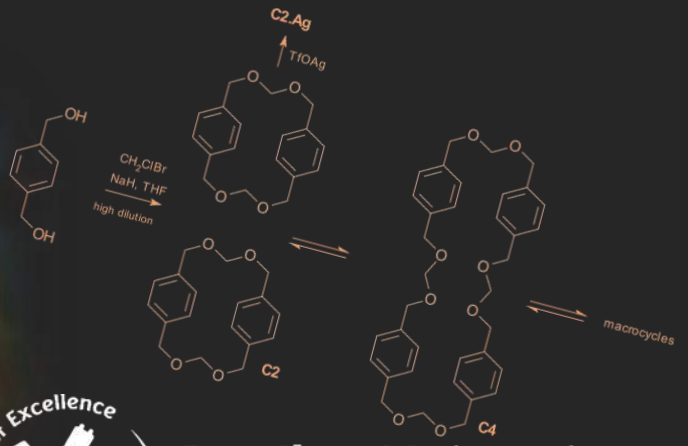
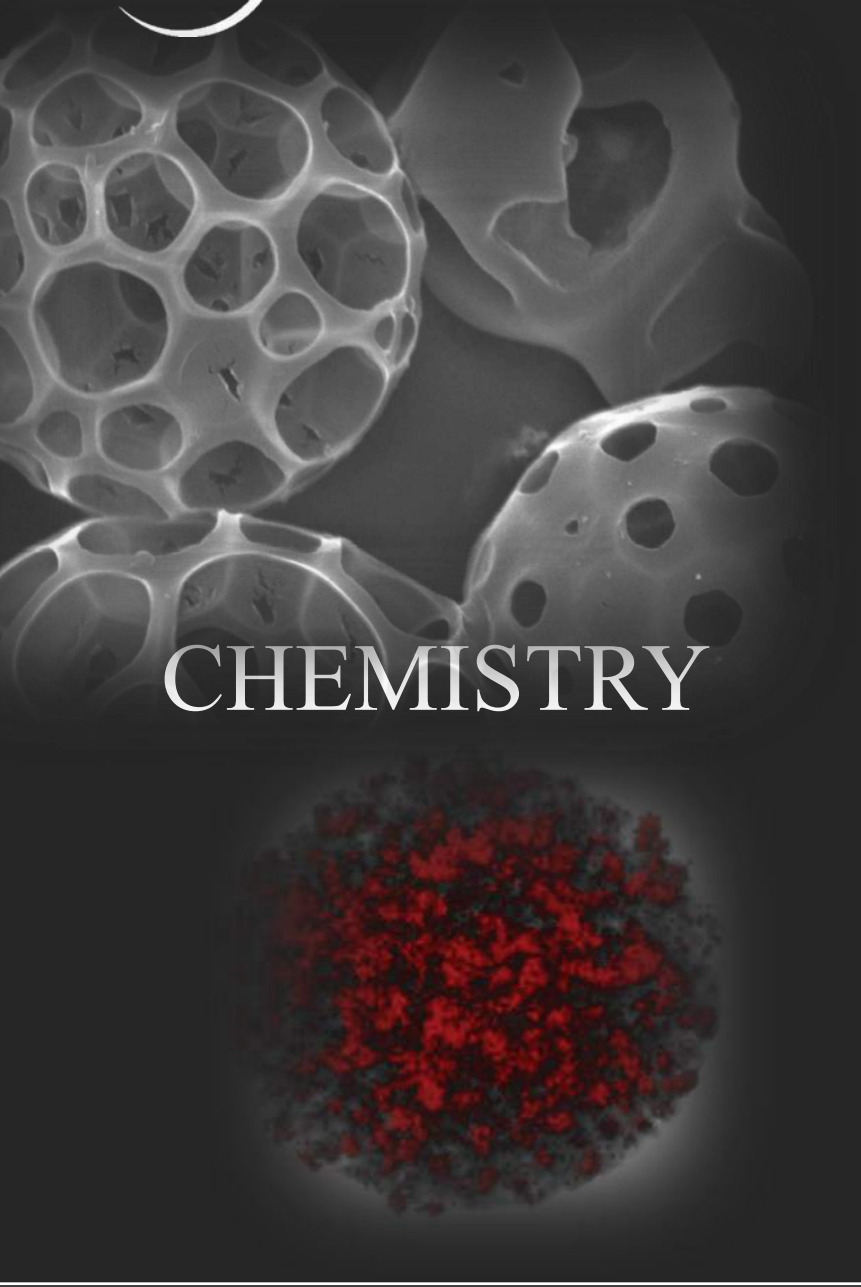


Tradition of Excellence

Bar-Ilan University
אוניברסיטת בר-אילן



CHEMISTRY

Department of Chemistry

Chemistry was one of the first subjects to be taught at the inauguration of BIU in October 1955.

The Chemistry Department is currently in an unprecedented growth phase. The department has recruited several young researchers, branched into new research fields, and completed the building and staffing of the BINA nano-technology center.

The department offers three undergraduate programs - a comprehensive chemistry track, medicinal chemistry and material chemistry.

In addition, the department offers graduate programs including an original dissertation in a wide variety of disciplines such as medicinal, theoretical and computational, biological, organic and inorganic, physical and polymer chemistry, as well as nano-chemistry, and solar and renewable energies.

Two major changes in recent years have propelled the department forward. Twelve new faculty members have been recruited in a variety of disciplines of chemistry. The department now possesses new capabilities in fields such as computational chemistry, structural biology, magnetic resonance, bio-inorganic chemistry, and nano-materials and devices, alongside the more established fields of medicinal chemistry, organic, inorganic and physical chemistry.

No less important was the founding in 2007 of BINA, the Bar-Ilan Institute of Nanotechnology and Advanced Materials. This enterprise, with which 12 chemistry research groups are affiliated, is committed to advancing scientific achievements in the areas of nano-materials, nano-medicine, nano-energy, nano-magnetism, nano-photonics, and nano-cleantech. In October 2009 six research groups moved into state-of-the-art laboratories in the Nanotechnology Triplex building. The BINA center brought with it courses, study programs and scholarships for students in the fields of material science, and strengthened the chemistry department considerably.

Scientific Equipment Center

Nuclear Magnetic Resonance

Bar Ilan's nuclear magnetic resonance (NMR) unit is one of the largest in Israel and includes 6 Bruker spectrometer devices (frequencies of 200-700MHz for protons), with one of the instruments dedicated for solids, and the other with a cryo probe for work with proteins and samples at low concentrations. All devices are suitable for 2D experiments and are suitable for nuclides such as ^{13}C, ^{15}N, ^{31}P, ^{25}Mg, ^{27}Al etc.

Mass-Spectrometry

The unit provides mass spectra (MS) analysis for solutions, gases and solids. This unit is equipped with GC-MS, HPLC-MS, MALDI and TGA-MS. A variety of quantitative and qualitative analyses (such as HRMS and MS/MS) are provided for both synthetic and natural substances. Professional consultation and interpretation will be given on demand.

SQ 6120 (ESI/APCI), by Agilent
Q-TOF 6545 (High Resolution) LC-MS (ESI/APCI/ASAP), by By Agilent
Autoflex III smartbeam MALDI TOF/TOF, by Bruker
TGA-GC-MS (EI/CI) Clarus 680/Clarus SQ 8C, by Perkin Elmer

Elemental Analysis

The center for Chemical Services is equipped with a Thermo CHNS-O elemental analysis device, model EA 1110, capable of detection of the elements C,H,N,S and O.

Inductively-Coupled Plasma (ICP)

Different elements, including halogens can be detected using the ICP technique, with a SPECTRO ARCOS ICP-OES Multi view device.

BET

Surface area measurements and adsorption isotherms can be performed for solids and powders using a Quantachrome NOVA 3200E device.

Optical Spectroscopy

In the unit for Chemical Analysis, different optical measurements can be performed using diverse techniques, such as:

Micro Raman spectrometry by JOBIN-YVON
FT-IR by Thermo Scientific
UV-Vis-NIR
Circular Dichroism (CD) spectroscopy- Chirascan ByApplied photophysics

X-Ray Diffraction (XRD)

Analysis of the structure and composition of crystalline and amorphous materials using X-ray diffraction measurements are performed at our center using a Bruker XRD device, model D8 Advance (powder analysis).

X-Ray Photoelectron Spectroscopy (XPS)

The XPS method allows study of the chemical composition of the surface of materials. Information obtained by this method includes the identification of different elements (except hydrogen) and relative quantity. The Center employs a Kratos Analytical XPS instrument, model AXIS-HS.

Electron Paramagnetic Resonance (EPR)

The center for EPR (or ESR) owns modern equipment that provides the necessary resources for contemporary research in organo-metallic chemistry, organic radicals, radicals in biology research, antioxidants, electrochemistry, radicals in nano-chemistry and protein research. The center possesses an advanced Bruker, ElexSys 500 instrument (4°- 300 ° K) and an EPR spectrometer – the Bruker EMX 100d.

Molecular modeling and computer-driven materials design

Using molecular modeling computer software has a proven potential for streamlining and optimizing development processes such as pharmaceuticals and nanomaterials. The Department of Chemistry owns an advanced computational platform, both on the hardware and software level, enabling a wide variety of structural and energetic calculations (quantum computations, minimization of energy, conformational searches, molecular dynamics, anchoring, statistical modeling and more) on systems ranging from the atomic level to the crystal lattice cell unit. The calculations are carried out by several research groups with many years of experience.

Institute for Nanotechnology and Advanced Materials

Bar Ilan's Institute for Nanotechnology and Advanced Materials (**BINA**) is a dynamic and growing scientific community. At BINA, a renowned research staff – including a large number of young faculty members recruited from abroad – educate Israel's next generation of nanoscience professionals, while collaborating with academic and industrial experts on nano-based approaches to energy, magnetism, optics, clean tech and biomedicine.

Established in 2007 and housed in the Leslie and Susan Gonda (Goldschmied) Nanotechnology Triplex, BINA boasts 40 cutting-edge laboratories as well as state-of-the art "Scientific Service" facilities for electron microscopy, nanofabrication, surface analysis, fluorescence, and magnetic measurement, all of which are available for use by the wider scientific community.

BINA's remarkable productivity – in publications, grants, patents, and in the creation of successful start-ups from basic science breakthroughs – have made BINA highly sought after as an R&D partner. In addition to academic collaborations with some of the world's top research institutes, BINA currently partners with leading multi-national corporations including GM, Tadiran, Samsung, CIVAN and Joma.

BINA offers a comprehensive set of educational frameworks, including PhD and MA studies, and a selective program for BIU undergraduates majoring in the sciences.

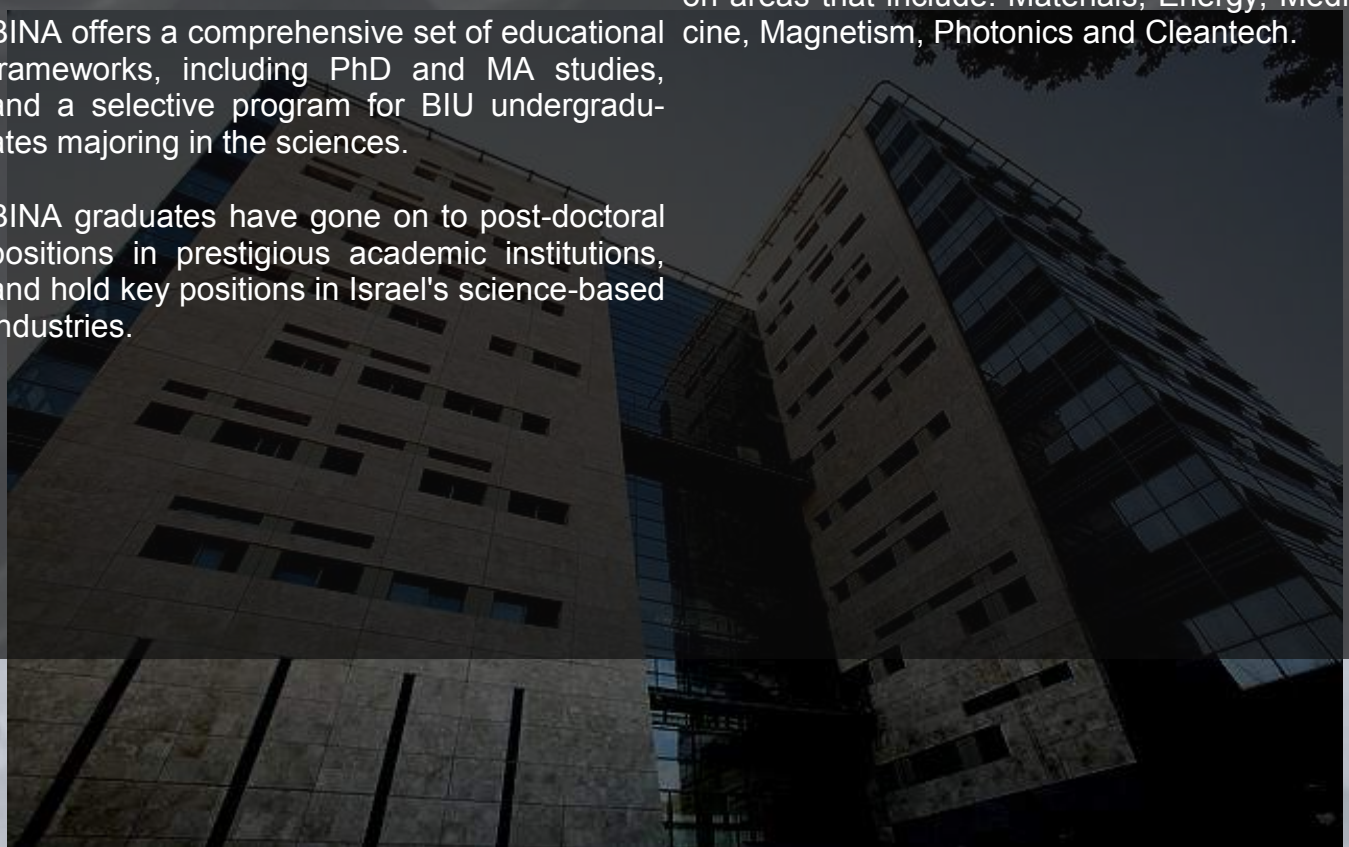
BINA graduates have gone on to post-doctoral positions in prestigious academic institutions, and hold key positions in Israel's science-based industries.

BINA comprises almost 60 research groups in which veteran scientists have been joined by a bumper crop of new faculty members – mostly "returning" Israelis as well as new immigrants – who trained at top-flight institutions like Harvard, Stanford and MIT.

BINA researchers are making important contributions to fundamental nanoscience, while producing practical applications in the marketplace – everything from electric vehicle batteries, to energy-saving digital lighting displays, to medical nanoparticles for the targeted eradication of the herpes simplex virus and cancer. BINA's experts in magnetism and optics are laying the groundwork for tomorrow's computers, while materials science breakthroughs are being applied to everything from agricultural irrigation to space satellites.

Collaborating with the world's most respected research centers – as well as multi-national corporations such as General Motors, Tadiran, and Samsung
– Bar-Ilan is leading the charge toward a future in which the potential of nanotechnology makes life better – for all of us.

BINA researchers are currently exploring a vast number of basic and applied projects, focusing on areas that include: Materials, Energy, Medicine, Magnetism, Photonics and Cleantech.



Nano Research Centers

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Nano Research Centers

Materials

BINA is a world leader in materials science research. BINA researchers have been appointed as members of editorial boards in prestigious journals and have been awarded prizes such as IVS and ICS. Their discoveries are fueling practical advances in a wide range of areas including energy, computers, communication and health care.

Innovative methods for nanoparticle fabrication
Synthesis, characterization and biomedical applications of functional nanoparticles
Self-assembled monolayer films
Nanoscale organic and inorganic coatings
Functional and chiral self-assembly monolayers
Nanostructures – from individual nanoparticles to functional materials
Carbon nanotubes growth mechanisms
Carbon nanotubes synthesis and functionalization
Colloidal models of phase transition in nano-scale systems
Computational nanotechnology

Energy

From its earliest days, BINA researchers have played a vital role in the development of renewable energy applications. Focusing on photovoltaics, energy storage, solar thermal energy, energy conservation – as well as basic research – BINA's nano-energy experts are world leaders in the techniques that are forging a path toward practical and green solutions for a sustainable future.

Advanced materials for rechargeable battery systems and super capacitors
Dye-sensitized solar cells
Nano-based optics for photovoltaics
Low cost, multi-band-gap photovoltaic systems
Carbon engineering and electrochemistry for EDL capacitors
Electrical and optical properties of carbon nanotube structures
Carbon nanotube-based electrodes for batteries and super capacitors
Solid-liquid interfaces of ionic liquids

Medicine

BINA scientists are uncovering fundamental principles that govern human health and disease, while creating the path-breaking medical technologies that will save lives. From specially-designed nanoparticles for diagnostics and targeted drug delivery, to innovative approaches to neurodegenerative disease, viral infection and cancer, BINA laboratories are producing the basic science breakthroughs that will serve as a springboard for tomorrow's therapeutic strategies.

Nano-based methods for targeted drug delivery
Innovative methodologies for diagnostics
Active oxygen chemistry and biochemistry within liposomal and membrane bilayers
Liposomes as nanometric "drug vehicles" and models for living cells
Microfluidic-based studies of virus-host interaction
The use of nanoparticles for cytoplasmic and nuclear gene silencing
Structure and function of ion channels
Nanoparticles for improved CT imaging
mRNA dynamics in living cell systems in the single-molecule, single-gene and single-cell level
Neuronal nano-engineering
Protein-DNA interaction on the single-molecule level
Organization of the genome in the nucleus and its disruption in cancer cells
Nanoparticle-based methods for the imaging and treatment of brain tumors

Magnetism

From fundamental studies of the magnetic properties of materials, to the fabrication of new materials for use in spintronics-based applications, to the integration of these materials in advanced devices, researchers in the BINA Nano-Magnetism Center are making dramatic contributions to the science that will lead to novel devices for communication, medicine and industry.

Low-dimensional magnetism and superconductivity
Nano-sized electronic systems
Transport properties of disordered and granular films
Magneto-transport in thin films of magnetic perovskites
Giant planar Hall effect in manganites
Ferromagnetic-superconducting hybrids
Magnetic properties in nanoparticles
Theory of single-molecule and single-photon spectroscopy
Statistical mechanics and transport phenomena in meso- and nanosystems
Spintronics of nano-scaled lateral structures, phenomena and applications

Photonics

Research in BINA's Nano-Photonics Center encompasses two main areas: imaging and vision, and optic information transport. BINA scientists are improving imaging techniques for biological materials, while examining the atomic-level magnetism that may someday allow computer engineers to exceed the classical bounds of processing speed and information bandwidth. By combining experimental and theoretical approaches, BIU researchers are helping to advance our understanding and control of the quantum behavior of light.

Super-resolution imaging
Fiber devices
Silicon and RF photonics
Optical data processing
Precise optical detection of DNA-protein interactions
Precision measurement and control of quantum matter and quantum light
Short laser pulses for controlled heat and mass transfer within optical nano-composite materials
Light-matter interactions in molecular solids
Organic optoelectronics
Silicon photonics

Cleantech

Members of BINA's Nano-Cleantech Center are advancing the knowledge – and developing the materials and methodologies – that will lead to a sustainable, environmentally-friendly society. Their combined efforts – related to alternative energy, climate change, pollution and "green" chemistry – are at the heart of many promising industrial collaborations.

Development of new approaches for breaking down hazardous bio-films
Micro-porous, double-layer carbon electrodes for water de-ionization and desalination

Equipment Facilities at BINA

Since 2008, the Bar Ilan Institute of Nanotechnology and Advanced Materials (BINA) Center for Scientific Instrumentation has been providing world-class service to scientists from both academia and industry. Housed within the largest nanotechnology complex in the State of Israel, its laboratories and advanced instrumentation are among the most sophisticated in the world, offering the highest standards of scientific performance. Its five facilities include Electron Microscopy, Nano Fabrication, Surface Analysis, Magnetic Measurements, and Fluorescence Measurements. The Center is staffed with dedicated, expert, PhD-level scientists who work closely with researchers, providing guidance on experimental design, optimal equipment operation, sample preparation, and analysis of results. Its infrastructure, including the vibration-free Invariant Zone, offers reliably stable laboratory conditions for all aspects of nanotechnology research.

The range and quality of advanced instrumentation at the BINA Center for Scientific Instrumentation makes it one of the world's leading facilities for nanotechnology research and development.
The Center is divided into five main facilities:

- Electron Microscopy
- Nano-Fabrication
- Surface Analysis
- Magnetic Measurements
- Fluorescence Measurements

Equipment Facilities at BINA

Electron Microscopy

The Electron Microscopy (EM) Facility, equipped with a variety of scanning and transmission electron microscopes (SEM's and TEM's) is a sophisticated facility for advanced imaging and analysis. It can provide 3D morphology and topography information, as well as 2D imaging with nanometric spatial resolution. They offer high resolution, bright and dark-field imaging, Electron Diffraction (ED) including crystallographic information, phase and structure identification and determination of unit cell parameters and analytical capabilities using Energy Dispersive X-ray Spectrometry (EDS). Both the scope and sophistication of its equipment make the EM facility an invaluable resource for researchers in semiconductors, ultra-fine grain materials of thin films, solar cells and many other fields that are based on nanotechnology, nanodevices, and materials science.

Surface Analysis

BINA's Surface Analysis Facility has a an established reputation for solving a variety of problems in materials science including analysis of polymers, metals, semiconductors, corrosion coatings, thin films, glass and ceramics. Of particular expertise is in the analysis of discoloration, contamination, and adhesion problems. The types of analysis most frequently performed in this facility include atomic force microscopy (AFM), ion beam analysis (IBA) and X-ray diffraction (XRD).

AFM is based on scanning probe microscopy and provides unique data about atomic scale surface topography, as well as electrical, magnetic and mechanical surface properties. AFM offers sub-nano scale surface analysis and detection of adsorbed molecules, as well as manipulation of small structures for a wide range of lithography applications.

IBA is a cluster of analysis techniques that utilizes high energy (MeV) acceleration ion beams to probe elemental composition (including hydrogen and different isotopes) as a function of depth to several microns with a typical depth resolution of 2-3 nanometers. These methods have certain advantages over conventional spectroscopies and offer unique capabilities as near-surface compositional probes. Such techniques are, in general, non-destructive and capable of yielding absolute concentrations, frequently at the sub-monolayer level. Particularly, IBA provides full information about material composition, matrix and impurity depth distributions and depth profiles for investigation of semiconductors and composite materials. This allows estimation of their composition and damage for improvement or modification of their properties. Hydrogen and other light elements contained in different materials such as plastics, polymers and biomaterials can be analyzed using this method. Quantitative information about film thickness, with high precision and without special pretreatment of the sample, including multilayers, is also possible.

A state-of-the-art powder and thin film diffractometer (XRD) (also can be configured as a reflectometer) provides x-ray reflectivity measurements for thin film thickness, roughness and density determinations; full pole figures and phi scans for crystallographic texture analysis; high-resolution rocking curves for film and crystal quality measurements; automated X-Y mapping of wafers; stress measurements; grazing incident angle diffraction for polycrystalline thin film.

Nano Fabrication

The BINA Nano Fabrication Facility provides state of-the-art tools, such as: Focused Ion Beam (FIB), helium ion microscope (HIM), e-Beam lithography, photolithography, and a range of deposition tools like Atomic Layer Deposition (ALD), Pulsed Laser Deposition (PLD), and advanced sputtering & evaporation systems for thin layer fabrication of a wide variety of material and compositions. The BINA Fabrication facility also includes clean rooms (Class 100 and 1000) equipped for a variety of fabrication processes. Using these capabilities, the BINA Center offers patterning and crafting devices on a nanometer scale resolution, as well as several Failure Analysis (FA) processes such as cross sectioning, TEM lamellas preparation, circuit editing and nano probing. Moreover, our professional staff offers creative solutions for a wide range of fabrication processes.

Magnetism

BINA's Magnetic Measurements Facility offers comprehensive magnetic characterization, including information about electrical properties, heat capacity, and magnetization. It provides magnetic imaging capabilities over a wide range of temperatures. The facility is equipped with a Magnetic Force Microscope (MFM) – a fully operating Atomic Force Microscope (AFM) capable of working in high magnetic fields (up to 8 Tesla), a wide range of temperatures (2K to 400K), and high vacuum. The MFM is used to study magnetic, electronic and morphologic properties of surfaces and devices, with nanometric resolution.

Fluorescence

BINA's Fluorescence Facility offers basic and advanced fluorescence measurements for a variety of applications in biomedical and biophysical research. The combined skills of its biologists, physicists, and engineers enable precise visualization and quantitation, in keeping with the best measurements available today. The instrumentation in the Fluorescence Facility enables the performance of fluorescence excitation & absorption spectroscopy, time-resolved fluorescence correlation spectroscopy, fluorescence recovery after photo-bleaching, 3D-FRAP, FRET and single molecule FRET. Imaging modules, stop flow time-resolved measurements and spectral imaging are also offered.

The Bernard W. Marcus Center for Medicinal Chemistry

The Bernard W. Marcus Center for Medicinal Chemistry is based in the Chemistry Department of Bar-Ilan University and has as its research core the groups of Professors Abraham Nudelman, Alfred Hassner, Bilha Fischer, Gerardo Byk and Amnon Albeck. The Center serves as a focal point for research in drug development, studies of mechanisms of drug action, enzymatic mechanisms, drug-receptor interactions. The sponsored investigations address problems involving basic research on the elucidation of drug action as well as applied research involving the development of novel drugs.

The fields being investigated include: Antibiotics, anticancer agents, enzyme inhibitors, antidiabetics, drugs for the treatment of AIDS, neuroprotectants for treatment of Alzheimers and Parkinson diseases, antivirals, drugs for the treatment of neuropathic pain, anti-schizophrenics, drugs useful in photodynamic therapy, anti-glaucoma drugs, anti-oxidants, cholinergics, nano-biotechnology: development of high throughput methods for fast screening of small molecules, development of computational tools for drug design and development of novel diagnostic techniques

The Research Objectives of the Center are:

- To study the basic mechanisms of drug action.
- To develop new drugs for the treatment of diseases which affect large numbers of patients.
- To identify small molecules for tumor imaging and drug targeting.
- To instruct undergraduate and graduate students on all stages of drug development.
- To develop novel drug design tools
- To develop novel diagnostic tools

Presently one of the drugs synthesized is about to complete a Phase II clinical trial for the treatment of schizophrenia.

It should be noted that a considerable number of the graduates of the Division of Medicinal Chemistry of the Bar-Ilan Chemistry Department are employed by the pharmaceutical industry in Israel.

M.Sc. Program

The Department of Chemistry offers a study program that includes conducting research and submitting a written thesis. The duration of the studies is 2 years.

Areas of specialization

Physical chemistry.
Organic chemistry.
Inorganic chemistry.
Theoretical chemistry.
Physical-organic chemistry.
Electrochemistry.
Medicinal chemistry.
The chemistry of materials.
Bio-organic chemistry.
Biophysics.
Polymers.
Nanotechnology.
Computational chemistry.

Admission requirements

Bachelor's degree in Chemistry with a grade average of at least 85%.

Bachelor's degree in Biophysics with a grade average of at least 83%.

Graduates of other universities whose Bachelor's degree studies are not identical to the Department's program, holders of a Bachelor's degree from Bar-Ilan from previous years and holders of a Bachelor's degree from Bar-Ilan in a course of study other than the one they have chosen for their Master's degree studies will be required to study supplementary courses, to be determined on an individual basis.

All applicants in all courses of study are required to find a supervisor from among the department's faculty members before applying.

Acceptance to the department is conditional on the presentation of a medical certificate confirming fitness to study in the department, including participation in labs. The certificate is to be presented no later than on the registration day of the study program. Bar-Ilan students registering for Master's degree studies immediately after completing the Bachelor's degree are exempt from presenting such a certificate.

Course and seminar requirements

Regular program

14 credits as follows:

10 credits – elective courses in chemistry (or outside the department with the approval of the teaching committee).

2 credits – seminar in one's area of specialization.

2 credits - participation in the departmental colloquium.

Knowledge of languages

English for Master's degree.

Students who studied a foreign language (English) as part of their obligations for their Bachelor's degree will be exempt from a foreign language for Master's degree.

Final exam

The final exam will be based on the thesis and on the bibliography that served as the basis for the research.

Ph.D. Program

Requirements for the Ph.D. Degree in Chemistry

The Department of Chemistry will accept candidates having a B.Sc. or M.Sc. in Chemistry with a minimum average grade of 85% for the Ph.D. degree. The degree requirements are divided into two parts: research and coursework.

Research

Each student is required to engage in an original research project under the supervision of a faculty advisor and present the results in the form of a thesis at its conclusion.

The branches of chemistry offered in the department include: physical, theoretical, computational, inorganic, organic, physical-organic, physical-inorganic, bio-organic, bio-inorganic, medicinal, materials and nano chemistry.

The Department offers students the opportunity to pursue doctoral degrees in the following areas:

Organic Chemistry: Synthesis, physical-organic chemistry, reaction kinetics, NMR and mass spectrometry, stereochemistry, combinatorial chemistry, polymers, organo-metallic reactions, singlet oxygen and superoxide radical ion reactions.

Physical Chemistry: Medical applications of lasers, spectroscopy, basic and applied electrochemistry, inorganic-physical chemistry, sonochemistry, conversion and storage of energy – rechargeable batteries (Li, Li ion, Mg), super capacitors, photovoltaic cells, solar cells

Theoretical and Computational Chemistry: Quantum chemistry, electronic structure, molecular orbitals, multi-photon processes, interaction between light and matter, reaction dynamics, intramolecular energy transfer, semiclassical approximations in molecular dynamics, computational models for enzyme mechanisms and enzyme inhibition, computational models for chemical reactions, computational models in materials science

Medicinal and Bio-Organic Chemistry: Anticancer drugs, antibiotics, drugs for the treatment of Alzheimer, Parkinson and diabetes, adrenergic and cholinergic drugs, enzyme inhibitors, ligand-receptor interactions, immobilized enzymes, drug delivery systems, enzymatic mechanisms, peptides and peptidomimetics, computational models for drug development

Materials Science, Polymers and Nanotechnology: Thin layers, functional nanospheres, heterogeneous polymer systems, surface chemistry, bioactive polymers, sonochemistry, nanoparticles, complex metal-polymer materials, solid state chemistry and crystallography

Biophysics: Interaction between electromagnetic radiation and biological systems, treatment of cancer cells with radiation, protein structure determination and interactions of proteins via NMR spectroscopy, interactions of proteins and peptides with inorganic surfaces.

Coursework

Each Ph.D. student is required to complete 6 credits of courses as well as actively participate in 3 graduate seminars in one's field of specialization and in the departmental colloquium throughout his period of study.

The Graduate Program

Graduate Stipends

Scholarships (including full tuition) are generally granted to students having an undergraduate average of 85 and above (subject to change from year to year). The amount of the stipend is determined according to the student's year of study in a particular degree.

Masters students with an undergraduate average of 90 or above will receive the second year stipend at the beginning of their first year.

Additional scholarships are available for superior students – further information can obtained from the department chairman.

In recent years, the university has invested considerable resources into encouraging research students, by offering, among others, President's scholarships of NIS 40,000 annually to outstanding students for Ph.D. degree, which are granted on a competitive basis, in addition to an exemption from tuition fees, subject to the student's commitment to complete the Ph.D. degree within a period of four years.

Application and Admission

For further information, or if you have any questions, please contact:
Academic Program Coordinator
Phone: 410-516-7427
Fax: 410-516-8420
E-mail chem.grad.adm@jhu.edu
Faculty members are also happy to answer questions about their individual research interests; their e-mail addresses are included in the faculty research section of this brochure.

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Amnon Albeck

Organic chemistry, Peptides and peptidomimetics, Biochemistry, Enzymology, Enzyme mechanisms, Enzyme inhibition, Proteases, Computational biochemistry

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Professor, Department of Chemistry

Ph.D., The Weizmann Institute of Science

Post-doctorate, Brandeis University

Vice Rector, Bar-Ilan University, since 2014

Weizmann Post-doctoral Fellowship

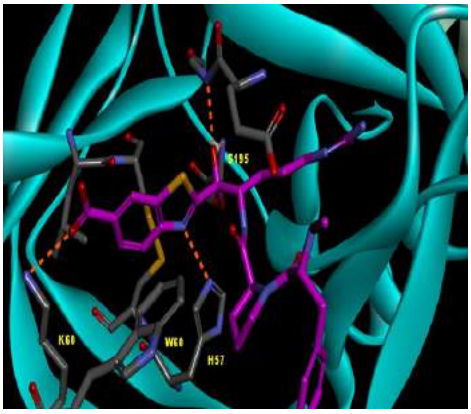
Alon Fellowship for young scientists

Member of the Marcus Center for Medicinal Chemistry, Bar-Ilan University

The laboratory of Prof. Amnon Albeck at the Department of Chemistry, is trying to understand enzyme mechanism and inhibition and to design and develop drugs targeted towards enzymes. The research is interdisciplinary in nature, combining synthetic organic chemistry, biochemistry, enzymology, computational chemistry, and cellular biology.

Enzyme Reaction Mechanisms

Understanding the mode of action of enzymes at the molecular level has important potential applications, as it opens up possibilities to selectively control or modulate such activities. This approach is essential for basic research, as well as for the development of new drugs and other biologically active compounds.
Albeck and his team study proteolytic enzymes, enzymes that hydrolyze (cleave) proteins and peptides which are involved in many biological processes. The research combines experimental research with computational biochemistry. Experiments include biochemical analysis, enzyme kinetics, chemical synthesis, and analytical techniques such as NMR and X-ray crystallography.



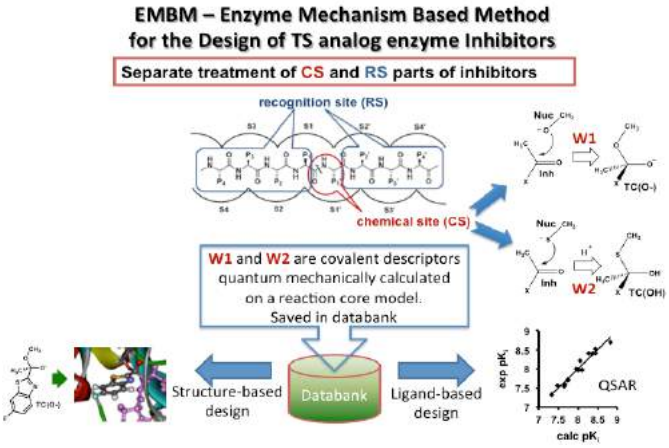
Representative 3D structure of enzyme active site (cyan) interacting with its inhibitor (magenta). The structure emerged from computational studies.

Drug Design and Delivery Research

This research involves the design and synthesis of enzyme inhibitors, drug candidates and drug delivery systems, as well as evaluation of their activity at various levels, from in-vitro studies to in-vivo animal model experiments.
One project, in collaboration with Prof. Gary Gellerman from Ariel University, focuses on the development of novel methodologies for the preparation of targeted multi-drug delivery systems, with the aim of recruiting anti cancer drugs and drug candidates that failed clinical trials due to their toxicity.
Another project, with Prof. Ilana Nathan from Ben-Gurion University and Soroka Medical Center, concentrates on understanding basic biological processes involved in necrotic cell death and on the development of protease inhibitors to treat necrosis. This project has produced very encouraging in-vivo results in three animal model systems.
A decade-long collaboration with Prof. Michael Albeck and Prof. Benjamin Sredni from Bar Ilan University deals with the development of tellurium-based bioactive compounds as potential anti-cancer and anti-viral drugs. Here, too, animal studies demonstrated the therapeutic potential of these compounds.
Other projects in the pharmaceutical field and in an industrial application are underway in the Albeck laboratory.

Computer-Assisted Drug Design Tools Development

One central research direction in Albeck's lab involves the development of novel computer-assisted drug design (CADD) tools to assist medicinal chemists and the pharmaceutical industry in the design of new bioactive compounds.



A description of the EMBM methodology for virtual screening and rational design of protease inhibitors

In a project that may help to overcome the problem of mutational drug resistance, Prof. Albeck, in conjunction with Dr. Michael Shokhen, is developing computational tools for the design of new antibacterial and antiviral drugs based on enzyme inhibitors. Common drug design tools deal with non-covalent inhibitors, which eventually suffer from mutational drug resistance. The emergence of resistant bacterial and viral strains, as well as cancer cells, has become a major problem in modern medicine. The methodology developed by Albeck's group is applicable to transition-state analog enzyme inhibitors. These reversible covalent inhibitors interact directly with the catalytic machinery of the enzyme, which is not subject to mutations. While the common CADD tools are either structure-based or ligand / pharmacophore -based methodologies, Albeck's approach can be classified as a mechanism-based drug design tool. Indeed, previous mechanistic studies on enzyme catalysis and inhibition, conducted by Albeck and coworkers, provided the basis for the development of this novel CADD methodology.

Peptidomimetics

Peptide analogs, in which one or more functionalities have been altered, are promising for many applications in drug development, diagnostics, and mechanistic studies. Albeck's lab develops innovative methods for the preparation of such peptide analogs, applying them for the synthesis of novel enzyme inhibitors.
These inhibitors may serve mechanistic research goals, or may be developed for drug discovery projects. Their functional alterations may include the introduction of reactive functional groups to covalently interact with a target enzyme, conversion of a peptide bond to a metabolically stable isostere, or design of scaffolds that mimic small peptides.

Looking to the Future

As a research group that combines both experimental and computational research tools, and that emphasizes both basic-mechanistic and applied research, Albeck's lab is committed to the improvement and further development of its drug design computational methodologies and their application in practical drug development projects. Ongoing projects as well as future projects are expected to yield biochemical information and bioactive compounds that together will provide the grounds for the development of new drugs.

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Doron Aurbach

Materials Science, Nanotechnology, Renewable Energy

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Professor, Department of Chemistry

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E.B. Yeager award of the International battery association (IBA), 2014

Award of the Electrochemical Society battery division, 2013

Kolthoff prize in chemistry, of the Technion, 2013

Israel Chemical Society (ICS) prize of excellence, 2012

Landau Prize for Green Chemistry, 2011

The Edwards Company Prize of the Israel Vacuum Society (IVS) for research Excellence, 2007

The Technology Award of the Battery Division of the Elec-

Aurbach and his team study the electrochemistry of active metals and polar aprotic systems, the development of spectroscopic methods (in situ and ex situ) for sensitive electrochemical systems, and the electrochemistry of modified electrodes.

They conduct basic studies of electrochemical intercalation processes and work to develop rechargeable high energy density batteries and EDL capacitors.

They also work on electronically conducting polymers and activated carbon electrodes, and their engineering, characterization and applications. Aurbach's group also studies water desalination by electrochemical means.

Materials Science

Aurbach is best known for the important role he played in acquiring the basic science that was needed for the development of commercial lithium ion batteries, which is now standard issue in cellphones and computers. He was involved himself in a pioneering development of commercial rechargeable Li (metal) batteries, together with the Israeli company Tadiran Inc.

Today, research in his lab focuses on several important topics, including the development of new materials for advanced, high energy density Li ion batteries for electric vehicle (EV) applications in collaboration with General Motors (GM) USA and the biggest chemical company in the world – BASF , Germany. The group is actively collaborating in Israel with ETV energy, a start-up company that develops novel power sources, Elbit-systems, Tadiran-batteries and electric fuel.

The group also develops electrochemical storage technologies for sustainable energy (solar, wind). These include magnesium-based batteries, invented by Aurbach's group that can be cycled thousands of times. In another project, the group works on the development of electrode materials and methodologies for water desalination.

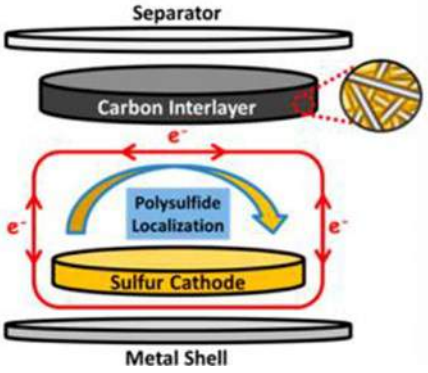
Nanotechnology

Currently, approximately one-fifth of the world's population lacks dependable access to clean drinking water. To address this pressing issue, Aurbach and his team use nanoporous carbon electrodes to create novel technologies for water desalination and purification.

Their work focuses on capacitive deionization (CDI), a process in which voltage applied to saline water selectively moves salts through electrochemical filters, leaving fresh water behind. The systems they develop intend to provide relatively fast and cost-effective means of water desalination and purification. In addition, these systems can be selective enough to prevent the removal of the alkaline earth ions, namely important nutrients such as calcium and magnesium ions from drinking water.

Renewable Energy

Aurbach's group is also working on new technologies for storing the nonpolluting energy harvested from wind turbines and solar power stations. They are working on "load leveling" technologies, which would allow power station activity to fluctuate in accordance with consumer demand. Such technologies would provide a method to store energy when it is created and allow it to be delivered according to the desired level of energy consumption. Aurbach's group collaborates with a number of leading industrial concerns on several electrochemical technologies for the storage and conversion of sustainable energy.



Carbonized interlayer system for intercepting the migrating polysulfide species

Scope of Collaborations

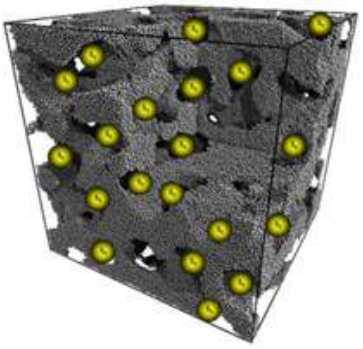
Aurbach's group has active and formal collaborations with leading giant companies including BASF and General Motors (GM) in the US, on new materials for EV batteries. The group collaborates with prominent research groups from Canada, the US, Germany, Switzerland and Japan on advanced materials science for new power sources within the framework of a scientific network supported by BASF.

The group also collaborates with Elbit, Tadiran-battery division and Vulcan Israel on R&D of new power sources. D. Aurbach is the leader of INREP – Israel National Research center for Electrochemical Propulsion (since mid-2012), which includes now 16 research groups from BIU, Tel-Aviv University, the Technion and Ariel University.

Looking to the Future

Aurbach's group plans to maintain its position of world leadership in the research and development of novel devices for energy storage and conversion. The group aims to be in the center of national efforts to change the energy economy to a lesser dependence on fossil fuels.

They also intend to play a major role in the revolutionary move of ground transportation from propulsion by internal combustion engines to electric vehicles. One of their goals is to demonstrate new approaches for water treatments (desalination, removal of poisons) by electrochemical means.



Sulfur encapsulation into the porous carbon matrix

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Nano-biomaterials for drug discovery; Gene therapy; Modern methods for organic synthesis of natural compounds.

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Yigal Alon Fellowship 1998-2002

TEVA centennial award to young investigator 2001-2004

Schmidt Prize from Weitzman Institute to the best PhD thesis in Organic Chemistry in Israel, 1991

Member of the Marcus Center for Medicinal Chemistry, Bar-Ilan University

Nanobiotechnology: high-throughput technologies for life cell and in vivo screening of small molecules for drug discovery.
The laboratory develops novel nanoparticles by a new fabrication mechanism that allows obtaining core-shell like nanoparticles of varied sizes all of them composed by the same polymeric shell. In a recent research [1-2], we have presented a new type of NPs with varied sizes (from 20 to 400 nm) having the particularity of being generated from very same materials combined in a core-shell like structure composed of a core, rich in poly-N-isopropyl acrylamide- polypropylene oxide (PNIPAAM-PPO), and a shell, rich in polyethylene oxide (PEG) well-known as one of the most biocompatible materials. The NPs are obtained by a mechanism where a mixture of monomers and macromonomers form first self-assembled micelles at high temperature facilitated by the thermo-responsiveness of the monomers mixture. Different ratio of the monomers in the mixtures allows generating micelles of different sizes at high temperature. The presence of an initiator and cross linker freeze the micelles' structure by radical polymerization producing NPs of varied sizes (see mechanism in figure 1).

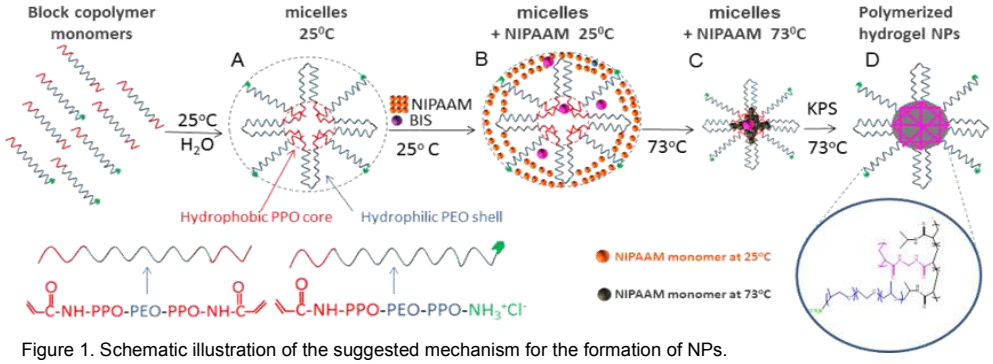


Figure 1. Schematic illustration of the suggested mechanism for the formation of NPs.

The peculiar composition allows keeping intact the biocompatibility along the different sizes of NPs as proved by their lack of cell toxicity (tested up to 5 mg/ml concentration) and their in vivo compatibility in zebra fish model (see figure 2).
The shell of the NPs bear free amino groups that can be used for labeling or peptide synthesis. Furthermore, the NPs are robustly cross-linked to permit repeated chemical reactions on their surface using organic solvents without promoting their chemical/physical degradation. Fluorescently labeled NPs were injected to zebra fish embryos at one cell stage and observed in real time along the development of the animals. No apparent toxicity could be established: the animals developed normally (see figure 2) and interestingly, the fluorescent NPs were distributed into different organs in their body (see figure 3). These results suggest that the NPs can be used for in vivo tracking of stem cells loaded with NPs without significant risk of toxicity.

The suitability of the NP's for biological applications motivated developing a new method for peptide synthesis on nanoparticles [1, 3]. We have developed a strategy for multiple peptide synthesis by embedding the nanoparticles into a magnetic inert matrix that allows reacting the NPs with different reagents and their easy removal by magnetic field. At the end of the process the magnetic matrix is removed and the synthetic peptide remains on the surface of the nanoparticles. (see scheme 1).

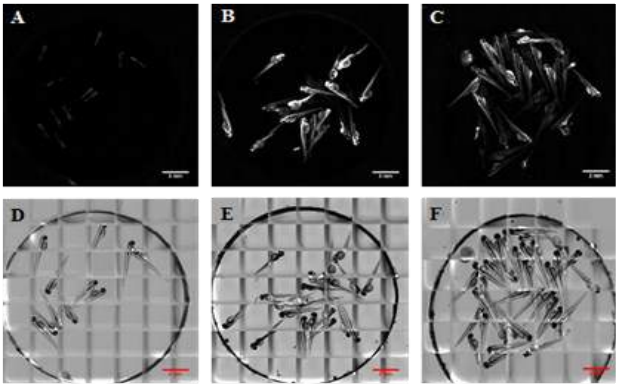


Figure 2. (a) Fluorescence and (d) bright-field channels of single cell water injected embryos at ~65 hpf. (b) Fluorescence and (e) bright-field channels of single cell (Alexa Fluor® 488)-labeled NPs injected embryos at ~65 hpf. (c) Fluorescence and (f) bright-field channels of yolk (Alexa Fluor® 488)-labeled NPs injected embryos at ~65 hpf. Scale bar: 2 mm.

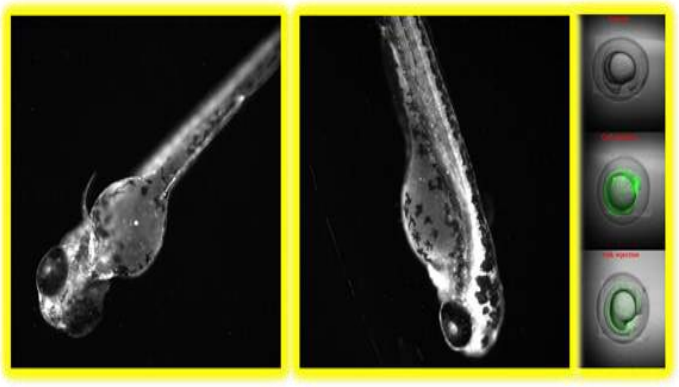


Figure 3. The NPs were tested in vivo using the zebrafish model system. The impact on embryonic development was observed (right panel). 20 nm NPs were labeled with Alexa Fluor® 488 (λex = 488 nm, λem = 519). The qualitative toxic effect of two kinds of administration was monitored: 1) microinjection into the yolk sac (right panel bottom) and 2) microinjection directly into the zygotic cell (right panel middle). In addition, the NPs were tracked in vivo and their intra-body fate in the developing embryo was assessed in both cases

Gene therapy: design and development of non-viral vectors for gene delivery and expression of foreign genes for gene therapy.

In recent publications [4-6] non-viral vectors were synthesized and conjugated to genetic material and observed in vivo for their intra body localization using an MRI probe (see figure 4).

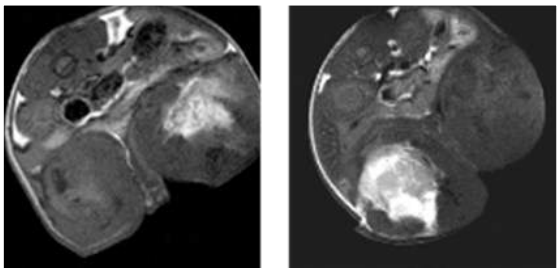
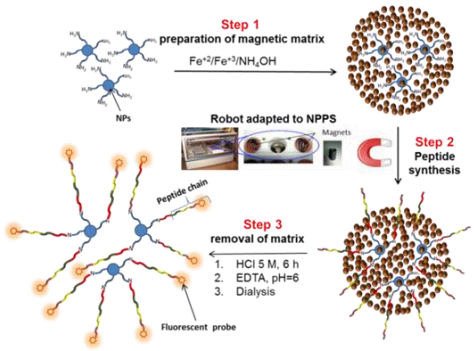


Figure 4: MRI Images of mice. left: 48h after injection of the left side tumor with MCO-I-68-Gd/DOPE/ DNA complexes. Right side tumor is the non-injected tumor control. right: 48h after injection of the right side tumor with



Scheme 1. Nanoparticle peptide synthesis (NPPS) process.

Modern organic Synthesis: Total synthesis of natural compounds with biological activities

Novel methodologies especially employing microwave energy and design of novel multicomponent reactions are being developed in the laboratory for the synthesis of biologically relevant natural compounds. Synthetic products are characterized molecules for the final validation of the natural compounds structure. For more details see references 7-11.

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Jordan Chill

Structural biology; biomolecular NMR; membrane proteins; intrinsically disordered proteins; protein-protein interactions

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EMBO Long-term Post-Doctoral Fellowship, NIH

NIDDK Scientific Director's Fellowship Award

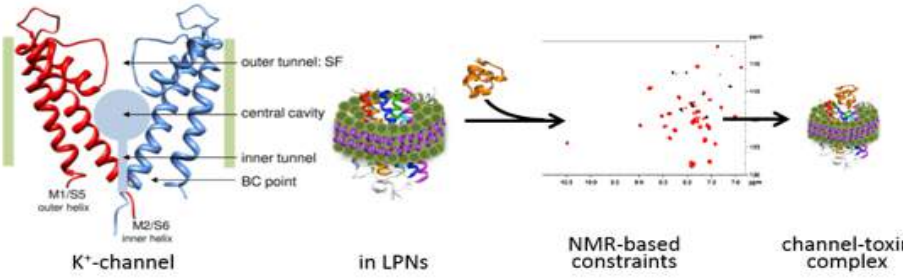
Chill's research group applies nuclear magnetic resonance (NMR) to study the structure, dynamics and function of proteins with an emphasis on possible applications to health and disease.

Biophysics Research

The structure and motions of proteins are key to the multitude of critical functions they fulfill in the biological setting. NMR is well suited to capture the biophysical nature of these cellular events and thus provide insight into the molecular mechanisms that make proteins work. State-of-the-art isotopic labeling methods and NMR methodologies allow NMR to access proteins ranging from highly flexible disordered proteins to the slowly-tumbling membrane-associated proteins.

Membrane-Embedded Proteins

Membrane proteins are extremely important as guardians of the cell and have many biological roles, yet defy structural study because they must be examined in a cumbersome hydrophobic medium which mimics the membrane. Chill's team applies a combination of protein expression and sample preparation methods to create detergent- or lipid-solubilized MPs which can be studied using NMR, and then tries to shed light on their structure, dynamics and function. An important focus in the group is upon ion channels and their interactions with natural and synthetic ligands capable of blocking channel function. Since over 50% of all drugs target membrane proteins such as channels, transporters and G-protein coupled receptors, understanding the structural basis for binding of inhibitors to these proteins will be absolutely essential for efficient drug development. Chill seeks to bridge the gap between this vital need and the lack of reliable structural data for most membrane proteins.

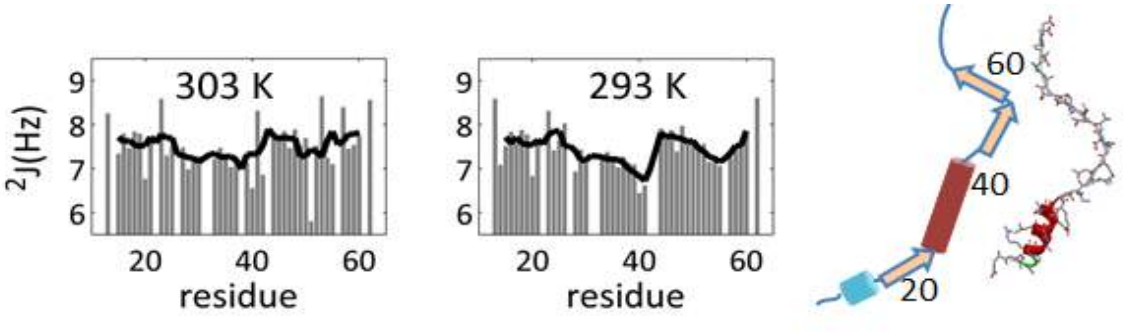


From left to right, a potassium channel allows K+ to enter the cell in a specific and controlled manner, biosynthetic channels expressed in bacteria are incorporated into lipoprotein nanodiscs (LPNs) which stabilize the channel outside the membrane, the NMR spectrum detects which signals coming from the channel are affected by addition of a channel inhibitor and maps the inhibitor binding site, the structure of the complex between inhibitor and channel is determined using this information and sheds light on the molecular basis for inhibitor binding thus assisting future drug design.

In another concerted effort, the group is also examining the ability of viral particles to enter through the membrane hinging upon two membrane-spanning proteins assembling into a heterodimeric complex. Having succeeded in preparing these membrane domains and determining their global assembly in membrane-mimicking micelles, Chill and his team now aim to determine the molecular interactions that mediate their dimerization. Ultimately this could suggest possible inhibitors that will halt progression of the disease which currently has few effective therapies.

Intrinsically Disordered Proteins (IDPs)

Quite different from their membrane counterparts, IDPs are a curious case in which residues of the protein dictate that it remains unfolded in solution. Once considered to have little biological function due to their lack of structure, they are now recognized as important players in protein-protein interactions, and it is estimated that over 30% human proteins contain a disordered domain. Whereas their inherent flexibility defies study by crystallography or electron microscopy, solution NMR is perfectly suited to address the challenges such proteins pose. The Chill group has participated in world-wide efforts to adapt NMR methods to the unique needs of such proteins. In addition, two disordered protein domains in human T cells have been fully characterized using these methods, showing that (i) disordered proteins actually do exhibit transient structure which echoes their eventual conformations in the bound state, and (ii) unknown functional epitopes can be identified using NMR, thus better defining regions of importance in these proteins and facilitating the structure-based design of therapeutic agents capable of targeting specific protein-protein interactions.



Couplings between magnetic nuclei, here the two-bond 15N-13Cα coupling, are strongly related to protein structure. By measuring these at two temperatures we identify structural propensities in the disordered N-terminal domain of human WASP-interacting protein (WIP), and these echo the structural elements found upon binding to actin.

Future Outlook

Challenges in sample preparation and NMR data acquisition must be overcome in each of the protein systems studied in the Chill group in order to provide the comprehensive structural understanding required for future practical applications. Equipped with a state-of-the-art magnetic spectrometer, Chill and his graduate students are confident that they can contribute to a better understanding of these systems at the molecular level, facilitating future drug-design efforts. In addition, the group aims to incorporate complementary experimental biophysical methods and molecular dynamics calculations to support the NMR efforts and propel the group and its students towards these ambitious goals.

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Elazari-Shalom, H.; Shaked, H.; Esteban-Martin, S.; Salvatella, X.; Barda-Saad, M.; Chill, J.H.* New insights into the role of the disordered WIP N-terminal domain

Lior Elbaz

Development of bio-inspired non-precious catalysts for oxygen reduction reaction. Improving precious metal based catalysts for fuel cells. New materials for alternative energy technologies (fuel cells, batteries and photovoltaics). Carbon supports for alternative energy applications (electrodes, electron acceptors). Electronically conductive ceramics

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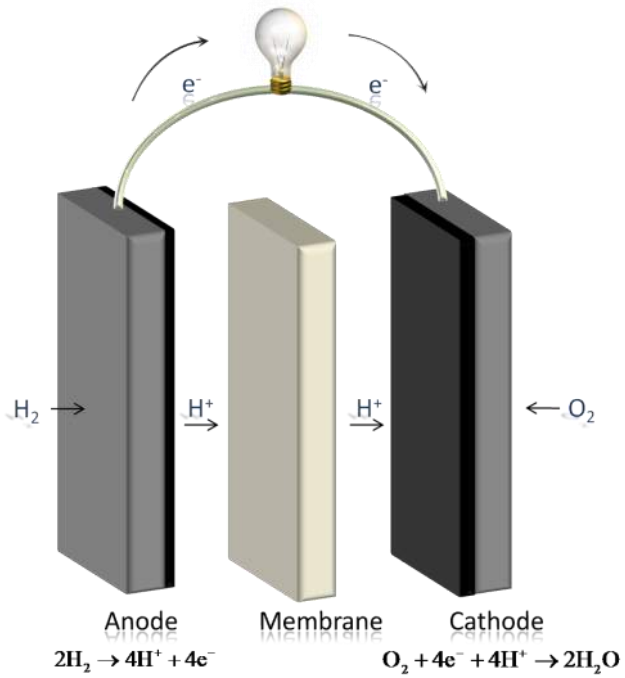
Carasso award for prospective new faculty members

The dependence of the free world on fossil fuels is increasing rapidly, whereas the world's reserves are diminishing. Moreover, the effect of using such fuels on climate change, public health and nature is detrimental. The best way to reduce this dependence and even eliminate it is the further development of renewable energy technologies such as solar cells and fuel cells, which have the potential to power our automobiles, households and industry. In order for them to take over the energy market, scientific breakthroughs are needed.

A fuel cell is a device that converts chemical energy into electrical energy. The energy conversion in a fuel cell continues as long as the fuel and the oxidizing agent are fed to the fuel cell; that is, in principle indefinitely. One of the most popular fuel cells today is polymer-electrolyte fuel cell (PEMFC) which uses hydrogen as fuel and oxygen from air as oxidant. The only product of the electrochemical reaction in this fuel cell is pure water.

In addition to their most obvious application – transportation, due to their very small foot print, low maintenance and environmental friendliness in comparison to batteries and combustion engines, fuel cells are also expected to replace the noisy, expensive and polluting diesel generators and battery stacks used as backup power in industry and remote locations, such as small villages in third-world countries and cellular antennas.

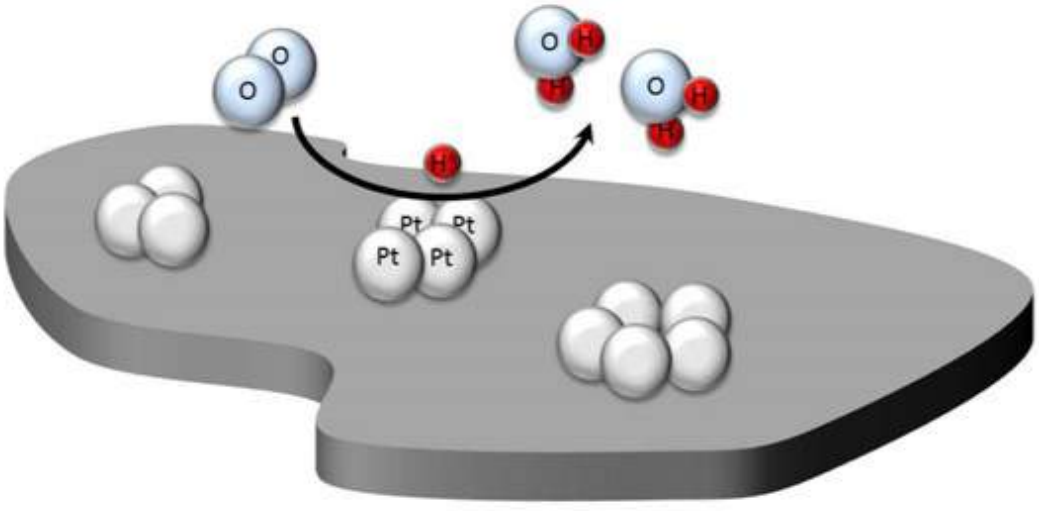
The advancement in the commercialization of fuel cells is hampered by the high cost of their components, and especially the catalysts - Pt in most cases. Although it is the premium catalyst both at the anode and cathode of most low temperature fuel cells, the notion that even the most ingenious improvements in platinum nano-structure and alloying synthesis cannot dispel the issue of this catalyst scarcity and cost escalation, it is a prudent endeavor to develop inexpensive catalysts for oxygen reduction (ORR) which can be obtained from abundant and sustainable sources in order to realize the eagerly anticipated mass commercialization of fuel cells.



H_2/O_2 polymer electrolyte membrane fuel cell

Since the discovery of their ability to catalyze the ORR and up until today, there has been a continuous growth in the interest in macrocyclic compounds. Researchers in various fields, from biology to physics and chemistry, have investigated the ORR mechanism and modified the macrocyclic structures and transition metal complexes to achieve better catalytic performance. While good catalytic activity was demonstrated under certain conditions, further development is needed in order to make them competitive with platinum based catalysts.

Our projects aim at developing bio-inspired catalysts for ORR as well as improving precious metal based catalysts for fuel cells. We also study and develop new materials, based on ceramics, for fuel cells and batteries that could extend their durability and increase their activity.



Oxygen reduction on platinum nano-rafts (3-6 atom clusters of Pt)

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Bilha Fischer

Drug development; Development of diagnostics methodologies; Nucleoside/nucleotide/ oligonucleotide chemistry; Bio-inorganic chemistry

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Professor, Department of Chemistry

Ph.D., Bar-Ilan University

Postdoctoral, NIH

Teva Company Award for excellent young scientists, 1995

Juludan Prize for the Application of Exact Sciences to Medicine, 2006

Shoham Prize for the Arts, 2008

Selected as one of the 50 influential women in Israel (Globes Magazine), 2014

Nature is economy, efficiency, and elegance. Indeed, a limited number of small molecules play numerous functions in life. In our research we have selected natural mononucleotides, di-nucleotides, nucleoside-bisphosphates, and oligonucleotides as scaffolds for the synthesis of novel chemical entities, and the development of novel building blocks and synthetic methodologies. Those new molecules target various applications in the field of medicinal chemistry including diagnosis (probes for detection of mRNA cancer markers towards personalized medicine, SNP-typing probes, and detection and quantification by improved RT-PCR probes), and drug development (treatment of diabetes Type 2, glaucoma, Alzheimer's disease, inflammatory bowel diseases, and osteoarthritis).

Drug Discovery Research

Prof. Bilha Fischer, designs and develops drugs for the treatment of Type II diabetes, Alzheimer's disease, glaucoma, osteoarthritis, and inflammatory bowel diseases.
Most of these drugs share common nucleotide scaffolds.

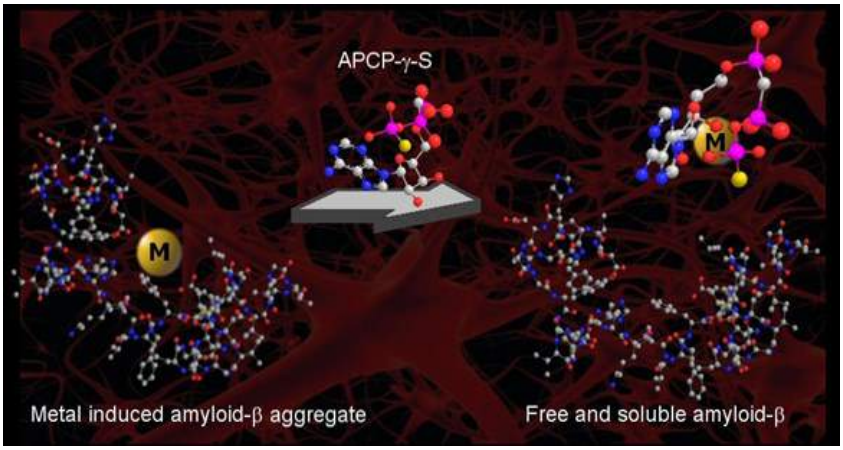
Their targets are either extracellular nucleotide metabolizing enzymes or purinergic receptors that are activated, or antagonized, by extracellular nucleotides.

In her laboratory, Fischer has introduced modifications into natural nucleotides that make them more stable, and allow them to bind and to activate or deactivate specific targets – both qualities vital for effective drug interaction.

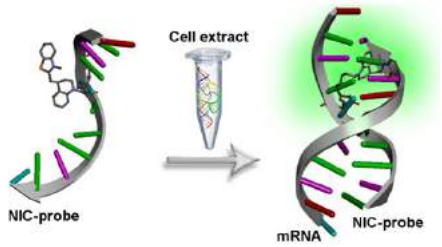
Drugs for the treatment of Alzheimer disease

Fischer and her team have synthesized and identified protective agents that may minimize the devastating effects of Alzheimer's disease. Unlike other potential drugs that target individual factors associated with this disease, Fischer's protective agents are capable of addressing several drug targets at once.

In in-vivo studies in an aggressive AD mice model, Fischer has demonstrated how her protective agents prevent oxidative damage to neurons, as well as the pathological build-up of plaques, leading eventually to almost normal behavior, learning and memory.



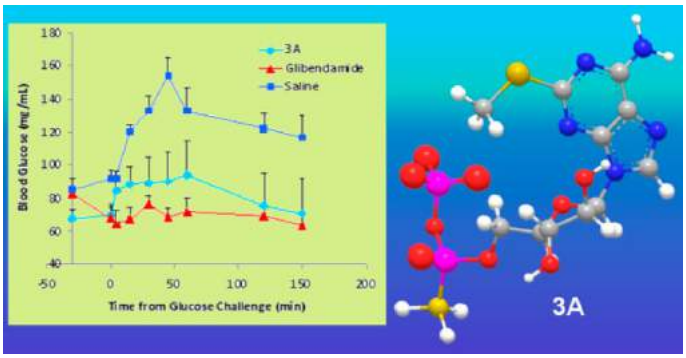
Nucleoside-5'-phosphorothioate Analogues are Biocompatible Antioxidants Dissolving Efficiently Amyloid Beta – Metal Ion Aggregates



Detection of Cyclin D1 mRNA by Hybridization
Sensitive NIC - Oligonucleotide Probe

Insulin Secretagogues for Type 2 Diabetes

Fischer's group has successfully identified a safe and potent insulin secretagogue for the treatment of Type 2 diabetes.
The efficacy and potency of this P2Y1 receptor-selective ligand was demonstrated in diabetic mice and rats, conducted in collaboration with a pharmaceutical company. In these animal models, the compounds were found to be a superior and safer alternative to current insulin secretagogues for reducing glycemia to normal levels without the risk of hypoglycemia.



Insulin Secretagogues for Type 2 Diabetes

Drug Candidates for Glaucoma

Fischer's team has also designed a highly efficacious drug candidate for the treatment of glaucoma. This nucleotide-analogue reduced intraocular pressure in normal rabbits by 45%, through activation of P2 receptors. This analogues was found to be a promising alternative for the treatment of ocular hypertension and glaucoma to the leading drug, timolol maleate, which cannot be taken by patients suffering from cardiovascular problems, diabetes, or asthma.

Diagnostics of Breast Cancer towards personalized medicine

Fischer and her group develop novel fluorescent probes and methodologies for the early detection and identification of certain types of breast cancer based on detection of mRNA markers in total RNA extracts of cancerous cells.

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Gil Goobes

Associate Professor, Department of Chemistry

Ph.D., Weizmann Institute of Science

Postdoctoral fellow, University of Washington, Seattle Wa

Crown Foundation Career Development Awardee

Solid state NMR spectroscopy; Tools for molecular structure and binding characterization of proteins bound to the surfaces of solid substrates; Advanced nanomaterials for use in contemporary batteries

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The Goobes group develops and applies new solid-state NMR techniques to address important questions related to surface phenomena and interfaces between different materials. Research in the group in the last few years has encompassed biomaterial interfaces such as protein-mineral interactions that are important in hard tissue formation; polymer interfaces for use in function nanomaterials; heterogeneous catalysis and advanced materials for lithium batteries.

Developing grounds for multidimensional NMR of protein-biomaterial systems

The main objective of research in the group in the last few years has been to apply advanced solid-state NMR techniques for high resolution structural biology characterization of biomolecules bound to solid surfaces. These measurements provide extensive atomic view of protein structure while immobilized on material surfaces and its orientation and interaction interface on the surface. These studies are used for identifying the means that proteins utilize to recognize surfaces of biomaterials and materials in general. Following initial studies on model proteins, recording multidimensional NMR data, the focus shifted to functional proteins and peptides that are viable for material synthesis in Nature, such as biomineralization proteins.

Designing experimental setups for bio-material preparations

An apparatus for controlled preparation of biomaterials in particular apatite, calcite, aragonite and biosilica was constructed by researchers in the group in order to allow for mineral growth in the presence of the functional proteins from bone and dentine, corals and silica diatoms.

Biomimetic porous silica was synthesized using modified template molecules to control the chemical characteristics of the silica surface formed. Using NMR work, the structure and dynamics of organic tethers on the synthetic silica surfaces were characterized. These surfaces were later tested for protein adsorption to maximize loading of biomolecules.

Biosilica inspired by diatoms was recently prepared by polymerizing silicon oxide in the presence of peptides derived from the diatom's biosilicification protein, silaffin, similar to the natural process. This allows us to examine the properties of functional proteins and peptides as they participate, catalyze and regulate silica deposition processes in organisms such as diatoms and other silica mineralizing organisms.

Coral inspired aragonite is currently being prepared with recently discovered coral proteins in collaboration with Dr. Tali Mass from the University of Haifa. The coral calcification process regulated by these coral proteins is used as a proxy for the effect of increase in carbon dioxide production and subsequent climate changes on the mineralization processes in reef inhabitants.

Studying advanced battery materials for design of Li-ion electrodes

Solid-state NMR techniques are employed in the group to examine materials used in future lithium-ion batteries. Surfaces and interfaces, between electrodes and electrolytes i.e. the solid electrolyte interphase, through which lithium ions migrate during battery work cycles are studied in atomic detail to give a comprehensive picture of the processes associated with efficient shuttling of lithium ions inside batteries, and to aid in the prevention of electrode material deterioration. We utilize both low field and moderate field NMR measurements to characterize paramagnetic and diamagnetic electrode materials and are making important contributions to the design of next-generation lithium battery electrodes.

Studying polymer-molecular interfaces

In comb polymers, small pincer molecules, mixed with polymers, align the polymer chains and generate better-defined molecular structures without cross-linking. The molecular interface formed between a polymer with aromatic repeat units and the head group of a pincer molecule made of a metal center bound to three aromatic rings, was revealed and the driving forces for their co-assembly into a mesomorphic structure were defined. In collaboration with Professor Shenhar from the Hebrew University in Jerusalem, we determined that ring stacking provides the dominant mechanism for assembly, and followed the molecular rearrangement that occurs with time through the organization of this unusual phase. Solid NMR quantification of order/disorder in these materials has proven invaluable for other work analyzing the degree of crystallinity in composite biomaterials.

Measuring heterogeneous catalysts by NMR and other techniques

Quantifying the activity of proteins as heterogeneous catalysts, i.e. bound to surfaces is a major pre-requisite complementing the structural work carried out via solid NMR on enzymes that interact with synthetic surfaces in bio-electronic devices. Using real-time microcalorimetry, the activity of the silica-bound ribonuclease was characterized. The mechanism of operation of the enzyme immobilized on mesoporous silica MCM41 was shown to be modified by trapping on voids on the porous silica surface that are commensurate with the size of the enzyme. Modified binding of substrate and product probably due to structural changes in the immobilized enzyme, cause a change in the mechanistic operation of ribonuclease. Applications which seek to sequester operation of this enzyme which degrade RNA molecules can utilize the insights gained from this work.

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Arie-Lev Gruzman

Development of novel drug candidates, using multidisciplinary approaches such as organic synthetic chemistry, medicinal chemistry, analytical chemistry, biochemistry, pharmacology, molecular biology, cell and animal models for drug candidates screening, and nanotechnology. Creation of therapeutic agents for treatment of several human devastating diseases: among them Amyotrophic Lateral Sclerosis, diabetes and cancer

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Senior lecturer,
Department of Chemistry

Ph.D., The Hebrew University of Jerusalem (Summa cum Laude)

Postdoctoral,
University of California, and Research Institute of Pacific Medical Center at San Francisco, 2004-2007

Vice president of the Medicinal Chemistry section of the Israel Chemical Society, 2010-2015

D-cure (Israel Diabetes Association). Young investigator award, 2013

D-cure (Israel Diabetes Assotiation) and EFSD (European Foundation of study of Diabetes) Young Investigator Award for Collaborative Diabetes Research between Israel and EU, 2010

"Faculty of 1000 best world publications in biology, in 2007"

Our research focuses on development of novel drugs against diabetes, ALS and cancer.

Development of novel drugs against Amyotrophic Lateral Sclerosis (ALS)

ALS is a fatal neurodegenerative disease characterized by progressive muscle weakness and reflective loss of upper and lower motor neurons, predominantly in the spinal cord. We have developed novel in vivo active chemical chaperones that increase the degradation of disease related mutated proteins and increase the survival of motor neurons by enhancing the degradation of misfolded proteins. We plan to continue synthesizing new chemical chaperones that are active at low concentrations, with long half-lives, high potency and efficacy that may lead to new ALS treatment.

Development of novel antidiabetic therapeutic strategies

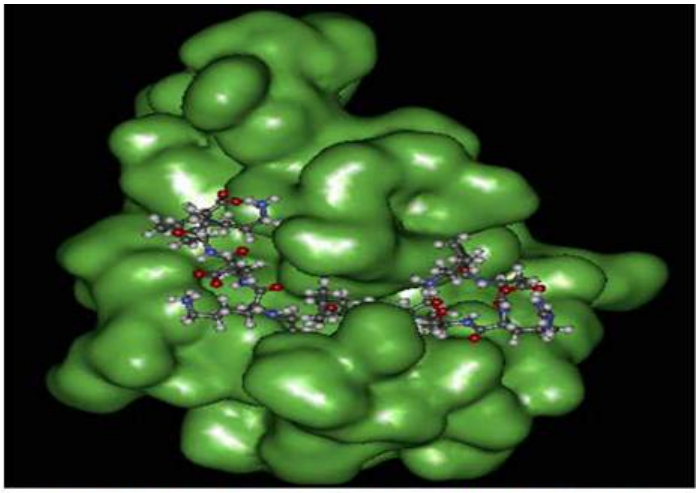
Non-insulin dependent diabetes mellitus (type 2 diabetes) affects tens of millions of people worldwide. The search for novel antihyperglycemic compounds and drugs to treat diabetic patients is paramount in diabetes research. We have found that several novel thiolane derivatives increase the rate of glucose transport into insulin-sensitive cells such as skeletal muscles, but not into insulin-insensitive cells, such as vascular cells. In addition such molecules augment insulin secretion and protect beta-cells (the cells in the pancreas that make insulin) in the pancreas against oxidative stress. We have synthesized potent thiolane derivatives with favorable pharmacokinetic and pharmacodynamic parameters and tested these molecules in both in vitro and in vivo systems. We are currently further investigating the cellular and molecular mechanisms of action of these compounds and developing more potent antihyperglycemic agents.

Despite important advances in the past three decades that have begun to elucidate how and why beta-cells lose the capacity to produce and secrete sufficient insulin, there are fundamental unanswered questions with regards to how beta cells function and why they gradually fail in diabetes. Since beta-cells descend from the same precursor cells as neurons, we investigated a class of neuronal proteins known to be important for the development and operation of cellular functions in neurons that closely resemble beta-cell functions critical for insulin secretion. Our team has focused on neuronal synaptic proteins called neuroligins and neurexins. It was found that insulin secretion by beta-cells and the proliferation rate of the cells are increased when beta-cells are co-cultured with other cells that express high levels of neuroligin. Moreover, these co-cultured beta cells were less vulnerable to oxidative stress, a major factor causing diabetes-induced cell toxicity. In addition, beta-cell precursor cells made from human embryonic stem cells exhibited increased levels of maturation when exposed to neuroligins. We hypothesize that, by using small molecules derived from neuroligin's structure, we will be able to stimulate insulin secretion, protect beta-cells from the oxidative stress, and possibly induce beta-cell proliferation. We expect that these same molecules would aid in the development of transplantable β cells produced from human stem cells. A molecule combining these three effects would constitute an extremely powerful therapy for diabetes. Using molecular modeling and nanotechnology methods, we have synthesized several clustered neuroligin -based peptides attached to nanoparticles that showed a stimulatory effect on insulin

Ultimately, this work is expected to lead to new approaches in diabetes treatment, including the design of novel drugs.

Development of novel antiprostate cancer drugs

Many aspects of prostate cancer pathogenesis remain a mystery, including the early triggers for malignant transformation and the basis for progression to androgen independence, two critical milestones in the etiology of prostate cancer. Prostatic acid phosphatase (PAcP) has long been recognized as important diagnosing prostate cancer. Studies have shown PAcP to be a critical androgen-dependent regulator of prostatic epithelial cell growth. PAcP has at least two functional folding forms. The extracellular secreted form causes unregulated cancer growth of prostate epithelial cells and the intracellular form inhibits it. These two functional forms of PAcP differ in their glycosylation pattern. In normal prostate epithelial cells, this protein is secreted into the seminal fluid. In early prostate cancer, PAcP is secreted into the bloodstream. The progression of prostate cancer is marked by the loss of expression of PAcP. This period of time between detecting PAcP secretion in the blood until its disappearance, marks the transition between a treatable prostate cancer with a good prognosis and a non treatable cancer with a very poor prognosis. Our working hypothesis is that PAcP is the key protein which converts the differential androgen sensitive cancer cells to non differential non androgen sensitive cancer cells. We have designed and synthesized different compounds that prevent the generation of the pro-cancer PAcP secreted isoform. These new synthetic classes of PAcP-release inhibitors will hopefully be the basis for new therapeutic approaches to treat prostate cancer.



Development of anti-prostate cancer novel therapeutic agents. In silico design of an inhibitor of signal peptidase 1

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Eckshtain-Levi M.; Lavi R.; Yufit D.; Arora H.; Daniel B.; Green O.; Richman M.; Rahimipour S.; Gruzman A*.; Benisvy* L. A Versatile Water-Soluble Chelating and Radical Scavenging Platform. ChemComm, 2016, 52:2350-2353.

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Jean-Paul (Moshe) Lellouche

Surface nanoscale structuration and chemical engineering of functional nanoscale materials towards innovative drug delivery, catalytic, electro-conductive and antibacterial improved systems

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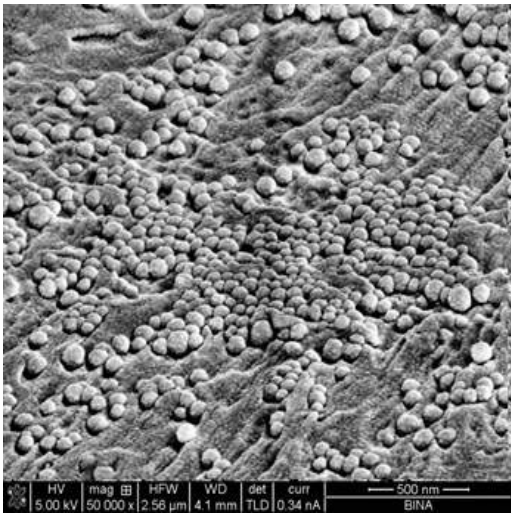
Lellouche's main research interests include the chemical design, fabrication, and characterization of a wide range of functional nanomaterials for various energy, biomedicine, and (bio) sensing-driven applications.

Functional Conducting Polymers (CPs)

Lellouche's group has successfully performed multi-step chemical synthesis of various pyrrole (Pyr), thiophene (Th), and carbazole (Cbz)-containing (electro) oxidizable monomers, which has led to the development of different nanosized materials such as polyPyr/polyTh/polyCbz-multi-walled carbon nanotubes. These materials are useful for (i) surface nano-structuration in sensing devices and sensors, (ii) mechanical re-enforcement of polymeric matrices, and (iii) securing conductivity features in polymeric matrices (PMMA, epoxies, PCs). This work is primarily based on an innovative, patented process they developed, called "CP polymer growth from surface." This process has solved the major limiting issue of phase separation, and has recently been adapted for the development of highly hydrophobic scratch-resistant polymeric coatings.



FIB (SEM) microphotograph (tilt image) of a Parylene C coating functionalized by UV-photoreactive SiO_2 nanoparticles

Hybrid Inorganic Nanosized Materials

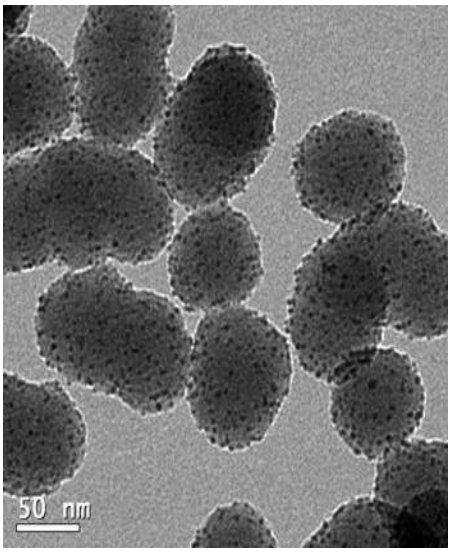
Lellouche and his team also developed an original co-hydrolysis method using variously modified bifunctional silicate species for the development of a number of hybrid silica (SiO_2) nanoparticles. These particles possess very useful features, such as simultaneous hybrid FT-IR and fluorescence imaging capabilities, and photoreactivity for covalent attachment/surface modification. As a result, they are currently implementing R&D applications that deal with in vitro and in vivo bi-modal cancer cell/tissue imaging as well as the development of a new generation of catalytic metallic nanosized conductive inorganic/organic nanoparticulate systems for fuel cell technology.

In addition, they are working on the surface modification/nanostructuration of non-functional biocompatible parylene C-D polymers (biocompatible implant technology), and the surface nanostructuration/chemical engineering of QCM sensing resonating crystals/electrodes for early cancer detection using an acoustic non-contact methodology.

Magnetic Iron Oxide (Magnetite/Maghemite) Nanoparticles

The fabrication of high quality, non-aggregated iron oxide-based nanoparticles is useful for major biomedicine applications such as cell sorting, magnetism-mediated drug delivery, cancer hyperthermia, and magnetic resonance imaging.

However, nanoparticle aggregation has been a major obstacle for the success of these applications. In this context, Lellouche's laboratory team has developed an innovative process towards non-toxic hydrophilic maghemite (ã-Fe2O3) nanoparticles that demonstrate complete control of the NP aggregation level. Rather than involving surface-passivating bifunctional ligands or routinely used physically adsorbed natural/non-natural polymers, the process makes use of a new concept of surface doping using Ce3+ cations for electrostatic stabilization of resulting Ce3+-doped particles.



Innovative composite SiO_2-Pt(o) nanoparticles of a core-shell morphology prepared by reductive UV-photochemistry - Application in effective catalytic reduction of nitro-phenols

Innovative Nanosized Formulations for Gene/Sirna and Antimicrobial Agent Delivery

Lellouche and his team are currently developing various polymeric and inorganic nanosized formulations in order to effectively deliver biologically significant cargos into diseased cells. Examples of these include gene silencing RNA sequences and FDA-approved antimicrobial agents.

Polymeric polyethyleneimine nanoparticles fabricated by the group using an innovative "intra-chain collapse" method have achieved significant cell penetration and total RNA delivery, illustrating their great potential for gene silencing.

In addition, they have demonstrated that "trojan horse"-like silica (SiO2) and polyacrylate (PAs) nanosized formulations of typical FDA-approved antimicrobial agents have bacteria killing capabilities that are greater by a 105/6 factor, as compared to free agents (triclosan case). Current studies aim at further developing this nanotechnology-mediated approach tohybrid/multipotent antimicrobial particles as a potentially useful solution to human health-threatening bacterial diseases.

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Yitzhak Mastai

Chirality
Chiral self-assembled monolayers
Liquids and water in nanoporous materials
Biomimetic Chemistry
Nanomaterials

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Professor, Head of the Chemistry Department

Ph.D., Weizmann Institute of Science

Postdoctoral, Max Planck Institute

Minerva fellowship for Postdoctoral research

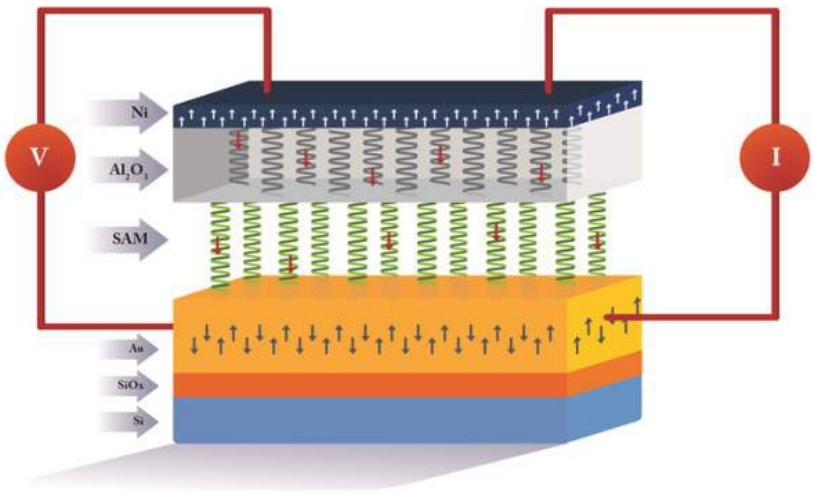
My primary field of research is chirality at the nanoscale, with a focus on preparation and application of nano-chiral surfaces for enantioselective processes. My research interests can be divided into several areas:

Chiral surfaces based on self-assembled monolayers

This research concerns fundamental studies of chiral surfaces based on ultrathin molecular architectures, such as self-assembled monolayers (SAMs), on solid supports. We were pioneers in the study of chiral SAMs for the preparation of chiral nanosurfaces for chiral resolution by crystallization. In a series of papers, our research group has shown that chiral SAM surfaces can be employed as resolving auxiliaries in the crystallization of amino acids from solutions.

Chiral polymeric nanoparticles and mesoporous materials

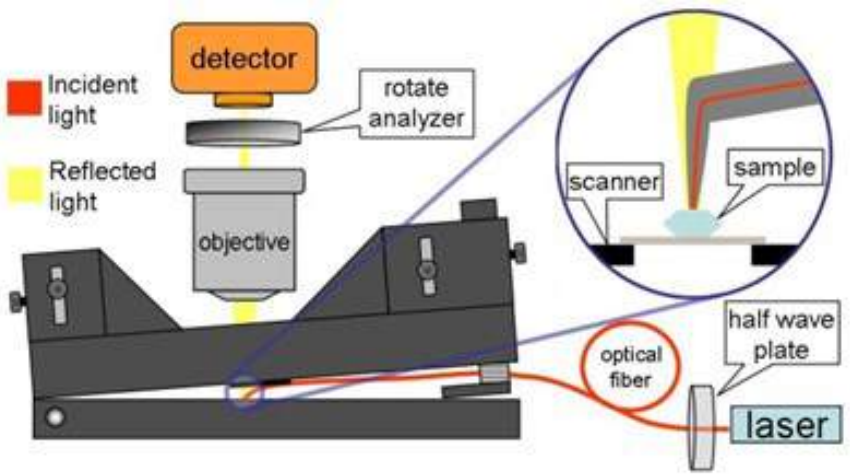
This research concerns the development of polymeric nanoparticles fabricated using emulsion (mini or micro) polymerization. For example, we developed chiral polymeric nano- and microspheres that can act as chiral auxiliaries and be utilized for enantioselective crystallization. We are also developing chiral polymeric nanoparticles of controlled size and shape for other chiral applications such as a chiral stationary phase for chromatographic separations and as catalytic systems for stereoselective reactions. Our group is also involved in the development of chiral mesoporous silica by chiral imprinting or by cooperative self-assembly of chiral amphiphiles and silica precursors. Recently we presented an innovative new type of chiral surface based on a chiral SAM coated with ceramic nanolayers that preserves the enantioselectivity nature of the chiral SAM and enables its protection. These surfaces can lead to a new class of chiral nano-surfaces with the improved characteristics that are necessary for any chiral application.



Scheme of chiral thin films of metal oxide based on the chiral SAM/coated by ceramic nanolayer surfaces. This device and of the four-probe measurement of Au/chiral SAM/Al_2O_3/Ni device is constructed on a Si/SiOx substrate. The chiral SAM/Al_2O_3 tunneling barrier polarizes the spin distribution of transmitted electrons, and it is probed by the magnetic field dependence of the resistivity through the Ni layer.

New chiral analytical techniques

The group is also working on the development of new analytical methods to probe chirality at the nanoscale. We pioneered the development of near-field scanning optical microscopy (NSOM) and isothermal titration calorimetry (ITC) for the determination of chirality at the nanoscale.



Schematic illustration of the near-field scanning optical microscopy (NSOM) for studying chirality at the nanoscale.

Antifreeze Proteins

Other aim of Mastai's research laboratory is to advance the understanding of the structure and behavior of water and the interactions of macromolecules with water. To this end, they use synthetic macromolecules, e.g. double-hydrophilic block copolymers and peptides, which mimic the structure and functionality of antifreeze proteins (AFP). Recently they demonstrated high antifreeze activity of short segments of type I antifreeze protein instead of the whole protein. Their approach of using short segments of the protein simplifies the correlation between antifreeze protein characteristics such as hydrophilicity and hydrophobicity and the effect of those characteristics on the antifreeze mechanism. In addition, it enables the preparation of large quantities of short AFP segments at low cost and with high antifreeze activity. This combination of benefits facilitates development of the commercial potential of AFPs.

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Dan Thomas Major

Computational Chemistry, Computational Biochemistry, and Computational Nanotechnology

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Associate Professor, Department of Chemistry

Ph.D. , Bar-Ilan University

Postdoctoral,
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Fulbright Scholarship, 2003-2004

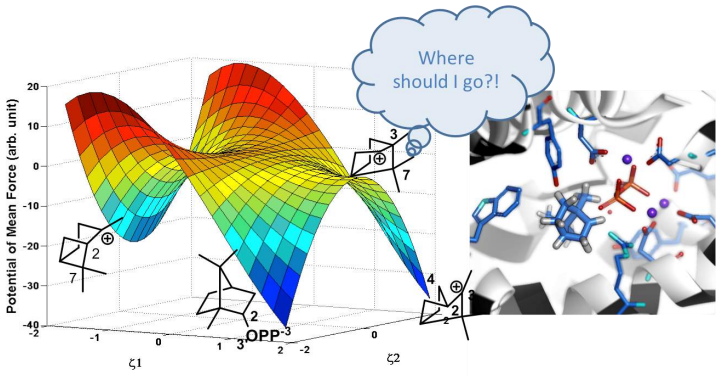
Yigal Alon Fellowship, 2008-2010

Krill Prize (Wolf Foundation), 2009

Major and his research team engage in interdisciplinary research, encompassing chemistry, biochemistry, and nanotechnology. The group tackles questions at the frontier of these areas using a variety of simulation approaches, with the ultimate goal of understanding the intimate functional details at an atomic and sub-atomic level. The group is also actively involved in developing new methods for the study of biological systems and nano-materials.

Computational Chemistry, Computational Biochemistry, Computational Nanotechnology

The Major group develops classical and quantum simulation tools for *in-silico* enzyme studies, developing and incorporating several novel methods into software platforms for bio-simulations. This entails the development of new path-integral methods for the simulation of zero-point energy and tunneling effects in condensed phase environments, as well as multidimensional free energy approaches.



Dynamic effects determine product distribution in a terpene synthase.

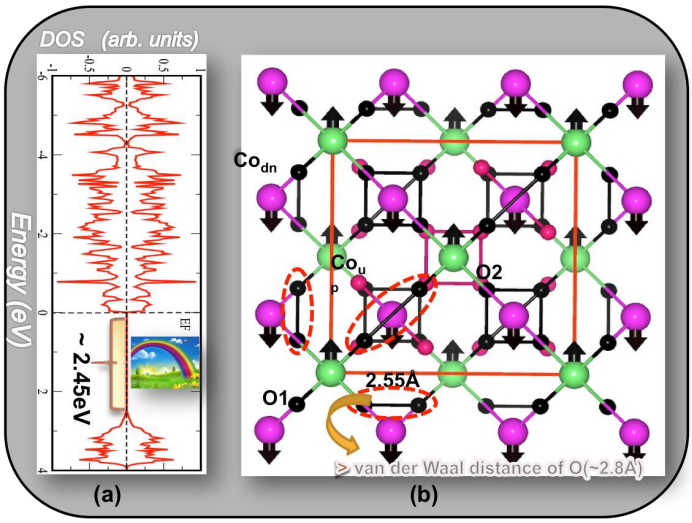
The development of novel methods has facilitated groundbreaking studies on numerous enzymes. Indeed, using novel theoretical tools, the group has managed to elucidate the role of tunneling and dynamic effects hitherto unknown to exist in enzymes. In particular, the group has unveiled the catalytic role of tunneling in a proton transfer in the enzyme nitroalkane oxidase (*PNAS* 2009) and the role of chemical dynamics in complex terpene synthase reactions (*JACS* 2010, 2012). Additional studies focus on the connection between nuclear quantum effects and protein dynamics, employing the hydride transfers in dihydrofolate reductase and formate dehydrogenase as the model chemistry.

The group has also developed methods for heavy atom kinetic isotope effects, which can be used to delineate complex enzyme mechanisms. This type of approach has been used to study the reaction mechanism in deaminase and decarboxylase enzymes.

Tunneling in the dihydrofolate reductase

In addition to the biomaterial research, the Major group also engages in numerous projects on nano-materials applicable as renewable energy sources. In particular, the group carries out first-principles studies on materials for rechargeable batteries, such as Li-ion batteries. Such work is crucial as part of a global effort to move from vehicles powered by traditional combustion engines to full electrical vehicles. Additionally, the group studies numerous metal-oxide materials in search of promising photovoltaic alternatives. This work focuses on promising photovoltaic materials such as iron and cobalt oxides. In particular, the group attempts to engineer properties, such as band-gaps, via computer simulations and hence propose new, novel materials.

In both of these energy projects, the Major researchers employ density functional theory methods to search for new, efficient, and economical alternatives to the current state of the art.



Looking to the future

Major's group continues to expand its pool of theoretical methods, enabling the group to tackle even greater challenges. The group envisions being able to treat bio-molecular and nano-material processes with greater accuracy and with more realistic *in -silico* models in the future.

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Gilbert Daniel Nessim

Laboratory for the synthesis of nanostructures: catalysis, growth mechanisms, functionalization, and integration into devices (electrical, electrochemical, medical, etc.)

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Ph.D., Massachusetts Institute of Technology (MIT)

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M.Sc. Electrical Engineering, Politecnico di Milano

Postdoctoral, Massachusetts Institute of Technology (MIT)

Intel Fellowship (2006-2008)

Marie Curie, European Union Reintegration Grant, 2010-2014

The goals of our laboratory for the synthesis of nanostructures are: (1) to better understand the complex mechanisms of growth of nanostructures such as nanotubes, nanofibers, graphene, and other 2D-materials, (2) to functionalize the synthesized nanostructures, and (3) to integrate them into useful devices.

The amazing properties of carbon nanostructures

The synthesis of carbon nanotubes (CNTs), carbon nanofibers (CNFs), and graphene from catalyst on substrate using chemical vapor deposition (CVD) has massively progressed in the past decade, especially the ability to control the nature of these structures on many length scales and in many aspects of their composition and morphology. Their pristine exceptional mechanical, thermal, and electrical properties, coupled with the possibility of chemical functionalization to alter their bulk or surface properties (e.g., superhydrophobicity), make them a candidate of choice for a wide array of applications, such as additives or scaffolds for battery and supercapacitor electrodes, reinforcing elements of electrically-conductive polymer composites, sensors, future electronics, medical devices, etc. We are currently partnering with various universities to integrate our carbon nanostructures into more efficient electrochemical devices. We are also partnering with a start-up to use a sophisticated array of nanostructures for a medical application.

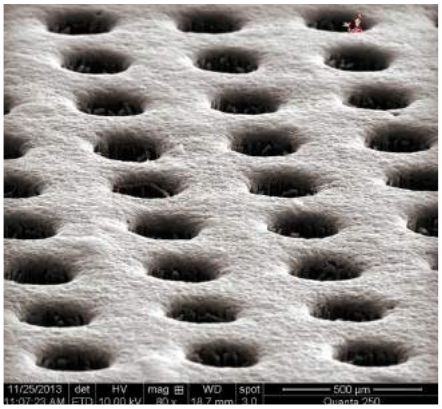
The fascinating science of catalysis and growth of carbon nanostructures

On the scientific side, after focusing on the synthesis of carbon nanotubes (CNTs) and making significant contributions on the role of catalysts, underlayers, and gases, our current research focus has expanded towards (1) studying the influence of what lies below the underlayer or above the catalyst layer in the synthesis of CNTs, (2) synthesizing new types of nanostructures (other 1D materials, graphene, and non-carbon 2D materials), (3) chemically functionalizing the nanostructures, and (4) integrating the nanostructures in devices (batteries, supercapacitors, sensors, etc.).
For instance, we recently showed how a “reservoir” layer (iron thin film) positioned below the underlayer influenced the dewetting/coarsening at the catalyst level, thus leading to an increase in CNT yield (up to 2X). In a second study, we showed the growth of millimeter-tall dense arrays of CNTs on copper using an intermediate thin layer of aluminum oxide, while maintaining electrical conductivity between the CNTs and the substrate; this is an important result in the quest of growing long arrays of CNTs on metals for electrical and electrochemical application.

Recent studies on carbon nanofibers (CNFs) and graphene

Regarding the synthesis of new types of nanostructures, we recently focused on carbon nanofibers (CNFs) and graphene. In collaboration with Professor Ralph Spolenak (ETH Zurich), we showed the growth of ultra-dense arrays of CNFs. The originality lied in the growth mechanism where thin film alloying and fragmentation led to bi-directional CNF growth. In a second study, we showed how a thin adhesion layer was used to let the catalyst/underlayer stack delaminate during the synthesis, leading to a completely new mode of growth of a ready-made mat of CNFs with a yield up to 35× compared to the “standard” growth mode (without delamination).

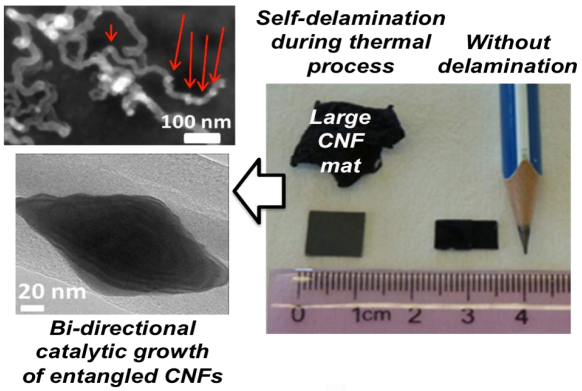
Finally, we demonstrated fully repeatable synthesis of better quality graphene at lower temperature by preheating the incoming gases. This study led to some pointers to which carbon species are really important for graphene growth (e.g., large polycyclic aromatic hydrocarbons (PAHs)).



Patterned CNT carpets (collaboration with O2Cure ltd.)

Broadening the scope to non-carbon nanostructures

Two-dimensional monolayers of transition metal dichalcogenides have attracted significant attention due to the wide range of possible bandgaps. Capitalizing on our expertise in CVD and using our state-of-the-art plasma-enhanced CVD system (Blackmagic from Aixtron) and our thermal CVD system now couple with a temperature-controlled bubbler system to allow in-situ functionalization, we plan to focus add a new focus on these new materials and tuning their properties via functionalization.



High-yield of superhydrophobic CNF mats via self-delaminating catalyst layer

Millimeter-tall carpets of crystalline and vertically aligned carbon nanotubes synthesized on silicon substrates

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Shai Rahimipour

**Neurodegenerative diseases (Multiple Sclerosis, Alzheimer's Disease, Parkinson's Disease);
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Fulbright Postdoctoral fellowship, 2000

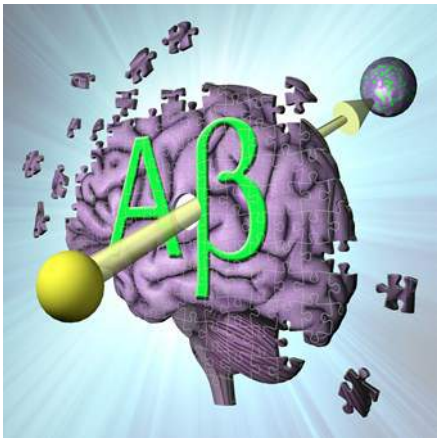
Human Frontier Science Program (HFSP) long-term fellowship for postdoctoral research, 2003-2004

One of the major goals of Rahimipour's group is to better understand and utilize self-assembly processes in order to design new modalities for arresting amyloid formation, and to enhance the biological activity and multimodal activity of different pharmacophores by inducing multivalency.

Drug Discovery, Design, and Delivery Research for Amyloidogenic Diseases

An increasing body of evidence suggests that protein misfolding and self-assembly into aggregates and fibrils is the fundamental cause of many amyloidogenic diseases. Rahimipour and his team are trying to develop a supramolecular-based platform that can be used as a general scaffold for design and discovery of novel therapeutic agents with potential application in different amyloidogenic diseases, such as Alzheimer's disease (AD) and Parkinson's disease (PD).

By using a wide range of biochemical and biophysical methods, the group has recently discovered that there are immense structural and functional similarities between AD-associate amyloid b (Ab) protein and their novel self-assembled cyclic D,L-a-peptides, which led to their cross-reaction with Ab and inhibition of its aggregation and toxicity both *in vitro* and *ex vivo*. Moreover, the discovered cyclic peptides also inhibited the aggregation and toxicity of other structurally related pathogenic amyloids, such as PD-associated a-Syn, tau and insulin. The team strongly believes that these studies may shed light on the ethiology of misfolded proteins and provide additional directions to tackle other important topics in the field, such as the infectious nature of the amyloids and their cell-to-cell spreading ability.



Sonochemically prepared protein microspheres whose surfaces are modified with an Ab recognition peptide bind with high affinity and selectivity to Ab, sequester it from the medium, inhibit its aggregation, and directly reduce its toxicity toward neuron-like cells.

Rahimipour's group is also involved in developing new chemical methods to induce multivalency effects, which is frequently used by nature to dramatically increase the bioactivity of ligands with intrinsic low activity. These methods include the development of a new and straightforward sonochemical method to generate nano- and micro-sized particles, the surface of which is covalently attached to multiple copies of a bioactive element. Using this technology, the group has shown that particles expressing multicopies of an anti-amyloidogenic peptide KLVFF can strongly bind Ab, inhibit its aggregation and reduce its toxicity to the cells. Moreover, the particles could simultaneously reduce the Ab-associated inflammation and stimulate the immune system to clear Ab from the media. The initial *in vivo* toxicity experiments suggested that the particles are biocompatible even after repeated intravenous injections of high amounts of the particles and could also be used as potential contrasting agents. Bio-distribution and pharmacokinetic studies are now in progress.

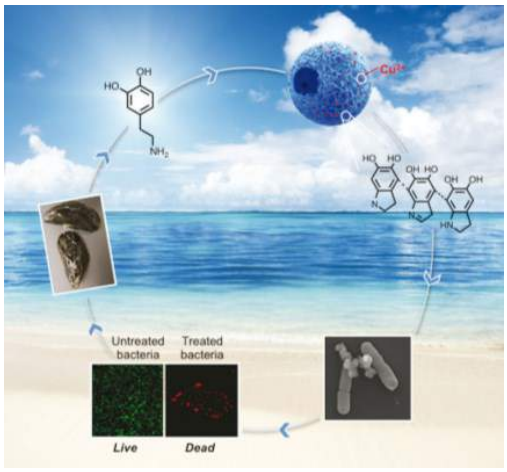
Utilizing Multivalency and Supramolecular Chemistry toward Inflammatory Disease Research: Type II Diabetes and Multiple Sclerosis

Different aspects of oxidative cellular stress are associated with the pathogenesis of several devastating human diseases, including diabetes, AD, PD, and multiple sclerosis. It is well known that the generation of reactive oxygen species (ROS) in abnormal amounts or an impairment of the cells' anti-oxidative protective systems can lead to cellular and tissue damage.

In a recent study, Rahimipour's group has demonstrated that multivalent presentation of histidine residues induced by the self-assembly of an abiotic cyclic D,L-a-peptide supramolecular structure can led to the generation of multifunctional agents that catalytically decompose intercellular ROS and induce cell protection. In particular, they showed that treatment of muscle cells with such permeable Histidine-rich cyclic peptides protects the cells against oxidative stress induced under hyperglycemic conditions and increases the uptake of glucose from periphery by increasing the translocation of glucose transporters 1 and 4. More importantly, they were able to show that the peptides possess potent anti-inflammatory, anti-oxidant and anti-excitotoxic activity to neuronal cells, and protect them against axonal damage, *in vitro*. In a pilot study carried out in collaboration with Teva Pharmaceutical Industries Ltd., the group also demonstrated that the discovered cyclic peptides exhibit potent neuroprotecting activity in an animal model of multiple sclerosis (EAE) and significantly reduce the symptoms.

Utilizing multivalency toward Infectious Disease Research

Rahimipour and his team are also utilizing the multivalency effect induced by surface-modified particles to develop new modalities against bacterial and viral infectious. In one example they have shown that multivalent presentation of mannose on the surface of the protein particles could cause the tight binding of the bacteria expressing mannose-binding receptors to the surface of the particles, which was used to detect the low number of bacteria in solution. Moreover, the group demonstrated that encapsulation of the particles with the common antibacterial drug, tetracycline, significantly enhanced the antibacterial activity of the encapsulated drug. Similar results were also observed when the surface of the particles was covalently modified to express multiple copies of mercaptoethane sulfonate to inhibit HSV-1 infection.



Sonochemically produced polydopamine nanocapsules with selective antimicrobial activity

In another avenue, the group utilized mussel adhesive protein mimics (polydopamine) and sonochemistry to generate nanocapsules that preserve all the characteristics of polydopamine, including adhesivity to different surfaces and reactivity to different nucleophiles, which was used to introduce new functionalities to the particle's surface. More interestingly, the group demonstrated for the first time that presence of Cu or Ag ions during the sonochemical irradiation generates particles that exhibit potent antibacterial and antifouling activity, without inducing any toxicity to mammalian cells. These particles could be potentially applied to different surfaces by a paint-like procedure and be applied on large surfaces to inhibit bacterial growth.

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Sharon Ruthstein

Protein structure and function, structural biology, magnetic resonance, metalloproteins

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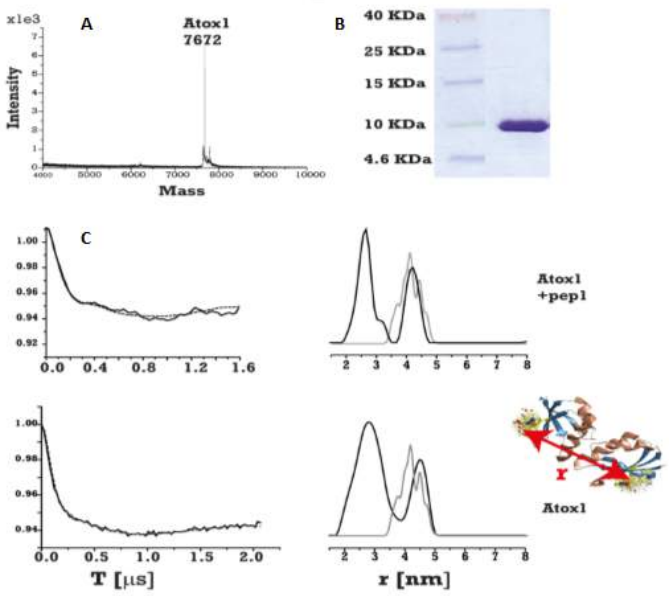
Krill Prize in Science - 2015

Ruthstein's research aims to exploit biological pathways in human and bacteria cells, which involve metal ions, using pulsed Electron Paramagnetic Resonance Spectroscopy (EPR). In her new lab –Ruthstein hopes to get a clearer picture of the metal-related processes that can lead to disease.

Metals, Magnetism and the Structure of Human Health

Metals are cofactors for many cellular enzymatic, catalytic, and oxygen reactions. Despite the important roles of metal ions, the underlying mechanism regarding the role of metal ions in promoting protein conformational changes as well as influencing subsequent chemical/biological pathways is poorly understood. It is crucial to comprehend how cells harness the power of essential metals to their proper function, while preventing toxicity, and how they defend against determinants of their functionality. Although, most of the proteins that are involved in a specific cellular metal transport are believed to be identified, little is known about how proteins regulate a particular metal cycle, what are the conformational changes that proteins should assume in order to initiate a transfer mechanism, and what are the key amino residues that control this cycle. This lack of knowledge is due to the difficulties associated with gaining structural information on integral proteins, and the absence of a biophysical system designed to systematically study cellular metal transport. One of the least resolved pathways in the human cell is related to the copper cycle. Copper is essential trace element involved in key biological processes, on the other hand, copper can be extremely deleterious, leading to neurological diseases and disorders.

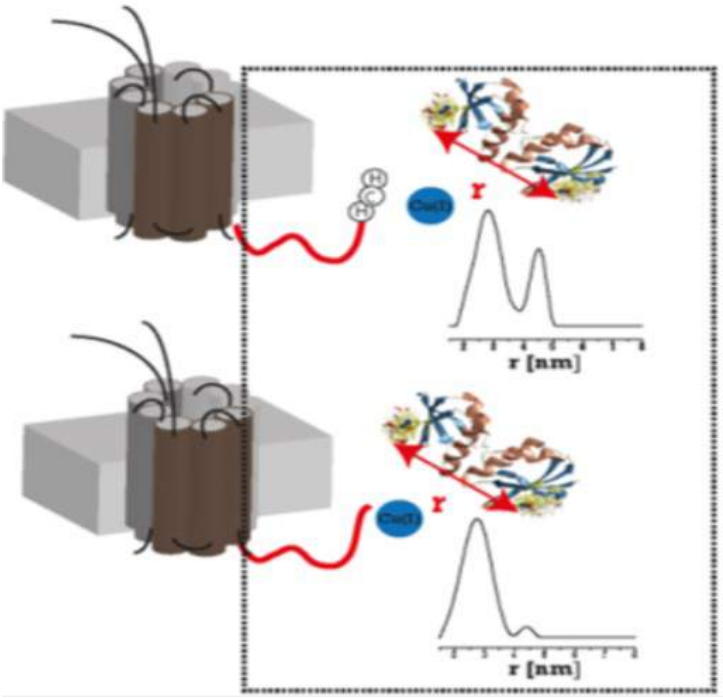


EPR signals and corresponding distance distributions for: Atox1, Atox1+pep1 (pep1 is the cytoplasmic domain of CTR1, SWKKAVVVDITEHCH), and corresponding distance distribution functions.

To comprehend such processes it is necessary to be sensitive to the structural changes that occur in the protein upon metal binding and upon protein-protein interaction. The main biophysical tool that is used in the lab of Dr. Ruthstein's lab is pulsed EPR spectroscopy. The power of EPR lies in the sensitivity to both atomic level changes and nanoscale fluctuations. In addition, EPR is not limited to the protein's size and does not require crystallization.

To date, it is known that the copper cycle (Cu(I)) in the human cell involved three different pathways: to the cytochrome C, to SOD, to the Golgi apparatus. The Ruthstein group is currently concentrating on the transfer mechanism of copper from the copper transporter CTR1, through the Atox1 metallochaperone, and to ATP7B in the Golgi apparatus.

Mutations in the ATP7B were found to be responsible to the Menkes and Wilson diseases. However, the methodology developed in the lab will lay the groundwork for other future mechanistic and structural studies of other unresolved biological pathways; such as the cycle to the SOD, and to the cytochrome C.



The distance distribution functions obtained for spin-labeled Atox1 at position Cys41, in the presence of the cytoplasmic domain of CTR1, SWKKAVVVDITEHCH, and the domain without the last three amino residues, SWKKAVVVDITE.

In one of their works, the Ruthstein lab suggested close and specific interaction between proteins that are involved in the human copper cycle. In a recent paper, they followed the copper import mechanism from the CTR1 cytoplasmic domain to the metallochaperone Atox1. In this work, they expressed, purified, and spin-labelled Atox1 at the Cys41 position with nitroxide spin-labels. They showed that the EPR signal initiated bimodal distance distribution functions. They explained it by two conformation states that the Atox1 can assume. Moreover, in the presence of the CTR1 cytoplasmic domain, 15 amino acids segment (pep1), the conformation of the Atox1 is restricted resulting in a narrower distance distribution functions. This research found that the Atox1 is sensitive to its environment, and that structural changes that this protein undergoes during the copper transfer mechanism can be followed by EPR distance measurements. This work also showed that mutating C189 of CTR1 strongly affects the structure of Atox1. This suggests that C189 is an important residue for the copper transfer mechanism, and mutation in this residue can affect the transfer mechanism.
The group is also investigating the effect of competitive metal ions on the copper cycle. They hypothesize that the presence of competitive metal ions such as: Ag(I), Zn(II), cisplatin drug, or Cu(II) ligands, can affect the copper cycle, and by adding them to the cell, one can control the rate or the pathway of the cellular copper metal ion.

Looking to the future

The interactions between proteins that are involved in the metal cycle are often difficult to study since the affinity between the proteins is low. Moreover, upon metal coordination, the protein assumes only minor conformational changes, which can be targeted only by high resolution biophysical tools. The Ruthstein lab is also aiming to increase the sensitivity and resolution of the current EPR methods, and to develop new methodologies that will be able to probe and follow a cellular biological process at the molecular level *in vitro* and in the cell environment.
The success of their research will create substantial progress in the biophysics and medicinal chemistry communities, and will provide a spectroscopic tool that can follow the transfer mechanism of any metal, ligand, or therapeutic drug, providing a detail mechanism and molecular knowledge on the pathway of this ligand.

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Plasmonics, hybrid materials for renewable energy, light matter interaction, aerogel, metallic nanostructures, SHG, surface chemistry, photochemistry

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Current research in Salomon's lab is on interaction between molecules and light at the nano scale, and real time imaging of electrode surfaces as part of INREP–Israel's National Research Center for Electrical Propulsion .

Salomon is applying her complementary knowledge of optics and surface chemistry to the development of hybrid materials for renewable energy and photochemistry on surfaces. By fabricating metallic nanostructures, she captures light energy that can be used as a tool for controlling processes in molecular systems. She is also working on batteries, as part of INREP, using an optical technique to look inside the battery electrode at the nanoscale during the electrochemical reaction. Such a technique will help us understand the structural degradation occurring during the charge/discharge cycles.

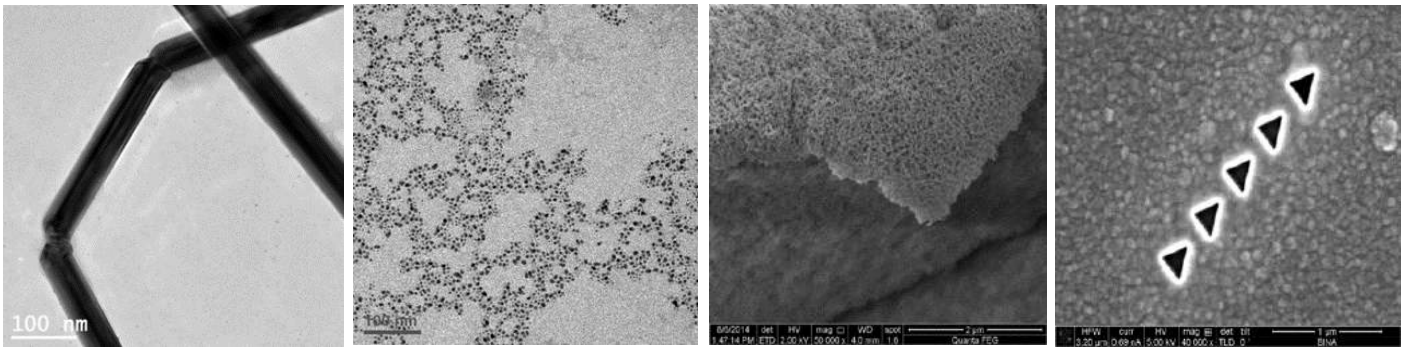
The Salomon lab combined unique expertise both in surface chemistry and in nanophotonics. They design and synthesize hybrid materials which are based on adsorption of molecules on metallic nanostructures, aiming for new molecular systems with specific optical properties.

Using state of the art fabrication technique available at the BINA nanocenter and wet chemistry, we fabricate metallic nano-structures; particles; holes and aerogels. Such metallic nanostructures act as antenna for the light energy and thus enhance and focus the light field at specific frequencies, much depending on the metallic geometrical parameters. Molecules located in proximity to such surfaces experience a very strong field and thus their physical/photo-physical properties are altered. We studied those unique properties using optical set-ups available in our lab where the idea is to achieve control of the photo-chemical processes of the studied molecular system.

Long range energy transfer processes between molecules, photochemistry on surfaces, energy conversion systems and nonlinear optical properties are examples of on-going research projects in the Salomon lab.

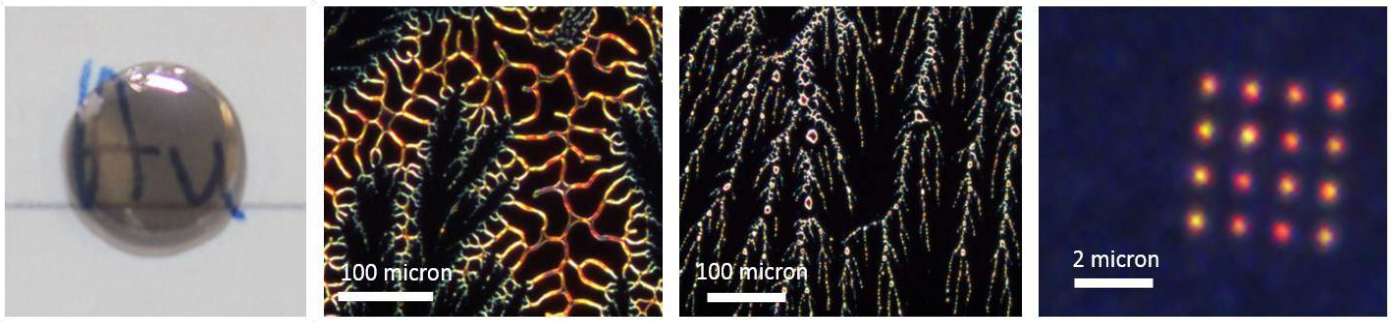
Fabrication of Metallic nanostructures

These are the metallic structures we synthesize and fabricate in our lab taken by electron microscopy. They are all with features which are much smaller than the optical wavelengths. We use silver gold and aluminum .



Properties of metallic nanostructures

Some examples from daily life in our lab:
The colors images below are of the metallic structures we fabricate. One of our goals is to synthesize transparent conductive metal with unique catalytic properties .



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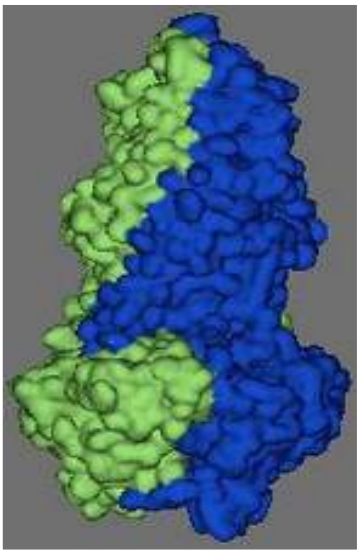
Our laboratory combines basic scientific research with translational research for the development, implementation and application of new computational methodologies in drug and material design. For drug design our research involves modeling the structure and mode of action of pharmaceutically relevant bio-targets using advanced computational methods, studying the factors governing the interactions between such targets and their potential ligands, virtually screening for and designing new ligands and predicting the pharmacological profile of drug candidates. We work on proteins involved in multiple pathologies such as Cystic Fibrosis, cardiovascular diseases, calcification-related diseases, and neuro-degenerative diseases.

In the area of material design we primarily use statistical methods to study arrays of materials (material libraries) and to design materials with improved properties.
Our research is interdisciplinary, at the interface between chemistry, biology and computer science, and is done in close collaboration with experimentalists.

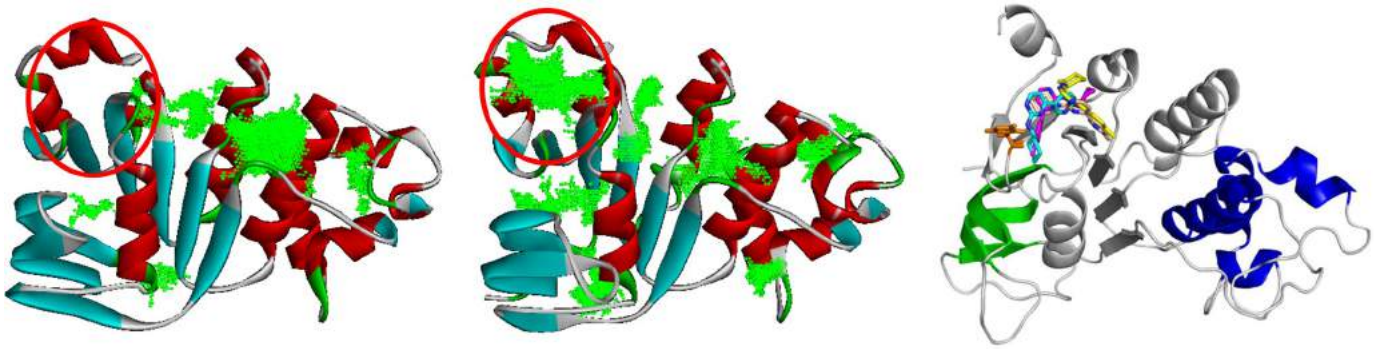
Cystic Fibrosis (CF): Searching for the Cure

Cystic Fibrosis (CF) is the most common lethal genetic disease among Caucasians with an estimated worldwide patient population of 70,000 and a median survival age in the late thirties. The only available treatments for most CF patients are symptomatic and the disease has no cure. CF is caused by mutations to the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) chloride channel, which typically lead to a misfolded, non-functioning protein.
Our lab is part of an international consortium, whose mission is to obtain the 3-dimensional structure of CFTR, study the structural manifestations of its most prevalent mutations, and rationally design small molecules that would correct its folding defect and potentially cure CF.



A 3-dimensional model of the Cystic Fibrosis. Transmembrane Conductance Regulator (CFTR), the main protein implicated in Cystic Fibrosis (CF). Such a model could help in the rational design of CFTR modulators as potential therapies for CF.

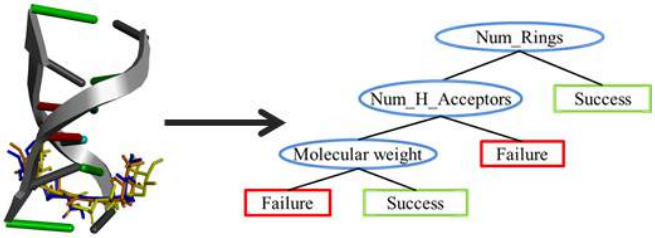
As part of our efforts we have extensively characterized CFTR and its domains using molecular dynamics (MD) simulations and identified several new ligands that bind CFTR and correct its impaired chloride conductance.



Left: Binding sites (green) identified on the crystal structure of F508del-NBD1. Middle: Binding sites (green) identified from molecular dynamics simulations of F508del-NBD1. The red circle indicates the binding site of CFFT-001 which is only apparent from the REMD simulation. Right: CFFT-001 docked into its binding site.

Work on DNA

DNA is an important target for the treatment of multiple pathologies, most notably cancer. In particular, DNA intercalators have often been used as anti-cancer drugs. In our research we have analyzed the binding of intercalators to DNA using docking simulations and identified factors responsible for their activity. This knowledge could be used to design better intercalators.



Left: Intercalatros bound to DNA. Right: A decision tree predicting the success of docking simulations to accurately dock ligands into DNA.

Cheminformatics and Quantitative Structure Activity Relationship (QSAR): Development and Applications

Cheminformatics involves the usage of computer and information techniques to transform data into knowledge for solving various problems in chemistry. These techniques are used both in the academia and in the industry, for example by pharmaceutical companies.

One of the most common cheminformatics techniques is QSAR. QSAR is a general name for a host of methods that try to correlate a specific activity for a set of compounds with their structure-derived descriptors by means of a mathematical model. This technique has been widely applied in many fields including chemistry, biology, and environmental sciences. Over the last few years our group has been engaged in the development of new QSAR methodologies. In particular we have developed new algorithms for the rational partitioning of a data set into a training set and a test set and for the removal of outliers. These algorithms are key in the development of reliable QSAR models.

These new algorithms were incorporated into a newly developed workflow which was applied for the study and design of photovoltaic (PV) cells. Such cells have the potential to meet future demands for clean affordable energy. In particular, cells made entirely of metal oxides (MO) have many favorable properties. We have developed multiple QSAR models which will predict several solar cells properties (for example, voltage and current) and used them for solar cells design.

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Directed Materials Assembly, Influencing Polymerization & Phase Separation Processes with Optical and Acoustic Tweezers, Controlled Hybrid formation, Directional Surface Treatment

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Shpaisman's lab is devoted to generating novel techniques for fabricating micro/nano-scopic structures, and for examining ways that these new structures could be further manipulated. The novelty arises from combining various methods from the fields of chemistry, physics and material science. The goal is to achieve a better understanding of the underlying scientific principles that govern such processes, while at the same time, developing custom-designed materials for use in various nano-technological applications.

Controlling Material Formation with Acoustic and Radiation Forces

Light and sound waves can influence materials in various ways. One influence, that is usually neglected due to its small impact at normal conditions, is a physical force that pushes or pulls materials. But, if light or sound waves are tightly focused, one can manipulate these waves to trap materials in three dimensions. These methods were coined "optical tweezers" and "acoustic tweezers". Shpaisman and his group are exploring how these tweezers can effect material formation.

The group has shown that if a chemical reaction such as emulsion polymerization is taking place while the optical tweezers are present, the tweezers will direct the chemical reaction to take place at certain locations. As these forces influence a wide variety of materials, creating interesting hybrid structures (that are not easily achieved by other techniques) is possible. The resulting structures could be custom-designed (size, shape, density, composition, material distribution profile etc.) for use as catalyst support, magnetic recording media, templating materials and biomedical/pharmaceutical applications.

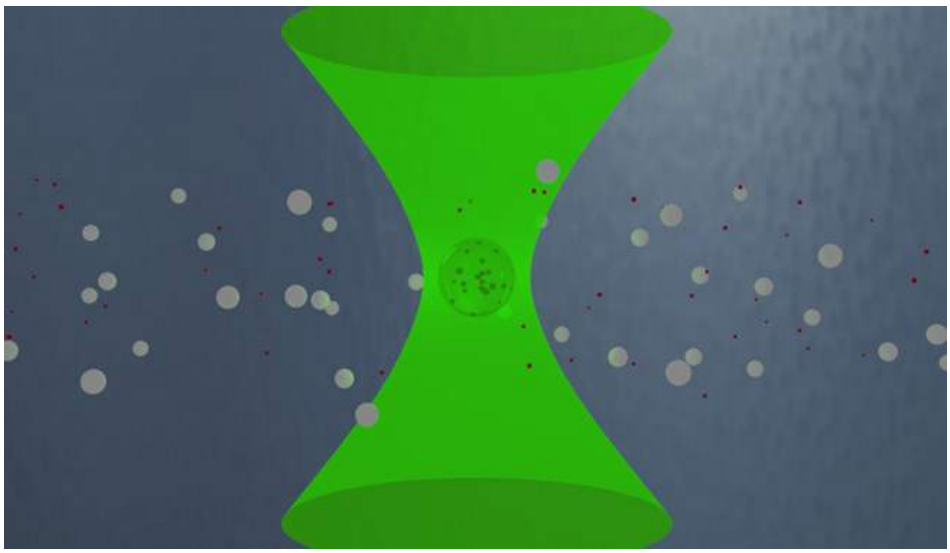

Illustration of hybrid (organic-inorganic) colloidal formation with optical tweezers. Greyish spheres represent organic nucleation sites and micelles, while smaller reddish particles represent inorganic nanoparticles

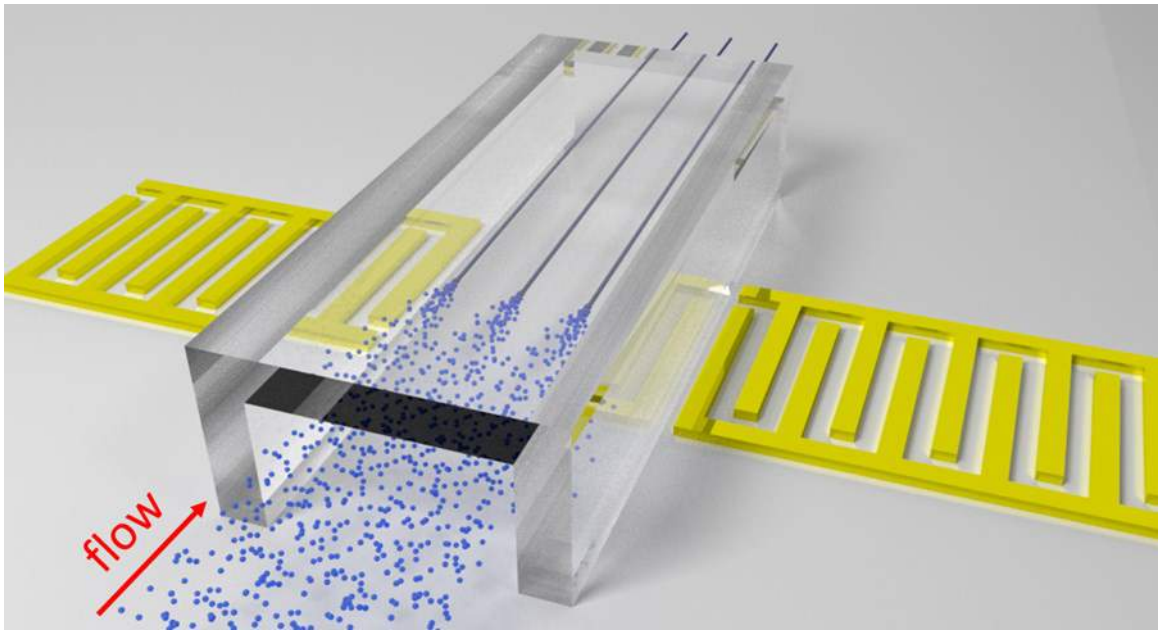

Illustration of fiber formation due to the effect of a standing surface acoustic wave on metallic nanoparticles under constant microfluidic laminar flow

Directional Surface Treatment in Microfluidic Channels

Shpaisman's lab has recently introduced a new design of a microfluidic device allowing a selective treatment of part of a colloid's surface. This treatment is achieved by transferring a minute amount of the precursor solution through a nozzle onto the surface of the colloid. Sequential functionalization with different precursors from different directions would generate colloids with the potential of forming on-demand 3D colloidal assemblies for applications in photonics, plasmonics, or catalysis.

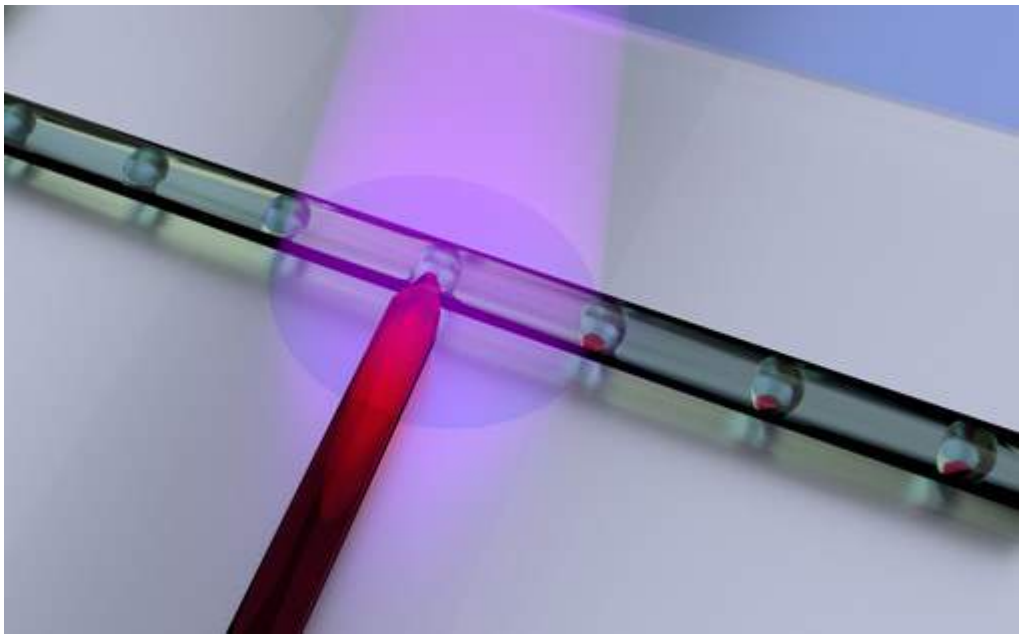

Illustration of the directional surface treatment system

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Guastella Foundation Fellow

Fulbright Research Fellow

NIH-Research Career Development Awardee

Research in Sukenik's lab focuses on understanding the chemistry of ordered organic assemblies with special emphasis on self-assembled monomolecular films and other nanostructured interfaces including hybrid organic/inorganic composites and functionalized nanoparticles. Current research projects address a number of important applications of this thin film chemistry with an eye towards problems in biomaterial design, sensors, and nanoscale devices.

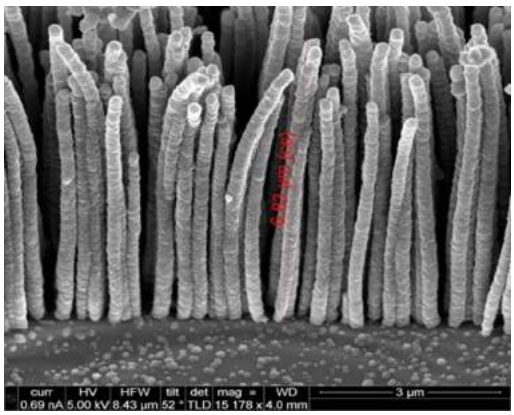
Nanotechnology and Materials Science

Sukenik and his group are exploring various approaches to the surface modification of engineered materials. To this end, monolayer assemblies provide a structurally well-defined means of changing surface properties of materials without altering their bulk properties. Both organic and inorganic thin films have been developed as tools for controlling the surfaces of both metals and polymers.

Monolayer assemblies are being used for anchoring biologically active molecules on a variety of metal and metal oxide surfaces. The stability, uniform thickness, and controlled chemical composition of siloxane anchored and phosphonate anchored self-assembled monolayers make them ideal vehicles for the application of novel anchoring chemistries with control over biomolecule orientation and activity.

The group has used monolayer films as templates for the growth of a wide range of metal oxide thin films. These ceramic materials are remarkably uniform and pore free. Moreover, by patterning the monolayer, Sukenik and his team can pattern the ceramic overlayer. Monolayers with specially designed chemical reactivity have also been applied as nanometric glues for electronic and photonic materials.

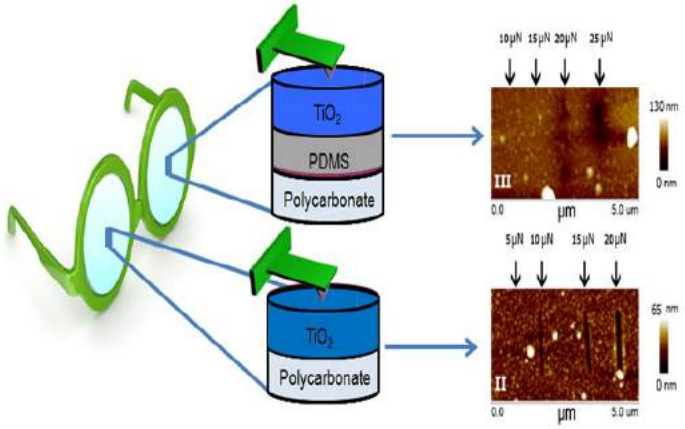
Methodology for applying ceramic thin films on surfaces have been developed using a variety of liquid phase and gas phase methodologies. The films are typically very adherent to the solid substrates even in the face of aggressive thermal or chemical post-deposition treatments. Sukenik and his group are currently exploring the physical and chemical properties of these films, as well as their potential use as ultra-thin barrier layers.



Carbon Nanotubes (CNTs) coated with a uniform 60 nm shell of TiO_2.

In related work, thin film coatings are being tested as novel tools for modifying surface properties of micron to nanometer scale devices. Such applications focus on the electronic, mechanical, wetting, and lubrication properties.

Sukenik and his group have used thin oxide films to repel bacteria when applied to the silicon rubber used in medical devices such as catheters. Interestingly, the same method for fabricating thin oxide films has been used to improve the stability of polymer composites and protect satellites from the erosion that occurs in low earth orbit.

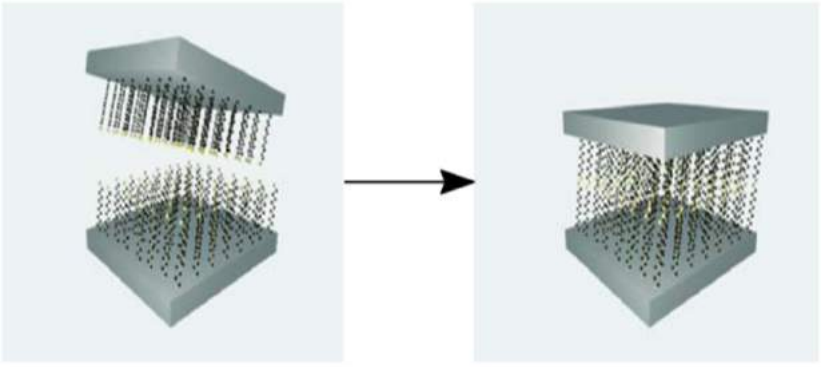


Oxide nanometric overlayers on top of an initial soft polymer coating introduce a "cushioning effect" for application to optical lenses to improve scratch resistance.

Researchers in Sukenik's lab also collaborate with Dr. Avi Zadok, of the School of Engineering and BINA, on silicon photonics research. Together, they have fabricated layered "sandwiches" of electronic and photonic materials, resulting in a new paradigm for wafer processing with the potential for the creation of advanced opto-electronic devices. Among the goals of their silicon photonics research is to develop optical communications components for use in future multi-processor computer systems.

Looking to the Future

Sukenik's group continues to expand its repertoire of nano-fabrication tools with the addition of techniques like atomic layer deposition (ALD). Surface chemistries that impart new reactivity to otherwise inert polymer surfaces are being developed alongside new strategies for modulating mechanical properties of interfaces. The combination of various solution and vapor phase-based processing methodologies provide new kinds of surface structures and offer new insight into chemistry at interfaces.



A method for the bonding of dissimilar materials at low temperatures, based on the application of chemically active, self-assembled-monolayers on the surfaces to be bonded.

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Yaakov Tischler

Coherent light-matter coupling in molecular systems: Polaritons, J-aggregates, Organic Lasers. Near-Field scanning microcopy and ultra-fast non-linear spectroscopy. Applications of Raman scattering for energy sustainability and biotechnology

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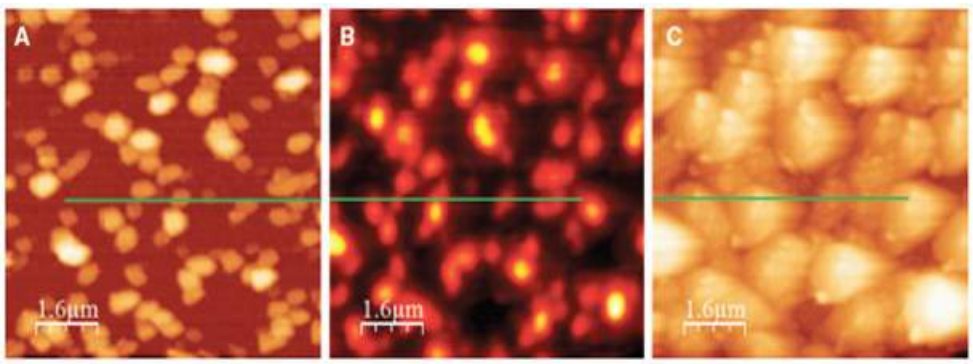
As one of the world's foremost experts in molecular photonics, Dr. Tischler combines his knowledge and skills in two distinct fields of research-materials science and spectroscopy. Under his direction, the Molecular Photonics Laboratory (MPL) is conducting experiments in coherent excitonic coupling using semiconductor microcavity lasers. They also synthesize organic nanoscale thin films, layers of carbon-based materials which range in thickness from 1 molecule to about 100 molecules.

Photonics and Optics Research

In Tischler's lab, the team is engaged in studying fundamental interactions between light and matter. They believe these investigations will lead to deep insights into the way that nano-materials exchange energy with light, and they expect to arrive at new solutions to important scientific and technological challenges.

The interactions between light and matter can occur so quickly that rapid detection mechanisms are often required. The light-based methods used in MPL are effective for characterizing molecular based photonic devices that may ultimately lead to future optical switches, chemical sensors, and new coherent light sources.

Tischler's team uses ultra-fast laser spectroscopy to characterize the properties of light-activated materials arranged in films only one molecular layer thick, and he has shown that such "monolayers" generate new optical resonances. This discovery may lead to improved sensors for a variety of applications. In addition, they are working on the development of next-generation nano-lasers for the promotion and control of chemical sensing.



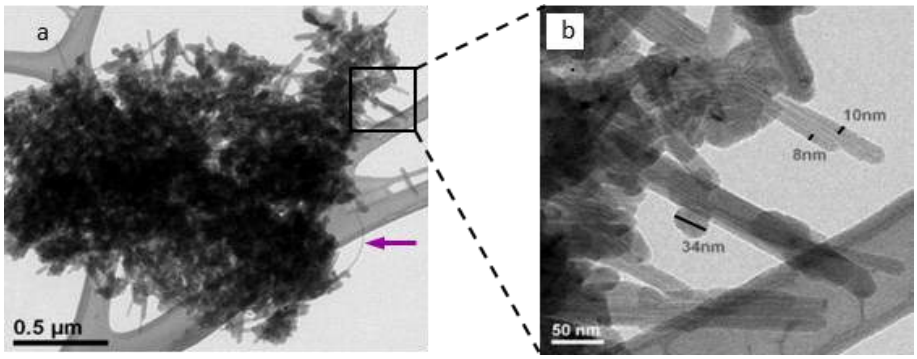
Dual-Tip AFM/NSOM SPM results for thin film of Lumogen Red doped into a Lumogen Organge matrix (5%/95%). (A) Topography obtained from AFM tip in soft-contact with NSOM probe, (B) Simultaneously measured near-field fluorescence signal obtained from NSOM probe showing spatial heterogeneity of the NSOM fluorescence in the image, (C) topography obtained from NSOM probe

Capturing the Sun's Energy

Tischler and his researchers are experts in characterizing next generation solar cell materials using Raman scattering spectroscopy. They also study energy-transfer dynamics in J-aggregates and other light-harvesting materials utilizing time resolved near field scanning microscopy.

Practical Applications

Tischler and his team are researching scientific problems where breakthroughs will lead to new technology. Some of this technology has applications that will touch everyday lives, such as chemical and explosives detectors based on infrared spectroscopy to increase security in public spaces or solar cells that convert sunlight into electricity. Future applications of Tischler's work also include protein sequencing and tunable lasers. Some of these developments are already patent-pending and licensed by the Organic Light-Emitting Diode (OLED) display industry.



TEM images of C8S4 J-aggregates: a. A stack of circular and fibrous aggregates of C8S4. The arrow indicates an unfolded fiber. b. Zoom-in on the edge of the stack shows the fibers are folded, and their size is on the order of 10 nm. In addition, a dot aggregate can be seen.

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Arie Zaban

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Ph.D., Bar-Ilan University

Postdoctoral, US National Renewable Energy Laboratory (Denver, CO)

ICS Prize of Excellence , 2014

The IVS Research Excellence Prize, 2011

Michael Landau Research Prize in Renewable Energy, 2007

Israel Chemical Society Prize for Outstanding Young Scientist

Rothschild Fellowship for Postdoctoral Research

Levi Eshkol Scholarship for outstanding student

Renewable energy; All Oxide Photovoltaics; Perovskite Sensitized Solar Cells; Quantum-Dot Sensitized Solar Cells; Transparent electrodes and current collectors; Metal-air batteries

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Zaban's research interests are in the field of materials science for a sustainable world, with a focus on renewable energy resources. Recent achievements concentrate on: (i) All-oxide photovoltaics (ii) mechanisms in ferroelectric based solar cells e.g. perovskites, (iii) built-in QD antennas for photovoltaics, (iv) high conductivity transparent electrodes for optoelectronics, and (v) high energy density metal-air batteries.

All Oxide Photovoltaics via Combinatorial Material Science

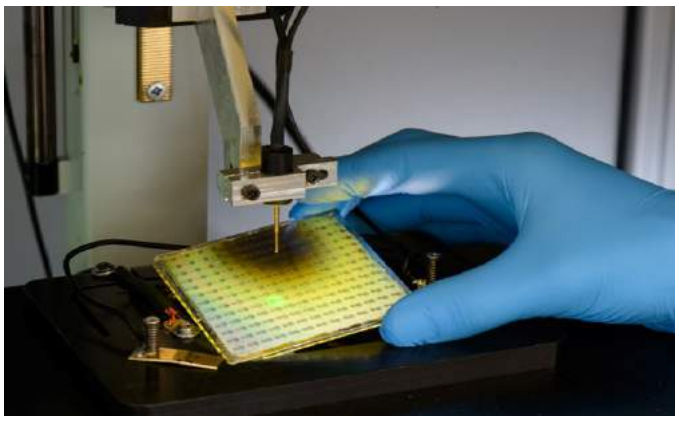
Zaban's group uses combinatorial material science to answer renewable energy's need for new materials. The combinatorial approach is an efficient way to discover compounds with unique characteristics. The current focus is metal oxides that can perform as light absorbers and/or electron/hole conductors in PV solar cells.

The team has created a "materials data factory" for metal oxides that generates information on new compounds and their functionality in devices on a daily basis. The Metal Oxides family includes billions of materials, however only ~30,000 have been studied so far. Using a high throughput combinatorial method the group has discovered new exciting metal oxide materials that have never been considered before in the photovoltaics industry. A good example is the novel heterojunction solar cell based on Co_3O_4 and TiO_2 that displays photovoltaic activity. In order to optimize the performance of such devices the team utilizes high throughput methods to determine the ideal thicknesses of layers as well as deposition conditions. The newly discovered light absorber material, Co_3O_4, is an excellent starting point from which the laboratory is expanding its combinatorial study of metal oxide materials for binary and ternary systems that can use similar crystal structures, or as a material's building block.

Another example of the power of combinatorial material science is the ability to isolate the functionality of a specific phase out of many, for example the three oxide phases of copper include Cu_2O, CuO, and Cu_4O_3.

The group has also demonstrated the ability to translate findings from ultra high vacuum fabrication techniques to vacuum free techniques, which are far more cost efficient and relevant for large scale industrial processes.

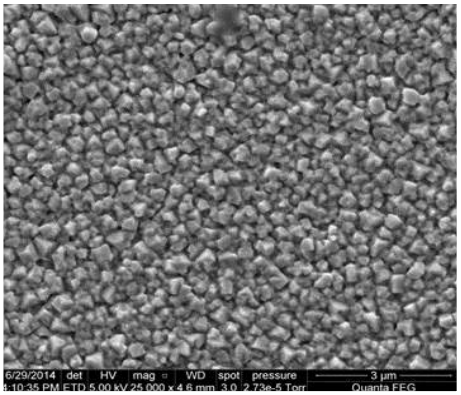
Prof. Zaban and his team believe that through the use of combinatorial material science and big data tools, they will create new insights, new materials, unique devices, and possibly new physics, in the field of photovoltaics.



High throughput IV-scanner

Perovskite sensitized solar cells

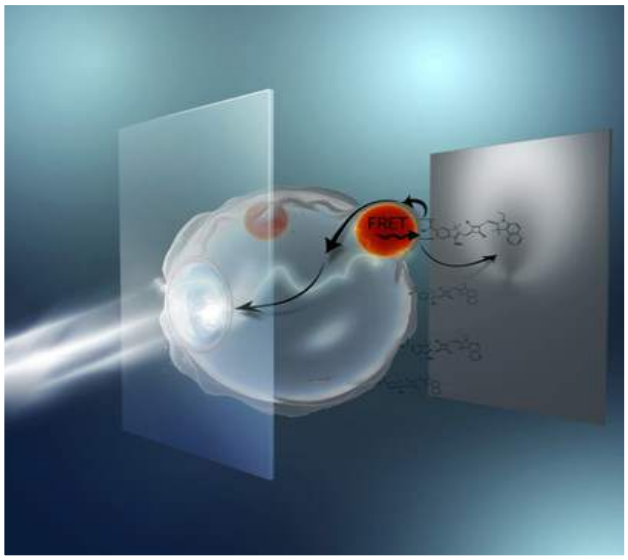
Zaban's group also studies a family of solar cells, based on hybrid organic-inorganic perovskite absorbers. Progress of PV devices based on these absorbers and their solar to electrical power conversion efficiencies was unprecedentedly high, in a period of only three years. Despite the rapid increase in solar cell efficiency that is associated with device evolution, optimization and full characterization of these devices needs to be undertaken to fully utilize perovskite absorbers. Zaban's research focuses on the fabrication of high efficiency perovskite ($MAPbX_3$) based solar cells, and the study of cell operation mechanisms and interfaces, using photo-electrochemical and photo-physical methods. Zaban's group also studies the properties of $MAPbX_3$ thin films under solar cell working conditions, without typical selective (n- and p-type) contacts.



SEM image of $MAPbI_3$

Quantum Dot Sensitized Solar Cells

Zaban and his group study mono- and poly-dispersed quantum-dot-sensitized solar cells (QDSCs), focusing on stability, coating methods and performance. In one of these studies, Zaban and his collaborators Professors David Cahen and Dan Oron from the Weizmann Institute developed a new design combining the broad absorption spectrum of QD's with the evolved charge transfer mechanism of DSSC. In their design, QDs serve as “antennas”, funneling absorbed energy to nearby dye molecules via FRET, a non-radiative energy transfer, rather than being used directly as sensitizers. The QDs are incorporated into the nanoporous TiO_2 electrode with total isolation from the electrolyte, significantly improving their photostability. This new cell design enhances light absorption and broadens the absorption spectrum, effectively increasing the number of photons harvested by the dye sensitized solar cell .



QD antenna in Dye Sensitized Solar Cell

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David Zitoun

Synthesis of metallic colloids;
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Lithium-ion batteries;
Electrocatalysis.

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My main objective as a researcher is to synthesize novel inorganic and hybrid nanostructures with applications in colloidal science and electrochemistry.

The aim of the Zitoun's laboratory is to elaborate metallic and magnetic nanocomponents for batteries, fuel cells, sensors and biomedical applications. The laboratory works on the interface with micro and macro-scale environments.

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Postdoctoral,
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Senior lecturer, University Montpellier II, France, 2004-2009

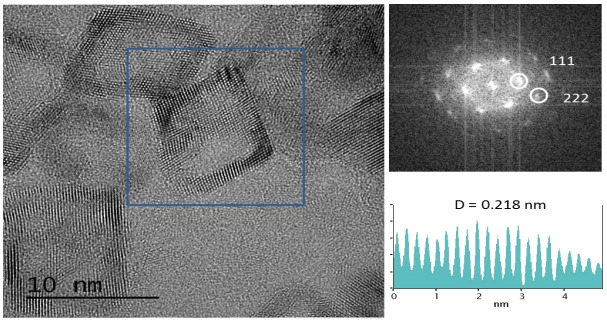
Associate Editor for Journal of Nanoparticle Research, 2014-present

Nanoparticles Synthesis: an organometallic approach

Zitoun's research group has developed new chemical routes using soluble organometallic or metal-organic precursors as an alternative to conventional colloidal chemistry and gas phase thin film deposition. We have explored the organometallic synthesis of metallic nanocrystals and the non-aqueous sol-gel synthesis along two major research axes. The first consists of the batch synthesis of nanospheres and nanowires which are then assembled. In the second approach, the organometallic precursor is directly cast on the substrate and reacts on the spot.

Dr. Zitoun's *group synthesizes reactive organometallic complexes and studies the thermolysis and chemical reduction of these complexes to yield nanostructures. They have demonstrated that properly designed, reactive, organometallic precursors could be decomposed to form metallic coatings directly on almost any substrate with unique control.*

This approach allows direct synthesis of metal films on plastic substrates, using standard coating equipment (e.g. spin coating). This synthetic pathway has been successful with manganese, cobalt, nickel and copper alloys and compounds. It has also enabled the discovery of size dependent electronic properties (magnetic moment, anisotropy, plasmon).



Hollow octahedral nanocrystals for hydrogen oxidation reaction in alkaline membrane fuel cell: HRTEM image with electron diffraction

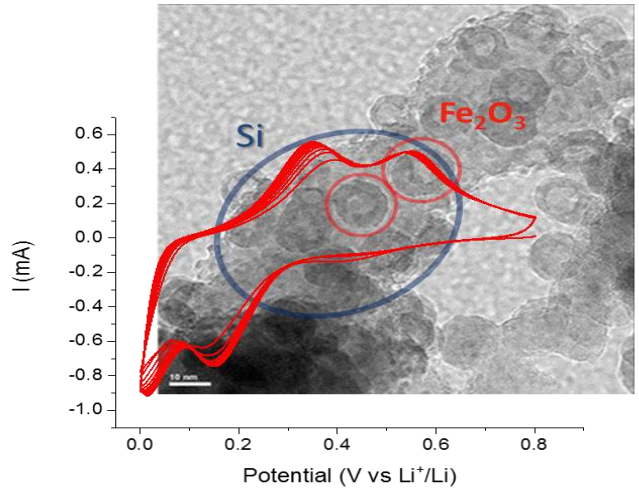
Electrocatalysts and Electrode Materials

The metallic nanoparticles are used as electrocatalysts or electrode materials in electrochemical devices (fuel cells or batteries). The organometallic syntheses described above lead to "clean surface" nanoparticles and tailored interfaces. Typically, colloidal syntheses have successfully controlled the size of nanospheres. We have brought such control to the shape and crystallographic facets of the nanocrystals. This approach has been applied to monometallic and bimetallic systems. The transition metal nanocrystals have been of particular interest in that they display high electrocatalytic activity in alkaline membrane fuel cells.

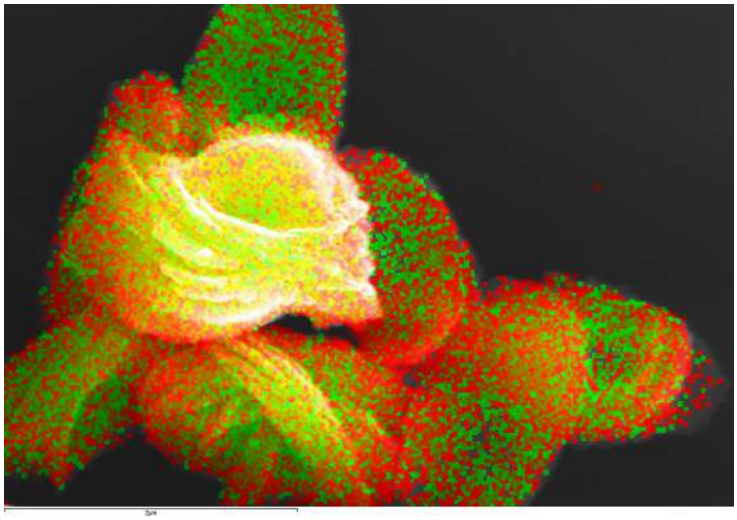
Electrochemical devices: understanding down to the nanoscale through electron magnetism

One of the challenges in energy storage research is the design and study of new electrode materials and efforts to understand their mechanism for lithium uptake. New ways to get real–time information on the performances of such batteries are continuously sought. The development of in-situ techniques can provide unique understanding of the mechanisms, successes, and failures of electrochemical devices. The development of in-situ (or in operando) characterization techniques provides uniquely valuable information about chemical processes since the interpretation of ex situ measurements can only offer a partial picture of the chemical reactions. We envision several future developments that would stem from our novel approach of bottom-up elaboration of nanomaterials. The nano-composites offer a unique platform with active elements and probes so that these real -time measurements actually map the electrodes and reveal the nature of their interfaces.

We were the first laboratory to introduce the use of electron magnetic measurements in post-mortem analyses of Li-ion batteries and the first group to publish the operando electron magnetic measurements. These in-situ measurements allowed us to propose a new electrochemical mechanism for the high energy density anodic material $FeSb_2$. Such approaches provide a deep understanding of the material response to electrochemical processes down to the nanoscale.



TEM image of hollow iron oxide/silicon composite as high energy density anode material for Li-ion batteries (cyclic voltammetry)



HRSEM mapping of core/shell high voltage olivine material for Li-ion batteries

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Critical onset of layering in sedimenting suspensions of nanoparticles
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Harold Basch (Emeritus)

Computational Chemistry

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Professor (emeritus),
Department of Chemistry

Ph.D., Columbia University

Postdoctoral,
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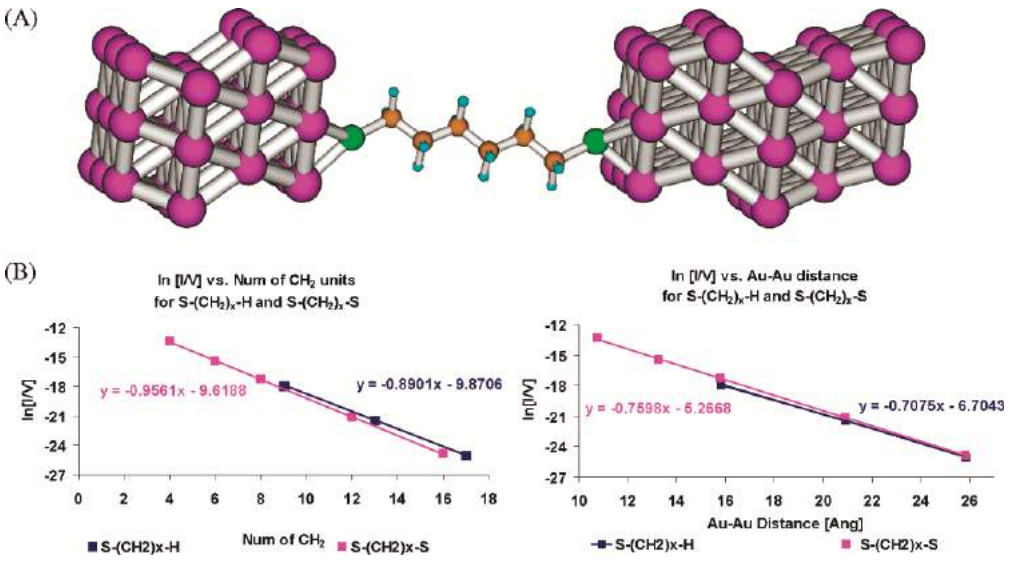
Member of the National Council for Higher Education, 1985-1991

Dean, Bar-Ilan Faculty of Exact Sciences, 1987-1989

Vice President for Research of BIU 2005-?

The uses and applications of computers in Chemistry as a ubiquitous research tool has been extensively developed and applied routinely only for the past decade, when fast computers and reliable and stable computer codes were developed which could be safely used scientifically as "black boxes" by non-experts such as experimentalists. Prof. Harold Basch was, and continues to be, a pioneer in computational quantum chemistry, developing methods and innovative applications of theoretical concepts and equations to solving problems in Chemistry.

Already in 1962, as a beginning graduate student at Columbia University in New York, Harold Basch recognized the potential use of the computer (which then filled a whole building), in chemical research. The methods and paradigms he developed are used today in modern software packages for the calculation of molecular properties. The list of applications he has been involved in include electron, electronic and photoelectronic spectroscopies, energetics, geometric and electronic structures, chemical reaction paths, intermediates and transition states, metal-ligand, metal-metal and metal cluster bonding, and active site reactions in metalloenzymes. The theoretical methods include single and multi-configuration molecular orbital theory, valence bond theory, and effective core and effective fragment potentials.
Current computational research efforts are directed towards finding appropriate molecular bridges that can serve as nano-conducting and switching elements in electronic devices (molecular electronics). These nanotechnological bridges will allow the further shrinking of electronic components, leading to much faster and more compact devices (including computers).



(A) The assumed transport geometry of a representative dithiolated alkane for which the I-V was calculated. The 3-fold site is a face centered cubic (fcc) hollow site. (B) The calculated length dependence of the transport in mono- and dithiolated alkane junctions as a function of the number of methylene units and of Au-Au distance. β=0.71 and 0.76 1/Å for monothiolated alkanes and dithiolated alkanes, respectively. Calculations used V) 1V.

Aryeh A. Frimer (Emeritus)

Professor (emeritus), Ethel and David Resnick Professor of Active Oxygen Chemistry

Ph.D., Harvard University

Postdoctoral, Weizmann Institute of Science

Sr. Medical Scientist, Medical Department, Brookhaven National Laboratory, Long Island, NY, 1982-1983

Sr. Research Fellow, Materials Division, NASA Glenn Research Center, Cleveland OH, 1990-2004

NASA-OAI Collaborative Aerospace Research Faculty Fellowship, 1997-2004

NRC-NASA GRC Senior Research Associateship Award, 1990-1996

Active Oxygen Species in Biochemistry, Electrochemistry and Aerospace Research

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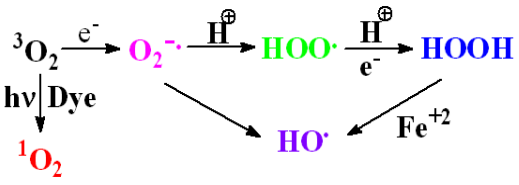
The Frimer group explores the chemistry of Active Oxygen Species (AOS) within the cell membrane, attempting to fight disease, inhibit aging and control natural autoxidative deterioration.

Chemistry of Active Oxygen Species

Free radicals are molecular fragments with unpaired electrons. Despite the pivotal role of free radical processes in nature, free radical damage presents a serious and constant threat to living organisms. One of the clearest sources of radicals in the body is superoxide anion radical [O_2-], which is formed in many biologically important reactions in both enzymic and non-enzymic processes. Frimer's Active Oxygen Group has been studying the organic chemistry of superoxide, hydroxyl, peroxyl and hydroxyalkyl radicals, and singlet oxygen with various organic substrates intercalated in the lipid bilayer of liposomes, biological membranes and erythrocyte ghosts. Our goal is to understand the mechanism of action of these active oxygen species within cell membranes.



Active Oxygen Species

Biophysics Research: Determining the Quantitative Depth of Intercalants within the Lipid Bilayer

Decades of research have elucidated the fundamental role played by the lipophilic cell membrane in regulating the transport of chemicals and nutrients into and out of the cell. Using both chemical and spectral techniques (NMR, ESR and fluorescence), Frimer has been developing chemical probes and a "molecular ruler" to measure the angstrom depth of intercalants and active oxygen species within the lipid bilayer of liposomes and biological membranes. The ultimate objective is to demonstrate a correlation between the location/orientation of the substrate/intercalant within the bilayer and its reactivity.

Advancing Lithium-Oxygen Battery Research

Interest in active oxygen chemistry has blossomed recently in a totally different field – Lithium-Oxygen (Li–O_2) batteries. The latter show tremendous promise in the critical area of electrochemical energy storage. The high energy density of Li–O_2 battery can aid in extending the driving distances between charges which is very close to that of gasoline. Our current research has been focused on the interaction of reduced oxygen species with non-aqueous electrolytes used in Li–O_2 batteries.

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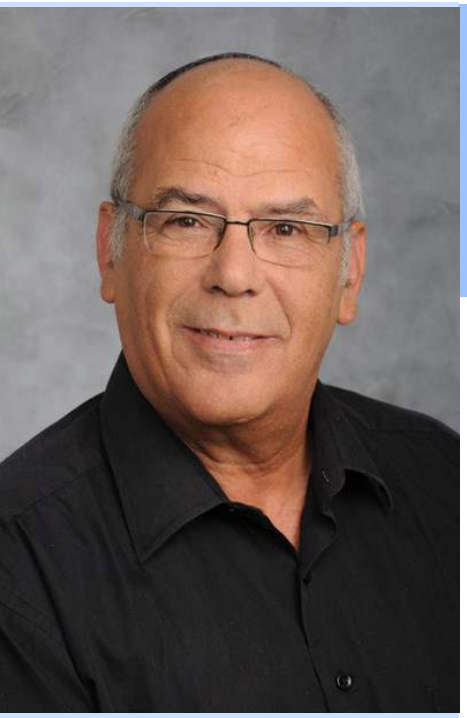
Aharon Gedanken (Emeritus)



Developing methods for the fabrication of nano-materials and their application in various fields

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Dean, Bar Ilan Faculty of Exact Sciences, 1995-1996

Prize of the Israeli Vacuum Society, 2009

Prize of the Israeli Chemical Society, 2013

Representative of Israel to the EC committee on Nano, Materials, and Processes (2009-2013)

Serves on the Editorial Board of 7 Journals

Awarded the prize for excellence in research by the Israel Vacuum, 2009

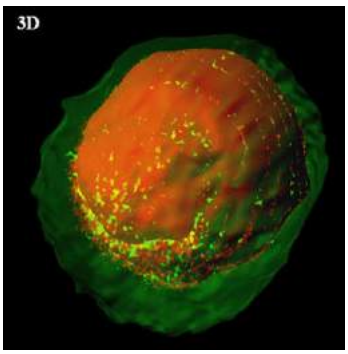
Recipient of the President of Israel Achievement Award for coordination of a European Funded Research

Gedanken is a pioneer of sonochemistry – a discipline in which chemical reactions are accelerated through the application of ultrasonic sound waves. His synthetic specialties include also Microwave Superheating, Sonoelectrochem-istry, and Reactions under Autogenic Pressure at Elevated Temperatures. He has published more than 770 papers in peer-reviewed Journals his H-Index is 81.

Nanotechnology Research

Gedanken is an expert in the fabrication of nanostructures with special properties such as antibacterial, antiviral (i.e. Swine influenza), antifungal and antibiofilm. Some of his antibacterial nanoparticles kill not only regular bacteria but also bacteria that are resistant to antibiotic.

Among his discoveries is the fact that ultrasound radiation can coat a large variety of solid surfaces such as metals, ceramics, polymers, glass, textiles, and even paper, enabling him to impart a variety of properties to the substrate.



Confocal microscopy images of CY3-RNA (red) encapsulated within FITC-BSA (green)

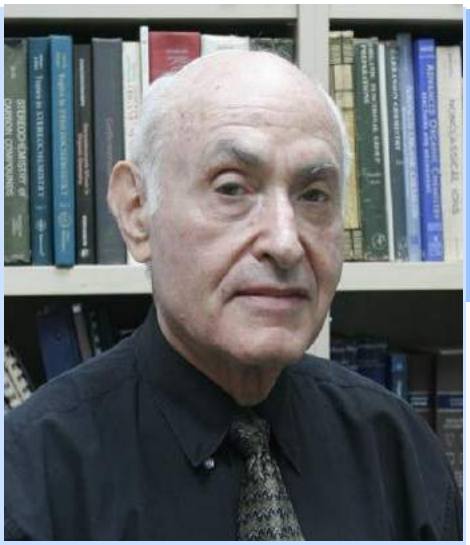
The EC has announced a "success story" a grant that Gedanken has leads (Oct. 2009-Sept. 2013), with 17 partners from academia and industry. The consortium was focused on the Hospital of the Future, in which all textiles such as bed sheets, pajamas, pillow covers, curtains, doctors' robes, will be antibacterial. Due to deep embedding of antibacterial nanoparticles in the textiles, their antibacterial properties are maintained even after 65 hospital washing machine cycles at 92°C. Results obtained in a Bulgarian hospital where 22 patients were dressed and slept on coated textiles has shown a decrease of nosocomial infections as compared to patients that slept and dressed with regular textiles. Together with Prof. Shulamit Michaeli, Gedanken has also recently fabricated RNA-based nanoparticles that can "silence" specific genes and are kept stable at room temperature even after a week.

The same coating method was used to coat medical devices such as Catheters, Contact lenses, and Silicon implants.

Drug Discovery, Design, and Delivery Research for Anti-Cancer Drugs

Gedanken uses sonochemistry to produce micro and nanovehicles that deliver antibiotics and anti-cancer drugs in a rapid-release mode. These drugs are encapsulated in proteinaceous micro and nano spheres. Finally, one of his metal oxide nanoparticles has shown very efficient killing of pancreatic cancer cells.

Alfred Hassner (Emeritus)



Organic Chemistry, Stereochemistry, Medicinal and Heterocyclic Chemistry, Synthetic Methods

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Professor (emeritus), Department of Chemistry

Ph.D., Univ. of Nebraska (Cromwell)

Postdoctoral, Harvard University

Professor, University of Colorado Boulder, 1957-1975

Leading Professor, SUNY Binghamton, 1975-1984

Humboldt Fellow,

National Cancer Inst. Fellow

Lady Davis Fellow

A.W. Killam Award

I.C.S. Prize for Excellence

Fulbright Senior Award,

Fellow Royal Soc. Chemistry,

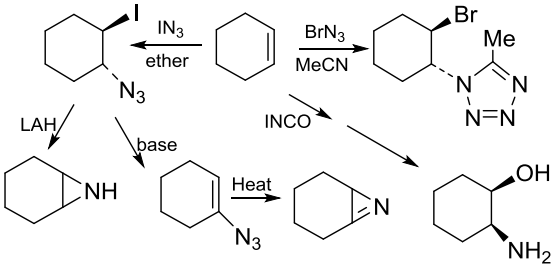
Past President Israel Chem Society,

Editorial board of 4 journals

With more than 300 research articles in print, Professor Hassner has had a major impact on chemical science, particularly on organic synthetic methodology and small ring heterocyclic chemistry.

Some of his major contributions include the stereoselective introduction of nitrogen functionality, such as nitro, azido, isocyanate and nitrile oxide, into organic molecules. His group pioneered in azide chemistry and discovered stereoselective and regioselective halogen azide additions to multiple bonds. They were able to establish that such additions can proceed either by an ionic or a free radical mechanism leading to different isomeric products, depending on solvent polarity. This led Hassner to propose the concept of regioselectivity, now a universally used terminology in organic chemistry.

In addition to halogen azides, his group examined the synthetic utility of other pseudohalogens like iodine isocyanate, nitrosyl chloride, iodine isothiocyanate, chlorosulfonyl isocyanate, carbomethoxysulfamoyl chloride and nitrile iodide in reactions with multiple bonds. Other studies established the stereochemistry and regiochemistry of ring opening of three-member rings, including small rings fused to larger rings, as well as the intermediacy of iodonium ions and nitrilium ions in these reactions.



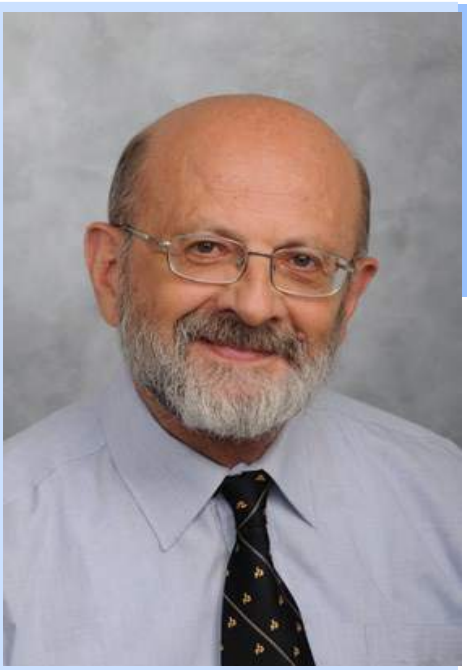
Hassner's group pioneered in methodology for synthesis of small ring heterocycles such as aziridines, azirines, azetines, as well as of larger ring heterocycles including azepines. In the steroid field, he developed the synthesis of steroido-heterocycles and was one of the first to recognize the application of NMR half-widths to stereochemical structure assignments before high resolution NMR became available.

In parallel with Steglich, Hassner showed that 4-dimethylaminopyridine (DMAP) and in particular 4-dipyrrolidinopyridine (DPP) is a useful super-acylation catalyst that can enhance many fold the direct esterification of carboxylic acids by alcohols including hindered alcohols.

$$R\text{-}CO_2H + t\text{-}BuOH \xrightarrow[25^{o}]{DMAP,\ DCC} R\text{-}CO_2\text{-}t\text{-}Bu$$

Professor Hassner's research on regioselective [2+2] ketene – olefin cycloadditions led to synthesis of steroidal cyclobutanones. He also developed stereo- and regioselective [2+2] ketene – olefin cycloadditions and proposed a preference for axial approach in the cycloaddition of ketenes to six-member ring alkenes.

Shmaryahu Hoz (Emeritus)



Professor (emeritus), Department of Chemistry

Ph.D., Bar-Ilan University

Postdoctoral,
University of California

Vice President for Research of BIU 1996-2001

Presently, senior advisor to the university president and the Head of the Responsa Project

Mechanistic Chemistry of SmI_2
Mechanics of Nano Rods
Effect of electric fields on structure and reactivity
Nucleophilic Reactions

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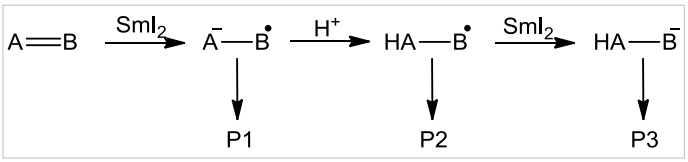
Our research is focused on three main topics: The chemistry of SmI_2 – mechanism and the mechanistic basis for its utilization in synthesis; the mechanics of nano – molecular rods and the effects of electric fields on structure and reactivity.

Mechanistic Chemistry of SmI_2

In our lab we have striven to understand the driving forces behind the chemistry of SmI_2 and the origins of its versatility. Its high versatility results from the fact that unlike reductions by metal hydrides which generate a single anionic intermediate, reduction by SmI_2 may generate three different intermediates, each of which may lead to a different product (P1 – P3).



We focused on developing ways to channel at will the reactions leading to one of the three possible products.

Mechanics of Nano Rods and Electric Field Effects

Using the combination of mechanical engineering methods and quantum mechanical calculations, we have shown that the hardness of polyyne rods along the long axis is 40 times that of a diamond – the hardest known material in nature. Another type of molecular rods, prismanes, was shown to demonstrate auxetic behavior. Namely, contrary to expectations, they become thicker when stretched, and thinner when compressed. This is the first time that the auxetic effect has been demonstrated at the molecular level.

Carbon nanotubes are known to be homogeneous along their long axis. By applying an electric field along this axis, we were able to induce regio-selectivity towards nucleophilic and electrophilic reagents in model polyynes, thereby enabling the barcoding of nanotubes.

We induce chirality in non-chiral molecules such as glycine, by applying an electric field directed along one of the C-H bonds, thus rendering the two hydrogen atoms non-equivalent and we bent polyyne rods substituted at their terminal carbons by an electric field perpendicular to their long axis.

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Deciphering a 20 Year Old Conundrum: The Mechanisms of the Reduction by the Water/Amine/SmI2 Mixture. Sandeepan Maity and Shmaryahu Hoz, Chem. Eur. J. 2015, 21, 18394-18400.

Kenneth G. Kay (Emeritus)

Theoretical chemistry; dynamics of chemical reactions; semiclassical approximations for the dynamical behavior and static properties of atoms and molecules.

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Professor (emeritus), Department of Chemistry

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Postdoctoral,
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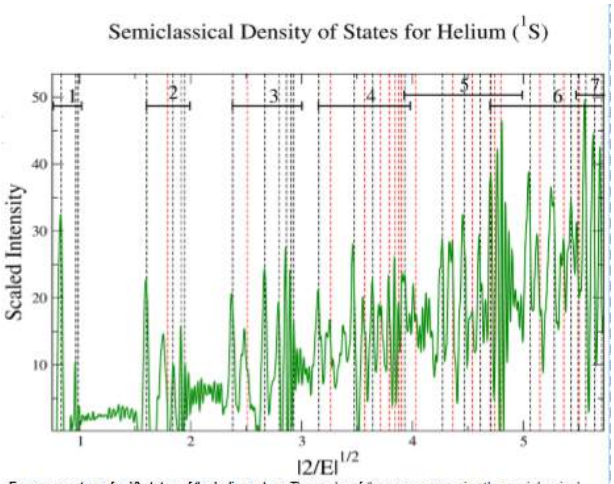
Professor of Chemistry, Kansas State University, 1971-1987

Visiting Professor of Chemistry, University of Toronto, 1982-1983

Visiting Associate Professor of Chemistry, Tel Aviv University, 1979-1980

It has been known since the early years of the 20th century that the classical mechanics of Newton is unable to correctly describe the motion and properties of the fundamental building blocks of chemistry, atoms and molecules. However, quantum mechanics, which indeed provides the correct treatments, is difficult to apply computationally and, in many respects, hard to understand intuitively. Semiclassical mechanics is an approximation that uses ordinary classical mechanics to obtain quantum mechanical information. Semiclassical calculations can be much simpler and faster than ordinary quantum computations, allowing one to explain the properties and dynamical behavior for much larger chemical systems. Also, because such calculations are based on classical descriptions of the motion for electrons and nuclei, the results can be understood more intuitively, in terms of familiar concepts, leading to explanations of physical and chemical phenomena that are clearer and easier to grasp. Finally, semiclassical mechanics serves as a bridge between quantum mechanics and classical mechanics. Its study allows one to address intriguing issues about how the quantum wave description of matter tends to the much more familiar classical picture, as particles become more massive or energetic.

Professor Kay's research focuses on the development and application of such semiclassical treatments. Broad topics of interest include development of useful semiclassical approximations for the treatment of: (1) the electronic structure of atoms and molecules, (2) tunneling dynamics in molecular systems, and (3) classically chaotic systems that defy application of many current practical semiclassical techniques.



Energy spectrum for ^{1}S states of the helium atom. The peaks of the green curve give the semiclassical energy levels in atomic units and the drop lines give the quantum values. The numbers across the top identify the Rydberg series of the levels (the principal quantum number for the inner electron).

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Rachel Lubart (Retired)

Associate Professor (Retired),
Department of Chemistry

Post-Doctoral studies:
Department of Physics, Bar-Ilan University

Light devices in the visible range for wound healing, bacteria killing, and for increasing the fertilizing capability of sperm cells. Nano-particles like ZnO and Cupric oxide doped with Zinc as a source for oxy radicals for killing bacteria and fungi. Nano organic drugs.

Lubart's group is focused on visible light- tissue interaction. In order to interact with the living cell, light has to be absorbed by intracellular chromophores.

Infectious Disease Research via Light –Tissue Interaction

Lubart 's group They have suggested that endogenous porphyrins, mitochondrial cytochromes flavoproteins, and the NADPH-oxidase system, can be targets of light. Following illumination these intracellular chromophores generate reactive oxygen species (ROS). Using the EPR spin trapping technique, Lubart has characterized the various ROS formed in many cells like skin, muscle, sperm, bacteria, and fungi. While light-induced ROS at small quantities stimulate cell activities, high concentrations are lethal to the cell.

Photo-Bio-Stimulation with a Novel Light Device

Lubart developed a new light device that emits a broad band of wavelengths at targeted intensities, and thus capable of cell activation through small amounts of ROS formation. The device was found to mimic laser light functions in the area of photo-bio-stimulation, such as acceleration of cell proliferation for wound healing and enhancement of the fertilization rate of damaged sperm cells.

Using High Intensity Visible Light to Kill Bacteria

Lubart also designed high intensity visible light devices that produce high amounts of ROS that can be used for killing bacteria and fungi without the addition of exogenous photosensitizers as used in photodynamic therapy (PDT).

Treating Acne with Nano-particles

Recently Lubart and her team have loaded nano-particles like ZnO and Cupric oxide doped with Zinc (CuO/Zn) as a source of oxy radicals into various pathogens for killing them. They have found that nano CuO/Zn is an excellent agent for treating Acne vulgaris.

Nano organic materials

In recent years nanoparticles of organic materials have become very attractive due to their increased biological activity and penetration depth into human tissues. Recently Lubart and her colleagues have prepared nano Vitamin B12 and Penicillin and demonstrated their enhanced biological activity. The size and morphology of the nano Penicillin and Vitamin B12 were investigated using electron microscopy as well as dynamic light scattering techniques. The increased penetration depth of these organic nano particles was estimated using an optical iterative method. We believe that nano organic drugs would have a great impact on the medical field.

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Enhanced pharmacological activity of Vitamin B12 and Penicillin as nanoparticles. Inbar Yariv, Anat Lipovsky, Aharon Gedanken, Rachel Lubart, Dror Fixler, International Journal of Nanomedicine 10 3593–3601 (2015).

Shlomo Margel (Emeritus)

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Postdoctoral,
California Institute of Technology (CALTECH)

Senior Scientist, California Inst. of Technology, Jet Propulsion Lab., Pasadena, CA, 1978-1979

Associate Professor, Weizmann Institute of Science, 1985

Dean, Bar-Ilan Faculty of Exact Sciences, 2002-2004

President of the Israel Chemical Society, 2006-2009

Dean of Students, Bar-Ilan University, 2010-2012

Polymers and Biopolymers, Functional nano/micro-particles for industrial and medical applications, Polymers and biopolymers, Magnetic materials, Environmental chemistry

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Margel's research focuses on the synthesis, characterization and biomedical and industrial applications of functional micro and nano-particles of narrow size distribution, as well as selective marking and drug delivery for diagnostics and therapy.

Nanotechnology Research

Recently, Prof. Margel established a new startup company, Nano Thera Ltd., in collaboration with Prof. Chaya Brodie, dedicated to treating brain cancer with bioactive iron oxide nanoparticles.

New Polymeric Uniform Nanoparticles and their Applications

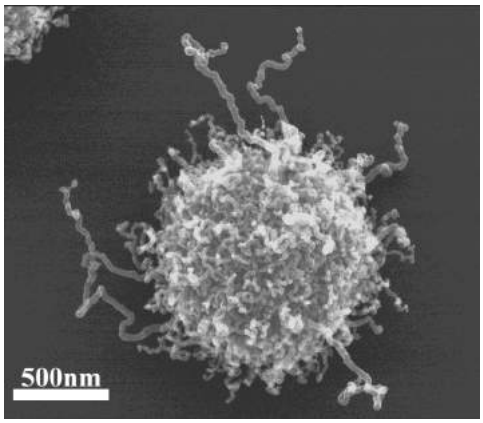
Over the past ten years, Margel and his team have pioneered the development of uniform polymeric nano/micro-spheres ranging in size from a few nanometers to a few microns. These particles may be magnetic and non-magnetic, fluorescent (e.g., near IR) and non-fluorescent. The functional groups of the particles have been used, via different activation procedures, for covalent binding of ligands such as drugs, proteins, enzymes, antigens and antibodies to the particles' surface.

These were then used for applications such as water purification, heavy metal ions detoxification, antibacterial and antifouling applications, specific cell labeling and cell separation, diagnostics, affinity chromatography, cell growth, specific blood filtration by hemoperfusion, enzyme immobilization, carriers for oligonucleotide synthesis, drug targeting for cancer therapy (glioma, bone and intestine) , tissue engineering, biological glues, imaging and various biochemical reactions.

Materials Science Research: Biological Glue Based on Thrombin Conjugated Nanoparticles

Currently available hemostatic preparations using collagen, gelatin, or oxidized regenerated cellulose do not have an immediate effect. In addition, a new generation of biological glues based on fibrin has significant drawbacks. Margel has developed a form of thrombin conjugated to biodegradable or non-biodegradable nanoparticles that is significantly more stable in various conditions, e.g. inhibitors, bacteria, increased temperature, storage time, pH, light, lyophilization, etc.

The hemostatic uses of Margel's formulation may be applicable for all areas of surgery, home care, clinics, army services, industry, etc. It may also be useful for controlled release, drug targeting, tissue adhesive, and wound healing.



Typical SEM micrographs of core shell SiO_2/Fe/carbon nano tubes "medusa-like" microspheres prepared by annealing the core shell SiO_2/IO microspheres in ethylene atmosphere at 600 °C

Abraham Nudelman (Emeritus)

Medicinal Chemistry – Anti-inflammatory drugs, anticancer agents, antischizophrenics, drugs for induction of hemoglobin synthesis, drugs for the treatment of neuropathic pain and for the treatment of anemia, antibiotics. Prodrugs, drug delivery systems, organic syntheses

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Head of Marcus Center for Medicinal Chemistry, BIU

Prof. (Emeritus) Abraham Nudelman, Founder of the Medicinal Chemistry Division at BIU's Department of Chemistry, and Founding Director of the Bernard W. Marcus Center for Pharmaceutical and Medicinal Chemistry, has generated a rich pipeline of potential drugs to combat diseases such as cancer, schizophrenia, and inflammatory illnesses.

Drug Discovery, Design, and Delivery Research

Having published more than 130 articles, mostly in areas of organic chemistry and drug development, Nudelman's laboratory continues to discover and develop a variety of medicinal compounds as well as drug delivery systems and novel, efficient methods for synthesis of commercially available drugs. Nudelman has 84 patents in his name, all in the field of drug research.

Anti-inflammatory Compounds

In collaboration with Prof. Marta Rosin at the Hebrew University, Prof. Nudelman is developing a family of neuroprotectant compounds that have shown promising anti-inflammatory, anti-oxidant and cholinesterase inhibitory activities in initial in vitro studies. Currently, the group is proceeding with further development of the compounds for in vivo evaluation as anti-inflammatories, in particular for the use of the treatment of Crohn's disease and colitis.

Anti-cancer Agents

A novel family of anti-cancer agents developed by Nudelman in collaboration with Dr. Ada Rephaeli at Tel Aviv University is derived from known histone deacetylase inhibitory (HDACI) molecules linked to acyclovir. The new compounds have demonstrated potent anti-cancer activity both in vitro and in vivo and were well tolerated in initial safety studies. A second family of drugs, which display promising activity for the treatment of superficial tumors, base of the Photodynamic Therapy technology, have been discovered and these compounds are being evaluated for cancer activity as well as potentially active agents for the treatment of anemias. In collaboration with Prof. Ammie Hodak, head of dermatology at Beilinson Hospital and with Dr. Ada Rephaeli from Tel Aviv University, a potent histone deacetylase inhibitory agent labeled AN-7, is undergoing evaluation for the treatment of cutaneous t-cell lymphoma.

Areas of Interest

Other medicinal drugs being investigated by Nudelman's team include novel compounds for photodynamic therapy. These compounds have been patented and are undergoing extensive studies for further development.

Selected Recent References

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Indoline-3-propionate and 3-aminopropyl carbamates reduce lung injury and pro-inflammatory cytokines

Avigdor Persky (Emeritus)

Professor (emeritus), Department of Chemistry

Ph.D., (Summa cum Laude), Weizmann Institute of Science

Postdoctoral, California Institute of Technology (Caltech)

Senior Scientist, Weizmann Institute of Science, 1970-1974

Research Collaborator, Brookhaven National Laboratory, 1992-1993

Fulbright-Hays Research Scholar Fellowship

Molecular dynamics; Experimental kinetic studies of atom-molecule reactions in the gas phase; Theoretical molecular dynamic studies of atom-molecule reactions; Quasiclassical trajectories calculations.

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The research of professor Avigdor Persky involves experimental and theoretical studies of the dynamics of atom – molecule reactions in the gas phase, which are of fundamental importance for the development of chemical dynamics theory, or are of practical interest.

Experimental kinetic studies

The experimental projects are directed towards the determination of accurate rate constants of atom – molecule reactions over wide temperature ranges. Kinetic results, which have been obtained over the years, are considered to be accurate and reliable and are often used for critical testing of predictions based on various theories. Experimental measurements were performed in fast- flow systems, with online analysis of reactants and products by quadrupole mass spectrometers, which are interfaced with microcomputers, for controlled operation and for real-time calculations of kinetic data.

Special attention was given to reactions of fluorine atoms. The available reported results for such reactions are mainly for room temperature, often with wide error limits and, in many cases, with significant differences between various research groups. This is due to the high reactivity of fluorine atoms. It is rather difficult to avoid the occurrence of secondary reactions of the fluorine atoms with the products of the primary reactions and this affects significantly the experimental results. Special techniques and procedures were developed in Persky's laboratory, in order to minimize the interfering effects of such reactions.

Theoretical dynamic calculations

In the theoretical projects, the quasiclassical trajectories method (QCT) was employed extensively, in order to explore the dynamics of atom-molecule reactions. A variety of potential energy surfaces were employed, mainly semi-empirical surfaces. The quantities obtained from the computations include reaction cross sections, rate constants and the energy partitioning among the products, for a variety of initial conditions. The calculated results were compared to available experimental data and conclusions were drawn concerning the accuracy of the potential energy surfaces and of the assumptions made in the calculations.

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Arlene Wilson-Gordon (Emeritus)

Professor (emeritus), Department of Chemistry

D.Phil., Oxford University

Postdoctoral,
Hebrew University of Jerusalem

Nonlinear optics; Quantum optics;
Coherent effects in interaction between light and matter

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The work of Prof. Arlene Wilson-Gordon spans several branches of chemistry and physics. Working at the atomic and molecular level, she and her research team make discoveries that transfer from the theoretical to the practical.

Nonlinear and Quantum Optics

The focus of Wilson-Gordon's work is in the field of theoretical nonlinear and quantum optics. In particular, she is interested in effects involving quantum interference and coherence and their potential applications.
Some of the topics her research team has explored are pump-probe and four-wave mixing spectra in simple systems such as two-level systems, three-level systems in Lambda and Vee configurations, and four-level systems in N and double two-level configurations.

In recent years, her group has been interested in pump-probe spectra of degenerate two-level and three-level Lambda systems, such as those that occur in alkali metal atoms. They have constructed computer programs that can simulate these systems--which are complicated due to their many sublevels-- and allow interpretation of the results in terms of simple level schemes.

Of particular interest are effects such as coherent population trapping (CPT), where all the population is trapped in the ground state, and the related phenomenon of electromagnetically induced transparency (EIT), in which a strong pump laser renders an atomic system transparent to a weak laser (which would be absorbed in the absence of the pump laser).

Another effect extensively studied by the Wilson-Gordon group is electromagnetically induced absorption (EIA), in which the weak laser experiences additional absorption due to the presence of the pump laser.

In addition, several aspects and applications of an effect that can occur in solids, such as ruby crystal or NV diamond, called coherent population oscillation (CPO) have been studied. CPO is similar to EIT in several ways but has important differences. Recently, it has been shown that CPO can also occur in atomic systems usually characterized by EIT. In order to switch from EIT to CPO, an external magnetic field is applied and linear rather than circular polarization is used. Efforts to characterize these systems and explore their quantum features are ongoing.

Recently, the group has collaborated with an experimental group to study a very thin layer of chiral molecules adsorbed on a gold surface. By comparing the theoretical values of various spectra with the experimental ones, they were able to determine the orientation of the molecules on the surface.

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Antibacterial, antiviral and antifungal nanoparticles; sonochemical deposition of nanoparticles on surfaces; DNA and RNA nanospheres and their application for gene expression and gene silencing; conversion of biomass to biofuels.
Equipment: - TGA and DSC; reflection spectrometer; IR spectrometer; microwave ovens; sonicators of powers at 600-2500 W; roll to roll sonochemical coating machine.

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Medicinal chemistry. Highly potent agents for the treatment of neurological and inflammatory diseases (Parkinson's, Alzheimer's and colitis). Novel anticancer agents and inducers of biosynthesis of blood cells (hematopoiesis). New compounds directed to the treatment of neuropathic pain. Agents for protection against nerve gases.

65 **Prof. Avigdor Persky**
Molecular dynamics; Experimental kinetic studies of atom – molecule reactions, in the gas phase, over wide temperature ranges; Theoretical molecular dynamic studies of atom – molecule reactions, mainly by the quasiclassical trajectories method; The effects of reactants vibrational and rotational excitation, steric requirements, isotopic substitution and features of the potential energy surface on the dynamics.

66 **Prof. Arlene Wilson-Gordon**
Theoretical nonlinear and quantum optics, coherent light-matter interaction in model and realistic atomic and solid-state systems, second-harmonic generation of chiral surfaces, propagation, solitons, four-wave mixing.

Bar-Ilan University

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