The Institute of Chemistry
Annual report
2018

More details on the institute and chemistry studies can be found on: https://chemistry.huji.ac.il
Preface

The Institute of Chemistry was founded in 1923 with the goal to provide academic education in Chemical Sciences. It was the first School of Chemistry in Israel, founded even before the official establishment of The Hebrew University and the State of Israel. The founding father of the Institute of Chemistry, Prof. Andor Fodor, was recruited for this project by Profs. Albert Einstein and Chaim Weizmann. The first scientific paper of the Institute was submitted for publication in January 1924.

At present, the Institute of Chemistry has 34 faculty members and 20 active emeriti professors, all performing research in a variety of fields. These include theoretical and computational chemistry, physical, analytical, organic, inorganic, bioorganic, atmospheric and material chemistry, as well as nanoscience. The Institute is a vibrant education and research center, offering B.Sc., M.Sc. and Ph.D. degrees in chemistry. Currently, it is comprised of more than 250 undergraduates, about 200 research students and 100 Post-doctoral researchers from all over the world.

The Institute equips its graduates with advanced scientific and technological skill sets, and has evolved into a center of excellence in various areas of chemistry with emphasis on multidisciplinary research programs. The Institute provides a rich environment for teaching and research, with first-rate infrastructure and state-of-the-art instrumentation. The excellent research conducted at the Institute is reflected in the great number of publications in top journals and the many patents and industrial activities that have evolved from it, including the development of new processes and products and the establishment of start-up companies.

This annual report summarizes the recent activities of the Institute of Chemistry. We hope you will find it informative, useful, and inspirational.

Prof. Meital Reches  Prof. Shlomo Magdassi  Prof. Norman Metanis
Nano-catalysis

Prof. Raed Abu-Reziq
Email: Raed.Abu-Reziq@mail.huji.ac.il

Group Research:

Our current research activity focuses on the developing different types of polymeric or inorganic nano- and microcapsules containing dissolved catalysts or dispersed metal nanoparticles in their cores. These catalytic nano- and microreactors shows a unique reactivity and selectivity in different organic transformations. Recently, we have developed a method for preparing new chiral materials based on encapsulation of chiral ionic liquids (ILs) and deep eutectic solvents (DES) within silica microspheres. In addition, we have developed a method for preparing chiral periodic mesoporous organosilica (PMO) nanoparticles consisted of 100% chiral bridged-silane precursor. These chiral PMO nanoparticles exhibited a large surface area that reached up to 1776 m²g⁻¹ and they were utilized to host metal nanoparticles such as ruthenium and platinum nanoparticles.

Preparation of micro- and nanoreactors for effective catalysis

Specific current research topics:

- Development of smart nanosystems for the slow-release of pheromones
- Catalytic nano- and microreactors
- Magnetically separable nanocatalysts.
- Particulated ionic liquids and deep eutectic solvents.
- Catalytic periodic mesoporous organosilica (PMO) nanospheres.
- Catalytic solid lipid particles.
- Nano- and microencapsulation methods.
List of selected publications in the last three years (2015-2018)


List of Patents (2015-2018)

Protons in liquid water, gas-phase clusters and biological systems

Prof. Noam Agmon

Email: agmon@fh.huji.ac.il
Website: http://vintage.fh.huji.ac.il/~agmon/

Research Summary

A. Infrared spectra of protonated water clusters.

We were able to compute and assign the complex infrared spectrum of the protonated water trimer, H+(H2O)3 in the gas phase (Figure 1). This unit serves as a “water wire” for short range proton transport within proteins, for example, from the chromophore of the Green Fluorescent Protein (GFP), Figure 2. The analysis shows that the difficult to assign spectral range, 1800-2300 cm⁻¹, arises from strong Fermi resonances between the concerted “proton transfer mode” and two different combination bands. These may temporarily impede proton transport through this wire.

Figure 1. 2nd order vibrational perturbation theory (VPT2) explains the IR spectrum of (a) the gas-phase H+(H2O)3 cluster and (b) its deuterated isotopologue.
B. Water-wires in GFP.

The GFP chromophore emits a proton following photoexcitation, and the resulting anion fluoresces green. We have used molecular dynamics to search for water-wires that could serve as putative proton transporters. We have found one short wire that may transport the proton outside the protein (Figure 2), and a long wire along the protein axis (not shown) through which a new proton may be recruited. These findings prompted us to suggest a new mechanism for proton migration in GFP.

C. Small, neutral water clusters are prevalent in the atmosphere, forming rings at very low temperatures. Recently it was demonstrated that their IR spectra at elevated temperatures exhibit some interesting blue shifts. We have shown computationally that these shifts are due to ring expansion rather than to their cleavage.

Selected publications (2016-2017)

Surface photophysics, photochemistry and catalysis group

Prof. Micha Asscher

Email: micha.asscher@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/surface-asscher/index.html

Research interests

1. Model heterogeneous catalysis is studied under ultra-high vacuum (UHV) conditions on top of alloy bimetallic nano-clusters (e.g. Au-Cu and Cu-Pd) grown via buffer layer assisted growth method in UHV. In situ Auger and thermal desorption methods are used to follow reactivity and selectivity. High pressure-low pressure apparatus is uniquely used to study the thermal and photo-excited catalysis.

2. Local (transient) electric field effect on photo-induced and electron-induced reactivity of caged molecules within solid water films on surfaces is studied near sharp edges and by growing model in-vacuum nano-capacitors by trapping electrons in ice.

3. The effect of solid water growth temperature on the nature of charging and transmission of electrons through such films reveals strong temperature dependent binding of the electrons to water. These trapping sites were not reported before.

4. The role of plasmonic giant field enhancement near metallic (Ag) nano-particles on photo-reactivity vs. the effect of hot excited electrons on surface photochemistry has been...
investigated. Its potential enhancement in photo-catalysis when embedded within TiO$_2$ films has also been investigated.

**Selected publications (2015-2018)**

Materials science: Metals and ceramics, Chirality and symmetry

Prof. David Avnir

Email: david.avnir@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/avnir

Research Summary

Current scientific activities include organically doped metals, theoretical and experimental aspects of chirality, theoretical studies in symmetry, and sol-gel organic hybrid materials and biomaterials. Earlier major interests included fractal theory in chemistry and physics, and far-from-equilibrium phenomena such as chemically driven hydrodynamic instabilities.

Selected publications (2015-2018)

   - Science: http://news.sciencemag.org/biology/2015/05/silver-turns-bacteria-deadly-zombies
   - One of the top 100 read Scientific Reports articles in 2015, out of 11,000.C&EN: http://cen.acs.org/articles/93/i18/Reason-Silver-Nitrates-Prolonged-Microbial.html
   - Popular Science: http://www.popsci.com/bacteria-acts-exactly-zombie
3. V. Vinogradov and D. Avnir, “Enzyme renaturation to higher activity driven by the sol-gel transition: Carbonic anhydrase” Sci. Rep. 2015, 5, 14411, 1–7, Highlights:

Left: Silver within which polystyrene has been entrapped. Center: The degree of C2-symmetry of HIV protease, is determined. Right: Fluorescent laser dye entrapped within a sol-gel silica glass.
Roi Baer Research Group

Prof. Roi Baer

Email: roi.baer@huji.ac.il
Website: https://scholars.huji.ac.il/roibaer

Baer is the Ratner Family Chair of Chemistry and is the Director of the Fritz Haber Research Center of Theoretical Chemistry at the Hebrew University.

Summary Group Research:

Roi Baer is a theoretical chemist, developing new theories and computational methods to predict the properties of molecules, nanocrystals and in general materials directly from the basic laws of quantum physics. His research focuses on the search of new ways for producing sustainable energy, including conversion of sunlight to electricity via solar-cells and the production of clean and efficient fuels from natural gas. Baer’s recent research involves development of new computational techniques for studying the behavior of charge carriers in nanocrystals and polymers. More recently he has developed superfast memory-compact algorithms, based on statistical polling, for performing electronic structure calculations on molecular systems of unprecedented size.

Specific current research topics:

- Stochastic density functional theory
- Stochastic many-body (GW and GF2) approaches
- Open-system quantum dynamics of Fermions
- Spontaneous charge-carrier localization in extended one-dimensional systems.

List of selected publications in the last three years (2015-2018)


Baer’s group includes a research associate, 6 PhD students and one MSc student.
Science and Technology of Nanocrystals

Prof. Uri Banin

Email: uri.banin@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/~nano/

Research Summary

Colloidal semiconductor nanocrystals, are a class of nanomaterials that manifest the transition from the molecular limit to the solid state. Control over their size, shape, composition and organization on the nanometer scale, enables unique tuning of chemical, optical, electrical, magnetic, mechanical and thermodynamic properties. The tunable properties along with the chemical processibility retains significant potential for using nanocrystals as building blocks for nano-devices in diverse applications such as solid state lighting, flat panel displays, solar energy conversion, optoelectronic devices and bio-medical applications. In our lab, we study the chemistry, physics and applications of nanocrystals. A focus of our work in recent years concerns hybrid nanoparticles, composed of two components of different material types that represent a frontier area of research in nanomaterials. This addresses a key goal of nanocrystal research in the development of experimental methods to selectively control the composition and shape of nanocrystals over a wide range of material combinations. A particular combination which we pioneered in 2004, concerns the growth of metal (Au) tips onto the apexes of semiconductor (CdSe) nanorods creating ‘nanodumbbells’. Since this discovery, we have been studying hybrid metal-semiconductor nanoparticle systems extensively. The ability to selectively arrange nano-sized domains of metallic, semiconducting and magnetic materials into a single “hybrid” nanoparticle offers an intriguing route to engineer nanomaterials with multiple functionalities or the enhanced properties of one domain.

Selected publications (2015-2018)


**List of Patents (2015-2018)**


**Industry-related stories:**

1. Licensing Agreements: Merck KGaA (see below)
2. Start up companies: Qlight Nanotech, a Start-up company which was fully acquired by Merck KGaA in 7/2015. Qlight is developing semiconductor nanocrystals for flat panel display and solid state lighting applications. Qlight Nanotech acts as a global R&D site for Merck on Quantum Materials. It operates within the Edmond J. Safra campus of the Hebrew University. The company at this site has currently ~30 employees in Jerusalem, most of which are R&D scientists and engineers. Qlight Nanotech was awarded the Nanotechnology Company of the Year prize at the 2014 Nano Israel conference.
1. Carbyne radicals
We study the formation and chemistry of free carbyne and carbene radicals in aqueous solution. These species are produced by degradation of metal complexes that contain triple or double metal-carbon bonds in water. An alternative route to obtain these extremely reactive species is by reacting tri- or di-halo alkanes with chromium(II) ions. Both carbynes and carbones undergo coupling reactions and produce alynes and alkenes respectively. In addition, they react with solvent molecules and produce a large variety of products.

We study the mechanism by which organo-metallic cluster complexes that contain alkylidyne ligands are formed. We believe that the origin of the alkylidyne group is a free carbyne that reacts with the tri-nuclear framework. We apply ion-exchange chromatography, GC-MS and X-ray crystallography techniques to elucidate the exact mechanism.

2. Organometallic complexes with alkylidyne ligands
We study the mechanism by which organo-metallic cluster complexes that contain alkylidyne ligands are formed. We believe that the origin of the alkylidyne group is a free carbyne that reacts with the tri-nuclear framework. We apply ion-exchange chromatography, GC-MS and X-ray crystallography techniques to elucidate the exact mechanism.
3. Ferric citrate

Ferric citrate complexes play an important role in the biological mobilization of iron in living cells. Ferric citrate preparations are used in medicine as iron supplements and for imaging purposes. Our goal has been the structural characterization of several ferric citrate complexes and the understanding of the role of each species in biological systems.

Specific current research topics

- Structural inorganic chemistry
- Synthesis and characterization of polynuclear metal complexes
- Production of nanometric metal alloys

List of selected publications (2015-2018)


Macromolecular networks in bacterial biofilms: structure, function, aggregation, interactions and biomineralization

Dr. Liraz Chai

Email: liraz.chai@mail.huji.ac.il
Website: http://lirazchai.huji.ac.il/

Research Summary

How do intermolecular interactions govern the formation of macromolecular networks? This is the basic question that we ask in the group. We currently implement this question on biopolymers from the extracellular matrix in bacterial biofilms. Biofilms are communities of microbial cells that grow on natural and synthetic surfaces. Irrespective of whether biofilms are beneficial or detrimental to the host, their extracellular matrix is critical to their development and survival. The extracellular matrix (ECM) is a mesh of biopolymers, mainly polysaccharides, proteins and nucleic acids that connects the biofilm’s cells together. We study the structure of the extracellular matrix components and the interactions between them and their precursors and relate these properties with their function. Our experimental toolset includes Atomic Force Microscopy and calorimetry (to study interactions), Circular Dichroism, Fourier Transform InfraRed spectroscopy, Nuclear Magnetic Resonance (to study structure), as well as fluorescence and light scattering techniques (to study the kinetics of the networks' assembly). Approaching complex biological structures from a basic perspective will allow the engineering of inhibitors that will prevent the formation of detrimental biofilms and encourage the formation of beneficial biofilms.

Specific current research topics:

- Structure and function of extracellular matrix proteins and polysaccharides
- Interactions between extracellular matrix peptides and proteins
- Biomineralization and biomaterials
List of selected publications in the last three years (2015-2018) (not more than 10)


Excitonic Solar Cells

Prof. Lioz Etgar
Email: lioz.etgar@mail.huji.ac.il
Website: http://lioz.etgar.huji.ac.il

Research Summary

Prof. Etgar research group is concentrating on investigating the optical, physical and photovoltaic properties of hybrid organic-inorganic perovskites. During the past few years, a breakthrough has occurred in the PV field by using organic-inorganic hybrid perovskite as the light harvester in the solar cells to achieve more than 20% efficiency. Our laboratory was the first to demonstrate that organic-inorganic perovskite could function simultaneously as a light harvester and as a hole conductor in the solar cell, making the solar cell more stable and simplifying its structure.

Selected publications (2015-2018)

8. Daniel Amgar, Tal Binyamin, Vladimir Uvarov, and Lioz Etgar. “Near ultra-violet to mid-visible band gap tuning of mixed cation \( \text{Rb}_{x}\text{Cs}_{1-x}\text{PbX}_3 \) \((X=\text{Cl or Br})\) perovskite nanoparticles.” *Nanoscale*, **2018**. DOI: 10.1039/C7NR09607K.


**List of Patents (last three years (2015-2018))**


3. Lioz Etgar, Shlomo Magdassi “Semi transparent perovksite solar cells”, Provisional.


7. Lioz Etgar, Daniel Amgar, provisional, title: Rubidium Lead Chloride Nanocrystals.
Using peptides to study and modulate protein interactions: from biophysical studies to drug design

Prof. Assaf Friedler

Email: assaf.friedler@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/~assaf/
From October 2016: Vice Rector, the Hebrew University of Jerusalem

Research Summary

Our group is interested in using peptides for the quantitative biophysical and structural analysis of protein-protein interactions (PPI) in health and disease. Based on this, we develop lead compounds that modulate PPI for therapeutic purposes. Peptides serve as major tools both for studying PPI and for modulating them (by inhibition or activation). Some examples are:

1. Development of new synthetic methods for peptide modifications. We developed a new approach for peptide cyclization during solid phase synthesis under highly acidic conditions using simultaneous in situ deprotection, cyclization and TFA cleavage of the peptide, which is achieved by forming an amide bond between a lysine side chain and a succinic acid linker at the peptide N-terminus. We also developed a new general N-acetylation method for solid phase synthesis. Malonic acid is used as precursor and the reaction proceeds by in situ formation of a reactive ketene intermediate. Another example is the development of a new method for covalent inhibition of proteins by succinimide-labeled peptides.

2. A new methodology for preparing multi-phosphorylated peptides: Multi-phosphorylation of proteins is one of the most important ways of regulating their biological function and for selecting between different signalling pathways. Multi phosphorylated peptides are the essential tools for studying the specific biological role of each phosphorylation pattern, however their synthesis is extremely difficult and in many cases impossible. We developed an efficient new strategy for the synthesis of libraries of multi-phosphorylated peptides with up to seven phosphorylated Serine (pSer) and Threonine (pThr) residues that are very close in sequence. Our new method was applied for the synthesis of a library of extremely difficult to synthesize multi-phosphorylated peptides derived from Rhodopsin C-terminal domain. Our results open the way for the synthesis of multi-phosphorylated peptides for a variety of applications, which was impossible until now, and enables studies of the mechanism of action of multi-phosphorylated proteins.

3. Intrinsically disordered proteins: About one third of the genome encodes for intrinsically disordered proteins (IDPs) or disordered regions in proteins (IDRs). These lack stable tertiary structures and are composed of a large ensemble of extended and flexible conformations interchanging dynamically. Our research focuses on the molecular mechanisms of action of the IDRs and how they mediate and regulate the interactions and activity of the protein. IDRs can either directly mediate the interactions of the protein or regulate that interactions and activity of the structured domains. IDPs are involved in many human diseases, making them attractive targets for drug design. However, more than 90% of current drug targets are enzymes or receptors and IDPs still cannot be targeted due to the lack of specific binding pockets for small molecules. Our ultimate goal is setting IDPs and IDRs as therapeutic targets. Three examples will be presented: (1) The
ASPP protein family, which regulates apoptosis; (2) The HIV-1 Rev protein, which mediates nuclear export of the viral RNA; (3) The centrosomal STIL protein, which is upregulated in cancer.

List of selected publications in the last three years (2015-2018)


Organometallic chemistry and catalysis

Prof. Dmitri Gelman
Email: dmitri.gelman@mail.huji.ac.il
Website: https://scholars.huji.ac.il/dmitrigelman/home

Group research

Generally, research in my group is focused on synthetic and mechanistic organometallic chemistry. The core of the work is the interplay between the structures and reactivity of organometallic compounds relevant to catalysis. We use a wide range of synthetic and spectroscopic methods for the manipulation and characterization of our targets: air-free techniques, NMR spectroscopy, X-ray crystallography, etc. The major current direction of our studies include: the design of new carbometalated transition metal complexes-based catalysts towards activation/formation of polar and nonpolar bonds.

We are interested in the design of novel catalytic systems for dehydrogenation of formic acid/hydrogenation of carbon dioxide and in the development of new generic transformations involving structural modification of functionalized hydrocarbon substrates using formic acid as a source of H₂ and CO₂.

We are interested in the design of new concepts in acceptor-free dehydrogenation of alkanes to alkenes and molecular hydrogen, as well as of new generic transformations involving structural modification of the resultant unsaturated hydrocarbon products (as a long-term target).

Specific current research topics:

- Synthesis and applications of 3-D pincer complexes
- Ligand-metal cooperating catalysts
- Enzyme-mimicking artificial catalysts

List of selected publications in the last three years (2015-2018)


**List of Patents (2015-2018)**


[http://hikari.co.il/About.aspx?l=2](http://hikari.co.il/About.aspx?l=2)
Chemical Reaction Dynamics and Spectroscopy of Complex Systems

Prof. Robert Benny Gerber

Email: benny@fh.huji.ac.il; bgerber@uci.edu
Website: scholars.huji.ac.il/robertbennygerber/home

Research Summary

1. Molecular mechanisms and dynamics of atmospheric reactions on water and on ice surfaces:
The chemistry of at the atmosphere is governed by a huge number of reactions, many of which take place in complex environments such as seawater. Molecular-level understanding of such processes is not yet at hand, and poses a major challenge for the field. Our theoretical work aims at providing microscopic understanding of such processes by first-principles simulations. The main methods we use combine many-atom dynamics simulations with quantum-chemical treatment of the forces acting on the atoms. Examples of important recent results include a description of hydrolysis and halide substitution reactions at surfaces of seawater.

2. Dynamics of photochemical reactions in complex systems: Photochemical reactions are among the most difficult types of chemical processes to understand microscopically and predict computationally, due to the challenges of treating excited-state potential energy surfaces in all but the simplest systems. We are developing new computational approaches for dynamics simulations of such processes, with direct use of quantum-chemical excited state methods for the potential acting on the atoms along the trajectories. We also pursue applications of the methods to challenging atmospheric processes: Photochemistry of aerosols and photochemistry of pesticides.

3. Quantum dynamics simulations of many-atom systems: Quantum effects such as zero-point energies, interference phenomena and tunneling can play significant roles in spectroscopy and dynamics of a range of chemical systems. We are developing new approximate quantum mechanical methods that can be used to describe the nuclear motions in such systems also when the number of degrees of freedom is large. A major area of application are time-dependent vibrational spectroscopies of peptides and proteins.

![Fig. 1. Theory predicts an important atmospheric process: N₂O₅ undergoes hydrolysis at the surface of a nanosize water aerosol. (a) Equilibrium structure; (b) Transition state and products.](image1)

![Fig. 2. Potential energy along the pathway for substitution and hydrolysis in (N₂O₅)(Cl)(H₂O). Timescales of some steps are shown.](image2)
Selected publications (2015-2018)


Organic Electronic Materials

Dr. Ori Gidron

Email: ori.gidron@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/gidron/

Research Summary

The main goal of our research is to discover new electronic and optical properties of conjugated organic molecules and polymers. In particular, we are interested in various aspects of conjugated molecules with axial chirality, and in their prospects as chiral organic semiconductors. In this respect, we introduced tethered twisted acenes with various torsion angles (left Figure). In addition, we have introduced oligofurans as platforms for the synthesis of various π-conjugated backbones (right Figure).

While the main part of our work involves organic synthesis of new materials, we also use computational tools to predict the properties of these materials, and materials characterization techniques such as electrochemistry, absorption and fluorescence spectroscopy, and circular dichroism, to gain deeper understanding of their structure-property relation.

Specific current research topics:

- Synthesis of nanocarbons using oligofurans as synthons.
- Helically stable chiral twisted acenes.
- Low-bandgap polymers with strong emission in the near-IR spectral region.

Selected publications (2015-2018)


**List of Patents (2015-2018)**


2. Ori Gidron, Sunita Gadakh, Or Dish, Method for the bottom-up synthesis of nanocarbons using linear and cyclic oligofurans, PCT Int. Appl. Filed on June 1st 2017. US 62/513532
Uncovering the basic elements that direct the reactivity of heterogeneous catalysts

Dr. Elad Gross

Email: elad.gross@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/gross

Brief Summary of research:

Heterogeneous catalysis is essential for the development of renewable and alternative energy resources. For example, catalysts can potentially transform biomass into biofuel, CO₂ into high added value products and split water into hydrogen and oxygen, thus providing new energy resources that will overcome our crucial dependence in fossil fuels.

The design of optimized catalysts that will effectively activate these challenging reactions requires better understanding of the ways by which the properties of catalytic nanoparticles direct their reactivity. This is the challenge that we tackle in my research group by addressing basic question in catalysis research, such as: Where and how do catalytic reactions evolve on nanoparticles? How the structure and composition of nanoparticles influence their reactivity? What is the mechanism of catalytic reaction and how can we better control it?

We use state-of-the-art spectroscopy and microscopy techniques to answer these fundamental questions and identify the elements that direct the reaction mechanism of catalytic nanoparticles. For example, we use IR nanospectroscopy measurements (see illustration) to identify how different sites on the surface of a single nanoparticle influence its reactivity. By using this approach we identified that highly defected surface sites are the one that that control the reactivity of nanoparticles.

Specific current research topics:

- High spatial resolution mapping of reaction on single particles
- Identifying the properties of surface-anchored N-heterocyclic carbenes
- Structure-composition-reactivity correlations in nanoporous networks

Selected publications (2015-2018)


Molecular Biophysics in Solution

Prof. Daniel Harries
Email: daniel.harries@mail.huji.ac.il
Website: https://scholars.huji.ac.il/danielharries
2018- Head of School of Chemistry

Research Summary

Our main interest is in the way biologically diverse environments create conditions for macromolecules to associate and dissociate and form complexes that carry specific functions in cells. Examples include receptors that bind or unbind ligands, and pass signals across cell membranes, proteins that fold and unfold in solution, and sometimes form aggregates such as amyloid fibers, or DNA that binds enzymes.

We have been following this theme in a number of biologically relevant systems that involve collections of macromolecules, such as peptide folding and aggregation, and viral assembly.

We emphasize theoretical approaches to help dissect the different contributing forces involved, while maintaining close contact to experimental findings.

Specific current research topics:

- Molecular crowding and osmotic effects on peptide folding and aggregation.
- Membrane interactions and properties of lipid bilayers.
- Depletion forces, solvation, and confinement effects in hydrogen bonding solvents.
Selected publications (2015-2018)


Automated Glycan Synthesis Group @ HUJI

Dr. Mattan Hurevich

Email: Mattan.hurevich@mail.huji.ac.il
Website: https://scholars.huji.ac.il/mattanhurevich/home

Group research

Carbohydrates are major components of biological systems and have many functions that range from purely structural ones to elusive fine-tuned communication ones. Carbohydrates (glycans), that is oligo- and poly-saccharides, are assembled from a monosaccharide building blocks that have multiple alcohol functional groups but vary in their structural features. This amazing variety accounts for the many roles of carbohydrates but makes their synthesis a very complex task because it requires the functionalization of a specific functional moiety in a sea of very similar groups. Chemical oligosaccharide synthesis using protecting groups is a strategy that is constantly being developed to allow accessibility to well-defined glycan structures.

Our group develops synthetic strategies to facilitate the procurement of oligosaccharides. We exploit the use of photochemical reactions for the synthesis of oligosaccharides in a very mild conditions and use of photo labile protecting groups (PPGs) that can be liberated using LED irradiation as attractive solution for oligosaccharide synthesis. We specialize in the state-of-the-art Automated Glycan Assembly (AGA) platform that enables fast and easy synthesis of complex glycans from simple monosaccharide building blocks. Our group utilizes flow chemistry, solid phase chemistry, photochemistry, automation and their combination for oligosaccharide and glycopeptide synthesis.
Selected publications


List of Patents

2017- 6315-00 United States Provisional Patent Application No. 62/549,452 "Sensor and uses thereof in detecting metal ions"
Laboratory of Environmental Chemistry And Advanced Materials

Prof. Ovadia Lev

Email: Ovadia@huji.ac.il
Website: http://chem.ch.huji.ac.il/ovadia/

Research Summary

ANALYTICAL CHEMISTRY: Electrochemical and mass spectrometric investigation of illicit drugs and emerging organic contaminants by mass spectrometry and/or by electroanalytical methods; Artificial tracer studies to quantify water sources; Sampling methods for the quantification of the chemical composition of pore water in the vadose zone.

ADVANCED MATERIALS: Hydrogen peroxide sol-gel chemistry; Coating of surfaces and particles by peroxy-nano particles. Use of reduced graphene oxide-coated by p-block elements, their oxides in crystalline or amorphous forms as lithium ion battery and sodium ion battery anodes. Development of nanostructured manganese oxide catalysts for water purification.

Specific current research topics:
- Lithium and sodium ion batteries
- Hydrogen peroxide sol gel chemistry
- Removal of manganese and arsenic from water sources
- Soil aquifer treatment

Selected publications (2015-2018)


**List of Patents (2015-2018)**

1. Yu; Yau Wai Denis, Batabyal; Sudip Kumar, Lev; Ovadia, Gun; Jenny, Prikhodchenko; Petr V., Method for forming a reduced graphene oxide/metal sulfide composite and its use as an anode for batteries Patent was granted, Sept. **2017** United States Patent 9,755,222

2. Lev; O; Sladkevich; S; Prikhodchenko; P; Gun; G, Process for the formation of metal oxide nanoparticles coating of a solid substrate, issued on November 6th, US patent number: 10/119,036

3. Alfonta, L Ravenna, YD, Gun, J, Lev, O, , Phenothiazine/phenothiazine – graphene oxide composite, Publication number: 20170173036, Type: US patent application Filed: July 21, 2015, Publication date: June 22, **2017**.
Chemical and biological Dynamics

Prof. Raphael D. Levine

Email: rafi@fh.huji.ac.il
Website: https://scholars.huji.ac.il/raphael.levine


List of selected publications in the last three years (2015-2018)

Science, Technology and Applications of Micro and Nanomaterials

Prof. Shlomo Magdassi

Email: magdassi@mail.huji.ac.il
Website: https://scholars.huji.ac.il/magdassi

Since 2016- Head of Institute of Chemistry, Hebrew University.
Since 2016- Head of the 3D and functional printing center of the Hebrew University.

Research Summary

The research group focuses on materials science and nanotechnology. The main research fields of the group are formation and stabilization of inorganic and organic nanomaterials, formulation of these materials in various delivery systems and inks, and their application in a variety of fields such as 3D and functional printing, solar energy and bio-medical systems. Current research projects include: conductive inks for printed electronics, transparent conductive electrodes, materials for 3D printing, inkjet inks formulations, coatings and inks for solar energy applications, nanoparticles for bio-imaging, drug delivery and cosmetic formulations. Based on some of the research projects, commercial activities evolved leading to worldwide sales and establishing new companies.

List of selected publications (2015-2018)

Selected Patents

6. PCT/IL(2016)/050693, Hybrid nanoparticles as photoinitiators.
7. PCT/IL(2016)/050019, Self-assembly of perovskite for fabrication of transparent devices.
8. PCT/IL(2016)/050509, 3D printing of shape memory polymers.
9. PCT/IL(2016)/050908, 3D polymerizable ceramic inks.

Success Stories:


1. Granalix, www.granalix.com: We have introduced a new concept in potential prevention and treatment of neurodegenerative diseases. A food supplement that utilizes a unique nano-delivery system composed of only food approved components and pomegranate oil as the active material was developed. The product, GranaGard, was shown to be active in animal studies and will be tested in clinical trial in the near future.

2. AMat, Asahi Solder: the company focuses on production of conductive inks composed of copper, for applications in the field of printed electronics.
Daniel Mandler research group

Prof. Daniel Mandler

Email: daniel.mandler@mail.huji.ac.il
Website: https://scholars.huji.ac.il/danielmandler

Research Summary

Mandler's research involves primarily electrochemistry and functionalized coatings. The research spans from micro and nanoelectrochemistry, where the aim is to control patterning and growth of nanoparticles on surfaces, to forensic studies of latent fingerprints by nanoscience. The "nano to nano" approach whereby electrochemistry drives deposition of nanomaterials from their stable dispersions has been developed. This has been applied for coating medical implants by functionalized hydroxyapatite nanoparticles, forming high efficient electrochromic displays and deposition of functionalized graphene and carbon nanotubes. Analytical chemistry is also part of the activity and comprises approaches for flow-through electrochemical membranes for the detection of metallic and organic species as well as for disinfection of drinking water. Furthermore, we have developed new approaches for selectively detecting nanoparticles based on nanoparticles imprinted matrices (NAIM) where nanoparticles are imprinted in a thin matrix and removed to form cages that can selectively reuptake the original nano objects. Last but not least, we have been working on solving one of the major problems of the Dead Sea, which is the huge excess of sodium chloride. We are currently developing the future materials for housing based on insoluble and stable NaCl bricks.

Selected publications (2015-2018)

List of Patents (2015-2018)

- PAT/210/13/15/PCT, Title: Electroactive Bioadhesive Compositions.
- Provisional Patent Application No. 61/950,279 filed on 10 March 2015, Invention: Stray Light And Solar Absorption By Black Coatings Based on Carbon Nanotubes (CNT) Formulations For Optical Systems And Thermosolar Collectors”.
- PCT Application No. PCT/SG2014/000426, “Electrochromic Device”.
- U.S Provisional Patent Appl. No.62/344,552, "Coated Compressed Salt Objects And Artifacts”.
Liquids and Solutions

Prof. Yizhak Marcus

Email: ymarcus@vms.huji.ac.il

Very Brief Summary of your research:

Solution chemistry: solvation of ions and non-electrolytes, binary solvent mixtures, concentrated electrolyte solutions, molten salts, solubilities. 
Thermodynamics: properties of gaseous ions, properties of liquids. 
Coordination chemistry: complexation in solutions, hydrometallurgical processes involving ion exchange or solvent extraction. 
Room temperature ionic liquids, deep eutectic solvents, supercritical fluids

Specific current research topics:

- Subcritical and supercritical water, methanol, ethanol and their mixtures: solubility in and extraction with
- Deep eutectic solvents: conventional ones and aqueous salt hydrates.
- The solubility parameter of carbon dioxide and its solubility in ionic liquids

List of selected publications in the last three years (2015-2018)

1. Y. Marcus “Internal pressure of neat liquids: a review”. In T. Letcher, E. Wilhelm, eds., Enthalpy and Internal Energy: Liquids, Solutions and Vapours, RSC, Cambridge, 2018, Ch. 18, 477-504.
2. Y. Marcus “Ionic liquid properties. From molten salts to RTILs” Springer Intl. Publ., Switzerland, 2016, 244 pp.
Research Summary

The synergy between Science and Art is the Mecca of our research. Therefore, we are actively engaged in the pursuit of innovative solutions to the enantio-selective synthesis of architectural complex molecules. The identification and investigation of transformative mechanisms, and the development of new chemo- and stereo-selective strategies in synthesis, is the principle driving force for our research program. Our program includes the applications of these new strategies for the synthesis of bio-active natural products cores. Moreover, we are interested in applying these new developments to the magical field of the hidden-chirality, which represents the state of the art of our scientific research, this cutting edge application provides more understanding and exposure of this challenging field of science. During the course of our studies, researchers will be exposed to all facets of organic synthesis including: studying reaction mechanism, reaction discovery and optimization, discovering unexpected reactivity, organometallic synthesis, physical organic chemistry, new methods for strong bonds (e.g. C-H, C-C, C-O) activation/functionalization, and medicinal chemistry exploration.

Overview: synthesis and reactivity of gem-diboryl alkanes
Specific current research topics:

- New reactivity, transformation, and application of gem-Diborylalkanes
- C-H activation/functionlization of phosphorus-compounds
- Hidden chirality in arylated compounds
- Synthesis of chiral tetra-arylmethanes
- Remote functionalization through Metal-catalyzed chain walking
- Chiral diarylmethane-phosphonium-salts: toward their preparation and transformations

Selected publications (2015-2018)


Research Summary

Proteins are the molecular machines of life. These amazing molecules responsible for transporting substances, minerals and building blocks for the cell, carrying the different chemical reactions, fighting foreign particles invading the body, or making part of the structural components of the cell, and many more.

Scientists have been using biological systems such as bacterial cells to put their hands on these great macromolecules in order to study their structures and their mode of actions. However, in the last two decades, chemists have made great advancement toward the preparation of proteins outside the cell, that is inside a test tube. Chemists have developed chemical protein synthesis, which uses principles of organic chemistry and chemical reactions to prepare the proteins of interest in good yields and homogenous forms. The chemical synthesis allow incorporation of building blocks that are not possible using biological systems, including D-amino acids.

We have expanded the native chemical ligation (NCL) reaction, one of the most useful way to synthesize proteins, but is typically limited to Cys ligation site, to Ala and Ser ligation sites. Ala and Ser are common amino acid in protein sequences. Using the reactivity of selenocysteine (Sec), a rare amino acid, we developed a deselenization reaction that converts Sec into Ala/Ser in the presence of unprotected Cys residues. More recently, we developed the selenazolidine (Sez) building block as a temporary protecting group for Sec, which is useful for the preparation of challenging proteins by chemical synthesis.
List of selected publications (2015-2018)


Group photo
NanoBioElectronics Group

Prof. Dr. Danny Porath

Email: danny.porath@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/porath/

2017-present Vice Dean Research, Faculty of Science, The Hebrew University of Jerusalem

Research Summary:

DNA is the most important biological molecule. Its double-strand recognition, as well as the ability to control its sequence and manipulate its structure open a multitude of ways to make it useful also for molecular electronics. By producing and measuring DNA-based building blocks we progress towards the construction of DNA-based programmable electronic circuits. Step by step we improve the synthesized constructs and the measurement methods of single DNA-based molecules in close collaboration with our partners.

In another research direction we use our physical approach and tools to address biological and medical challenges. We investigate DNA translocation through nanopores to develop methods for rapid DNA sequencing. We also develop ultrasensitive detection methods for biomarkers and proteins.

Development and investigation of DNA-based nanowires and nanodevices

Selected publications (2015-2018)


List of Patents (2015-2018)
• "On Demand degradable Medical Devices", Ofra Benny, Danny Porath, Oded Shoseyov, Yaron Bar-Lavie, Amos Ofer, PCT.
• "Hybrid Complexes of nucleic acid molecules and metal molecules", Alexander Kotlyar, Gennady Eidelshtein, Danny Porath, Dvir Rotem. PCT.
• “Peptide-modified nanopores and uses thereof”, Danny Porath, Dvir Rotem, Meital Reches, Abeer Karmi. Provisional patent.
• "Macro-molecules detection with single molecule imaging of nanoparticles", Yu Ju Chen, Assaf Friedler, Chun-Cheng Lin, Dvir Rotem, Danny Porath, provisional patent.
Structure, Interactions, and Dynamic Self-assembly of Biomolecules

Prof. Uri Raviv

Email: uri.raviv@mail.huji.ac.il
Website: https://scholars.huji.ac.il/uriraviv/home

Specific current research topics

- Dynamics of tubulin nucleation and assembly
- Multimode observation of virus assembly
- Structure and interactions between lipid bilayers
- Flagella-based polymeric materials
- Structural analysis of liposomal nanodrugs

Research Summary

Our lab is developing state-of-the-art measurements and analysis capabilities that enable us to study the structure and dynamics of self-assembled biomolecules in solutions. We are using a range of biophysical methods including solution X-ray scattering, time-resolved X-ray scattering, cryo-TEM, and osmotic stress to determine the structure, dynamics, and intermolecular interactions in complex macromolecular self-assemblies. We are investigating several purified biological relevant assemblies, including lipid membranes, viruses, tubulin, and microtubules.

Studying purified model systems, where fundamental physical chemistry questions can be addressed in great detail, is essential for understanding complex biological structures. Our lab is developing unique tools to resolve the high resolution structures in solution of complex biomolecular dynamic architectures at equilibrium, during assembly processes that can attain equilibrium, and under conditions that cannot attain equilibrium.
Selected publications (2015-2018)


Bio-Inspired Materials

Prof. Meital Reches
Email: meital.reches@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/~mreches/

Research Summary

1. Interactions of Biological Entities with Solid Surfaces: Understanding how biological entities such as cells, bacteria and proteins interact with various materials and surfaces is important for several areas. This includes the design of new implants and other medical devices, development of antifouling materials and design of composite materials. Many studies have been carried out to examine how these entities interact with solid surfaces; still, it is not clear how they “sense” a surface. The research in the lab focuses on the fundamental rules that govern the adsorption of cells, bacteria, proteins and peptides to solid organic and inorganic surfaces. Our approach includes the use of single molecule force spectroscopy with atomic force microscope.

2. Biomolecular Self-Assembly and Design of Functional Coatings: Based on our knowledge from single molecule experiments, we designed a short peptide (tripeptide) that can spontaneously form a coating that resists biofilm formation. Our results clearly demonstrate the formation of a coating on various surfaces (glass, titanium, silicon oxide, metals and polymers). In addition, we showed that this coating prevents the first step of antifouling, which involves the adsorption of bioorganic molecules to the substrate. Moreover, the coating significantly reduced the attachment of various organisms such as bacteria and fungi to surfaces.

Selected publications (2015-2018)


**Industrial Stories**

Founded the company *NanoAF* in 2014. The company licensed the technology to generate antifouling surfaces.
Computational and Theoretical Photochemistry

Dr. Igor Schapiro

Email: igor.schapiro@mail.huji.ac.il
Website: https://scholars.huji.ac.il/igorschapiro

Specific current research topics
- Spectral Tuning in photoreceptor proteins
- Excited state molecular dynamics simulations
- Hybrid Quantum Mechanics/Molecular Mechanics simulations

Research Summary

The objective of our research is to apply and develop computational tools to understand chemical reactions in biomolecules and organic molecules. On the application side our focus is on light-induced reactions, in particular in chromophore-protein complexes and solvated molecules. For this purpose we employ the QM/MM methodology which allows an accurate and efficient treatment of large systems. On the development side we are interested in computational tools to support our research on photochemical/photobiological systems. We have several contributions to the quantum chemistry packages with emphasis on multiconfigurational wavefunction methods.

We are currently working on the rational design of photoreceptor proteins. From a technological viewpoint photoreceptor proteins, the light-sensitive proteins involved in the sensing and response to light in a variety of organisms, represent biological light converters. Hence, they are successfully utilized in a number of technological applications, e.g. the green-fluorescent protein used to visualize spatial and temporal information in cells. We would like to derive a comprehensive understanding that would enable us to design these proteins with desired properties by mutations. The aim is that it will result in novel biotechnological applications, e.g. optogenetic tools, fluorescent probes and biosensors.

List of selected publications (2015-2018)

1. Wiebeler C., Rao A. G., Gaertner W., Schapiro I.: “The Effective Conjugation Length is responsible for the Red-Green Spectral Tuning in the Cyanobacteriochrome Slr1393g3.” Angewandte Chemie, accepted


Chemical Bonding and Reactivity:  
From Diatomic Molecules to Metalloenzymes

Prof. Sason Shaik  
Email: sason.shaik@gmail.com  sason@yfaat.ch.huji.ac.il  
Website: https://scholars.huji.ac.il/shaik  http://yfaat.ch.huji.ac.il/sason/  

- Recipient of the Alexander von Humboldt Senior Research Award; E. D. Bergmann Prize; ICS Excellence Award; Kolthoff Prize; Schrödinger Medal of WATOC; August-Wilhelm-von-Hofmann-Dekmünze, The Gold Medal of the Israel Chemical Society.  
- Fellow of the AAAS, Member of the International Academy of Quantum Molecular Science  
- Coauthored over 550 publications, has over 36,000 citations and holds h-index of 93.

Research Summary

The research group uses computational chemistry for understanding chemistry and discovering new chemistry, as well as for constructing new productive concepts. The research topics range from new bonding motifs in small molecules, through the creation of general models for chemical reactivity using valence bond diagrams, investigation of structure, reactivity and dynamics of metallo-enzymes, and all the way to the newest topic in the group; using oriented external electric fields (OEEFs) as smart reagents, which control, bonding reactivity and selectivity. The latter topic has been highlighted in a recent feature article (see Ref. 6, below). These various topics are described in the 10-selected papers [out of 74, including one book] published in the period 2015-2018.
List of selected publications in the last three years (2015-2018)

Nanoscale Assembly

Prof. Roy Shenhar
Email: roys@huji.ac.il
Website: http://chem.ch.huji.ac.il/shenhar-group/

Research Summary

We study the principles underlying the assembly of block copolymers (and other polymers) with functional components (e.g., nanoparticles, conductive polymers, etc.). Block copolymers give rise to a variety of periodic nanoscale morphologies that are accessible in a highly controlled fashion through a spontaneous process of phase separation, and therefore are attractive as structured matrixes for directing the two- and three-dimensional arrangement of nanoparticles in nanocomposite materials.

We have established the scientific foundations for the utilization of block copolymer templates for creating nano-patterned polyelectrolyte multilayers, and revealed unique phenomena in multilayer construction that directly relate to the effect of lateral nano-confinement on the growth of the deposited polyelectrolytes. This fundamental study now enables us to expand to various directions, including the creation of nanoparticle-based photonic surfaces and utilizing nano-patterned substrates for cell engineering.

Specific current research topics (titles):
- Polymer mediated nanoparticle organization
- Development of assembly strategies using block copolymers
- Combination of nanofabrication and self-assembly techniques

List of selected publications (2015-2018)


List of Patents (last three years (2015-2018))

Watching How Chemical Bonds Break

Prof. Daniel Strasser

Email: strasser@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/~strasser/

Research Summary

We develop methods that allow visualizing in "real time" how specific chemical bonds break and new bonds are formed.
We use intense femtosecond laser pulses to excite and probe ultrafast molecular dynamics leading to structural changes. Furthermore, we use molecular fragmentation to expand and magnify the instantaneous molecular structure from the sub-nanometer scale to the scale of centimeters. We develop cutting edge coincidence 3D fragment imaging methods to record and interpret fragment kinetic energy release and correlations in terms of molecular structure and dynamics.
The specific research projects are divided between two experimental setups:
In the first setup, we mainly investigate atomic, molecular and cluster anions interactions with intense femtosecond laser pulses. This unique experimental setup allows discovery and characterization of new mechanisms of nonlinear light-matter interaction. One example is enhanced multiple detachment of molecular and cluster anions that does not rely on the well described mechanisms of multiple ionization of neutral species.
In a different experimental setup, we use high-order harmonic generation (HHG) to produce ultrafast EUV pulses. This exceptional radiation source allows us to perform single-photon Coulomb explosion imaging that allows us to visualize the instantaneous molecular structure before, after and during a photochemical reaction.

Specific current research topics:

- Ultrafast EUV probe: Time resolved Coulomb explosion imaging
- Intense field interaction with atomic, molecular and cluster anions
Selected publications (2015-2018)

Synthetic Bioinorganic and Bio-inspired Coordination Chemistry

Prof. Edit Tshuva

Email: edit.tshuva@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/tshuva

Research Summary

The Tshuva laboratory investigates the coordination chemistry of transition metal complexes that have biological or medicinal applications. Our leading line of research involves the study of bio-friendly metals, such as Ti(IV) – despite its common hydrolytic instability limitations – as possible alternatives to the toxic Pt(II) for development of non-toxic anticancer chemotherapy. Throughout these studies, we have introduced a family of Ti(IV) complexes that are incredibly stable to hydrolysis, and are highly and widely active in vitro and in vivo. All 57 human cancer cell lines in the NCI-60 panel of the NIH, including multy-drug-resistant lines, responded to our Ti(IV) complex, with the least sensitive line producing a GI\textsubscript{50} value of 12 μM (average GI\textsubscript{50}: 4.7 μM representing slightly higher activity than that of cisplatin). Importantly, No clinical signs of toxicity were detected in treated animals, and no nephrotoxicity was observed.

Current studies in this project involve three main directions: further development of optimal compounds with activity, stability, and solubility; profound study of the mechanistic pathways involved in the reactivity of the Ti(IV) complexes through wide genome analysis as well as analysis of specific bio-interactions, accumulation, and reactivities; and development of custom-designed delivery vehicles to afford selective and tumor-targeted therapy.

List of selected publications (2015-2018)


**Patents (2015-2018)**

Tshuva, E. Y. & Hochman, J. Cytotoxic Titanium and Vanadium Complexes PCT/IL2013/05069 filed 15/08/2013; published under WO2014027355A2; filed in Europe (13830156.9) and US (14/421,258).
Interfacing Nanotechnology with Bioinspired Materials and Biomaterials

Prof. Itamar Willner

Email: itamar.willner@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/willner/

- Recipient of the Israel Prize in Chemistry, the EMET Prize, the Rothschild Prize and the Gold Medal of the Israel Chemical Society.
- Member of the Israel Academy of Sciences and Humanities, Member of the German National Academy of Sciences Leopoldina.
- Coauthor of over 780 peer reviewed publications, has over 60,000 citations and holds h-index of 129 (Web of Science), 149 (Google Scholar).

Summary of group research:

The laboratory activities include the development of topics related to nanotechnology, nanobiotechnology and “smart” materials related to catalysis and energy conversion. These activities include the development of stimuli-responsive hydrogels exhibiting shape-memory properties, self-healing functions, controlled release functions and triggered mechanical robotic functions. In addition, the development of nucleic acid catalysts (nucleoapzymes) or nanoparticle catalysts mimicking natural enzymes (nanozymes). Also, stimuli-responsive nanoparticle or microparticle systems for controlled drug release, catalysis and photocatalysis are being developed. These include the development of drug-loaded stimuli-responsive metal-organic framework nanoparticles, and micro- and nano-triggered microcapsules. Efforts are directed to the development of constitutional dynamic networks (CDNs), where adaptive, emergent and hierarchical compositions and functions are triggered by external signals. The evolution of networks and their replication as models for the origin of life are examined. The use of CDNs to develop new materials, sensors and logic gate circuits are explored. In addition, active research in “origami-chemistry”, plasmonic nanoparticles and their applications, and the development of artificial photosynthetic systems, is performed.

Specific current research topics:

- Stimuli-responsive metal-organic framework nanoparticles for controlled drug release.
- Stimuli-responsive microcapsules for controlled drug release.
- Inorganic nanoparticles and metal-organic framework nanoparticles for catalysis (nanoenzymes) and confined reaction media for programmed synthesis.
• Stimuli-responsive hydrogels for shape-memory, self-healing, and mechanical/robotic applications.
• Synthesis of functionalized nanoparticles (C-dots, semiconductor QDs, plasmonic nanoparticles) and their application for sensing, thermoplasmonic heating and photocatalysis.
• Synthesis and characterization of constitutional dynamic networks and their application in materials science, catalysis, and logic gate circuitries.

List of selected publications (2016-2018)

Materials chemistry, nanomaterials

Prof. Roie Yerushalmi

Email: roie.yerushalmi@mail.huji.ac.il
Website: http://chem.ch.huji.ac.il/~roie/index2.html

Brief Summary of research: The Yerushalmi group research topics are focused on materials science and chemistry with an emphasis on nanoscience and nanotechnology. The ability to synthesize nanostructures with controlled chemical composition and unique physical and chemical properties is vital to our research. Our work combines the use and development of novel synthetic methods for the production of nanostructures and the application of large arsenal of analytical methods for the characterization and exploration of nanomaterials.

Specific current research topics:

- **Hybrid Nanostructure synthesis**: We develop new methods utilizing vapor phase and condensed phase chemistry for the synthesis of new nanoscale hybrid materials with unique physical properties. Specifically, the formation of hybrid nanomaterials consisting of inorganic and organic parts. Our research has demonstrated the benefits of such materials in the context of photocatalysis and renewable energy sources. We study the reactivity, optical, and electronic properties of the Hybrid Nanostructures.

- **Bottom-up synthesis and assembly of nano architectures**: The developing of new bottom-up synthesis methodologies enabling the production of new semiconducting and hybrid metal-semiconducting nanosystems with controlled dimensions and composition. Our research focuses on utilizing non-lithographic methods for symmetry breaking and tailoring the structural details of complex nanosystems featuring unique optical and electronic properties utilized in chemical sensing, plasmonics, and more.

- **Catalytic properties of nanostructure arrays**: Nanomaterials exhibit unique catalytic properties that are very different from the bulk material properties. The distinct reactivity at the nanoscale enables new pathways for designing novel materials with tailored chemical reactivity. Our research focuses on the study of surface interactions at nanostructure interfaces in the context of photo-catalysis and electro-catalysis.

- **Development of advanced nanocomposite materials**

List of selected publications (2015-2018)


2. Z. Sun, A. Tzaguy, O. Hazut, L. J. Lauhon, R. Yerushalmi, D. N. Seidman “1D Metal Nanobead Arrays within Encapsulated Nanowires via a Red-Ox-Induced Dewetting: Mechanism Study by Atom-Probe Tomography” Nano Lett. 2017, 17, 7478.


List of Patents (last three years (2015-2018)

2. SMART INDICATORS FOR VOLATILE CHEMICAL TARGETS. 62/312,063

Industry-related Stories:

Research agreement with Elbit-Elop in the field of nano composite materials.
Bioelectronic Interfaces

Prof. Shlomo Yitzchaik

Email: shlomo.yitzchaik@mail.huji.ac.il
Website: https://scholars.huji.ac.il/profshlomoyitzchaik

Research Summary

Our research group is exploring the role of surface science in assembling novel classes of functional nanolayers and their implementation in molecular and biomolecular electronics and photonics. We investigate fundamental issues related to nanolayers structural organization and growth dictating rational design of a variety of new technologies. Our research is highly interdisciplinary and offers opportunities to advantageously combine principles of synthetic chemistry and materials science to build well defined architectures. The latter are helping us address key issues related to biomedical diagnosis, environmental sensors, unconventional computing, molecular electronics and photoactive materials. While design of new molecules and materials is at the core of our activities, the group is actively involved in a variety of state-of-art characterization studies, including advanced electrochemical methods, spectroscopic ellipsometry, nanoscale electrical measurements, and fabrication of prototype devices.

Scheme. Conformationally adaptive biosensors are exemplified schematically: These systems utilize the entropic component of the biomolecular recognition event for signal transduction.

Selected publications (2015-2018)


**List of Patents (2015-2018)**


More details on the institute and chemistry studies can be found on: https://chemistry.huji.ac.il