The 50th Anniversary of the School of Chemistry

1964-2014

יובל 50 לבית הספר לכימיה

TEL AVIV UNIVERSITY אוניברסיטת תל-אביב

Contents

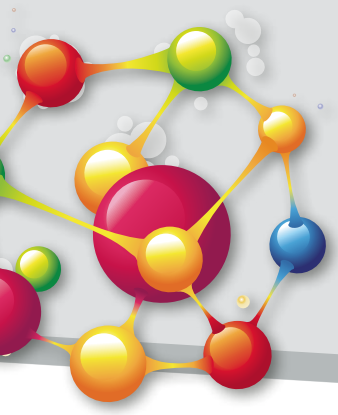
Our Mission 1

How it All Began 2

Our Research

- Bioorganic & Medicinal Chemistry 4
- Lasers in the Service of Chemistry 6
- Nanometric Devices 8
- Biophysics 10
- Green & Environmental Chemistry 12
- Alternative Energy 14
- Biomedical Diagnostics 16
- Theoretical & Computational Chemistry 18
- Advanced Materials 20
- Developing New Molecules 22

Faculty Members & Their Fields of Research 24



Our Mission

By **Prof. Gil Markovich**, Head of the School of Chemistry

In the dynamic, fast-changing and forward-looking reality of the 21st century, the discipline of chemistry is itself undergoing some fundamental changes:

First and foremost, the science of chemistry is no longer a world unto itself. Current-day chemists operate in an increasingly interdisciplinary environment, joining forces with scientists from other areas – most notably biology and material science. Moreover, as technology progresses, many fields of Chemistry once considered basic scientific research are rapidly turning into highly applicable endeavors, striving for the betterment of human lives.

This is the context in which we at Tel Aviv University's School of Chemistry celebrate 50 years of high achievement and great scientific impact – evidenced by our standing among our peers and in the global citation index (ISI). Proud of our past, we are driven constantly onwards: to contend with the deep and rapid transformations of the present, and prepare for the as yet unfathomable challenges of the future. This is our mission, and we labor every day to fulfil it, on several critical fronts:

Recruiting the best minds

The School's outstanding founding generation has by now retired for the most part, and we are gradually filling our ranks with some of Israel's finest young researchers. Many of our new staff members are returning scientists, recruited over the past few years from leading research institutions worldwide.

State-of-the-art research environment

To promote research and innovation, we provide our excellent chemists with advanced research laboratories, equipped with up-to-the-minute scientific instrumentation: NMR machines, mass spectrometers, ultrafast laser systems, X-ray diffractometers and high-power computer clusters. The latest addition to this powerful network is our new Analytical Chemistry Lab, currently under construction, which will offer frontline chemical analysis services. And three specialized in-house workshops – electronics, fine mechanics and glass blowing – are able to design and manufacture specifically tailored high- quality instruments at our scientists' request.

Reaching beyond our own premises, we were extensively involved in the establishment of TAU's Center for Nanoscience & Nanotechnology, and our researchers now have access to its cutting-edge facilities – such as top-class clean rooms, electronic microscopes and more. Other on-campus hubs – especially the university's Computation Center and the Wolfson Applied Materials Research Center – also provide us with crucial and highly advanced scientific services.

The most comprehensive teaching programs

The School of Chemistry, as its name suggests, places considerable emphasis on education. A major aspect of our mission is nurturing a new generation of excellent scientists, equipped with tools for shaping the future of chemical research.

To this end, we have constructed an academic program that is truly unique in both scope and depth. We offer our students state-of-the-art teaching labs in the full range of focal disciplines – General Chemistry, Physics, Physical Chemistry, Organic Chemistry, & Analytical Chemistry – and require them to take a record number of laboratory classes. The extensive hands-on experience and strong knowledge foundation acquired in this way is invaluable for their future professional lives – whether in academia or in industry.

In the interdisciplinary spirit of the day, many of our students combine Chemistry studies with other disciplines, such as biology and physics. Keeping abreast of global trends, we will launch a totally new Chemistry & Material Science and Engineering program in the 2014-2015 academic year. Another relatively new study program, entitled chemistry – Research Track, targets our very best B.Sc. students. First offered in 2010, this innovative program has proved immensely successful in cultivating talented research students, becoming a model for several other schools at TAU.

How it All Began

Science pioneers on a bare sandy hill

By **Prof. Joshua Jortner**, Founder of the School of Chemistry at Tel Aviv University

The Institute of Chemistry, founded in October 1964, was one of the first facilities established on the new campus of Tel Aviv University in Ramat Aviv. I had the great privilege of being there – right from the hopeful, if still humble start of this now globally renowned department. And I remember it all very well:

Earlier that summer, the phone rang in my lab in Chicago, where I was doing my post-doctoral work – following a PhD at the Hebrew University in Jerusalem. "My name is Dr. George Wise, and I am the President of Tel Aviv University," said the voice at the other end. All I could say was: "What's Tel Aviv University…?"

Dr. Wise, a great Zionist and a man of outstanding vision and leadership, came to see me in Chicago. His proposal was very compelling for a young and aspiring scientist: "Come to our newborn, forward-looking University, and help us build a brand new Chemistry Department – literally from scratch."

Several months later I found myself climbing a sandy hill – to one of the first two buildings raised on the bare plot that was to become a flourishing green campus. My partner in the other building was my good friend and colleague Yuval Neeman – one of Israel's greatest scientists and a future President of TAU – who was charged with establishing the new Physics Department.

And so, breaking away from the West-European tradition prevalent in Israel at the time, I set about structuring a new kind of Chemistry Department, based on the modern American model. No less than a revolution in Israeli science of the 1960's, this meant uniting all disciplines – Physical Chemistry, Organic Chemistry, Inorganic Chemistry & Biochemistry – under one roof, and allowing all senior researchers maximum independence in their scientific work. The new unified formation facilitated extensive interdisciplinary collaboration, significantly boosting scientific excellence and achievements. At the same time, a major recruitment effort brought some most

PhD candidate Aviv Amirav (left) explains the workings of a molecular beam system to visitors Menachem Begin (2nd from left) and Shimon Peres (4th from left). Amirav's supervisor Uzi Even (right) looks on. The picture dates back to around 1980.

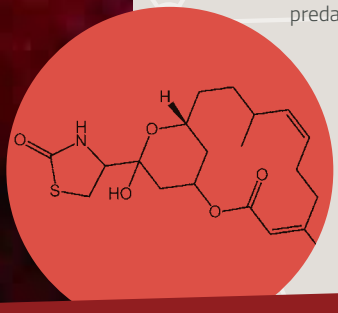
promising young chemists from Israel and abroad to the new Department in Tel Aviv, with each of our 30 scientists leading his own dynamic research group.

The new Department, it was decided, would blaze its own trails, focusing on fields that were as yet relatively untouched by other Israeli institutions – especially Chemical Physics, modern Physical Chemistry, Computational Chemistry & Electrochemistry, with NMR and Physical Organic Chemistry added a few years later.

The innovative model, experimental as it may have seemed in those days, proved highly successful. In 1968 the Department was simultaneously authorized by the Council for Higher Education in Israel to award all three academic degrees: BSc, MSc & PhD. By the mid-1970's, the Citation Index ranked our department 1st among all chemistry departments outside the USA. In 1985 Tel Aviv University recognized the accomplishments of its vigorous, world-leading Chemistry Department by granting it the status of School of Chemistry.

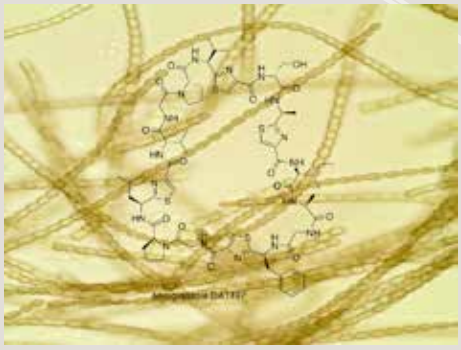
The President of Israel Chaim Herzog appoints Prof. Joshua Jortner President of the Israel Academy of Sciences and Humanities (1986). Over the years, scientists from TAU's School of Chemistry have won many prestigious prizes, medals, honorary degrees and memberships. The most notable of these have been: the Wolf Prize (Jortner), two Israel Prizes (Jortner, Nitzan), the EMET Prize, and many prizes from the American and Israel Chemical Societies.

The marine sponge Negombata magnifica pictured here produces Latrunculin toxins that inhibit the polymerization of Actin – a protein which plays a crucial role in muscle contraction and other critical functions. Latrunculins have become an important tool in cell biology research. In the photo, a shell-less mollusk (nudibranch) is seen feeding on the sponge, taking in the toxins as protection against predators (Prof. Yoel Kashman)



Bioorganic & Medicinal Chemistry

As science progresses, the borderlines between formerly very distinct fields of research grow increasingly hazy. In this interdisciplinary environment Bioorganic Chemistry serves as the interface between Chemistry and Biology, investigating biological processes with chemical tools and methods. Bioorganic chemists often apply their expertise to the development of novel pharmaceutical substances, a branch of science known as Medicinal Chemistry.

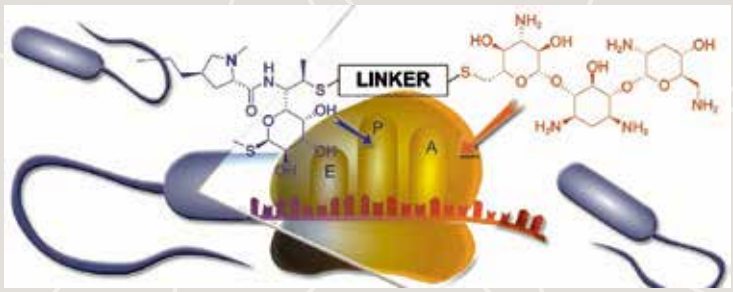


These new peptides, known as Aeruginazoles are derived from bloom-forming cyanobacteria collected in Israel. Recently isolated and characterized by chemists at TAU, they may serve as a basis for future medications. (Prof. Shmuel Carmeli)

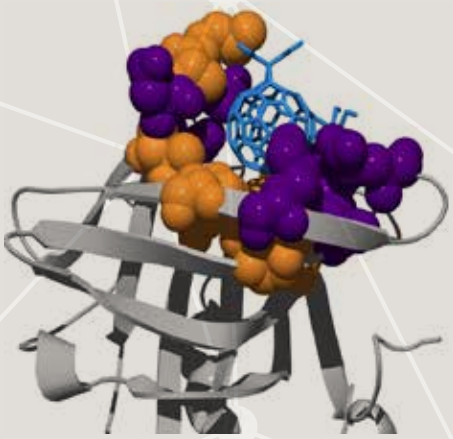
Our innovative research

Several Bioorganic Chemistry groups working at TAU's School of Chemistry propose a range of innovative approaches that may serve as a basis for effective future medications. These include:

- **Biologically active natural products** derived from marine organisms such as sponges and cyanobacteria. These powerful substances show substantial potential for treating a broad range of diseases, from cancer and neurological conditions to illnesses generated by microbes and viruses.
- **Self-immolative molecular systems,** an advanced type of targeted therapy. Once administered to the patient, these molecules remain inert and harmless until reaching their specific target – usually a tumor or infection. Here, special properties of the illness itself activate the system, causing it to disintegrate and release its medicinal 'cargo'.
- **Receptor-targeted drug delivery vehicles,** which, identified by the cell's outer defense systems, are able to penetrate the cell and effectively deliver the needed medication.
- **Anti-metabolic medication for cancer,** a novel strategy which blocks the malignant cell's energy-producing mechanisms by obstructing its ability to burn glucose (or other sources of energy) – thereby literally starving the ravenous tumor to death.
- **New antibiotics,** combating the ongoing process by which bacteria develop resistance to existing medications. These newly developed drugs target a range of infectious diseases that have been making an unwelcome comeback, killing millions every year.



Novel antibiotics, featuring a new approach to fighting infectious diseases. Small molecules developed in the laboratory penetrate the bacteria cell, fitting into specific cavities in the ribosomes responsible for constructing proteins. Here, the molecules are able to block the protein manufacturing mechanism, by either preventing the chemical reactions required for protein synthesis, or obstructing the nascent protein's movement. (Dr. Micha Fridman)



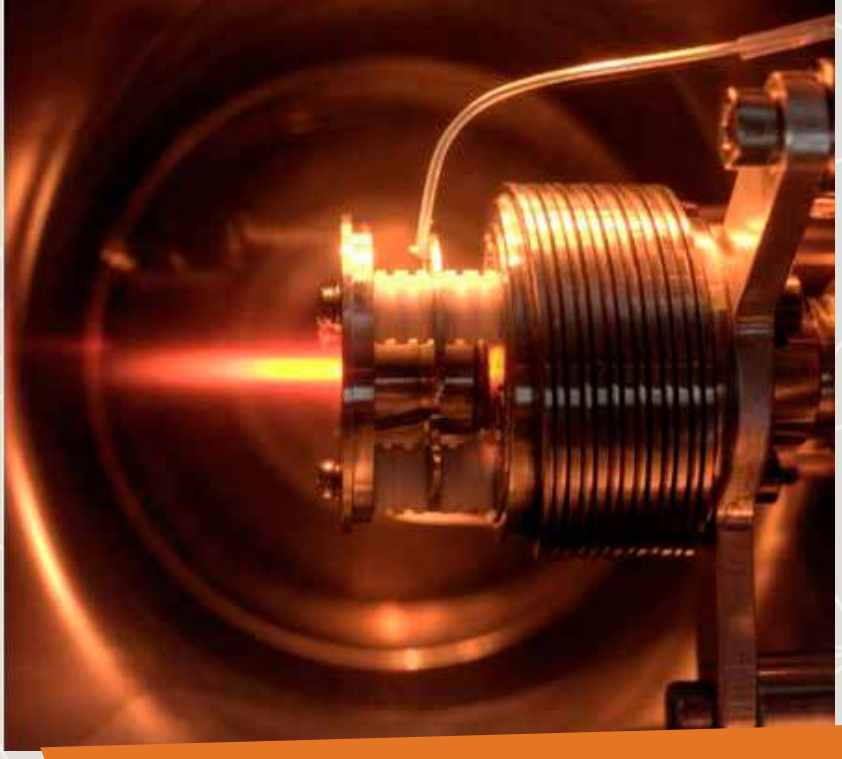
Studying the basis for toxicity of novel compounds. A new nanomaterial (blue) interacts with blood proteins (grey) and specifically with some of the proteins' amino acids (purple & orange) – in an experiment that tests whether the newly developed artificial substance is toxic or safe for use. (Prof. Michael Gozin)

Special achievements, patents & applications

Several drug developing groups at the School of Chemistry are collaborating with medical research groups for new drug development and testing. One study focuses on **new antipsychotic agents**, found to be efficacious against multiple schizophrenia-like symptoms, presumably through simultaneous action on a number of receptors in the brain. The prospective drugs are also intended to treat anxiety and depression, and to improve impaired social performance.

Our extensive research activity has already bred a number of patents, intended to bring these beneficial products and technologies to the medical marketplace:

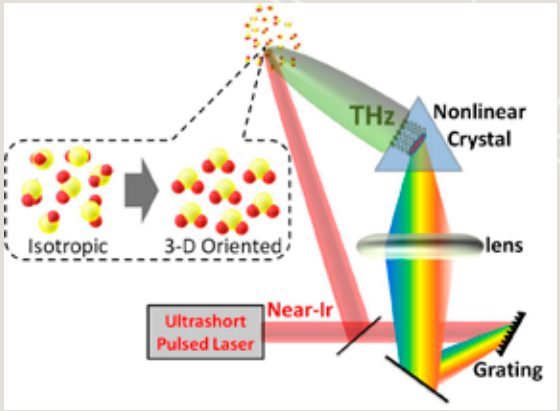
- A patent for effective anti-metabolic cancer treatments
- Patents for newly developed antibiotics



This unique pulsed gas valve, developed by researchers at TAU's School of Chemistry, is used in laboratories around the world. The valve forms an ultra-cold molecular beam that contains ions and radicals at a temperature below 1K. It serves as an important tool in fundamental studies of isolated molecules and their reactions, and is often used in conjunction with laser beams to probe the properties of cold molecular clusters. (Prof. Uzi Even)

Lasers in the Service of Chemistry

What happens when light meets matter? The answer to this intriguing question is fundamental to modern chemical research: interaction between light and matter reveals a great deal about the materials involved, and moreover, the energy of light can be used to actively change properties and behaviors of matter. To these ends, scientists use laser equipment which emits amplified beams of light, both within and beyond the visible spectrum. Advanced laser technologies implemented in today's laboratories include: spectroscopy, high resolution imaging, temporally ultra-short light sources, nonlinear optical processes and many more.

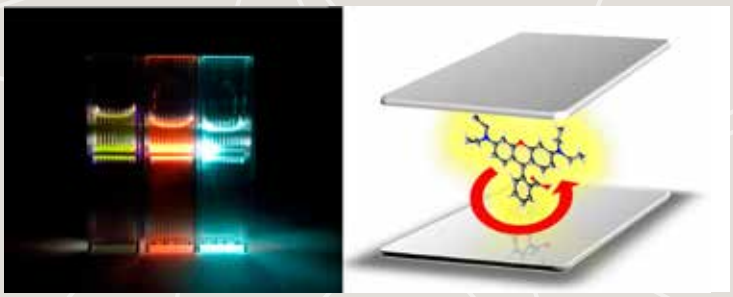


Controlling molecular dynamics – using strong laser fields to affect and study the molecular behaviors on ultra-short time scales (10^{-12}–10^{-15} seconds). In the proposed scheme, intense fields in the Near-Infrared and Terahertz regions of the electromagnetic spectrum provide two distinct 'control handles' over the molecular rotations, and their judicious combination is utilized for 3D-orientation of molecules in the gas phase – a goal pursued by scientists for many years. (Dr. Sharly Fleischer)

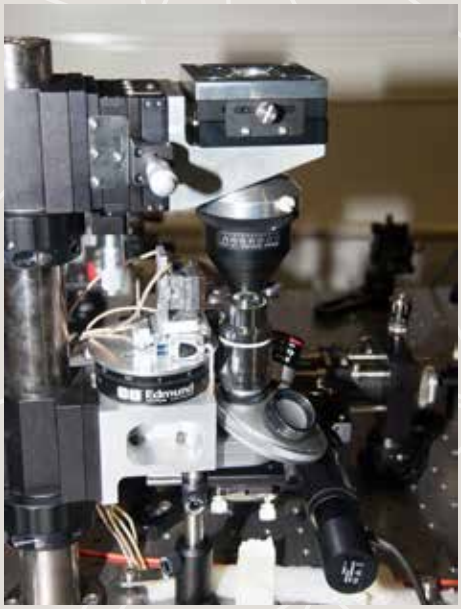
Our innovative research

Chemical physicists at TAU's School of Chemistry have been harnessing lasers to their multifaceted research for several decades. Studies that rely extensively on laser capabilities are:

- **Strong coupling** at the nanoscale, whereby light and matter become one entity.
- **Proton transfer,** using the energy of light to transfer a proton from one molecule to another within a solution, creating an acid for a very brief moment. This type of chemical reaction plays a central role in biology.
- **Controlling molecular dynamics** by energizing molecules in a gas or liquid phase, thereby studying their quantum properties.
- **Driving microscopic & macroscopic particles** in biological cells, for research in biophysics.
- **Flame spectroscopy,** exploring what happens to molecules under extreme conditions – as they burn.
- **Ultra-cold molecular beam spectroscopy,** investigating clusters of molecules at very low temperatures, near absolute zero.
- **Developing optical methods** for the study of phenomena at the nanoscale – capable of examining structures of no more than several dozen to a few thousand atoms.
- **Developing imaging & spectroscopy techniques** for investigating the chemical composition of DNA and other large bio-molecules.



Strong coupling. A light beam passing through organic molecules can interact with them to trigger fluorescence (left). When these molecules are placed between two mirrors (right) the emitted light is strongly confined, and the system of light & matter may start to behave as a single entity –with new quantum states and energy levels. This kind of coupling can be used to tailor photochemical reactions and molecular processes, possibly leading to novel types of organic light sources and light harvesting devices. (Dr. Tal Schwartz)

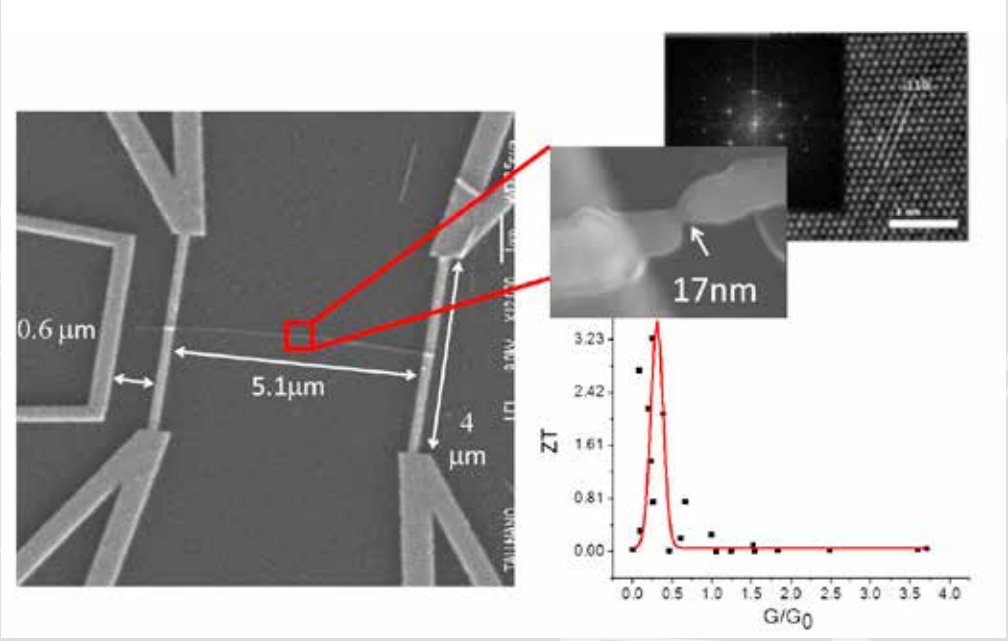


Super-resolution in microscopy of nano-objects. We develop novel microscopy techniques that allow us to observe nanoparticles one by one and study their properties, discerning details that cannot be seen with conventional microscopes. (Prof. Ori Cheshnovsky)

Potential applications

Laser-based technologies developed at the School of Chemistry may be used in the future to create a range of electronic, chemical and optical innovations, such as **ultra-sensitive sensors**, **photovoltaic materials** for harvesting solar energy, **organic light sources, clean combustion** and the chemical **mapping of DNA** – critical for advanced DNA-specific medicine.

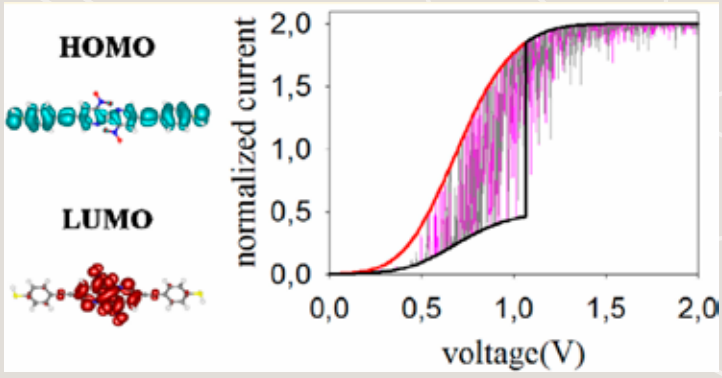
Other possible applications lie in the field of **terahertz technology**, which may enable highly efficient communication, harmless non-ionizing imaging and many other beneficial technologies.



An experimental circuit measures the efficiency of a one-dimensional thermoelectric cooler. Exhibiting unprecedented efficiency, such nanowire-based coolers may serve to cool nanoscale circuits in future nanoelectronic devices. (Dr. Yoram Selzer)

Nanometric Devices

Today's scientists are unraveling the secrets of the nano world – the minute dimension of molecules, atoms and their particles, seemingly governed by physical laws of its own. Here, in this emerging realm, materials behave very differently than they do in larger bulks, often revealing unexpected properties, which can be harnessed to produce an endless range of applications.

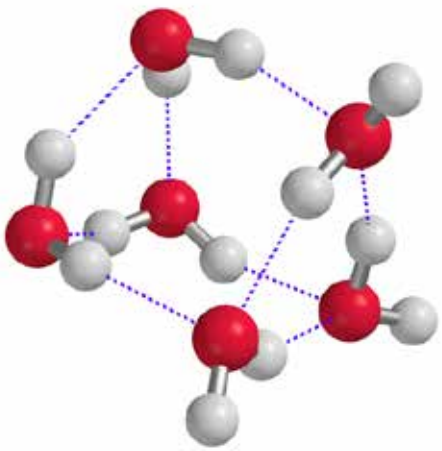


Different molecular states can be characterized by different localization properties of their electrons (left). These differences lead to a different ability to conduct (that is, to transfer electrons between two electrodes). Thus, molecular junctions made of varying molecular bridges can have several conduction states (right) – with potential applications in novel switching and memory devices. (Prof. Abraham Nitzan)

Our innovative research

Researchers at TAU's School of Chemistry have developed an impressive array of nanotechnological innovations. Their works focus on:

- **Developing nanoscale one dimensional materials for cooling and harvesting of thermal gradients for generation of electrical energy.** An innovative method to fabricate one-dimensional conductors with very high thermopower values and unusually low thermal conductivity are ideal for thermoelectrical applications, making the day in which such devices will replace household refrigerators much nearer.
- **Developing a range of highly sensitive chemical and biological sensors based on nanometric structures, each targeting a specific substance.** These cutting-edge sensors consist of semiconductor nanowires coated with a layer of miniscule receptors. The receptors detect and capture the target molecules and then send the message, through the wire, to the human user.
- **Developing methods for studying and measuring processes that occur inside a single molecule**. Trapping one molecule between two electrodes, researchers are able to study its reaction to various stimuli. An innovative technique developed in our labs exposes molecules to a combination of electric currents and laser spectroscopy – allowing scientists to examine and measure the molecule's dynamic properties, such as electric and thermal conductivity.
- **Studying electron transport dependent on magnetic fields at the nanoscale**. Researchers study magnetic properties and temperature-dependent magnetization dynamics in thin films of specially prepared magnetic nanocrystals.



The Water Prism. A 6 water molecule structure, one of many oligomers that populate surface and bulk water, first identified by thin film infrared spectroscopy, developed in TAU. (Prof. Edward M Kosower)

Special achievements & Applications

A number of **nanometric devices** originating from our laboratories are already being developed for the market by **commercial ventures**. To date, these novel applications include: an 'artificial nose' for detecting **explosives**, a straw that identifies GHB – better known as the the **date rape drug** – in a drink, a sensor that discovers malignancies through a simple **blood test**, and another that facilitates effective personalized **cancer treatments**.

In the field of **thermoelectricity**, the innovative methods introduced by our scientists could become essential in the development of highly effective nanoscale coolers for integrated circuits. Efficient cooling of hot spots that are prone to become failure points is critical for the prolonged high-speed performance of these circuits.

Films of **magnetic nanocrystals** prepared in our labs can be used as components in the fast developing field of **printed electronics**. For example, such films may serve to inexpensively ink-jet print magnetic field sensors for novel **contactless switches** and **motion sensing** applications.

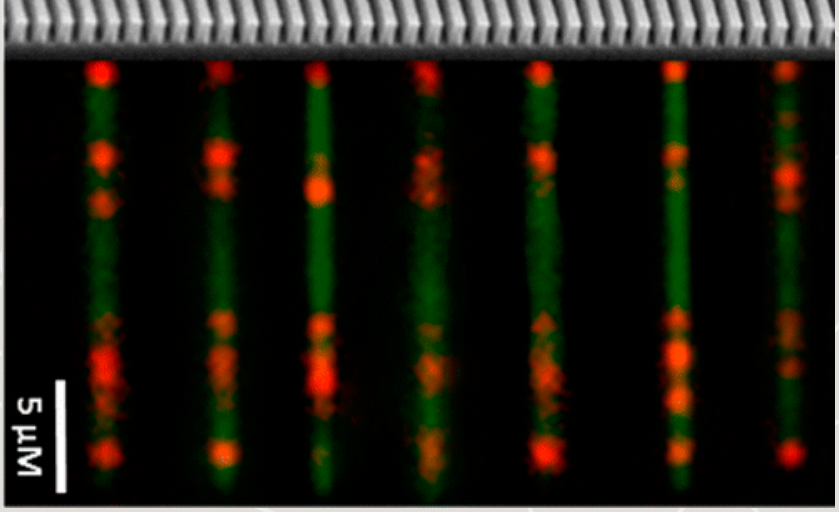


Image of DNA molecules, created with techniques of fluorescence microscopy. The red spots indicate genetic information, revealed as a fluorescent barcode along the DNA. Such views of individual DNA molecules enable the detection of rare sub-populations, carrying specific genes. (Dr. Yuval Ebenstein)

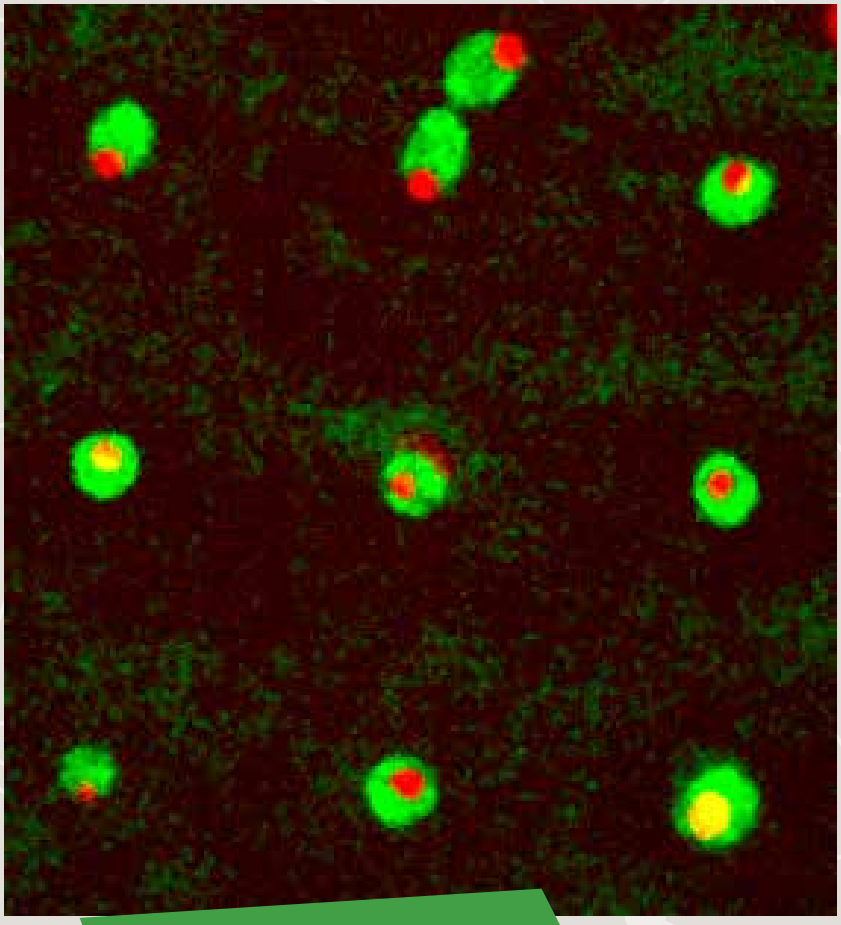


Image of yeast cells – their bodies dyed green with the nuclei in red. Arrays like this one, formed via a technique known as 'optical traps', are used to monitor cell growth, as researchers study the cells' reaction to various conditions and drugs. (Dr. Yael Roichman)

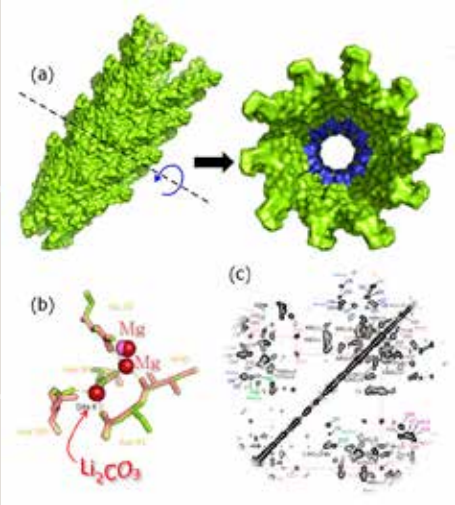
Biophysics

What can be more interesting than understanding the principles that govern life? This is precisely the mission of biophysics: searching for the simple, universal and quantifiable design of living cells and organisms – which are immeasurably more complex than the most sophisticated manmade technology. To do this, researchers employ tools created by many different scientific fields: from nanotechnology and biochemistry to fluorescence microscopy, NMR spectroscopy and advanced imaging techniques.

Our innovative research

At TAU's School of Chemistry, theoretical and experimental chemists collaborate closely with one another, complementing each other's efforts. Together they work to unravel riddles of the miniature realm of biological cells and their numerous components. Major issues addressed by their studies include:

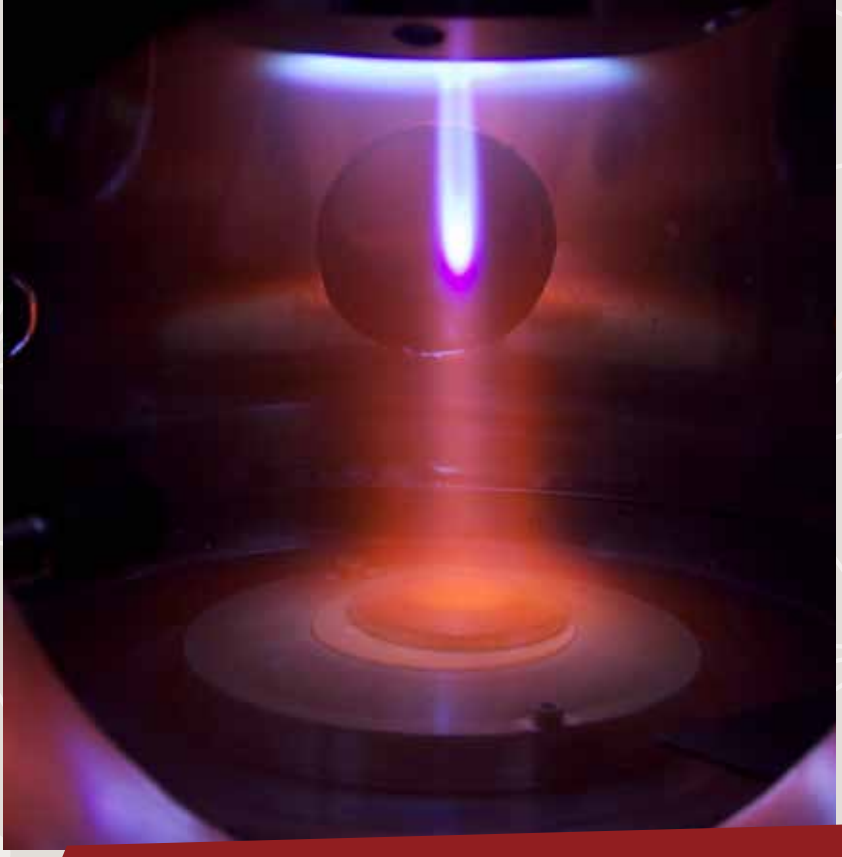
- **Biological molecules**, their structures and related chemical reactions. Main topics investigated involve the structure of DNA, protein structures, protein folding & unfolding and enzyme kinetics.
- **Biological cells,** their physical and mechanical properties. A special emphasis is placed on the outer membrane and cytoskeleton that hold the entire cell structure together, while facilitating the vital processes that take place inside.
- **Confinement & crowding,** their effects, mechanisms and possible roles in the functioning of biological cells. These studies carry special significance in living cells, wherein numerous proteins, nutrients, RNA molecules and a nucleus that contains a 2-meter-long DNA chain are all packed together in a very tiny space.
- **Inter-relations between the structure & function** of biological units. Researchers ask how nature designs specific structures to facilitate definite roles, focusing on a range of biological substances, such as enzymes, proteins and related bio-molecular complexes.
- **Transport in living cells.** Scientists investigate the movement of diverse biomolecules – inside the crowded cell, on its membrane, or passing in and out of the cell through the membrane.



NMR (Nuclear Magnetic Resonance) images of biomolecules and their chemical reactions: (a) The structure of a viral envelope. (b) Ions of lithium – the most common medication for bipolar disorder – bond with a specific protein. The NMR method allows researchers to follow the drug's mode of action. (c) Typical magnetic resonance spectra of various biomolecules – showing different frequencies for different atoms. (Dr. Amir Goldbourt)

Potential applications

Our research in biophysics may lead to the development of various **biomimetic products** – manmade machines and materials that imitate biological substances, principles or mechanisms. One of these, which already shows promising potential, is an innovative **nanoscale engine**, suitable for a range of useful functions.



Toward environmentally clean combustion. Spectroscopic flame chemistry research. (Prof. Sergey Cheskis)

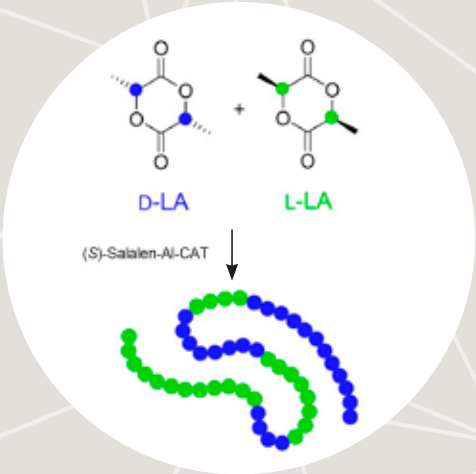
Green & Environmental Chemistry

Chemists play a major role in the global effort to protect our planet and minimize damage to the environment. Some, working in the field of Green or Sustainable Chemistry, develop new materials and processes that reduce the production of harmful substances; others, specializing in the related area of Environmental Chemistry, focus on the detection and analysis of chemical pollutants in our natural surroundings.

Our innovative research

TAU's School of Chemistry is the scientific home of several research groups in the fields of Green & Environmental Chemistry. Their innovations include:

- **Catalysts and catalytic processes that enhance the properties of polymers** (plastics)**.** Such catalysts affect the polymerization process, thereby changing the molecules' microstructure, and ultimately altering the material's properties. Controlling them enables developers to tailor polymers for specific applications – with environment- friendly attributes high on the priority list.
- **Catalysts leading to the production of novel forms of Poly(lactic-acid) –** a non-toxic, biodegradable plastic derived from annually renewable agricultural crops, such as corn or sugar beet.
- **Additives that change the solubility of substances in water.** This dramatic invention enables nonpolluting, recyclable water to replace highly polluting organic solvents as a medium for many chemical reactions. In the future, this innovation may contribute significantly to a reduction in industrial pollution.
- **Clean combustion** – improving the efficiency and reducing the polluting emissions of devices based on the combustion of fossil fuels, which currently account for nearly 90% of the world's energy supply.
- **Advanced instrumentation for the detection & analysis of environmental pollutants.** These state-of-the-art instruments, based on methods such as supersonic gas chromatography-mass spectrometry (GC-MS), enable faster and more accurate analysis of a greater range of substances.

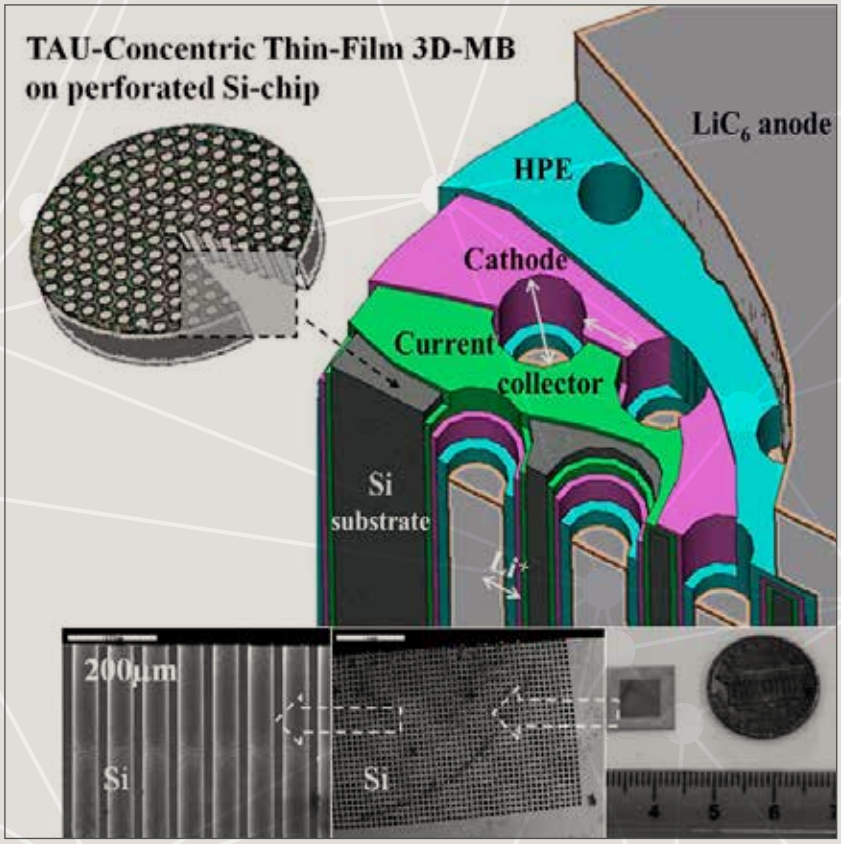


Molecules of the environment-friendly poly(lactic acid) polymers are manufactured through ring-opening polymerization. Induced by catalysts. This chemical process combines different monomers to form long chains – as shown in the illustration. Novel catalysts prepared at the School of Chemistry enabled the production of a new poly(lactic acid) with many potential applications. (Prof. Moshe Kol)

Special achievements & applications

Some of our innovations in Green & Environmental Chemistry are already proving useful in the universal drive for sustainability:

- **Catalysts developed in our laboratories have enabled the production of polypropylene with an exceptionally regular microstructure.** This novel polymer features superior physical properties, including the highest melting point ever recorded for plastic – 170°C. In the future, such strong, lightweight, transparent plastics may replace many traditional materials, improving both performance and efficiency, and reducing damage to the environment.
- **Many analytical instruments originating from our School are currently used worldwide to detect and monitor environmental pollutants.** Additional applications include field analysis of chemical warfare substances and the detection of drugs, explosives and pesticides.



An illustration of the 3D lithium-ion microbattery developed in our laboratories. Delivering the highest power and energy density values per area ever recorded, it may facilitate a range of medical and security-related applications, such as tiny ultra-sensitive sensors, cardiac pacemakers and other active medical implants. (Prof. Diana Golodnitsky and Prof. Emanuel Peled)

Alternative Energy

The modern way of life depends on power sources. From active medical implants to the latest smartphones, from solar and wind energy systems to the electric cars of the future – our cutting-edge devices all require new, efficient and environment-friendly ways to store energy and generate electric power. Looking for novel solutions, scientists around the world labor to develop high-performance batteries that are ever smaller, lighter, greener, more powerful, longer lasting *and* less expensive than any of their predecessors.

Our innovative research

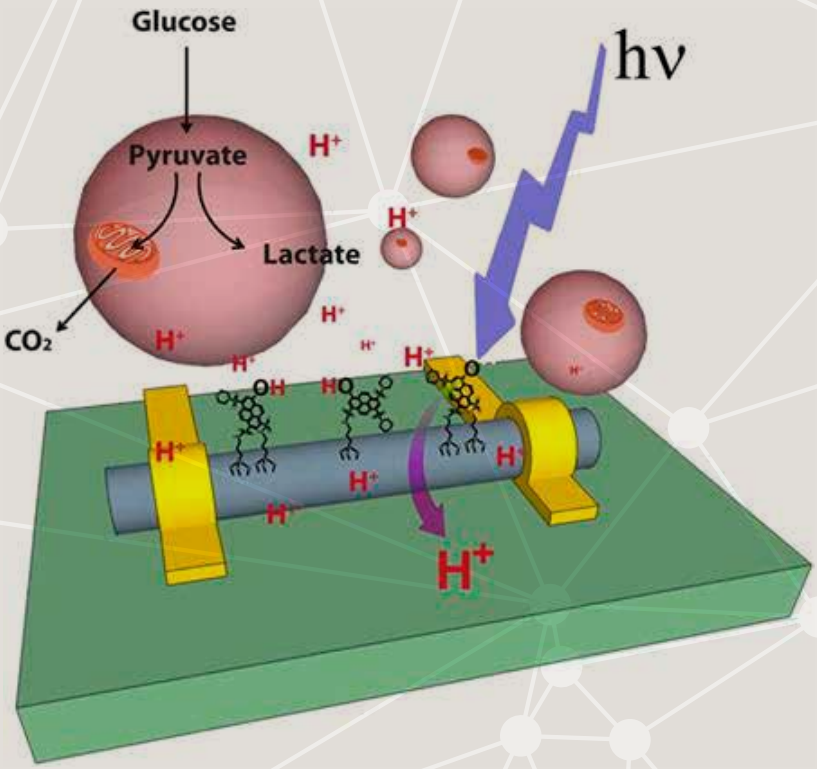
Researchers at TAU's School of Chemistry are responsible for some of the greatest advancements made in recent decades, with regard to power generation, energy storage and miniature sources of power. Their groundbreaking innovations include:

- **The revolutionary SEI model for lithium batteries,** which transformed the entire field of alkali batteries in 1979, ultimately enabling the development of a viable lithium battery. Approximately 200,000 studies presented since that time, and 75% of all relevant research papers published today, are based on this pioneering work.
- **The world's first 3D lithium-ion microbattery,** which has maintained its critical edge over all others for over a decade. The microbattery, which delivers the highest power and energy density values per area ever recorded, consists of a perforated silicon wafer with 10,000-30,000 through-holes, each containing a complete nanoscale lithium battery.
- **Innovative wide-operating-temperature-range fuel cells,** based on novel catalysts, nanotextured electrodes, fuels and membranes. These highly efficient and relatively inexpensive systems are capable of storing vast quantities of energy, and then transforming them into electric power.
- **Sodium-air batteries**, as well as critical improvements for **lithium-air** and **lithium-sulfur batteries**. All these innovative types of batteries are lighter, less expensive, more powerful and longer-lasting than the lithium-ion batteries used today.
- **Highly conductive solid polymer electrolytes,** enabling the development of safer lithium batteries that contain no inflammable solvents, and may be used, for example, in electric vehicles.

Achievements & applications

High-quality **lithium batteries** based on our scientists' SEI model are used today to power all mobile devices – including smartphones, laptops, iPads, digital cameras and more, as well as electric vehicles. Looking to the future, the **sodium-air, lithium-air & lithium-sulfur batteries** currently under development in our labs will provide improved performance, enabling electric vehicles to cover distances of up to 500 km without recharging.

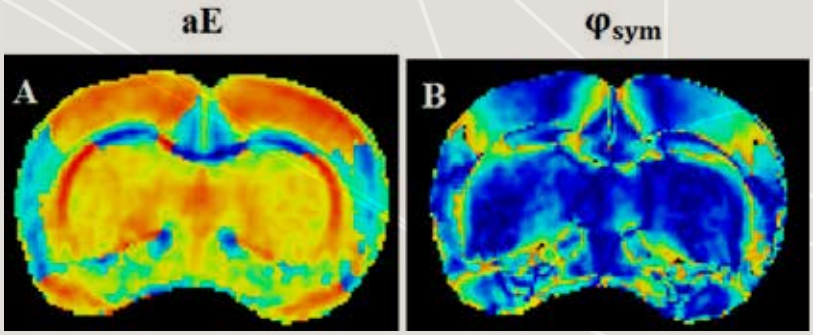
In addition, our advanced energy technologies have served as the basis for the establishment of three startup ventures, developing a range of novel solutions: fuel cells for storing vast quantities of energy produced by solar and wind farms; a device for measuring the time remaining in lithium batteries; and 3D lithium–ion microbatteries powering state-of-the-art security and medical devices – such as cardiac pacemakers and ultra-sensitive sensors.



A nano-sensor. The sensor captures biomarkers and reports its findings via an electrical current that runs through the nanowire. (Prof. Fernando Patolsky)

Biomedical Diagnostics

The critical field of biomedical diagnostics, focusing on the imaging and detection of specific conditions and pathologies in the human body, and is in many ways a form of analytical chemistry. Researchers involved in this area develop substances that mark or bond with the condition's indicators, as well as methods for delivering the findings in readable formats.

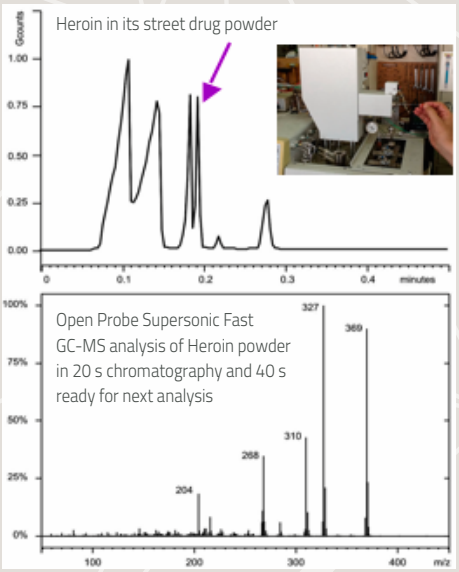


These advanced diffusion MRI images of a rat's brain were obtained by means of an innovative technology known as double PFG-MRI, which was developed, inter alia, at TAU's School of Chemistry. The method allows us to compute, for example, the apparent eccentricity – or deviation from a spherical shape – of various brain compartments. (Prof. Yoram Cohen)

Our innovative research

Work done today at TAU's School of Chemistry is recognized as the cutting edge of modern biomedical diagnostics. The novel approaches developed by our scientists include:

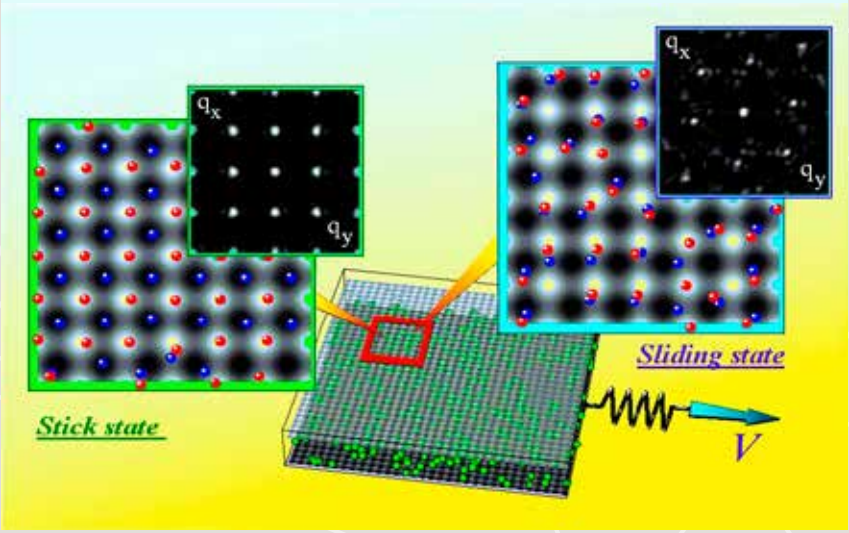
- **Specially tailored organic molecules and supra-molecular assemblies** to be used in diagnostic assays (test kits). Once exposed to the tested matter – such as a blood or urine sample – these innovative substances bond with the targeted biomarkers, quantify their presence, and then report their findings through various mechanisms (light, color change, electrical currents etc.), also incorporated into the diagnostic molecule.
- **Highly sensitive nano-sensors** consisting of nanowires encased in a layer of biological receptors**.** Biomarkers captured by the receptors change the sensor's electrical environment at the nanoscale, sending an indicative electrical current through the nanowire – to the human reader.
- **Groundbreaking methodologies enabling the examination of single DNA molecules.** Using chemical reactions to paint genetic information, researchers then squeeze the molecules 'in single file' through nanometric channels, and view them individually with a special microscope, equipped with advanced optical imaging. This novel technique attains unprecedented accuracy in analyzing DNA and detecting abnormalities along its molecules.
- **Innovative tools that enhance the effectiveness of NMR & MRI diagnostics.** These include: novel diffusion MRI methods to obtain microstructural information in the central nervous system (CNS) non-invasively, novel **contrast agents**, delivering magnetic resonance signals to indicate findings in the imaged tissues; advanced **algorithms** to control, process and interpret these signals; and new **imaging modes** for ultimately viewing the collected information.



These graphs, produced by a novel analytical instrument developed by our scientists, show positive ID of heroin powder. Such devices can also aid in the detection and analysis of a broad range of substances, including environmental pollutants, forensic samples, fuels, foods, medically significant agents and pharmaceuticals. (Prof. Aviv Amirav)

Achievements & potential applications

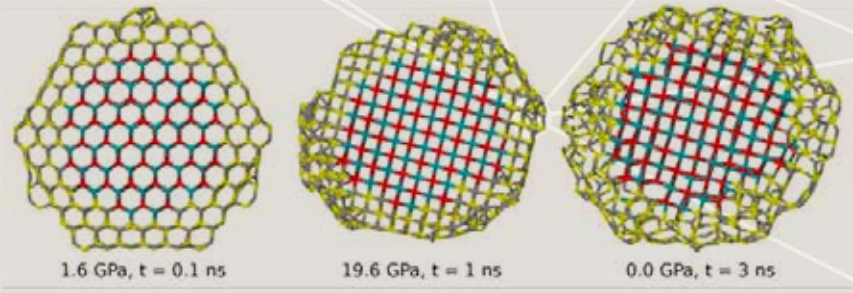
Future diagnostic techniques based on our novel methodologies may be used to detect a vast range of conditions – from cancer and diabetes to infections, pregnancy and many more. Due to their remarkable sensitivity, these technologies will be able to spot even minute signs of developing diseases, enabling medical professionals to diagnose pathologies at a very early stage. Our new diffusion MRI methods enable us to study of microstructural changes in the CNS totally non-invasively and to follow brain maturation and degeneration.



A nanoscale model of a lubricant in two different states: static and sliding. The lubricant, consisting of two types of molecules (red & blue), is applied in a single molecular layer (monolayer) between two surfaces. Organized in a tetragonal lattice in the locked state (left), the lubricant's structure changes to a hexagonal low-friction lattice when sliding (right). (Prof. Michael Urbakh)

Theoretical & Computational Chemistry

The great English physicist and 1933 Nobel Prize Laureate Paul Adrien Maurice Dirac wrote in 1929: *"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble..."* Dirac then tasked his scientific successors with developing "approximate practical methods" of application, and generations of theoretical & computational chemists have been striving to fulfill that mission ever since. Thus, over the decades – and especially with the advent of ever more powerful computers – many methods for modeling the properties of chemical systems have been developed, both predicting and explaining experimental results.



A computer simulation of cross sections of a rock salt nanocrystal, with its shell (yellow) and core (red & green) altering their structures under varying degrees of ambient pressure. (Prof. Eran Rabani)

Our innovative research

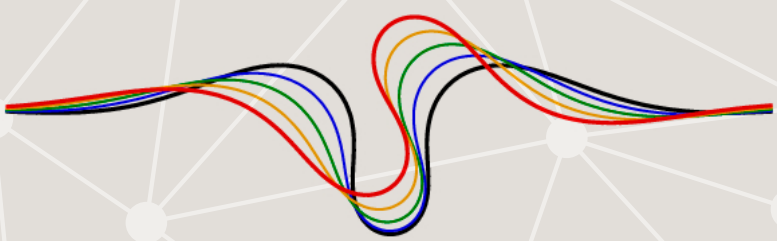
Since its early beginnings, TAU's School of Chemistry has been a world leader in the field of Theoretical & Computational Chemistry, establishing a proud tradition of outstanding, highly diverse research. Our significant contributions in this area include:

- **Laying the scientific foundations for the new field of molecular electronics**, which studies the conduction of electricity through single molecules and their application in future nanoelectronic devices.
- **Deciphering the dynamics of charge transfers in closed systems,** which play a major role in critical biological processes such as photosynthesis.
- **Modeling random walks** – conceptually simple and very powerful computational methods for obtaining important information about highly complex and typically random natural processes – in the realms of physics, chemistry and biology.
- **Predicting the structural and electronic properties of nanocrystals**, and how they self-assemble to form ordered arrays, such as spheres, rods and wires.
- **Understanding how soft biological materials and complex fluids are organized**, and how they respond to various forms of stress.
- **Basic and applied computational nanomaterial science,** modeling the mechanical, dynamic, electronic, magnetic, optic and conductivity properties of systems at the nanoscale, and how these properties may be tailored through chemical processes – to rationally design new materials with desirable attributes.
- **Studying the tribological properties of materials at the nanoscale** – namely developing methods for the modeling and simulation of friction, ware, and lubrication occurring at nanoscale materials interfaces.
- **Conversion of laser energy into nuclear energy via a Coulomb explosion of nanostructures** – ultrafast laser pulses driving tabletop nuclear fusion reactions by creating multi-charged states in nanostructures.

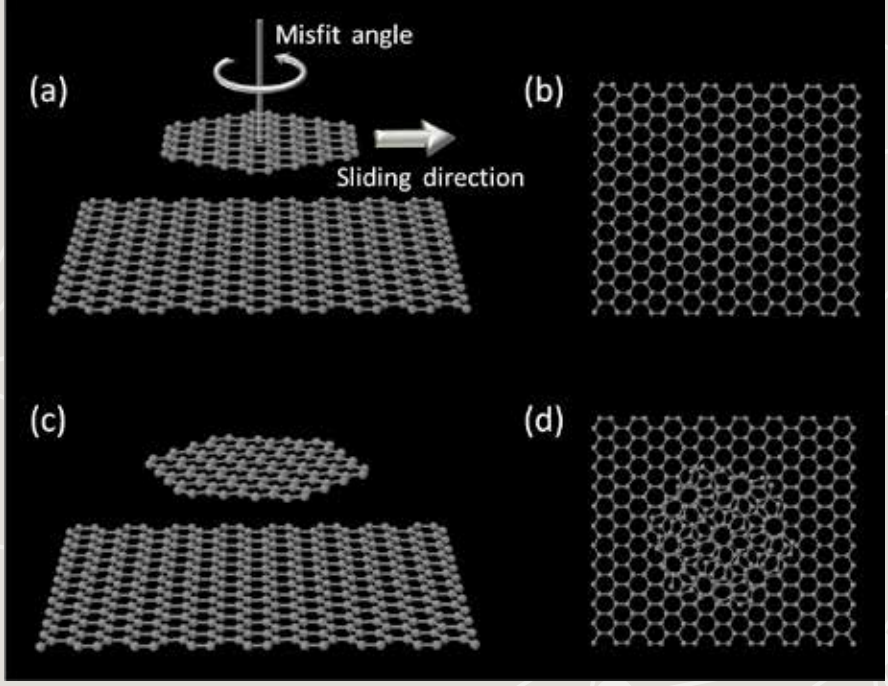
Potential applications

Our highly diversified research can lead to the development of a vast range of useful innovations such as:

Materials featuring exceptional **strength** and/or **flexibility**; materials with **no friction** at the nanoscale – for applications such as **dry lubricants** that reduce engine wear to a minimum; the new field of **molecular electronics**, enabling the use of molecules as components of novel computers and electronic devices; **molecular magnets** for next-generation computer **memories**; high-efficiency **solar devices** based on nanostructures; ultra-sensitive chemical **sensors** for a range of application such as detecting explosives; nanodiamond-based biological **markers** for high-resolution diagnostic **imaging**; artificial **membranes** for **medical** applications; and more.



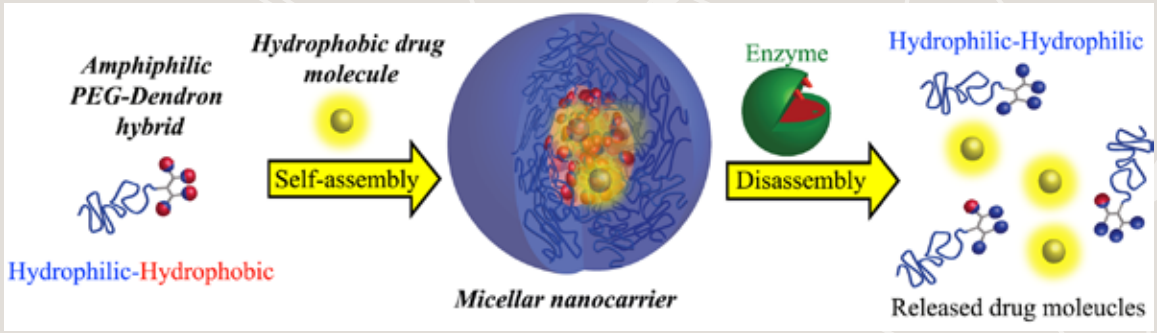
This figure represents a new mathematical model for folds formed in rigid thin sheets overlying fluid materials, when subjected to lateral pressure. The model, simulating processes in biological membranes and similarly structured composite materials, reveals a new type of symmetry, with the deformation changing continuously from a symmetric fold (black) to an anti-symmetric one (red), without any energy cost. (Prof. Haim Diamant)



Computational models of nanoscale superlubricity. In the model a hexagonal graphene flake slides atop a graphene layer at varying angles aiming to identify the conditions under which a frictionless interface may occur. (Prof. Oded Hod)

Advanced Materials

From the Stone Age through the Bronze & Iron Ages to the Modern Era, mankind's technological capabilities have always been governed by available materials and the techniques developed to process them. Today, living in what may be labeled the Age of Nanotechnology, we are no longer dependent on nature to produce our raw materials. Present-day scientists are able to design new materials at the most basic atomic or molecular levels, creating advanced materials with novel properties, tailored precisely to our needs.

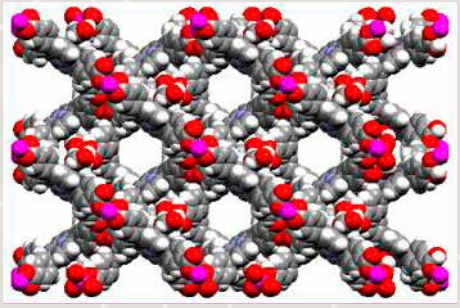


Enzyme-responsive drug carrier. Amphiphilic polymers self-assemble into carrier particles in a water-based solution, encapsulating the pharmaceutical substance (yellow). Encountering a specific enzyme (green) at the targeted site in the body (such as an infection or tumor), the particle breaks apart and releases the drug. (Dr. Roey Amir)

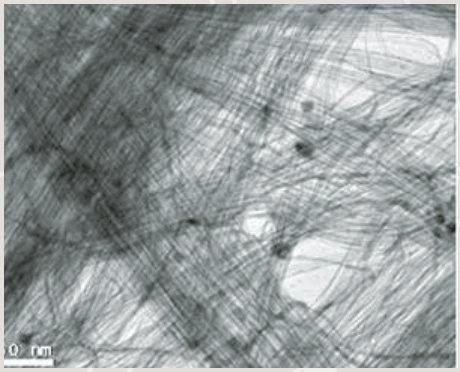
Our innovative research

Several research groups at TAU's School of Chemistry are laboring within the broad cutting-edge field of Advanced Materials, designing, synthesizing and characterizing a range of novel nanomaterials. Their varied investigations focus on:

- **New supra-molecular metal-organic frameworks (MOF) –** self-assembling meso- or nanostructures, in which various organic molecules serve as building blocks, bonded together by metal atoms;
- **Novel inorganic nanomaterials, nanocrystals and metamaterials,** their physical properties, such as electric conductivity, magnetism and optical features, as well as efficient chemical methods for manufacturing them.
- **Stimuli-responsive polymers & block copolymers** that self-assemble and then disassemble in the presence of specific enzymes.
- **Special properties of graphene –** a 2D sheet of carbon atoms, and other single-layer materials.



Robust 3D metal-organic framework (MOF) based on organic compounds known as porphyrins. The perforated diamondoid architecture is highly suitable for gas storage applications. (Prof. Israel Goldberg)

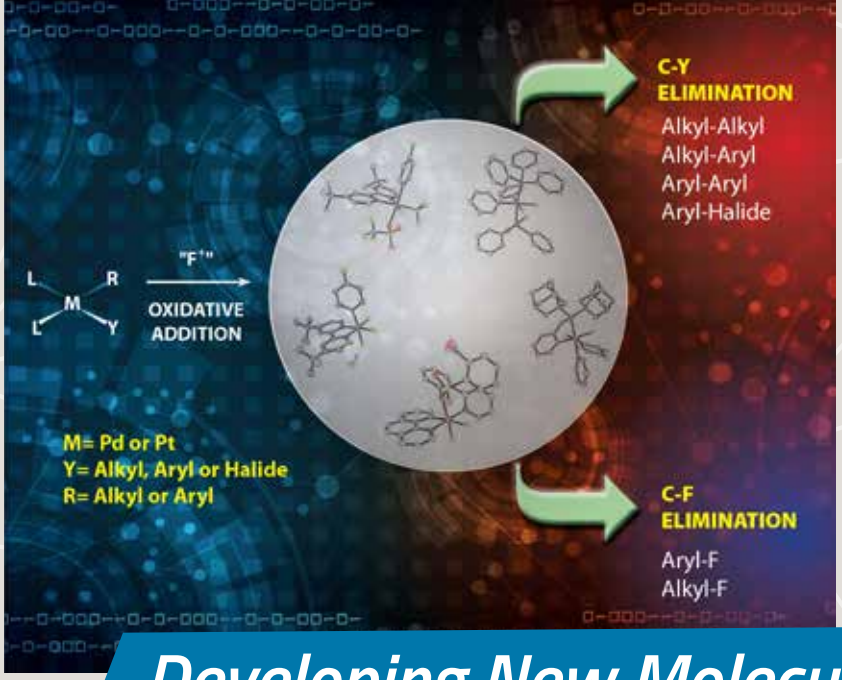


An ultra-thin film of gold nanowires – each only several nanometers thick. Such films may be used as transparent and flexible electrodes in various next-generation flat-panel displays and photovoltaic devices. The film is deposited on the relevant surface through a simple cost-effective process: printing or dipping in a water-based solution. (Prof. Gil Markovich)

Potential applications

The range of potential applications for the advanced materials developed and studied in our labs is immense:

- **Supra-molecular metal-organic frameworks** are essentially large perforated nets, within which various molecules may be trapped for storage – facilitating applications such as: enantio-selective catalysis; capturing CO_2 and transforming into fuel, thereby reducing the emission of greenhouse gases; high-efficiency photovoltaic cells; storing hydrogen to be used as fuel; and other gas storage applications.
- **Inorganic nanomaterials** may enable the development of numerous innovations such as: transparent and flexible conductors for displays in the next generation of electronic devices; giant solar panels; nano-antennas for high-efficiency photovoltaic cells; self-defrosting windows; new types of optical elements; and printable magnetic sensors for touchless switches and motion sensing.
- **Enzyme-responsive polymers** have great potential as synthetic drug carriers inside the human body. Harmlessly delivering encapsulated pharmaceutical substances, they will then break apart in response to specific enzymes produced by the targeted tumor or infection – thereby releasing the medication at precisely the right location.
- **Graphene** and other 2D nanomaterials may be used to develop chemical sensors with unprecedented sensitivity, as well as lubricants that reduce friction to negligible levels, preventing wear and saving energy in any number of future mechanical devices.



Synthesizing new organic molecules. By adding an atom of Fluorine (F) to an organometallic precursor molecule (far left), we can selectively and uniquely trigger the formation of new chemical bonds. The resulting molecules can contain fluorine (bottom) or other elements (top). (Prof. Arkadi Vigalok)

Developing New Molecules

Chemistry deals with the understanding of matter at the molecular level. For the past three and a half centuries, chemists have explored how molecules bond and dissociate, are assembled and disassembled, and interact with one another and with the environment. They have also investigated how properties of individual molecules translate into the properties of bulk materials – built of moles of those same molecules. Today's scientists take all this knowledge one step further: rather than study existing molecules, they seek to create new ones – with properties tailored at will, to serve numerous beneficial functions.

A dendrimer (a branched 'tree' molecule) used as a drug delivery vehicle for targeted therapy. Acting as a molecular amplifier, the dendrimer releases chemotherapeutic agents (blue) that attack the cancer cells. (Prof. Doron Shabat)

Our Innovative Research

Many scientists at the School of Chemistry, and particularly in the Organic Chemistry Department, are involved in cutting-edge projects for the development of new molecules. Their front-line inventions include:

- **Novel pharmaceuticals** targeting a broad array of diseases – from cancer and infections to schizophrenia and neurological disorders;
- **Chemically modified analogues of natural bioactive molecules** that may have medicinal qualities;
- **Molecular drug delivery systems** that release their medicinal cargo exactly where it is needed inside the body;
- **A range of smart molecules for medical imaging,** enhancing techniques such as MRI, CT, neuro-imaging and PET scans, and thereby enabling early and accurate detection of pathological conditions;
- **Molecular sensors for medical diagnostics** – such as detecting the presence in the body of hydrogen peroxide (H_2O_2), an important biomarker that could indicate abnormal physiological conditions characteristic to certain diseases;
- **Reagents enhancing fluorination processes** that are widely used in the pharmaceutical industry;
- **Reagents promoting oxidation processes** that significantly alter the properties of receiving molecules; among other effects, such reagents are able to improve semi-conducting properties of organic polymers for the future microelectronics industry;
- **Novel polymers** with exceptional physical properties, such as extra strength and a very high melting point;
- **Metal-based catalysts** facilitating the synthesis of innovative polymers and other new molecules with specially tailored properties;
- **Solid-supported catalysts** which can be easily removed once the chemical reaction has been completed, and in some cases even reused – promoting environmental friendliness;
- **Molecular sensors** for detecting very small amounts of various substances, such as explosives and air-polluting NO (nitric oxide) emissions.

Methodology for solid-phase synthesis of dendrons and their conversion into polymer-supported multivalent catalysts leads to more efficient and selective catalytic processes. (Prof. Moshe Portnoy)

The versatile nature of elemental fluorine. It can produce very important fluoro-organic compounds, in radical, nucleophilic or electrophilic mode at will, used, for example, as tracers for PET imaging. What is more, it is an unique tool for constructing important, but difficult to come-by, quite a few types of fluorine-free organic derivatives. (Prof. Shlomo Rozen)

Potential applications

New molecules developed by our scientists are geared for significant impact on a range of spearhead industries: **The biomedical industry**, constantly in search of new medications, more effective diagnostics and breakthrough drug delivery technologies; the **microelectronics industry**, urgently looking for totally new types of semiconductors and novel electronic components; and the **plastics industry**, striving to produce ever more durable, environment-friendly and cost-effective materials – to mention just a few.

Faculty Members & Their Fields of Research at the School of Chemistry

Amir Roey: Design and synthesis of advanced polymeric hybrids and their assembly into functional nanostructures for applications ranging from nanomedicine to materials science.

Amirav Aviv: Development of novel state-of-the-art analytical instrumentation.

Bar-Eli Kedma (Emeritus): Chemical oscillators.

Ben-Reuven Abraham (Emeritus): Bose-Einstein condensates and chemistry, quantum chaos.

Bixon Mordechai (Emeritus): Electron transfer in biomolecules.

Carmeli Shmuel: Natural products chemistry, chemical ecology, biosynthesis of natural products.

Cheshnovsky Ori: Raman spectroscopy of nanostructures, label free super-resolution microscopy, absorption microscopy of individual nano-objects.

Cheskis Sergey: Laser absorption spectroscopy, flame chemistry.

Cohen Yoram: Supramolecular chemistry, molecular capsules, diffusion NMR, diffusion MRI of the CNS, molecular and cellular MRI, contrast agents for MRI.

Diamant Haim: Structure and dynamics of complex fluids and soft matter.

Ebenstein Yuval: Nano-bio-photonics, single molecule genomics.

Even Uzi (Emeritus): Ultra cold molecular spectroscopy, quantum properties of clusters.

Fleischer Sharly: Coherent rotational control, THz spectroscopy and ultrafast molecular dynamics.

Fridman Micha: Glyco chemistry and biology, design of antitumor agents.

Fuchs Benzion (Emeritus): Supramolecular chemistry, macrocyclic systems stereochemistry, photochemistry, theory vs. experiment.

Gileadi Eliezer (Emeritus): Alloy deposition, studies of electrolyte/metal interface, theory of charge transfer in metal deposition and dissolution.

Goldberg Israel (Emeritus): Crystal engineering, supramolecular chemistry, crystallography, framework solids, porphyrin assembly.

Goldbourt Amir: Elucidation of structure and dynamics of biomolecules, biomolecular assemblies, and inorganic materials by magic-angle spinning solid-state NMR.

Golodnitsky Diana: Advanced materials, thin films for electrochemical energy storage and conversion.

Gozin Michael: Medicinal chemistry, protein chemistry, forensic chemistry, fullerene Chemistry.

Hod Oded: Computational nanomaterials science, physical and chemical properties of nanosystems, electron dynamics in open quantum systems, transport in molecular and nanoscale junctions.

Huppert Dan (Emeritus): Proton-transfer reactions, solvation dynamics, ultrafast events.

Jortner Joshua (Emeritus): Energy acquisition, storage and disposal in large molecules, clusters, nanostructures and biomolecules.

Kaldor Uzi (Emeritus): Structure and properties of heavy elements, quantum dots, relativistic effects.

Kashman Yoel (Emeritus): Marine natural compounds, peptide synthesis.

Kirowa-Eisner Emilia (Emeritus): Electroanalytical chemistry, under potential deposition, environmental studies.

Klafter Joseph: Anomalous kinetics, random walks, electron transfer & light harvesting, nanotribology.

Kol Moshe: Design of novel catalysts for polymerizations, asymmetric catalysis.

Kosower Edward (Emeritus): Surface-enhanced infra-red spectroscopy of thin films.

Markovich Gil: Magnetic and ferroelectric nanocrystals, metal nanorods and nanowires, nanoscale chirality and plasmonics.

Navon Gil (Emeritus): Biomedical applications of NMR and MRI.

Nitzan Abraham (Emeritus): Chemical dynamics, molecular electronics, transport phenomena at the nanoscale.

Patolsky Fernando: Design, synthesis and applications of nanostructured materials.

Peled Emanuel (Emeritus): Fuel cells, micro-batteries, thin-film cathodes, conducting membranes.

Portnoy Moshe: Synthesis on solid support, catalysis, dendrimer chemistry.

Rabani Eran: Stochastic electronic structure methods, nonequilibrium quantum dynamics, structure and electronic properties of nanomaterials.

Roichman Yael: Soft condensed matter, complex fluids, granular materials.

Rozen Shlomo (Emeritus): Fluorine chemistry and the art of inventing novel reagents for synthesis.

Schwartz Tal: Light-matter interaction in nanometric molecular systems.

Selzer Yoram: Molecular electronics, quantum transport in molecular systems, plasmonics.

Shabat Doron: Self-immolative dendrimers and polymers, chemical adaptor systems, molecular amplification, molecular probes for diagnosis and cancer imaging.

Shmueli Uri (Emeritus): Crystallography, symmetry- and composition-dependent crystallographic statistics, resonant scattering.

Urbakh Michael: Theory of atomic scale friction and interfacial electrochemistry.

Vigalok Arkadi: Green chemistry, metal-mediated formation of carbon-halogen bonds, calixarenes for catalysis and sensing.

The 50th Anniversary of the School of Chemistry