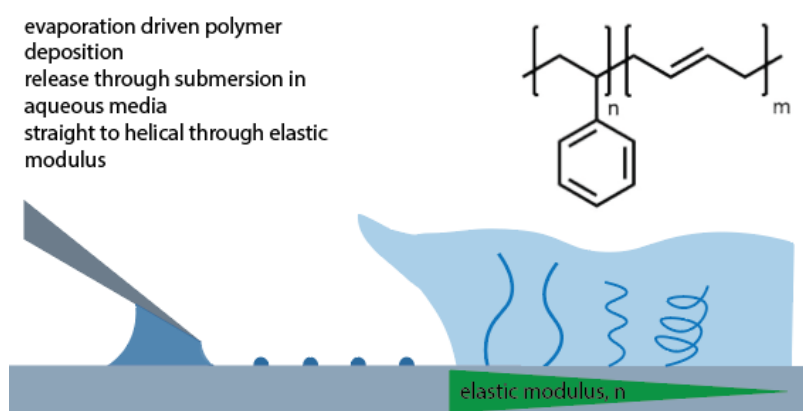

Thermal diffusivity area map of Bismuth Telluride
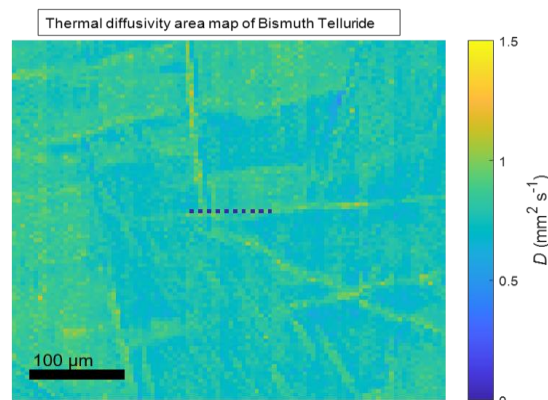
Cornelia Meissner

PhD student, Professor Alfred J. Crosby and Professor Todd S. Emrick, university of Massachusetts Amherst

Mesoscale Polymer Ribbons as Hierarchically Ordered Building Blocks

Active polymers are prevalent in biological systems spanning multiple length scales. Hierarchically ordered mesoscale building blocks are ubiquitous in nature such as tendons comprised of fibroblast bundles and cellulose nanofibrils bearing the load of trees. Ribbons fabricated via evaporative assembly combine nanoscale thickness with macroscale length, providing a unique opportunity to mimic mesoscale biological organization and dynamics. Many opportunities remain in the relatively under-developed field of biomimetics at the mesoscale, where elasticity, interfacial forces, and geometry all play important roles. Our work focuses on preparing highly adaptable mesoscale systems from industrially available block polymer. Polystyrene-block-polybutadiene (PS-b-PBd) ribbons can be fabricated with a majority glassy or rubbery component, tuning the elasticity of the mesoscale building blocks. The interplay of dewetting dynamics and mechanical stability of thin films allows for release of separate (distinct) mesoscale features into aqueous solutions. The preserved double bonds allow for facile photopatterning, enabling the introduction of site-specific mechanic properties. The hierarchical organization of mesoscale ribbons is anticipated to allow for synthetic polymers to achieve the strength, toughness, and resilience of biological materials.

evaporation driven polymer deposition
release through submersion in aqueous media
straight to helical through elastic modulus

elastic modulus, n

Sapir Willdorf Cohen

PhD student, Professor Dario R. Dekel and Professor

Charles E. Diesendruck, Technion

Ionomer Stability Studies for Anion-Exchange Membrane Fuel Cells

Anion-exchange membrane fuel cells (AEMFCs) have been attracting significant attention as a promising green and effective technology for energy conversion, suitable for both automotive and stationary applications. AEMFCs operate in an alkaline environment and thus allow the use of non-precious metal electrocatalysts from a wide selection of materials, as well as lower cost anion-exchange membranes (AEMs). In spite of the significant progress recently achieved, the commercial development of AEMFCs is hampered by AEM degradation process. The chemical decomposition of the AEMs during fuel cell operation is still considered as the main challenge that needs to be addressed. The combination of high pH environment and high current densities in the AEMFCs results in hydroxide anions with limited solvation, becoming extremely reactive towards positively charged quaternary ammonium (QA) salts.

In recent years, several new quaternary ammonium salts have been proposed to address this challenge, but while they perform well in ex-situ chemical studies, their performance is very limited in real fuel cell studies. Here, we use experimental work to show that water concentration in the environment of the hydroxide anion, as well as temperature, significantly impact its reactivity. We compare different quaternary ammonium salts that have been previously studied and test their stabilities in the presence of relatively low hydroxide concentration in the presence of different amounts of solvating water molecules, as well as different temperatures. Remarkably, with the right amount of water and at low enough temperatures, even quaternary ammonium salts, which are considered "unstable", present significantly improved lifetime.
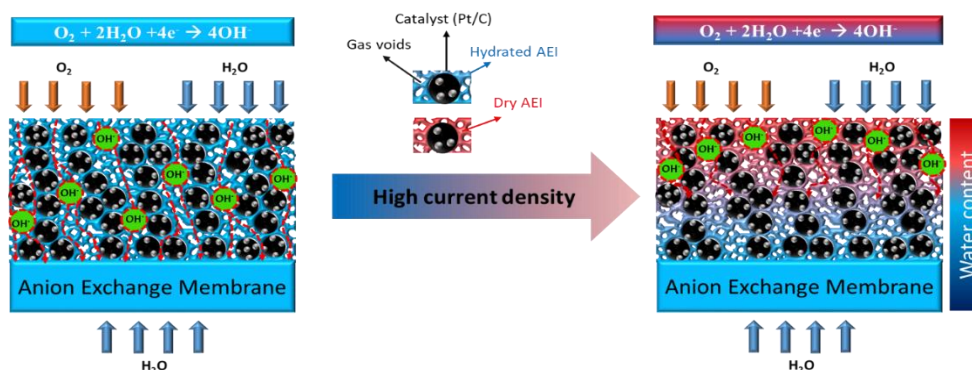
Noam Zyser

PhD student, Professor Vogt Charlotte, Technion

Linking Rational Activity and Stability Design in Catalytic Electrooxidation over Nickel

The rational design of catalyst stability, activity and selectivity is one of the major goals of catalysis research, and the description of surface energy lies at its heart. Approximations of surface energies in vacuum typically hold well for gas phase heterogeneous catalytic reactions, but at the electrified solid-liquid interfaces relevant to electrocatalysis current first principles descriptions are inaccurate. Here we use nickel oxyhydroxide (NiOOH) as a promising transition metal-based electrooxidation catalyst for several reactions deemed important in the energy transition such as the alkaline-based oxygen evolution reaction (OER), ammonia oxidation reaction (AOR), and the urea oxidation reaction (UOR) as a model system to extend the description of catalyst stability and activity from the localized atomistic, to bulk scale. Electrooxidation reactions over Ni generally occur spontaneously after NiOOH is formed by the electrooxidation of nickel hydroxide (Ni(OH)2), implying that the oxidation of the nickel catalyst itself is the rate-determining step. By systematically disentangling the effect of the numerous crystalline and amorphous phases of nickel, Ni(OH)2, and NiOOH from catalyst oxidation states, morphology, and structural disorders, a theoretical descriptor unifying these structural contributors is found, through mechanical concepts of elastic strain. By the application of several state-of-the-art characterization techniques, such as in-situ electrochemical quick-X-ray absorption spectroscopy (ec-QXAS) with sub-s time resolution, and electrochemical attenuated total reflection infrared spectroscopy (ec-ATR-IR) we demonstrate that the mechanical strain-descriptor theory allows us to describe and predict the stability and progress of reaction. We ultimately show that increased mechanical strain in the reversable Ni(OH)2 to NiOOH transition is negatively correlated to desirable lower onset potential and catalyst stability. We also show that shear, volumetric and longitudinal strain, which are quantifiable intrinsic parameters of the catalyst samples, influence the activity and stability through the same principle and affect the spectroscopically observed reaction mechanisms. The combined experimental and theoretical insights herein obtained into the effect of phase, transitional and inherent sample strain offer a novel approach to predict not only catalyst activity, but also its often-overlooked connection to stability.
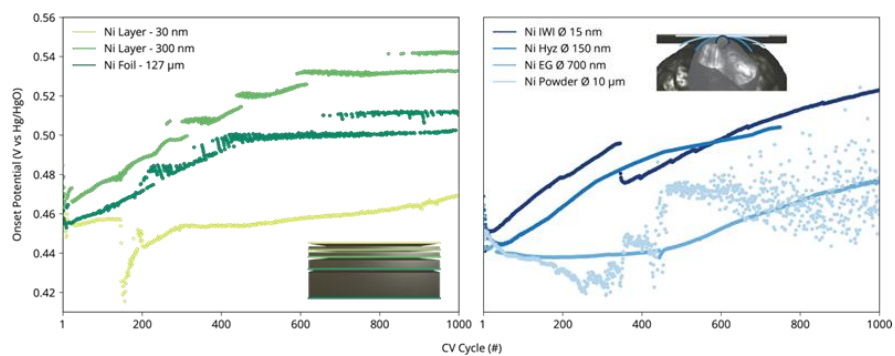
Figure 1. The influence of bulk-volume and surface curvature of Ni-based catalysts on the different activity descriptors controlling electrooxidation reactions in aqueous-alkaline conditions towards the strategic design of catalytic materials.

Timothy Little

PhD student, Professor Juliane Nguyen, North Carolina at Chapel Hill

Simultaneous dual epitope blocking CCR2 antibody to induce synergistic macrophage polarization

The CCR2 receptor and CCL2 chemokine are important regulators of macrophage recruitment during wound healing, inflammation, and infection, and their dysregulation is implicated in many diseases, including myocardial infarction, immunological diseases, and cancer. The CCR2-CCL2 axis has been shown to drive cancer metastasis by promoting invasion and migration through deleterious wound healing-like responses. Specifically, inflammatory monocytes are recruited to the tumor and polarized to a tumor-promoting M2 phenotype, also known as tumor-associated macrophages (TAM), via the CCR2/CCL2 axis in metastatic niches. TAMs are associated with poor clinical outcomes in various types of cancer. While many small molecule and antibody therapies targeting the CCR2/CCL2 signaling pathways have shown promise in clinical trials, none are FDA-approved yet. This may be due to the fact that most approaches target the N-terminal domain (NTD) of CCR2, while less is known about the function of the remaining extracellular loops as potential targets. To address this, we used phage display to identify antibody-derived single chain variable fragments (scFv) that specifically target the NTD, second extracellular epitope (ECL2), and third extracellular epitope (ECL3) of CCR2. We found that the NTD-scFv demonstrated higher inhibition of macrophage migration and induced higher M1-macrophage polarization compared to commercially available small molecule CCR2 inhibitors. Furthermore, simultaneous targeting and blocking of multiple CCR2 epitopes synergistically increased macrophage polarization to the M1 phenotype. We assessed macrophage polarization using various markers and found that the scFvs induced 6-9 fold higher polarization as shown by the iNOS/Arg1 and iNOS/Mgl2 ratios, and 20-30 fold higher polarization as shown by the IL-6/Arg1 and IL-6/Mgl2 ratios.

To further improve on our previous findings, we developed the second generation of CCR2 blocking agents. With recent advances in artificial intelligence technology, such as alpha fold, it has become increasingly easier to obtain high-quality three-dimensional structures of proteins and their targets. As a result, the molecular docking process has become more robust. We hypothesized that a bispecific antibody, which simultaneously blocks non-overlapping epitopes, could induce synergistic macrophage polarization. Before evaluating our new antibody construct in vitro, we modeled it in silico using alpha fold. This generated scFvs attached to a murine fragment, crystallizable region (Fc) domain via a flexible linker, and the murine CCR2 receptor. We used molecular docking software, such as Haddock, to determine the relative binding affinities of the NTD, ECL2, and ECL3 antibodies to their

respective epitopes (Kd = 48 nM, 0.85 nM, and 37 nM, respectively). The binding affinities from molecular docking were comparable to our in vitro ELISA data. We also introduced mutations in each Fc domain to ensure heterodimerization and confirm the bispecific antibody product, which we verified via western blot. Additionally, we determined if our bispecific antibody could inhibit CCL2 binding. We found that when one epitope was blocked by our antibody, CCL2's affinity towards CCR2 decreased by 1000-fold (0.21 nM to 430 nM) and up to 10,000-fold (0.21 nM to 2300 nM) when blocked by our bispecific antibody formulation. These studies demonstrate the benefits of molecular docking in accelerating drug discovery and provide insight into the effectiveness of simultaneous dual epitope blocking.
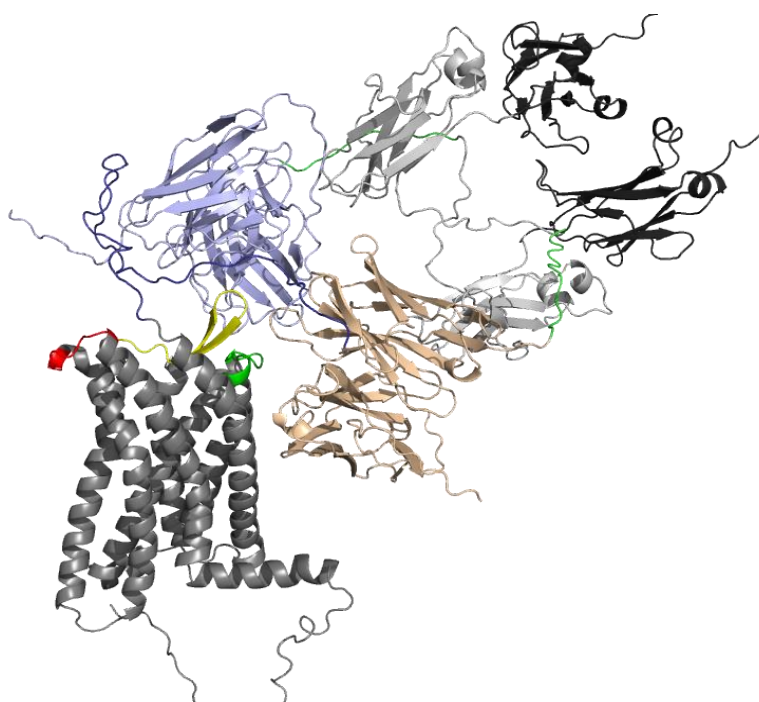
Or Peleg Evron

PhD student, Professor Havazelet Bianco-Peled, Technion

Crosslinking konjac-glucomannan with kappa-carrageenan nanogels: A step toward the design of sacrificial materials

Sacrificial materials are components used in a manufacturing process but are removed from the final product and do not remain part of it. The challenge in designing sacrificial hydrogels is to fabricate materials that are sufficiently crosslinked to be mechanically stable yet can be rapidly dissolved. My research aimed to meet this challenge by fabricating a new polymer-nanogel hydrogel based solely on hydrogen bonds between two polysaccharides. Notably, while many studies have explored hydrogel swelling behavior, only a few have focused on hydrogel dissolution. The study focused on hydrogels formed from soluble konjac-glucomannan and nanogels synthesized from kappa-carrageenan. This novel hydrogel exhibited self-healing and shear-thinning properties due to its weak physical interactions. The hydrogel dissolved simultaneously with its swelling. Changes in temperature or nanogel concentration, or the addition of potassium ions, altered the swelling and dissolution rates. The new formulation opens numerous possibilities as a potential sacrificial material for different applications since it is mechanically stable yet rapidly dissolves in physiological conditions without applying high temperatures or using chelating agents.
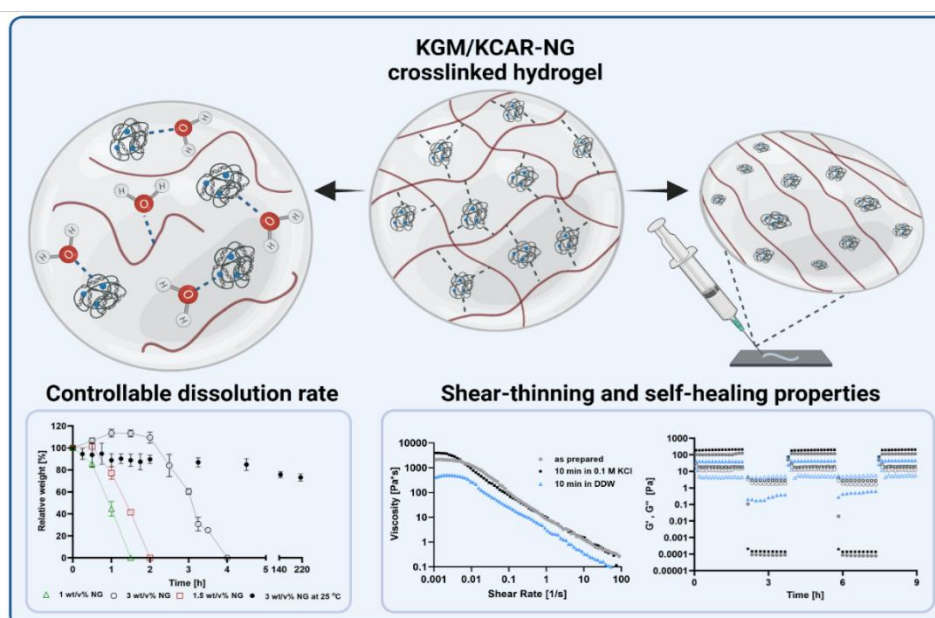
Melissa Bodine

PhD student, Professor Jeffry Ealm, Argonne National Laboratory and Professor Andrei Tomakoff, The university of Chicago

Development and Characterization of Electrodes with Atomic Layer Deposition for Two-Dimensional Infrared Spectroelectrochemistry

Despite the importance of electrochemistry in both the energy and chemical industries, very little is understood about the dynamics of water and electrolytes at electrode–electrolyte interfaces where there is an applied bias. While there is a significant amount of research using surface-enhanced IR and surface-enhanced Raman spectroscopy to investigate the electric double layer (EDL) of electrochemical interfaces, using ultra-fast IR spectroscopy to probe the dynamics of electrochemical interfaces introduces additional technical complications. Before two-dimesional IR (2D IR) spectroscopy can be used to experimentally investigate the structure and dynamics of the EDL, certain experimental challenges such as surface specificity, optimizing signal strength, and selecting materials that are both IR compatible and conductive must be overcome. Additionally, the interplay between the surface and solvent effects on the vibrational probes used in surface-specific IR spectroscopy is complex and to interpret these experiments we require a level of reproducibility between samples that cannot be achieved easily using methods such as vapor deposition or sputtering. By using atomic layer deposition (ALD) we have been able to create robust, reproducible, and 2D IR compatible electrodes. Here we will discuss the various considerations when designing 2D IR experiments of electrode interfaces and demonstrate a robust method for 2D IR experiments of electrode interfaces under applied potential that combines non-conducting Si ATR wafers with conductive ITO and thin nanostructured films of Au functionalized with 3-mercapto-2-butanone (MCB).
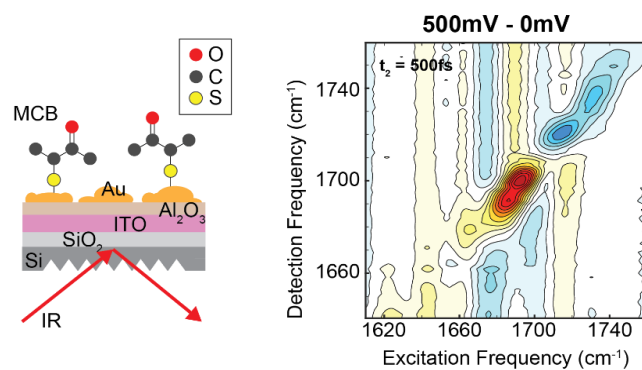
Figure 1. 2D IR difference spectra of the carbonyl stretch of 3-mercapto-2-butanone (MCB) shown for 500mV – 0mV applied potential. The cartoon depicts the electrode consisting of a commercial Si ATR wafer, ALD deposited ITO and Al2O3, and sputtered Au.

[1] Lotti, D.; Kraack, J. P., Surface-Sensitive Spectro-electrochemistry Using Ultrafast 2D ATR IR Spectroscopy. J. Phys. Chem. C 2016, 120, 2883-2892.

[2] Bhattacharyya, D. Et. Al. Sub-Nanometer Mapping of the Interfacial Electric Field Profile Using a Vibrational Stark Shift Ruler J. Am. Chem. Soc. 2022, 144, 14330−14338

Alexia Simon

PhD student, Professor Karin Oberg, Harvard University

Laboratory Investigation on Entrapment of Hyper-Volatiles in Interstellar and Cometary H2O and CO2 Ice Analogs: Importance on parameters dependence

Planets and planetesimals form from dust, ice and gas in so-called "protoplanetary disks", i.e. rotating circumstellar disc of dense gas and dust, around a young newly formed star. The resulting planet compositions depend on the abundance and distributions of volatiles (in gas and/or dust grains topped by icy grain mantles) compounds across the disk, which depend on the disk temperature profiles. From the radial temperature gradient in the disk, we expect more and more volatile species to freeze out further from the star, which will change the solid and gas compositions. Within the protoplanetary disk, ices at cooler temperatures (~10 to 200 Kelvin) are present as mixtures. If the ices are present as a mixture, entrapment of more volatile species in less volatile ice matrices will regulate the solid/gas composition within the disk. Entrapment mechanism will change the prediction of solid composition, since entrapment allows hypervolatiles to be present in solid form closer to the star, resulting in different radial profiles of common volatiles and elemental ratios than would otherwise be expected. Based on previous laboratory experiments, hyper-volatiles (CO, N2, CH4 and Ar) can become trapped in water ice. More recently, we showed that in addition to water, entrapment in CO2 ice may be important for the distribution of volatiles in disks. Indeed, CO2 traps CO volatile more efficiently than the analogous water ice. In this study we use laboratory experiments to extend and explore the ability of abundant interstellar and cometary ice matrices, H2O and CO2, to trap the hypervolatiles, CO, CH4, N2 and Ar, for a range of experimental conditions: ice thicknesses, mixture concentration and deposition temperatures. Entrapment efficiencies are experimentally measured through temperature programmed desorption (TPD) to determine the entrapment dependencies on the parameters. We find that ice entrapment efficiencies increase with ice thickness, up to a certain thickness, and ice mixing ratio to a maximum of ~65% for all hyper-volatiles.

Entrapment efficiencies are comparable for all hyper-volatiles, and for the two ice matrices. We further find that the entrapment efficiency is relatively insensitive to the ice deposition temperature between 10 and 30 K, suggesting that hyper-volatile entrapment at low (< 30 K) temperatures is a remarkably robust and species-independent process. We will present how hyper-volatile entrapment depends on the ice matrix properties, as well as the hyper-volatile properties itself, and the potential competition for multi-component vs. binary mixtures for which species can be trapped in a given volume of ice. The implications for the compositions of planet-forming solids in disks will be discussed.

Star

H₂O
snowline

CO₂
snowline

Hyper-volatiles snowline

Icy mantle:
H₂O, CO₂

Hyper-volatiles:
CO, CH₄, N₂, Ar

grain

CENTER FOR ASTROPHYSICS
HARVARD & SMITHSONIAN
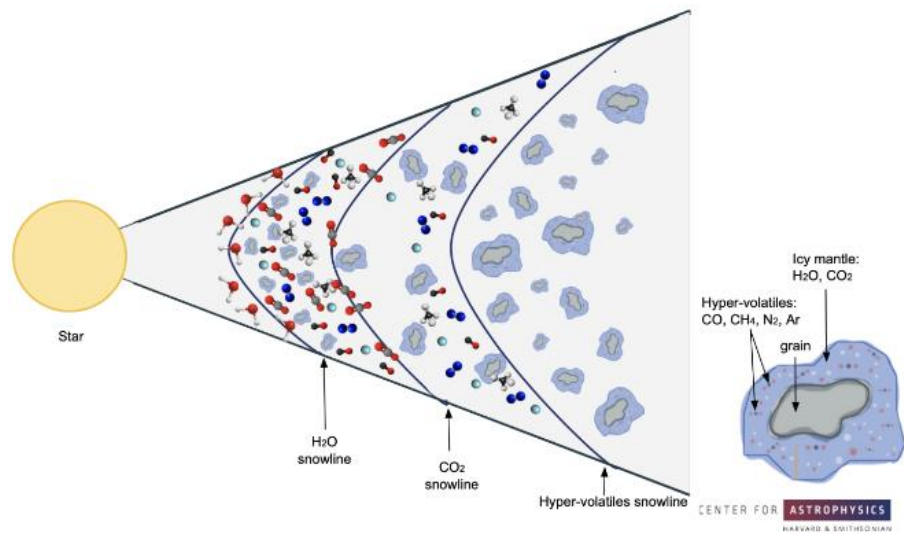
Yael Hershkovitz Pollak

PhD student, Professor Hossam Haick, Technion

Volatile Markers as Intercellular Communication Agents of Apoptosis

Communication between cells and metabolism within the cells are essentials to activate and regulate apoptosis, a process essential for the maintenance of human health. Traditional proteomic and genomic approaches are insufficient to understand intercellular communication in its entirety, as they may not be sensitive enough to
detect low levels of molecules, are expensive, complex, and may not reflect the reality of the whole body. Furthermore, they do not supply complete information on all the molecules used for communication. For this reason, it is necessary to develop another method to detect intercellular communication, one which does not include isolation or the exploration of genes and proteins. In this research, we study the possibility of volatile organic compounds (VOCs) acting as communication molecules for apoptosis. We conducted experiments in the BEAS-2B cell line using fluorescence microscopy and gas chromatography-mass spectrometry (GC-MS) and carried out cross-talk experiments between monocultures, co-cultures of the same cells, and co-cultures of different cells, and obtained different patterns of VOCs. Discovering specific VOC patterns involved in intercellular communication could add new biomarkers of biological pathways based on VOCs, aiding us to understand the biochemical processes
behind apoptosis and the interplay with cancer cells. Moreover, VOC-based intercellular communication offers the advantage of allowing communication over long distances, both between cells inside and outside the body.

Yuejun Yu

PhD student, Professor Yaron Paz, Technion

Developing and study of an automatic on-line micro-biotoxicity sensing and control unit for wastewater treatment, based on a cell viability monitoring assay

Wastewater streams contain quite often a large number of contaminants, part of which can be quite toxic for the working bacteria in bioreactors, thus might hamper the efficiency of the bioreactors. In such cases, pretreatment by an Advanced Oxidation Process (AOP) might be needed. Since, in general, biotreatment is more economic than AOP, it is sensible to design the integrated system in a manner that would reduce the load on the AOP as much as possible. This could be a very difficult task, especially when the total concentration of the toxic compounds varies over time. The problem is aggravated by lack of inexpensive and fast technologies that are able to evaluate the toxicity under conditions in which the nature of the toxic compounds is unknown.

Here we report on the developing of a unit that automatically measures the extent by which polluted water might put at risk a biological treatment unit. The sensing unit is based on PrestoBlue, a cell viability monitoring assay, and Bacillus Subtilis as reporting bacteria. The toxic compounds were modelled by three antibiotics (chloramphenicol, tetracycline and ciprofloxacin). The potential of embedding the sensing unit in a multi-technology system (AOP-biological) was demonstrated by connecting the sensing unit to a photocatalytic reactor and controlling the number of operating lamps in the photocatalytic reactor autonomously according to predesigned toxicity setpoint under both feedforward and feedback modes of control.

Two controlled water-treatment systems discussed above was constructed and connected to the wastewater outlet of Yoseftal Medical Center, Eilat and a wastewater treatment plant in Almedralejo, Spain. Experiments were made to verify the reliability of the sensing system.

Jonathan Prilusky

Msc student, Professor Lena Yadgarov, Ariel university

Enhanced photocatalytic activity of Cs4PbBr6/WS2 hybrid nanocomposite

Photocatalytic processes are among the prime means for mitigating the pollution caused by toxic effluents. In this context, photocatalysis presents a promising path and undergoing rapid evolution. Halide perovskites (HPs) are excellent candidates due to their negative conduction band minimum and low work function, which are essential for photocatalysis. Interestingly, HPs performance significantly improves by introducing transitional-metal dichalcogenides as a co-catalyst, which enables suppressed charge recombination. Here we investigate the photocatalytic performance of Cs4PbBr6/WS2 nanocomposites towards organic dye degradation under visible light illumination. We found that the nanocomposite with WS2 nanoparticles and nanotubes significantly increases the degradation rate compared to pristine Cs4PbBr6 nanocrystals. The transient absorption measurements reveal charge transfer from Cs4PbBr6 to WS2. Our study's results imply that the nanocomposites' boosted photocatalytic performance is due to the reduced carrier recombination. Our findings pave the way for implementing Cs4PbBr6/WS2 nanocomposites as superior photocatalysts.
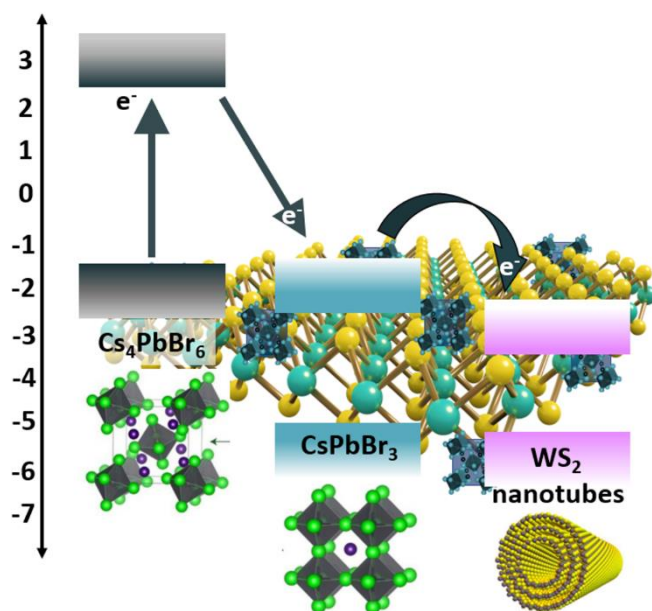
Matthew S. Johnson

PhD student, Professor Judit Zádor, Sandia National Laboratories

Pynta: A software for automatic calculation of microkinetic rate coefficients on metallic surfaces

Many important industrial processes rely on heterogeneous catalytic systems. However, these systems can be incredibly time consuming and expensive to optimize experimentally. Microkinetic models can be used to efficiently optimize reaction conditions, however, they require estimates of many thermochemical and kinetic parameters. Manually calculating these parameters using ab initio methods can be incredibly tedious and error-prone involving many interdependent calculations. In particular, generating saddle points (SP) guesses that reliably converge to transition states that both lead to the target reactants and products and are low in energy is nontrivial. We present Pynta (https://github.com/zadorlab/pynta), a software for automating the calculation of thermochemistry and rate coefficients for reactions on surfaces. Pynta can handle monodentate, bidentate and gas phase species on a given facet of a crystal lattice reacting through arbitrary reaction classes. Given 2D graph structures for the atom-mapped reactants and products it automatically identifies and evaluates all unique adsorption site configurations for adsorbates and SPs. We generate SP guesses using a new technique we term harmonically forced SP searching (HFSP). HFSP defines harmonic potentials based on the individual interaction characteristics along all bonds that break/form in the reaction. Raw initial guess structures are then optimized combining these harmonic potentials with the GFN1-xTB semi-empirical method to obtain SP guesses. We then filter this set of SP guesses based on the harmonic potential's contribution to the total energy to obtain a tractable set of low-energy SP guesses. Optimized SPs are confirmed using intrinsic reaction coordinate calculations. The results of reactant, product, and SP calculations can then be used to compute thermochemical and kinetic properties for the reactions.
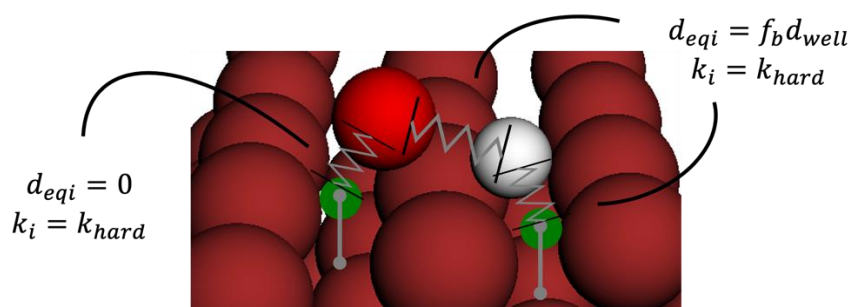
$$d_{eqi} = f_b d_{well}$$
$$k_i = k_{hard}$$

$$d_{eqi} = 0$$
$$k_i = k_{hard}$$

Emily Hanhauser

PhD student, Professor Rohit N Karnik, Massachusetts Institute of Technology

Creating Monitoring Paradigms and Sensors for Decentralized Settings: From Water Quality Monitoring to Clinical Diagnostics

Decentralized settings, those that have minimal infrastructure due to distance and/or resources such as rural towns, ad-hoc testing sites, and unpiped water sources, have unique needs in sensing applications, which are distinct from centralized settings. These requirements can make analytical processes suitable for well-resourced hubs practically useless in decentralized settings. Centralized processes can require multiple steps and specialized instrumentation requiring skillsets which can be a challenge to find in decentralized labor pools. Especially when coupled with poor infrastructure, physical distance can make timely transport of samples, replacement parts or reagents difficult. Because of this mismatch between standard analytical processes and the reality of operating in decentralized settings, monitoring water quality, food safety and human and animal health often suffers, contributing to poorer health outcomes, environmental pollution and a lack of actionable data. The challenge facing engineers is to design systems that deliver similar performance as gold standard techniques but at a cost and ease-of-use profile that suits the needs of decentralized settings. Towards this goal, this talk will present technologies developed for two applications, monitoring water quality and healthcare diagnostics.

Trace and emerging water contaminants are a class of chemical compounds that exist and cause harm at very low (parts per billion [ppb] or lower) levels. Aside from the challenge of the number of contaminants in this class, current methods are ill-suited for the needs of distributed monitoring that can detect trace contaminants, understand contamination events, and respond to these events in real-time. Field test kits have limitations for trace contaminants, and long-distance transport of large-volume water samples to centralized labs for analysis using high-throughput spectroscopic methods is difficult. Towards filling this gap, we created solid phase extraction, preservation, storage, transport and analysis of trace contaminants (SEPSTAT1), an alternate paradigm that facilitates water quality analysis via dry preservation. I will discuss insights from fieldwork that led to the inception of this framework and the development of a supporting technology for heavy metals, which can stably preserve heavy metal ions for up to two years and permit quantification at or below the maximum acceptable contaminant concentration.

Sandwich assays are the current gold standard in point-of-care (POC) healthcare diagnostics for protein analytes. The ASSURED criteria from the WHO2 sets goals for these devices, but current sandwich assays do not meet all of these targets. Despite progress towards this POC ideal, microfluidic assays face barriers to translation in part due to the instrumentation required for assay operation, often including bulky fluidic pumping. To overcome these challenges, we created an integrated platform that combines analyte capture by bead settling and non-fluidic manipulation in a single device that can determine analyte concentration at pico- to femtomolar sensitivity in less than 30 minutes. I will discuss the considerations that led to the conception of this platform and the specific demonstration of our device in the quantification of cardiac troponin I at clinically relevant levels, suggesting its utility as a diagnostic for resource-constrained settings.
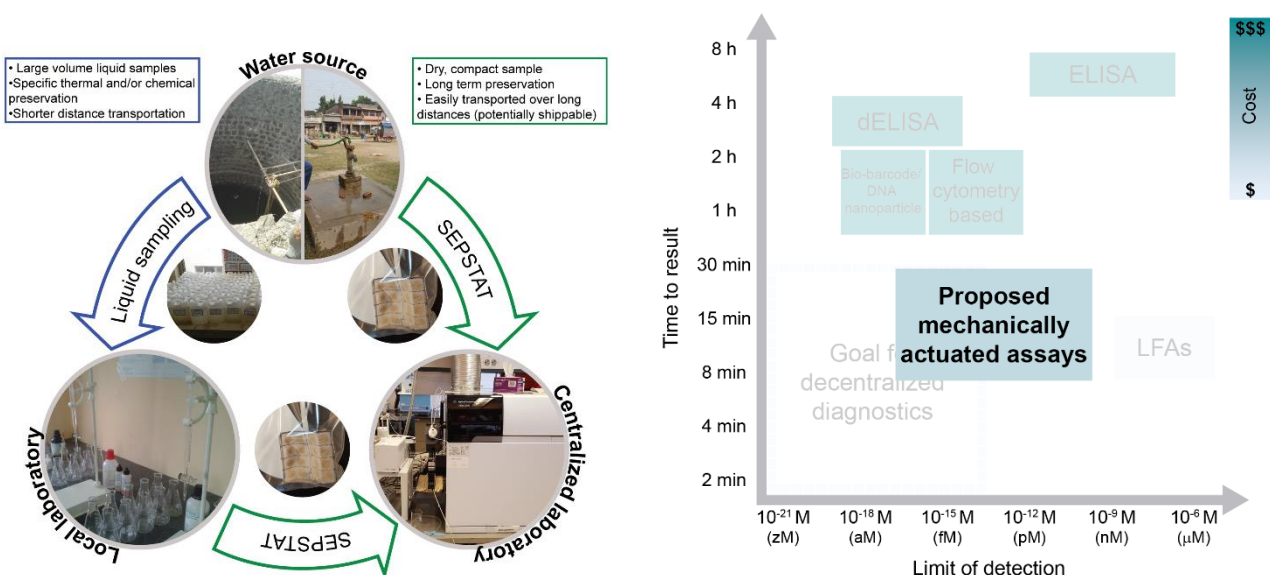
Figure 1. Systems and sensors for monitoring water quality (left) and healthcare diagnostics (right).

Chen Benafsha

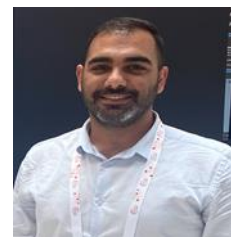**PhD student, Professor Joseph Kost, Ben Gurion University**

Enhancing HNSCC therapeutic efficiency by overcoming cetuximab resistance using modified Q-Starch/siRNA particles decorated with cetuximab as a targeting agent

Head and neck squamous cell carcinoma (HNSCC) is the sixth most common type of cancer worldwide and is usually characterized by the overexpression of epidermal growth factor receptor (EGFR). HNSCC management utilizes surgery (limited by the tumor's anatomical scope), radiation, and chemotherapy agents. One chemotherapeutic drug is cetuximab, an FDA-approved EGFR inhibitor that inhibits cell proliferation and enhances apoptosis. One of the main issues related to this treatment is that along the treatment course, patients develop resistance since the cancer cells become tolerant to the antibody and retain uncontrolled proliferation.

Currently investigated high potential approach to treat cancer is using RNA interference (RNAi) mechanism as a therapeutic tool for downregulating proteins involved with cancer cascade. Since the delivery of RNAi to cancerous cells is challenging due to several intra and extra-cellular barriers during the RNA pathway, considerable effort is invested in enabling its potential. The most common approach is to encapsulate the siRNA molecules into nano-sized particles with physicochemical properties that will allow the delivery and release of RNAi in the cell cytoplasm.

Our study aim is to exploit the RNAi process using modified polysaccharide carriers, based on chemically modified starch. The starch is able to form complexes with siRNA, which are used as a non-invasive, non-viral delivery system to downregulate specific oncogenes present in cancers. Our starch carrier is also conjugated to cetuximab antibodies which provide targeted delivery capabilities, cancer specificity and selectivity, thus increasing the efficacy of systemic administration.
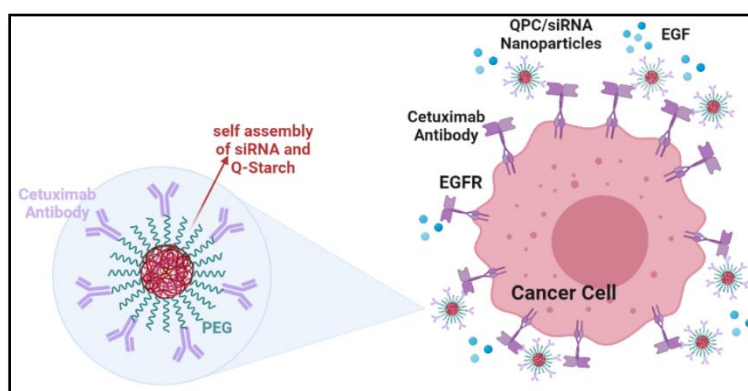
David Attia

PhD student, Professor Rachel Yerushalmi-Rozen, Ben Gurion University

Chiral Interactions and Assembly of Cellulose Nanocrystals Mesophases

Cellulose Nanocrystals (CNCs) are charged chiral rod-like nanoparticles that form electrostatically stabilized suspensions in aqueous media. CNCs suspensions undergo liquid-liquid crystalline phase separation into optically isotropic phase and cholesteric phase (chiral nematic, N*), upon increasing concentration. The effect of various parameters on the self-assembly and phase behavior of CNCs has been extensively investigated. However, the mechanisms of chirality transfer from the individual rod to the mesophase are not yet resolved. Herein, we report experiments indicating that the self-assembly and phase behavior of CNCs in aqueous media show chiral selectivity: using D- and L-Alanine (or D- and L-Leucine) as additives, we find that while L-Alanine does not affect the formation and characteristics of the cholesteric CNCs, D-Alanine (and D-Leucine) reduce the Pitch of the cholesteric phase (the length in which the director fulfills a full helical rotation) and the volume fraction of the N* phase as compared to Alanine-free suspensions. Small-Angle X-ray Scattering (SAXS) measurements reveal that D-Alanine promotes the assembly of the individual CNCs rods into small nematic islands. Isothermal Titration Calorimetry (ITC) measurements show preferential adsorption of D-Alanine (as compared to L-Alanine) onto CNCs rods. The insights gained from the observations will be discussed in the context of the molecular origins of the effect and the mesoscopic level.
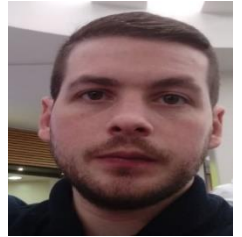
Roy Almog

PhD student, Professor Ronen Berkovich, Ben Gurion University

The effect of accelerated flow on the resuspension of small particles

Resuspension of deposited particles is a complex phenomenon that is incited when the sheer flow over a surface overcomes the adhesion force that attaches particles to this surface. Although this phenomenon has been extensively studied, some aspects of it are not fully understood. In particular, the information on the resuspension of particles with diameter smaller than 10 microns is rather scarce. The sporadic information is problematic since particles of these diameters are associated with increased health risks due to their high potential to penetrate the respiratory track. In order to study the resuspension of such particles in a controlled scenario, i.e., sparse distribution of particles over a clean and inert surface, high fluid velocities are required. In addition, the literature usually deals with fully developed flow conditions, where hardly any attention is given to the effect the fluid flow acceleration. Here we studied the resuspension of 9.0 microns in diameter silica glass particles, under three different accelerations: 0.3, 0.7, and 4.0 m/s^2. The spherical colloids were deposited onto a smooth glass slide and were exposed to increasing air velocities inside a specially designed wind duct with a cross section of 3.0 X 3.0 cm^2. After each acceleration cycle, when reaching final maximum fluid velocity of 85 m/s, it was consistently maintained for a relatively long time in order to evaluate the maximal possible resuspension under the applied conditions. The experiments showed that the highest levels of resuspension occurred during the lowest acceleration. While this is in accord with the literature, a noticeable difference was observed between an acceleration of 0.3 and 0.75 m/s^2, compared to the less pronounced difference between 0.7 and 4.0 m/s^2.
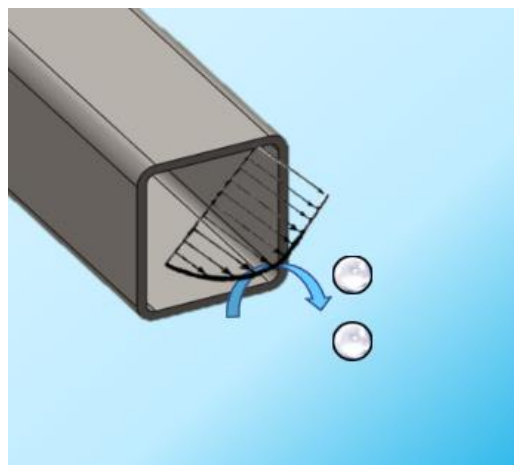
Yaniv Dror

PhD student, Professor Eran Edri, Ben Gurion University

Close-spaced sublimation of $(Bi_xSb_{1-x})2Se_3$ thin films for short-wavelength infrared photovoltaics

The effects of global warming and rising energy demand highlight the need to reduce fossil fuel usage and greenhouse gas emission. Photovoltaic (PV) technology offers a clean, sustainable, and cost-effective solution by directly converting solar energy into electrical power. Today, silicon(Si)- based single-junction solar cells are the most common commercially sold devices. Yet, their efficiency is limited due to carrier thermalization and loss of transmitted photons. Multi-junction solar cells can overcome this barrier and utilize a more significant portion of the solar spectrum for electrical power generation. Currently, tandem solar cells are too expensive for large-scale implementation. But recent progress in halide perovskite (HaPs)-Si tandems makes low-cost tandems commercially feasible. The next largely untapped portion of the solar spectrum is the short-wavelength IR region (0.7–0.95 eV; SWIR). However, suitable absorbers are looked-for. Antimony triselenide (Sb2Se3) is an earth-abundant and low-toxicity emerging PV absorber material. Sb2Se3 has a high absorption coefficient ($a>105$ cm-1), decent charge carrier mobilities (15 and 42 cm-1 ·V -1 ·s -1 for electrons and holes respectively), and an energy band gap of ~1.17 eV. Upon Bi-alloying, the band gap of Sb2Se3 is expected to decrease, and if a mixture rule is assumed, a band gap of ~0.7 eV is expected at (Bi0.48 Sb0.52)2Se3. Moreover, Sb_2Se_3 is potentially more defect-tolerant than conventional semiconductors due to its main group chemistry and unique crystal structure. In this presentation, I will present the fabrication of (BixSb1-x)2Se3 thin film using a simple and cost-effective close-space sublimation (CSS) method, producing continuous and phase pure thin films with various Bi concentrations, reaching up to 55 at% of Bi in Sb_2Se_3 [Bi/(Bi + Sb) = 0.55] and an optical band gap of 0.91 eV. A comprehensive characterization and optimization of the films' composition and microstructure was conducted. The $(B_{ix}Sb_{1-x})2Se_3$ thin films were incorporated into both superstrate and substrate PV device structuresto evaluate their applicability, as well as identify and address the limiting factors and mechanisms that restrict the device performance. For thin films with Bi-content of x>0.10, the best performing solar cell for film composition of (x=0.22) in a Mo/(BixSb1-x)2Se3/CdS/ZnO/AZO/Al device structure, exhibited a power conversion efficiency (PCE) of 0.10% with an open-circuit voltage (Voc) of 173 mV and short-circuit current density (Jsc) of 2.13 mA/cm2 . This study enables future development of SWIR-PV using $(Bi_xSb_{1-x})2Se_3$ thin films and using CSS to deposit thin film semiconductors with a controlled and variable composition.

(Bi,Sb$_{1-x}$)$_2$Se$_3$ film
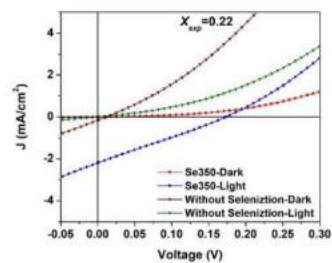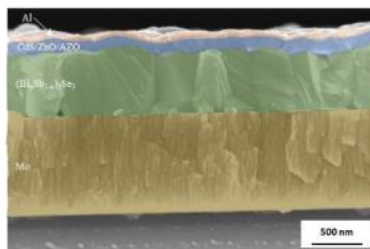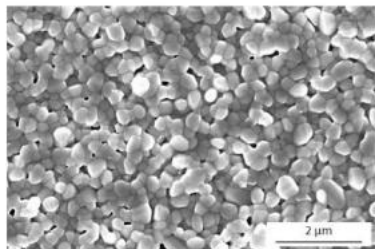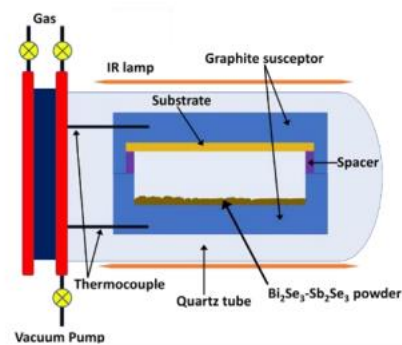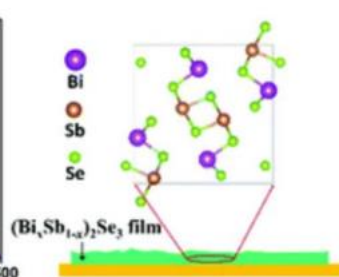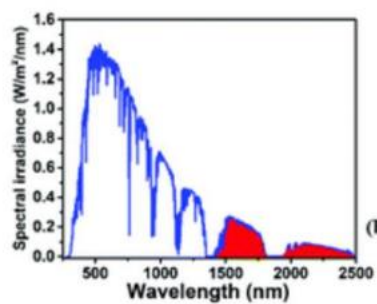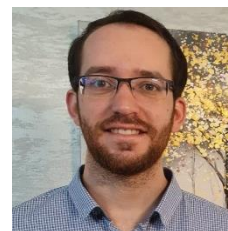
Yaniv Farkash

Msc student, Professor Gideon Grader, Technion

Nanofiber Electrodes for Efficient Decoupled Hydrogen Generation by the E-TAC process

There is a growing need for switching from fossil fuels to renewable energy sources, though the large-scale adoption of solar and wind energy is plagued by their intermittency, due to them being greatly affected by the seasons and the time in the day. Furthermore, any energy not utilized is wasted.

One way to remedy these issues is by using the excess energy to produce hydrogen, which can be stored and used in times when energy demand exceeds production.

Hydrogen has two main advantages over carbon-based fuel, having much higher energy density per unit of mass and producing only water during combustion. In addition, hydrogen can be produced in a rather simple process of electrolysis.

Electrolysis is not without disadvantages, namely the formation of both hydrogen and oxygen at the same time in the electrolytic cell. In order to overcome this, a decoupled water splitting process dubbed E-TAC (Electrochemical-Thermally Activated Chemical) has been developed. In this method the splitting process is broken up into two separate stages: an electrochemical step, in which the anode is oxidized, and gaseous hydrogen is produced, followed by a chemical step, in which the anode is reduced back to its initial state and oxygen is produced.

A key element in the E-TAC process is the anode, which needs to have a high capacity and at the same time be able to charge and discharge at a fast rate. This means that ideally the anode should be thin and consist of a high surface area material. For this reason, electrospinning was selected as the a method for producing nanofibers which are highly suitable as catalysts, due to their very high specific surface area.

Leo Giloni

PhD student, Professor Oz Gazit, Technion

Assessing acid – base cooperativity of layered oxides for biomass conversion

Introduction. Aldol condensation of biomass derived molecules is highly attractive for the upgrading of biomass to value added chemicals. While Aldol condensation can be promoted by acid or a base catalysts efficient acid-base cooperative interactions can facilitate lower activation barrier, lower reaction temperature, and better control over reaction selectivity. MgAlOx based Layer double hydroxides (LDH) act as a base catalyst for aldol condensation. If the LDH is deposited as thin (order of 1 nm) layers on the surface of an acidic metal oxide the material can have acid-base properties at the interface between the two oxides. In the current work, we study the acid-base functionalities of MgAlOx thin particles deposited on an underlying support (i.e., ZrO2). The catalysts are tested for the Henry reaction as a model reaction and the condensation of Furfural with Cyclohexanone.

Experimental/methodology. The catalyst was prepared through the synthesis of LDH thin sheets according to Yu et al.[2] and depositing them on either commercial oxides or dedicated zirconia which were prepared based on the protocol of Leib, E. W. et al.[1] Reaction testing was performed on a particulate catalyst while single particle characterization was performed by depositing the LDH thin particles on a zirconia coated Si-wafer. Reaction testing are performed in a batch mode and were analysed using 1H-NMR and GC-MS.

Results and discussion. Following catalyst preparation, we compared the performance of the calcined hierarchical catalyst (LDH/ZrO2, ZHOX) to that of the calcined native LDH (LDO) and ZrO2 oxides and their mechanical mixture in the Henry reaction, Figure 1. We find that the LDO (layered double oxide) is the most active with 0.032 mol/mgcat, the ZrO2 is the least active with 0.002 mol/mgcat and the mechanical mixture of LDO and ZrO2 is 0.003 mol/mgcat. The HOX catalyst per gram catalyst was slightly more active with 0.008 mol/mgcat. However, normalizing the conversion levels to the amount of LDO in each sample we find that the HOX out performed the LDO by almost 20-fold, Figure 2. This difference cannot be explained by surface area as the ZrO2 and HOX have roughly 10 m2/g and the LDO is about 140 m2/g. Hence, as the ZrO2 is almost inactive the higher activity of the HOX and mechanical mixture is postulated to originate from specific active sites generated at the interface between LDO and ZrO2. To better understand this effect we performed kinetic analysis, acid/base chemisorption at the macroscopic level and at the single particle level using AFM-IR. Work on the aldol reaction is in progress as well as additional analytical characterizations.
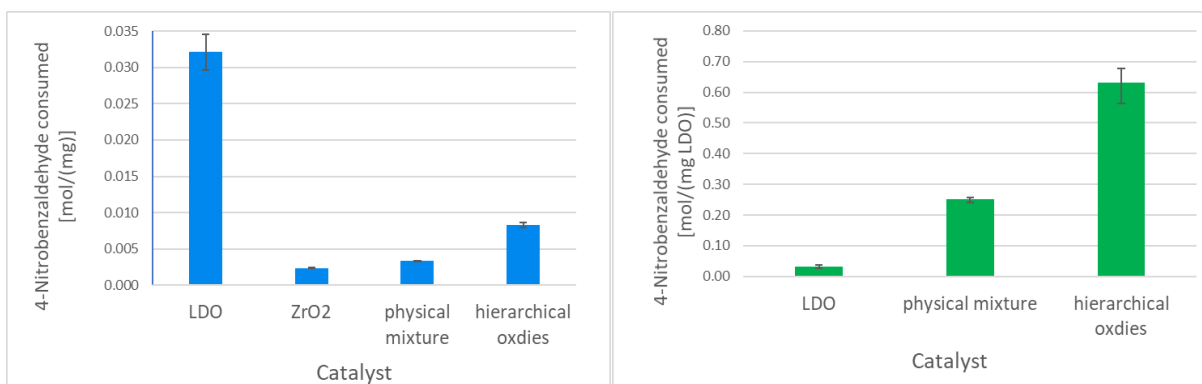
Figure 1. (left) Conversion per mg catalyst of Nitroaldol condensation reaction @15h at 80C
(right) Conversion per mg LDO of Nitroaldol condensation reaction @15h at 80C

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