

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. Matt Johnson- PhD student, Professor Judit Zador, Sandia National Laboratories.

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. Nitai Arbell - PhD student, Professor Yaron Paz, Technion.
5. Yuejun Yu - PhD student, Professor Yaron Paz, Technion.
6. Michal Levin - PhD student, Professor Noy Cohen, TecPhD studentthnion.
7. Noam Zyser - PhD student, Professor Vogt Charlotte, Technion.
8. Kfir Kaplan - Msc student, Professor Alon Grinberg Dana, Technion.
9. Sapir Willdorf-Cohen – PhD student, Professor Dario R. Dekel and Professor Charles E. Diesendruck, Technion.
- 10.Or Peleg Evron – PhD student, Professor Havazelet Bianco-Peled, Technion.
- 11.Yael Hershkovitz Pollak – PhD student, Professor Hossam Haick, Technion.
- 12.Yaniv Farkash – PhD student, Professor Gideon Grader, Technion.
- 13.David Attia – PhD student, Professor Rachel Yerushalmi-rosen, Ben Gurion University.
- 14.Roy Almog, PhD student, Ronen Berkovich, Ben Gurion University.

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.

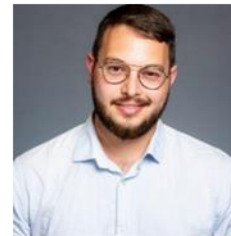
In the second part of my talk, I will introduce the field of Hydrodynamic Quantum Analogs, where small droplets placed on the surface of a vibrating fluid bath may propel themselves through a resonant interaction with their own quasi-monochromatic wave field. These “walking droplets” were shown to exhibit 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.

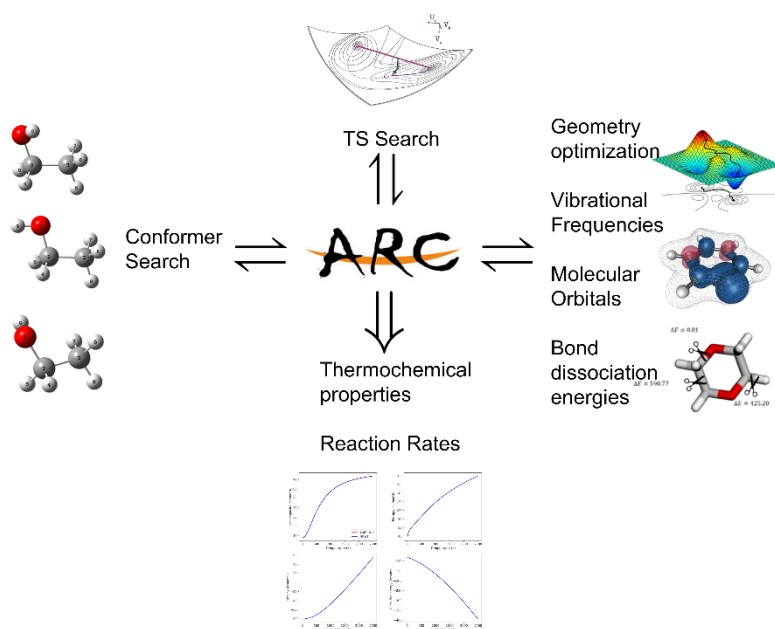
Kfir Kaplan

Msc student at Dr. Alon Grinberg Dana lab, Technion



Automated rate calculator (ARC): A tool for automated ab-initio 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-dimensional 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

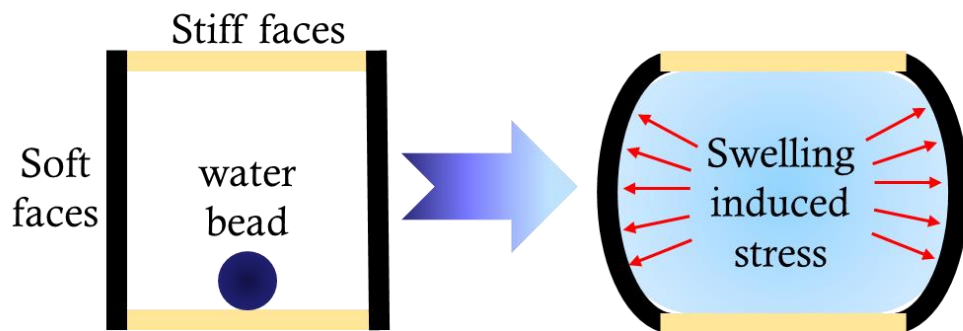
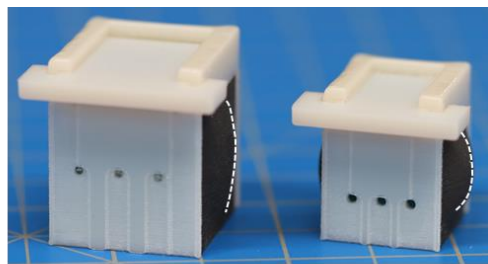
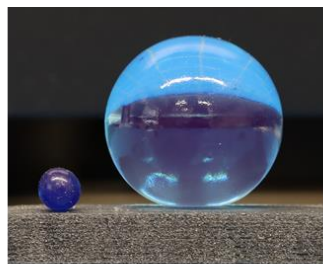


Measuring swelling induced stress of gels under constraints using 3D printing

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-induced 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

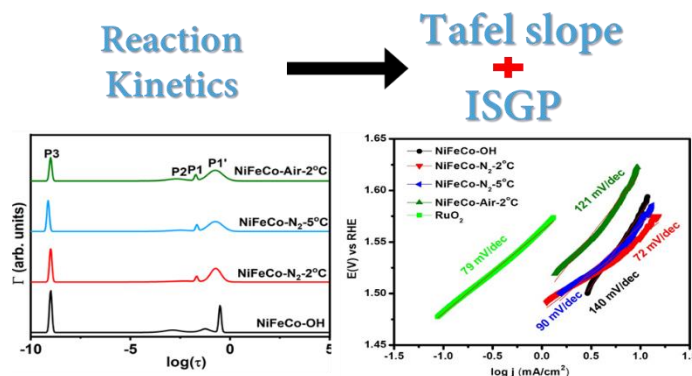
PhD student at Professor Yoed Tsur lab, Technion



Optimization of Metal Oxide/Hydroxide Catalysts for Oxygen Evolution Reaction by Relaxation Phenomena Analysis

Electrochemical hydrogen production is vital in eco-friendly energy storage and conversion applications. Water splitting is a sustainable approach for converting electrical energy into chemical energy (oxygen and hydrogen) without CO₂ emissions based on renewable energy sources. Two half-cell reactions occur during the water-splitting process: oxygen evolution reaction (OER) and hydrogen evolution reaction. Currently, the OER is the major challenging step since the reaction includes a high activation energy for the transfer of four electrons. Hence, finding an efficient catalyst with low activation energy is necessary. RuO₂, which exhibits a superior activity, is one of the common catalysts for OER reactions. However, the rarity and cost of this metal limit its application on a large scale. Trimetallic double hydroxide (NiFeCo-OH) family are appropriate candidates. We found it is interesting to control the heat treatment conditions to influence the stability of the catalyst, which is affected by the oxide-to-hydroxide phase ratio. Thermal and structural analysis reveal that the catalyst that has been prepared under inert atmosphere has mixed phases of metal hydroxide/oxide. In contrast, the catalyst that has been prepared under air atmosphere exhibits a single oxide phase.

As part of this study, we also examined the different contributions of electrochemical phenomena in OER using a distribution function of relaxation times (DFRT) modeling and well-known parameters like as Tafel slope to describe the reaction kinetics. Based on the results, we have initiated to re-examine the problems of Tafel slope. To bridge the gap in the information provided by a Tafel slope on reaction kinetics, we have offered a supportive approach with Electrochemical Impedance spectroscopy (EIS). EIS is commonly used to identify electrochemical phenomena occurring at the catalyst/electrolyte interface. Using a MATLAB-based genetic programming software, ISGP, the electrochemical phenomena can be separated and identified from EIS. ISGP provides an analytical form of the DFRT, when the DFRT modelling enables the kinetics evaluation of the catalysts. It is straightforward to extract from the DFRT the effective resistance and effective capacitance of each electrochemical phenomenon involved. In cases where Tafel slope fails, the ISGP can support or even be better.



Nitai Arbell

PhD student at Professor Yaron Paz lab, Technion



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

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

We demonstrated the capabilities of this approach using the dipeptide Leucylglycine as a model degradant, TiO_2 as the photocatalytic material, and Al_2O_3 as the inert overcoating layer, achieving a selectivity factor towards the degradation of the target enantiomer of up to seven, and an enrichment of a single enantiomer up to 85% from an initially racemic mixture [1]. The wide range of tweakable parameters in the system (photocatalyst, target molecule, concentration of imprinted sites, type of passivating layer, etc.), shows promise as a new possible industrial method for purifying racemic mixtures into enantiomerically pure compounds.

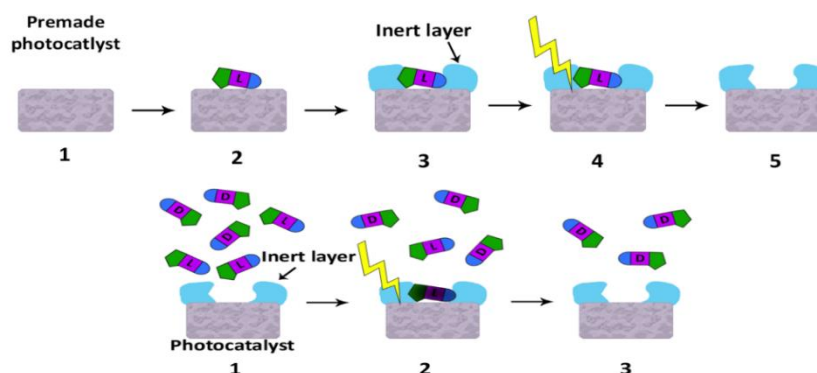


Figure 1. Schematic representations of (A) the preparation process of a PED and (B) its use for the enantiomeric enrichment of a racemic solution.

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

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)

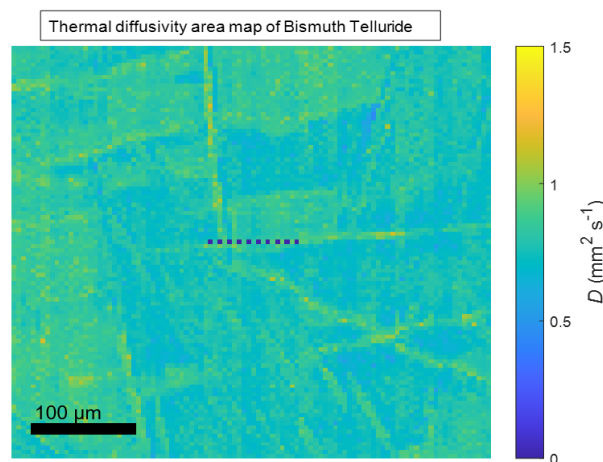


Microscale mapping of thermal diffusivity in thermoelectric materials using a micro four-point probe

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).

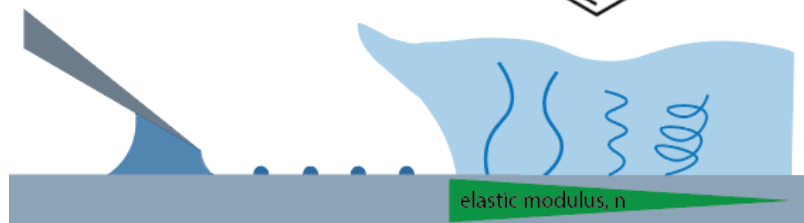
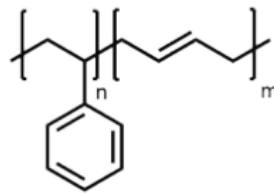
The μm -scale mapping of thermal diffusivity is arguably crucial for deeper understanding of thermal budgets of high-efficiency thermoelectric materials. The M4PP method proposed in this work provides rapid and accurate characterization of thermal diffusivity of such materials on the microscale.



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



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



Sapir Willdorf Cohen

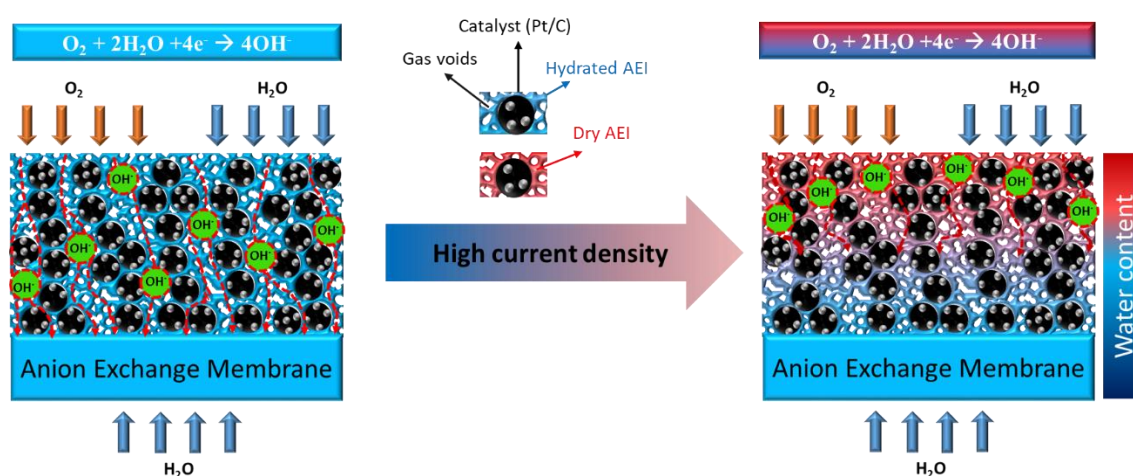
PhD student, Professor Dario R. Dekel and Professor Charles E. Diesendruck,
Technion



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 reversible 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.

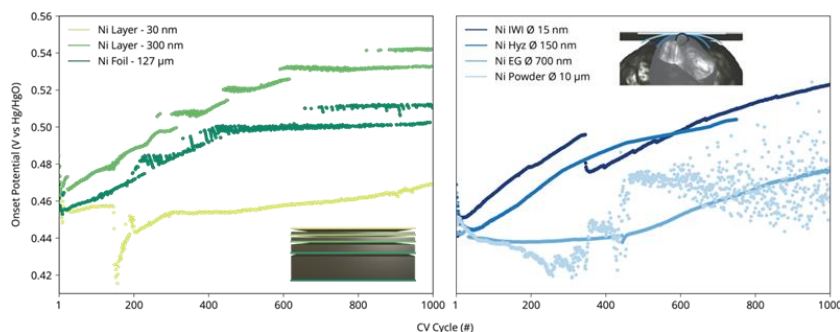


Figure 1. The influence of bulk-volume and surface curvature of Ni-based catalysts on the different activity descriptors controlling electrooxidation reactions in aqueous-alkaline conditions towards the strategic design of catalytic materials.

Timothy Little

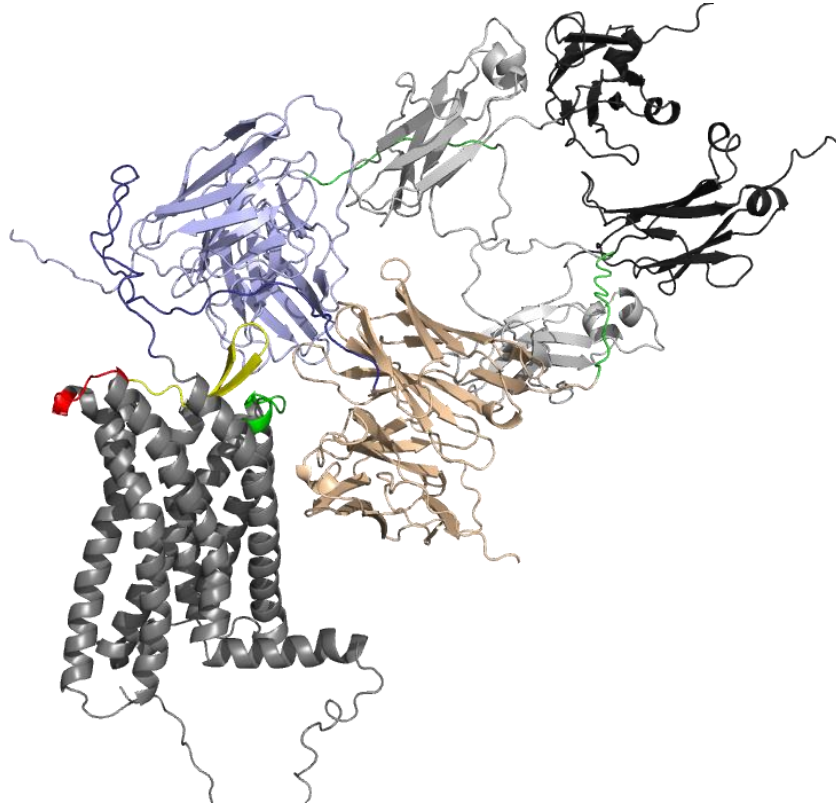
Professor Juliane Nguyen, North Carolina at Chapel Hill

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 ($K_d = 48$ 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.



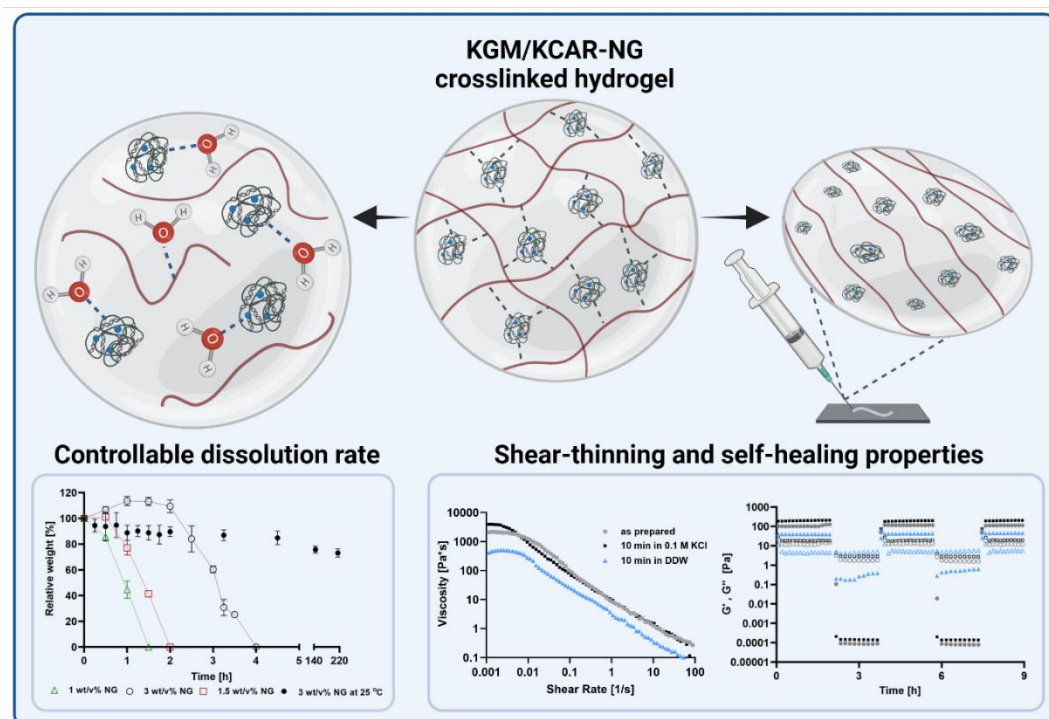
Or Peleg Evron

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-dimensional 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).

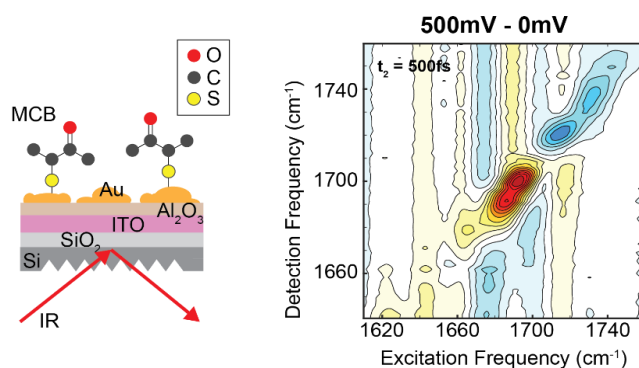


Figure 1. 2D IR difference spectra of the carbonyl stretch of 3-mercapto-2-butanone (MCB) shown for 500mV – 0mV applied potential. The cartoon depicts the electrode consisting of a commercial Si ATR wafer, ALD deposited ITO and Al₂O₃, and sputtered Au.

[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

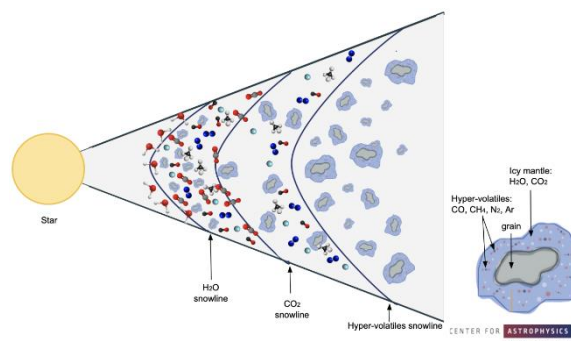
PhD student, Professor Karin Oberg, Harvard University



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.



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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.

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Developing and study of an automatic on-line micro-biototoxicity 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.