האקדמיה הלאומית הישראלית למדעים
المجمع الوطني الإسرائيلي للعلوم والآداب
THE ISRAEL ACADEMY OF SCIENCES AND HUMANITIES

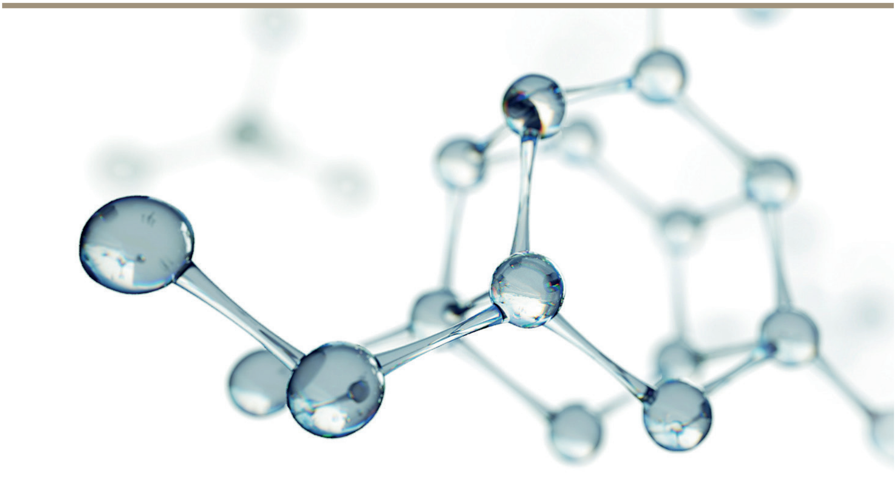
The Israel Academy of Sciences and Humanities

Celebrating the 70th birthday of the State of Israel

conference on

THE GRAND CHALLENGES IN THE CHEMICAL SCIENCES

Jerusalem, June 3-7 2018



Biographies and Abstracts

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Participants:

Dorit Aharonov
Takuzo Aida
Yitzhak Apeloig
Frances Arnold
Ruth Arnon
Avinoam Ben-Shaul
Paul Brumer
Wah Chiu
Nili Cohen
Nir Davidson
Ronnie Ellenblum
Greg Engel
Makoto Fujita
Oleg Gang
Leticia González
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Joshua Jortner
Jacob Klein
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Raphael Mechoulam
David Milstein
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Nathan Nelson
Hagai Netzer
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Geraldine L. Richmond
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Helmut Schwarz
Mordechai (Moti) Segev
Michael Sela
Dan Shechtman
Yaron Silberberg
Gabor A. Somorjai
Amiel Sternberg
Sir Fraser Stoddart
Albert Stolow
Zehev Tadmor
Reshef Tenne
Mark H. Thiemens
Naftali Tishby
Knut Wolf Urban
Arieh Warshel
Ira A. Weinstock
Paul Weiss
Shimon Weiss
George M. Whitesides
Itamar Willner
Xiaoliang Sunney Xie
Omar M. Yaghi
Ada Yonath

Biographies and Abstracts

(Arranged in alphabetic order)

Dorit Aharonov

The Hebrew University of Jerusalem

Quantum Physics through the Computational Lens

While the jury is still out as to when and where the impressive experimental progress on quantum gates and qubits will indeed lead one day to a full scale quantum computing machine, a new and not-less exciting development had been taking place over the past decade. Computational notions such as reductions, hardness, and completeness are quickly starting to be integrated into the very heart of the research of many body quantum systems. The computational perspective brings deep new insights into physical questions that seem completely unrelated to computers, including precision measurements and sensing, testing quantum mechanics, condensed matter physics and even black holes and quantum gravity. I will try to explain some of these intriguing connections and implicationsand time permitting, will ponder about what next.

Dorit Aharonov is an Israeli computer scientist from the Hebrew University of Jerusalem, who has made major contributions to the foundations of qua ntum computation, quantum fault tolerance and quantum Ham iltonian complexity. Growing-up in Haifa, she then moved to Jerusalem and received her BSc in Mathematics and Physics in 1994; after spending one year at the Weizmann institute's physics department, she continued to complete her PhD at the Hebrew University of Jerusalem under the supervision of Professors Michael Ben-Or and Avi Wigderson. She did one year of Postdoc at the IAS math department in Princeton, then completed another year of postdoc at the computer science department at UC Berkeley; in 2000 she joined the computer science faculty at the Hebrew University.
In 2005 Aharonov was profiled by the journal *Nature* as "one of four young scientists.... making waves in their chosen fields"; In 2006 she received the Krill excellence in research award, and in 2014 she received the Michael Bruno award.
Her current main interests are multiparticle entanglement, capturing the difference between quantum and classical physics through the computational lens, applying mathematics to philosophical and foundational physical questions such as testing quantum mechanics, Feldenkrais, Kung-Fu, Mountains, and other beautiful creations.

Takuzo Aida

Riken Center for Emergent Science; The University of Tokyo

Semibiological Robotic Nanocarriers Responsive to Endogenous Signals

Realization of "surgical nanomachines", proposed by physicist Richard Feynman, is undoubtedly one of the ultimate scientific challenges. Such nanomachines are expected to detect particular biological (endogenous) signals and judge necessary tasks to cure wounded tissues. Inspired by this vision, we developed the first robotic nanocarrier that senses ATP (adenosine-5'-triphosphate) and breaks up spontaneously to release a guest molecule. This unprecedented nanocarrier consists of tubularly assembled GroEL, a barrel-shaped chaperonin protein, ubiquitously present in the human body as an essential biomolecular machine that assists refolding of denatured proteins by trapping them inside its barrel. For GroEL to release refolded proteins from the cavity, it binds ATP, which is then hydrolyzed to create ADP, wherein GroEL undergoes a large conformational change. We took note of this ATP-fueled chemomechanical motion and hypothesized that if the mechanical force generated by this motion is large enough to cut non-covalent interactions, so that the tubular GroEL assembly may break up spontaneously into its monomer upon binding with ATP and release a guest molecule. We demonstrated that this idea works well. We also showed that the GroEL nanotube containing superparamagnetic nanoparticles respond to an applied magnetic field. Furthermore, the length of the nanotube can be controlled.

Takuzo Aida was born in 1956. He received his Ph.D. in Polymer Chemistry from the University of Tokyo in 1984, and immediately began his academic career as an assistant professor at the same university on precision polymer synthesis. In 1996, he was promoted to full professor in the University of Tokyo at the Department of Chemistry and Biotechnology. In 2008, he was appointed as a director for Riken Advanced Science Institute, and then in 2013, as a deputy director for Riken Center for Emergent Matter Science. In 2017, he moved his key role to Riken, while keeping the group in the University of Tokyo as a professor. His research interests cover molecular assembly, soft materials, and bioinspired systems, and he has done many seminal works such as extrusion polymerization using mesoporous silica (1999), bucky gels of ionic liquids (2003), self-assembled conductive nanotubes (2004), aqua materials (2010), and molecular/biomolecular machines (2003, 2015). More recent examples feature responsive materials of structural anisotropy (2011) and self-assembly under non-equilibrated conditions including the first chain growth supramolecular polymerization (2015).

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Yitzhak Apeloig

Technion - Israel Institute of Technology

Yitzhak Apeloig was born in Buchara, Uzbekistan (1944) and immigrated to Israel in 1947. He received his B.A. M.Sc. and Ph.D (1974) degrees in Chemistry (*summa cum laude*) from the Hebrew University in Jerusalem. In 1974-1976 he was a postdoctoral fellow in Princeton University. In 1976 he joined the Technion, becoming a full professor in 1988. Currently he holds the Nahum Guzik Distinguished University Professor Academic Chair.

Yitzhak Apeloig's research interests are in *Organosilicon chemistry*; *Computational quantum chemistry* and *Physical organic chemistry*.

He received many awards, among them: ACS Kipping Award in Silicon Chemistry, Wacker Silicone Award, Israel Chemical Society Prize and Gold Medal , Alexander von Humboldt Senior Scientist Award (3 times), JSPS Visiting Professor Award (3 times).

He is an Honorary Foreign Member of the American Academy of Arts and Sciences, a Fellow of the American Association for the Advancement of Science (2009), holds an Honorary Doctorate from TU Berlin and received the Order of Merit (First Degree) of Germany.

During 2001-2009 he was President of the Technion – Israel Institute of Technology. During these eight years he lead the Technion to higher levels of excellence in research and teaching and to increased involvement with the community. He led the Technion into new areas of science and technology and raised some $700 million dollars from private donors and foundations. During this period he continued to teach and to lead an active research group.

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Frances Arnold

California Institute of Technology

Engineering by Evolution: Bringing New Chemistry to Life

Not satisfied with nature's vast catalyst repertoire, we want to create new protein catalysts and expand the space of genetically encoded enzyme functions. I will describe how we use the most powerful biological design process, evolution, to optimize existing enzymes and invent new ones, thereby circumventing our profound ignorance of how sequence encodes function. Using chemical intuition and mimicking nature's evolutionary processes, we can generate whole new enzyme families that catalyze synthetically important reactions not known in biology. Exploiting the vast world of non-natural carbene chemistry, we recently reported the first enzymes that forge C-Si and C-B bonds in living cells and other enzymes that catalyze alkyne cyclopropanation to make highly strained carbocycles. We are also exploring enzyme-catalyzed nitrene transfer chemistry, to make new C-N bonds. Uncovering the mechanisms of these new enzymes derived from natural iron-heme proteins provides a basis for discovering yet more new biocatalysts for increasingly challenging reactions. These new capabilities expand the scope of molecules and materials we can build using synthetic biology and move us closer to fully DNA-programmed chemical synthesis.

(1) **S. B. J. Kan, R. D. Lewis, K. Chen, F. H. Arnold**. "Directed Evolution of Cytochrome c for Carbon–Silicon Bond Formation: Bringing Silicon to Life." *Science 354*, 1048-1051 (2016).

(2) **S. B. J. Kan, X. Huang, Y. Gumulya, K. Chen, F. H. Arnold.** "Genetically Programmed Chiral Organoborane Synthesis." *Nature 552*, 132-136 (2017).

(3) **K. Chen, X. Huang, S. B. J. Kan, R. K. Zhang, F. H. Arnold.** "Enzymatic Construction of Highly Strained Carbocycles." *Science 360*, 71-75 (2018).

Frances Arnold is the Linus Pauling Professor of Chemical Engineering, Bioengineering and Biochemistry at Caltech, where her research focuses on protein engineering by directed evolution, with applications in alternative energy, chemicals, and medicine. Dr. Arnold pioneered the 'directed evolution' of proteins, mimicking Darwinian evolution in the laboratory to create new biological molecules. Her laboratory has developed protein engineering methods that are widely used in industry and basic science.

Dr. Arnold received her B.S. in Mechanical and Aerospace Engineering from Princeton University and her Ph.D. in Chemical Engineering from UC Berkeley. She has been recognized by induction into the US National Academies of Science, Medicine, and Engineering, the American Academy of Arts and Sciences and the National Inventors Hall of Fame. Her awards include the Charles Stark Draper Prize of the National Academy of Engineering (2011), the Millennium Technology Prize (2016), the National Academy of Sciences' Sackler Prize in Convergence Research (2017), and the US National Medal of Technology and Innovation (2013). She has received honorary doctorates from Stockholm University, University of Chicago, Dartmouth University, and the ETH Zurich.

Dr. Arnold chairs the Advisory Panel of the David and Lucile Packard Foundation Fellowships in Science and Engineering and is a Trustee of the Gordon Research Conferences. She has co-authored more than 300 publications and is co-inventor on 58 issued US patents. Active in technology transfer, she co-founded Gevo, Inc. in 2005 to make fuels and chemicals from renewable resources and Provivi, Inc. in 2014 to develop non-toxic modes of agricultural pest control.

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Ruth Arnon

Weizmann Institute of Science

Copaxone – From Laboratory Polymer to Clinical Use

It all started with our efforts to understand the chemical basis of antigenicity of proteins, using the technology of amino acid polymerization developed by Ephraim Katchalski. The resulting synthetic antigens led to the understanding of the role of various molecular parameters in the immunological activity. Michael Sela and I were intrigued by the then newly developed animal model of multiple sclerosis, Experimental Autoimmune Encephalomyelitis (EAE), induced by a single protein of myelin - MBP- a very basis protein of pK 10.6. We hypothesized that a synthetic copolymer, endowed with the same basicity, may mimic its activity and serve as a research tool. Several basic copolymers we synthesized did not show any encephalitogenic properties; on the contrary, they were capable of competing with MBP, thus inhibiting or suppressing EAE in guinea pigs. Furthermore, the suppressive activity of the most effective of these copolymers, denoted Copolymer 1 (Cop 1), was demonstrated in many other animal species, including two species of primates – Rhesus monkeys and baboons. Following a Phase I clinical trial, a phase II trial performed by Murray Bornstein in the USA, demonstrated the efficacy of Cop 1 in MS patients -manifested in both reduction in the frequency of exacerbations and improvement of the disease clinical score. This led to the approval of Cop 1 by the FDA, under the trademark Copaxone®, for the treatment of MS. To date, it is used by several hundred thousand patients worldwide. Only after the approval of Copaxone for clinical use was the mechanism of its action explored in our laboratory, indicating that it exerts its beneficial effect by both immunomodulation and a neuroprotective activity, leading to neurogenesis and myelin repair in the brain.

Ruth Arnon, formerly Vice-President of the Weizmann Institute of Science (1988-1997), is a renowned immunologist. Prof. Arnon joined the Institute in 1960. Prior to her appointment as Vice-President, she served as Head of the Department of Chemical Immunology, and as Dean of the Faculty of Biology. From 1985 to 1994, she was the Director of the Institute's MacArthur Center for Molecular Biology of Tropical Diseases. Prof. Arnon has made significant contributions to the fields of vaccine development, cancer research and to the study of parasitic diseases. Along with her colleagues, she developed Copaxone® a drug for the treatment of multiple sclerosis which was approved by the U.S. Food and Drug Administration, and is presently marketed in the USA, Canada the EU, Australia and many other countries worldwide. Prof. Arnon is a member of the Israel Academy of Sciences and Humanities; she served as the Chairperson of its Sciences division from 1995-2001, and as the President of the Israel Academy of Sciences and Humanities in 2010-2015. On the world scene, she is an elected member of the European Molecular Biology Organization (EMBO). She has served as President of the European Federation of Immunological Societies (EFIS), and as Secretary-General of the International Union of Immunological Societies (IUIS) and as the President of the Association of Academies of Sciences in Asia (AASA). She served as a member of the European Union Research Advisory Board (EURAB). Her awards include the Robert Koch Prize in Medical Sciences, Spain's Jiminez Diaz Memorial Prize, France's Legion of Honor, the Hadassah World Organization's Women of Distinction Award, The Comet Award, the Wolf Prize for Medicine, the Rothschild Prize for Biology, The AESKU Prize for Life Contribution to Autoimmunity and the Israel Prize. She has an Honorary Doctorate from Ben-Gurion University of the Negev, Tel-Aviv University, Open University, Haifa University and Leuphana University (Germany), as well as from several colleges in Israel. She is a Member of the American Philosophical Society (APS), The European Academy of Science & Art as well as of the American Academy of Arts and Sciences (AAAS).

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Avinoam Ben-Shaul

The Hebrew University of Jerusalem

Avinoam Ben-Shaul is an (emeritus) professor at the Hebrew University of Jerusalem. He did his undergraduate and graduate studies at the Hebrew University, his postdoctoral work at the Technical University Munich, the Max Planck for Quantum Optics in Garching, and the University of Austin Texas. In 1974 he joined the Weizmann Institute and a year later moved to the Hebrew University of Jerusalem where he is ever since. He was as a visiting professor at the University of Los Angeles, and a visiting scholar at Columbia University, New York. His research is theoretical, mostly involving statistical thermodynamic theory and modeling of soft-matter, self-assembling and biophysical systems and phenomena, especially membranes biophysics and DNA and RNA in and out of viral capsids.

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Paul Brumer

University of Toronto

Seeking Quantum Effects in Biological Light-Harvesting Systems

Solar radiation powers some of the most fundamental processes in biology, from photosythesis to vision. A long-standing question, whether such processes display quantum effects such as interference, entanglement, non-locality etc. has now re-emerged due to developments in laser spectroscopy. Specifically, coherent pulsed laser experiments on photosynthetic light harvesting systems, as well as on light-induced processes in visual photoreceptors, have suggested a role for light-induced quantum coherences in Biology. We introduce the issues and show, using analytically soluble models, that such coherences will not occur in natural environments, where the turn-on time of the radiation is long and the light is incoherent. However, stationary coherences related to the open system character of such systems may well prove significant, both in Biology and in the design of efficient solar-driven devices.

Paul Brumer is a Distinguished University Professor and the Roel Buck Professor of Chemical Physics, Department of Chemistry, and University of Toronto. In over 300 publications and two monographs, he has successfully addressed a number of fundamental problems in chemical physics, including the role of nonlinear mechanics in chemical dynamics, and how to utilize lasers to control molecular processes -- the holy grail in chemistry. In the latter work, he and his colleague Professor Moshe Shapiro developed "Coherent Control", control scenarios based on quantum mechanical interference effects that are designed to alter dynamical pathways in molecules. In addition, Brumer has contributed to studies on quantum coherence, incoherence and decoherence in numerous processes, including those related to light-induced dynamics in biological systems.

Professor Brumer received his B.Sc. in Chemistry at Brooklyn College and his Ph.D. in Chemical Physics at Harvard University, followed by postdoctoral work at the Weizmann Institute of Science and at the Harvard College Observatory. His research has received recognition through numerous awards, including the Palladium Medal of the Chemical Institute of Canada, the Noranda Award of the Canadian Society for Chemistry, and the Killam Memorial Prize for Natural Sciences. He is a Fellow of the American Physical Society, the Chemical Institute of Canada, and the Royal Society of Canada.

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Wah Chiu

Stanford University

Cryo-EM, an Imaging Tool Beyond Crystallography

Electron cryo-microscopy (cryo-EM) is in the midst of a rapid advance in resolving biological structures of molecular machines and molecules previously either difficult or impossible to attain, at near atomic resolutions. We have solved different cryo-EM structures of molecular machines, including viruses, chaperonins, ion channels,

membrane proteins and RNA, to the level where full-atom models of the molecular components and ligands can be obtained from cryo-EM maps. Various quantitative measures have also been developed to evaluate the accuracy of the maps and models to allow the appropriate interpretation of the structures in context. In addition, electron cryo-tomography has opened an opportunity to visualize structure dynamics of macromolecules in cell while in action.

Wah Chiu received his BA in Physics (1969) and PhD in Biophysics (1975) from the University of California, Berkeley. He is a professor in the Department of Bioengineering, Department of Microbiology and Immunology and the SLAC National Accelerator Laboratory at Stanford University. He is a pioneer in methodology development for electron cryo-microscopy. His work has made multiple transformational contributions in developing single particle electron cryo-microscopy as a tool for the structural determination of molecular machines towards atomic resolution. Dr. Chiu's research, collaboration and training efforts have been recognized by his elected membership to the Academia Sinica, Taiwan (2008) and the United States National Academy of Sciences (2012) in addition to several honors including the Distinguished Science Award from the Microscopy Society of America (2014) and the Honorary Doctorate of Philosophy from the University of Helsinki, Finland (2014).

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Nili Cohen

President, The Israel Academy of Sciences and Humanities

Nili Cohen, Israel Prize Laureate in law research is currently the President of the Israel Academy of Sciences and Humanities. She was Benno Gitter Professor of Comparative Contract Law at Tel Aviv University and is the director of the Beverly and Raymond Sackler Fund for Human Rights in Private Law. She is a former Rector of Tel-Aviv University and was the first and until now the only woman to serve in this position at this university.

Nili Cohen earned her LLB magna cum laude, LLM summa cum laude and PhD at Tel-Aviv University. As a student, she was the founding and the first chief co-editor of the Law Faculty's publication. Her research interests are in contracts, torts, restitution, comparative law and law and literature. Since 2005 she has directed the conference series on Law and Literature within the Institute of Advanced Legal Studies at Tel-Aviv University.

Nir Davidson

Weizmann Institute of Science

Nir Davidson received a BSc from the Hebrew University of Jerusalem in 1982, an MSc from the Technion – Israel Institute of Technology in 1988, and a PhD from the Weizmann Institute of Science in 1993. After working for two years as a research fellow at Stanford University, he joined Weizmann's Department of Physics of Complex Systems in 1994. He became Dean of the Faculty of Physics in June 2015 and is the director of the André Deloro Institute for Space and Optics Research and the Center for Experimental Physics. He is the incumbent of the Peter and Carola Kleeman Professorial Chair of Optical Sciences.

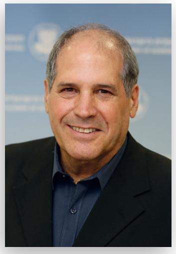
Prof. Davidson conducts research on laser physics and ultra-cold atomic physics. The world of ultra-cold matter is a fascinating place, because the behavior of matter at less than a millionth of a degree above absolute zero is ruled by the principles of quantum mechanics. At such temperatures, particles may combine into a new state of matter called Bose-Einstein condensate or BEC, a state at which quantum behavior can be observed. Prof. Davidson is interested in manipulating atomic motion using lasers, and in applying this manipulation to the atomic "traps" that induce the BEC state, as well as the use of such techniques for precision measurements of quantum phenomena. His ultimate goal is to establish ultra-cold atoms as a tool to study the transition from classical, Newtonian physics to quantum, nonlinear dynamics.

He is the recipient of the F.W. Bessel Award from the Alexander von Humboldt Foundation (2002), the Yosefa and Leonid Alshwang Prize for Physics from the Israel Academy of Sciences and Humanities (1998), the Morris L. Levinson Prize

in Physics, and the Rosa and Emilio Segre Research Award both awarded by the Weizmann Institute's Scientific Council (2001). In 2011, he was elected as a Fellow of the Board of Directors of the Optical Society of America (OSA). In 2007-2011 he was the President of the Israeli Laser and Electro Optics Society. Over the years, he has authored and co-authored over 200 scientific papers and holds 6 international patents.

Ronnie Ellenblum

The Hebrew University of Jerusalem



Ronnie Ellenblum – is a Professor at the Department of Geography at The Hebrew University of Jerusalem, specializing in Medieval Geographies, the History of the Levant in the Middle Ages, and the history of the Crusades. His latest studies deal also with Environmental and Climatic History and with the History of Jerusalem and the development of Historic Cities in general. Ellenblum headed the Vadum Iacob Research Project and was involved in the creation of several data bases dealing with the history of Jerusalem (together with al-Quds University); with the maps of Jerusalem and with English translations of documents and charters of the Crusader Period. Ellenblum has developed a comprehensive theoretical approach to 'Fragility,' claiming that a decade or two of climatic disturbance (droughts, untimely rains and severely cold winters) could lead to severe societal effects, and that the amelioration and even stabilization of climatic conditions for several decades can lead to a period of affluence. His theory of Fragility is based on a thorough reading of a wealth of well-dated textual and archaeological evidence, pointing to periods of Collapse (in the eastern Mediterranean and northern China during the Medieval Climate Anomaly), and affluence in the entire Mediterranean Basin during the Roman Optimum, and describing these processes yearly, monthly and even daily.

Greg Engel

University of Chicago

Design principles of photosynthetic light harvesting

Photosynthetic antenna complexes operate with near perfect quantum efficiency and steer excitonic motion with exquisite precision. The complex interplay between the chlorophyll molecules and their environment within the protein represents an entirely different approach to dictating energy transfer from what we create chemically in a beaker. We are developing new tools to isolate and copy the microscopic details of this process. We are particularly interested in how the electronic excitation couples to local molecular vibrations and how these vibrations can steer electronic dynamics. To this end, we build new spectroscopies, theoretical models, and model systems to test our ideas. I will discuss signatures of long-lived electronic coherence, how we measure dephasing rates and spectral diffusion to reveal how the protein environment dynamically perturbs the electronic states and drives energy transfer. We use this data learn how we can engineer similar effects into synthetic molecular systems.

Greg Engel was born in Pennsylvania in 1977. He obtained his B.A from Princeton University in 1999 and his Ph.D. from Harvard University in 2004. Working under Prof. James Anderson at Harvard University, Greg designed and built ultrasensitive spectrometers to enable in situ measurements of atmospheric tracers and isotopic fractionation profiles of water vapor in the tropical tropopause transition layer. In 2005, he moved to UC Berkeley as a Miller Fellow to study photosynthetic energy transport. Working with Prof. Graham Fleming, Greg discovered coherent excitonic energy transfer in photosynthesis by observing quantum beating signals with 2D electronic spectroscopy. Greg is currently a Professor at The University of Chicago in the Department of Chemistry, The James Franck Institute, and The Institute of Biophysical Dynamics and co-Director of the Graduate Program in Biophysical Dynamics. Engel's research group focuses on new strategies to observe, measure, and control excited state reactivity. Using spectrometers of their own design, the Engel Group explores bio-inspired design principles for steering excitonic transport, open quantum dynamics, and photochemical reaction dynamics. The group's scientific approach involves parallel efforts in theory, spectroscopy, biophysics, and synthesis.

Greg is past-Chair of the ACS Physical Chemistry Division and has served as chair of the ACS Biophysics subdivision. His research has been recognized with the Coblentz Award, DoD Vannevar Bush Fellowship, Sloane Fellowship, Searle Scholar Award, Presidential Early Career Award in Science and Engineering, DARPA Young Faculty Award, AFOSR Young Investigator, DTRA Young Investigator, Dreyfus New Faculty Award, World Economic Forum Young Scientist Program, and Scientific American's SciAm 50 Award. Greg's teaching has been recognized with the Quantrell Award for Undergraduate Teaching and the Camille Dreyfus Teacher/Scholar Award.

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Makoto Fujita

The University of Tokyo

Self-assembly Goes far beyond

Molecular self-assembly based on coordination chemistry has made an explosive development in recent years. Over the last >25years, we have been showing that the simple combination of transition-metal's square planer geometry with pyridine-based bridging ligands gives rise to the quantitative self-assembly of nano-sized, discrete organic frameworks. Representative examples include square molecules (1990),[1] linked-ring molecules (1994), cages (1995), capsules (1999), and tubes (2004) that are self-assembled from simple and small components. Originated from these earlier works, current interests in our group focus on i) molecular confinement effects in coordination cages, ii) solution chemistry in crystalline porous complexes (as applied to "crystalline sponge method"), and iii) and gigantic self-assemblies (Figure 1).[2] This lecture will feature a new family of non-Archimedian solids and their ability of protein encapsulation.

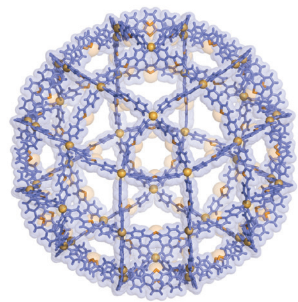

Figure 1.
X-ray structure of $M_{48}L_{96}$ complex.

(1) **M. Fujita, J. Yazaki, and K. Ogura** J. *Am. Chem. Soc. 1990*, 112, 5645-5647.

(2) **D. Fujita, Y. Ueda, S. Sato, N. Mizuno, T. Kumasaka, M.** Fujita, *Nature 2016*, 540, 563.

Makoto Fujita is Professor of Department of Applied Chemistry, School of Engineering, The University of Tokyo, Japan. He received his Ph. D. degree from Tokyo Institute of Technology in 1987. After working in Chiba University and Institute for Molecular Science (IMS) at Okazaki, in 1999, he was appointed as a full professor of Nagoya University. In 2002, he moved to the current position. His research interests include: (1) Coordination Self-Assembly: Construction of nano-scale discrete frameworks, including MnL2n Archimedian/non-Archimedian solids, by transition-metal ions induced elf-assembly. (2) Molecular Confinement Effects: Developing/creating new properties and new reactions in the confined cavities of self-assembled coordination cages. (3) Crystalline Sponge Method: Single-crystal-to-single-crystal guest exchange in the pores of self-assembled coordination networks is applied to a new X-ray technique that does not require crystallization of target compounds.

Selected Awards he has received are: Wolf Prize in Chemistry, 2018; Naito Foundation Merit Award, 2017; Medal with Purple Ribbon, 2014; Fred Basolo Medal (ACS), 2014; Arthur C. Cope Scholar Award, 2013; The Chemical Society of Japan (CSJ) Award, 2013; Thomson Reuters Research Front Award, 2012; Reona Ezaki Award, 2010; Japan Society of Coordination Chemistry Award, 2010; The Commendation for Science and Technology by MEXT, 2009; International Izatt-Christensen Award in Macrocyclic Chemistry, 2004: Silver Medal of Nagoya Medal Seminar, 2003; Japan IBM Award, 2001; Gold Medal of Tokyo Techno Forum 21, 2001; The Divisional Award of the Chemical Society of Japan, 2000.

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Oleg Gang

Columbia University - Center for Functional Nanomaterials; Brookhaven National Laboratory

Programmable Nano-Systems: form Designed Architectures to Controllable Processes

The ability to organize nano-components into the desired organizations is one of the major limitations for creating functional material systems. Our efforts are focused in establishing a broadly applicable DNA-based platform to address this challenge. DNA

provides powerful means for interaction encoding, and much progress was achieved in recent years in ability to tailor DNA structures. However, it is challenging to prescribe the behavior of the entire nanoscale system, built from DNA and other biotic and abiotic components, and to translate advances in DNA structuring into a material design.

Our research explores novel concepts for creating targeted static and dynamic nano-architectures by bridging DNA-encoded nano-objects with structural plasticity and programmability of DNA macromolecular constructs. Through establishing assembly approaches and revealing the principles governing systems with DNA-encoded interactions, we develop methods for creation of well-defined three-dimensional lattices, two-dimensional membranes and finite-sized clusters from the multiple types of the nano-components. Our recent progress demonstrates an integration of DNA with both inorganic and biological nanocomponents into well-defined objects with prescribed valency. We have established approaches for organizing such nano-components as nanoparticles and proteins into ordered 3D arrays with engineered crystallographic symmetries, and clusters with targeted architectures. As a next level of system control, we study approaches for programming a dynamic behavior: structural transformations on demand, specific triggering of desired configurations and regulated cascaded reactions. The applications of the DNA-based assembly platform for creation of nanomaterials with optical, mechanical, chemical and biomedical functions will be also discussed.

Oleg Gang is Professor of Chemical Engineering and of Applied Physics and Materials Science at Columbia University, and a Leader of Soft and Bio Nanomaterial Group at Brookhaven National Laboratory. He explores the soft matter, nanoscale and biomolecular systems, and develops novel strategies for creating nanomaterial based on self-organization. His research interests cover nanoparticle self-assembly, structural properties of polymers and biopolymers, and behavior of hybrid systems built from bioderived and nanoscale components. To probe materials in relevant environments, in action and in 3D, Gang uses and develops synchrotron methods and nanoscale imaging. The main objective of his research program is to establish approaches for creating targeted nanoscale systems with designed spatial organizations, programmable temporal behavior and prescribed reactivity. The developed material systems are applied for enabling new optical, mechanical and biomedical functions.

Gang earned Ph.D. (2000) from Bar-Ilan University (Israel) specializing in Soft Matter physics. As a postdoctoral Rothschild Fellow at Harvard University and Distinguished Goldhaber Fellow at Brookhaven National Laboratory (BNL), he studied nanoscale wetting phenomena and liquid interfaces. Gang became a leader of Soft and Bio-Nanomaterials group at the BNL's Center for Functional Nanomaterials in 2008. In 2016, Gang has joined Columbia University as a Professor of Chemical Engineering, and of Applied Physics and Materials Science. Gang has received numerous awards and recognitions, including Gordon Battelle Prize for Scientific Discovery and Department of Energy Outstanding Mentor Award, has been named Battelle Inventor of the Year, and he is a Fellow of American Physical Society.

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Leticia González

University of Vienna

Molecular Photochemistry

Life, at least as we know it, would not be possible without light. The sun is the driving force behind photosynthesis, which produces oxygen in plants, and without light there would be no oxygen and thus, no humans. Light also initiates many other chemical reactions which are vital in biology, utilized in medicine, chemistry, and information technology. To advance these many fields, it is therefore important to understand how molecules react to light and how molecular properties change when molecules are electronically excited –the realm of photochemistry. The field of computational molecular photochemistry still faces a number of challenges, dampening the intuitive development of photochemical materials with desired properties and the efficient harvesting of sunlight to initiate chemical reactions. To start with, textbook structure-function relationships, as they are known for the electronic ground state, rarely exist. Instead, the behaviour of a molecule under light irradiation is the intricate result of how different potential energy surfaces interact with each other. However, the available methods to compute such potential energy surfaces are still plagued of inaccuracies which grow with system size and energy range. As light triggers dynamical motion on the potential energy surfaces, theory also aims at providing a dynamical view of photochemistry by simulating how atoms directly move in real time. However, the simulation of photodynamics is still limited in system size and simulation times. This talk will review the recent progress and discoveries done in this exciting and rewarding field of research.

Leticia González is Full Professor at the University of Vienna since 2011 and works in the area of theoretical and computational quantum chemistry. Born in Madrid, Spain, she studied Chemistry. After one semester with Michael Robb at the King's College London, working on computational photochemistry, she earned her PhD at the Universidad Autónoma de Madrid under supervision of Otilia Mó and Manuel Yáñez. She then moved to the Freie Universität Berlin to work under the mentorship of Jörn Manz, where she became involved in the field of reaction dynamics and laser control of chemical reactions. She completed her Habilitation in the field of Theoretical Chemistry in 2004 and was appointed Professor for Physical and Theoretical Chemistry at the Friedrich-Schiller Universität in Jena in 2007. In 2011, she moved to Vienna where she is since then.

González has coauthored more than 200 publications and her research has been recognized by several awards, including the Dirac Medal from the World Association of Theoretical and Computational Chemists (WATOC) in 2011 and the Löwdin lecturer in 2014. Passionate about electronic excited states, her research combines highly accurate electronic structure methods and molecular reaction dynamical methods to discover photochemical mechanisms and eventually control chemical reactions using light. She has contributed to elucidate a number of photoinduced processes, in transition metal complexes, small organic chromophores, and biological building blocks.

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Hardy Gross

Max Planck Institute of Microstructure Physics; The Hebrew University of Jerusalem

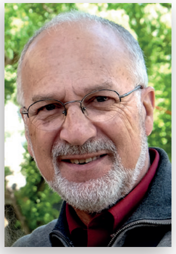
TDDFT: Simulating, Analyzing and Controlling Many-Electron Dynamics, from Photovoltaics to Laser-Driven Spin Switching

The microscopic description of electronic motion in real time is a fundamental step in understanding photo-induced processes such as the creation, travelling and splitting of excitons in photovoltaic systems, or the build-up of screening associated with a laser-induced insulator-to-metal transition. The basic equation describing such processes, the time-dependent many-electron Schrödinger equation, represents an exponentially hard numerical problem which cannot be solved with present-day computing facilities except for the tiniest systems. Time-Dependent Density Functional Theory (TDDFT) represents a viable and universally applicable ab-initio alternative. Since its formulation in 1984, TDDFT has conquered nearly all corners of chemistry and physics and is, by now, the method of choice to calculate any optical spectroscopies (stationary or time-resolved) of sizable molecules and solids. Some recent, non-standard, applications of TDDFT will be presented in this lecture. Those include the analysis of non-steady-state currents in molecular junctions, and the prediction of ultrafast laser-induced switching of magnetic order, e.g. from anti-ferromagnetic to ferromagnetic, which was confirmed experimentally after the prediction. While TDDFT is ideal for processes that are sufficiently fast so that nuclear motion can be ignored, the Grand Challenge is to predict, in an ab-initio way, the dynamics of matter beyond the Born-Oppenheimer approximation. Some steps towards this goal will be presented: Based on the exact factorization of electronic and nuclear degrees of freedom, we shall deduce a novel algorithm that combines a TDDFT description of electronic motion with a swarm of classical trajectories for the nuclei that neither requires surface-hopping nor decoherence corrections. To demonstrate the power of the new method, a simulation of the laser-induced ring opening of oxirane will be presented.

Hardy Gross received his MA (1976) and his PhD (1980) at the Goethe University in Frankfurt, Germany. After a postdoctoral stay with Walter Kohn and a Heisenberg Professorship at UC Santa Barbara, he returned to Germany in 1990 to be Fiebiger Professor at the University of Würzburg. In 2001 he became Chair of Theoretical Physics at the Free University Berlin, and since 2009 he is Director at the Max Planck Institute of Microstructure Physics in Halle, Germany. Since 2017 he is Professor of Chemistry at The Hebrew University Jerusalem. 2003-2004 he was foreign fellow at Trinity College, Cambridge, UK, and 2013-2016 he was Visiting Research Professor at the University of Hong Kong. He served as president of the Council of CECAM (Centre Europeen de Calcul Atomique et Moleculaire) from 2004 to 2008. Among his main recognitions are the 2004 Schlumberger Award at Cambridge University, the 2015 Tsung Ming Tu Prize (the highest distinction given by the Government of Taiwan to foreign scholars), the 2016 Bernie Alder CECAM prize (the most prestigious European distinction, awarded every 3 years, in the field of computer simulations) and he received an ERC Advanced Grant in 2018. He published 270 scientific articles and co-authored two textbooks. His primary field of research is electronic structure theory. He laid the foundation of time-dependent density functional theory with a theorem, now known as Runge-Gross theorem, developed a parameter-free *ab-initio* theory of phonon-driven superconductivity, and his most recent research focus has been the description of non-adiabatic dynamics in molecules and solids.

David Harel

Weizmann Institute of Science



David Harel is the Vice President of the Israel Academy of Sciences and Humanities, and has been at the Weizmann Institute of Science since 1980. He was Department Head from 1989 to 1995, and was Dean of the Faculty of Mathematics and Computer Science between 1998 and 2004. He was a co-founder of I-Logix, Inc., which is now part of IBM. He received his PhD from MIT in 1978, and has spent time at IBM Yorktown Heights, and sabbaticals at Carnegie-Mellon, Cornell, and the University of Edinburgh. In the past he worked mainly in theoretical computer science (logic, computability, automata, database theory), and he now works mainly on software and systems engineering, on modeling biological systems and on the synthesis and communication of smell. He is the inventor of Statecharts and co-inventor of Live Sequence Charts (LSCs), and co-designed Statemate, Rhapsody, the Play-Engine and PlayGo. Among his books are *"Algorithmics: The Spirit of Computing"* and *"Computers Ltd.: What They Really Can't Do"*. His awards include the ACM Karlstrom Outstanding Educator Award (1992), the Israel Prize (2004), the ACM Software System Award (2007), the Emet Prize (2010), and five honorary degrees. He is a Fellow of ACM, IEEE, EATCS and AAAS, a member of the Academia Europaea and the Israel Academy of Sciences, and a foreign member of the US National Academy of Engineering and the American Academy of Arts and Sciences.

Jim Heath

Institute for Systems Biology in Seattle

A Molecular View of Immuno-Oncology

At the heart of most cancer immunotherapies are specific molecular interactions between the principle cancer cell killers, T cells, and the tumor-associated peptide antigens that are presented within the tumor environment. Knowledge of these molecular details can provide deep insight into the nature of which patients do and don't respond to therapies, as well as guidance for designing therapies that range from vaccines to engineered T cells. I will discuss a number of single cell methods aimed at extracting the tumor-specific T cell receptor (TCR) $\alpha\alpha$genes and the peptide-major histocompatibility complexes (pMHCs) that they recognize. A more subtle challenge involves identifying those TCR-pMHC interactions that lead to activated T cells. It is not just the strength of the TCR-pMHC complex, but rather the lifetime of that complex, that is important. I will further discuss large scale molecular dynamics simulations we have carried out to identify a structural mechanism that uncouples TCR signaling from pMHC binding, and may provide insights into the exquisite sensitivity that characterizes these critical immuno-oncology interactions.

Jim Heath is President and Professor of the Institute for Systems Biology in Seattle, WA. He previously served as the Elizabeth Gilloon Professor of Chemistry at Caltech (2003-2018) and was Professor of Chemistry at UCLA from 1993-2002. Heath received his Ph.D. from Rice University in 1988, and was a Miller Postdoctoral Fellow at UC Berkeley from 1988-91, and a research staff member at IBM Watson labs from 1991-93. Heath has founded and serves on the board of several companies, including PACT Pharma, Isoplexis, Indi Molecular, and Sofie Biosciences. He directs the National Cancer Institute supported NSB Cancer Center, and is a member of the Parker Institute for Cancer Immunotherapy.

Joshua Jortner

Tel Aviv University

Joshua Jortner received his Ph.D. from the Hebrew University of Jerusalem in 1960. From 1973-2003 he served as the Heinemann Professor of Chemistry at the School of Chemistry of Tel Aviv University in Israel. He has held visiting Professorships at the University of Chicago, the University of Copenhagen, and the University of California, Berkeley. He was the Christensen Visiting Fellow at Oxford University, served in the International Research Chair "Blaise Pascal", France, and as a Humboldt Fellow at the Humboldt University, Berlin. Jortner holds honorary doctorates from seven Universities in Israel, France and Germany. Among his awards are the International Academy of Quantum Science Award, the Israel Prize in Exact Sciences, the Wolf Prize in Chemistry, the Honorary J. Heyrovsky Medal, the von Hofmann Medal, the Robert S. Mulliken Medal, the Joseph O. Hirschfelder Prize, the Maria Sklodowsky-Curie Medal, and the Lise Meitner Research Award of the Alexander von Humboldt Foundation. A member of the Israel Academy of Sciences and Humanities, Jortner is a foreign honorary member of the Academies of Sciences of Denmark, Poland, Romania, Russia, India, the Netherlands, the Czech Republic, the Leopoldina National Academy of Germany, the Italian Accademia Nazionale dei Lincei, the International Academy of Quantum Molecular Sciences, the American Philosophical Society, the American Academy of Arts and Sciences and the National Academy of Sciences of the USA. He held many honorary lectureships in Europe, Asia, the United States and Israel.

Jortner served as President of the Israel Academy of Sciences and Humanities (1986-1995), and as the Founding President of the Israel Science Foundation. He served as the President of the International Union of Pure and Applied Chemistry (1998-2000). His research centers on the exploration of the phenomena of energy acquisition, storage and disposal in isolated molecules, clusters, nanostructures, condensed phases and biophysical systems.

Jacob Klein

Weizmann Institute of Sciences

Hydration forces, Biolubrication and Gene Regulation: the Challenge of Osteoarthritis

As human longevity increases, diseases that affect joints, most commonly osteoarthritis (OA), have become a leading cause of pain and mobility-limitation in the elderly population, with over 250M people worldwide (and an estimated 0.8M in Israel alone) suffering from debilitating OA of the major joints (hips and knees). OA is a disease of the articular cartilage, the tissue coating our joints, which in its healthy state presents the most well-lubricated surface known in nature. Over the past 15 years we have elucidated the molecular origins of the low friction of healthy cartilage[1-6]: we find that it derives from the ångstrom-thick hydration shells exposed by molecules coating the cartilage surfaces, via the hydration lubrication mechanism. These molecules are primarily the proteoglycan lubricin, the polysaccharide hyaluronan, and especially phosphatidylcholine (PC) lipids. We find that PC lipids complex with the macromolecular components to expose their highly-hydrated phosphocholine groups at the slip plane between the sliding cartilage surfaces. OA is associated with the breakdown of such lubrication, both through wear-and-tear, and through the effect that the friction has on gene regulation via the mechanosensitivity of chondrocytes, the only cell type in cartilage. The talk will describe recent progress towards understanding and alleviating OA via better lubrication of cartilage.

(1) **Raviv, U. and Klein, J.**, 'Fluidity of bound hydration layers' – *Science 297*, 1540-1543 (2002)

(2) **Briscoe, W.H., Titmuss, S., Tiberg, F., McGillivray, D.J., Thomas, R.K., Klein, J.**, 'Boundary lubrication under water', *Nature 444*, 191-194 (2006)

(3) **Chen, M., Briscoe, W.H., Armes, S.P. and Klein, J.**, 'Lubrication at physiological pressures by polyzwitterionic brushes', *Science, 323* 1698-1702 (2009)

(4) **Ma, L., Gaisinskaya, A., Kampf, N. and Klein, J.**, 'Origins of hydration lubrication', *Nature Communications*, | 6:6060 | DOI: 10.1038/ncomms7060 (2015)

(5) **Seror, J., Zhu, L., Goldberg, R., Day, A.J. and Klein J.**, 'Supramolecular synergy in the boundary lubrication of synovial joints' – *Nature Communications*, | 6:6497 | DOI: 10.1038/ncomms7497 (2015)

(6) **Klein, J.**, 'Cartilage boundary lubrication and joint homeostasis', *Nature Reviews Rheumatology*, (2018, in press)

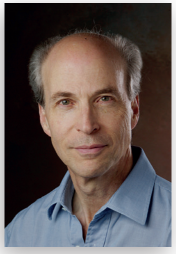
Jacob Klein is the Herman Mark Professor of Polymer Physics at the Weizmann Institute in Israel. Klein gained his BA in Physics at the University of Cambridge, where in 1977 he also received his M.A. and PhD at the Cavendish Laboratory. He did his postdoc at the Weizmann Institute in Israel, and from 1980-1984 was a Senior Scientist at the Weizmann Institute and a University Demonstrator at the Cavendish Laboratory. In 1984 he was appointed Professor at the Weizmann Institute (full Professor from 1987), and subsequently headed its Polymer Research department and was Chairman of its Scientific Council. From 2000-2007 Klein was the Dr. Lee's Professor of Chemistry at the University of Oxford and Head of its Physical and Theoretical Chemistry Department. His interests in soft matter have ranged from the dynamics and interfacial properties of polymers to the behaviour of confined fluids and biological lubrication. Klein has published over 260 papers, including over 25 in *Science* and *Nature*. His honours include the Charles Vernon Boys Prize of the Institute of Physics, UK (1984), the High Polymer Physics Prize of the American Physical Society (1995), the 2010 Prize of the Israel Chemical Society, the 2011 Soft Matter and Biophysical Chemistry Award of the UK Royal Society of Chemistry, the 2012 Tribology Gold Medal (world's top award in the field), the 2015 David Turnbull Lectureship Award of the Materials Research Society and the 2017 Liquid Matter Prize of the European Physical Society (awarded once every 3 years). In 2009 and 2017, he received ERC Advanced Grants. In 2013 he was elected to the European Academy and in 2016 he was elected to the Israel Academy of Science and Humanities.

Roger Kornberg

2006 Nobel Laureate in Chemistry; Stanford University

The End of Disease

Modern medicine is in a primitive state, due our limited knowledge of human biology. Most therapies are palliative and few diseases can be cured. Novel physics, chemistry and biology hold great promise for alleviating this condition. Recent advances are illustrative. Also arising recently, however, are major challenges to progress: biomedical and political myopia.



Roger Kornberg is Winzer Professor in Medicine and Professor of Structural Biology at Stanford University. He received a bachelor's degree in chemistry from Harvard College in 1967 and a Ph.D. in chemistry from Stanford in 1972. His first research was on the dynamics of lipid bilayers. He used nuclear and electron paramagnetic resonance to determine the rates of diffusional motions of lipids, termed flip-flop and lateral diffusion. He then turned to X-ray diffraction of chromatin and, in 1974, proposed the existence and structure of the nucleosome. This proposal was borne out in detail by subsequent structural studies. Kornberg moved to his present position in 1978, where his research has focused on the mechanism and regulation of eukaryotic gene transcription. Results of this research include the near atomic structure of RNA polymerase II, the elucidation of the RNA polymerase II transcription machinery, and the discovery of the Mediator of transcriptional regulation. Parallel studies of metal clusters have included atomic structures large gold nanoparticles by X-ray crystallography and aberration-corrected electron microscopy. Kornberg has received many awards, including the Welch Prize (2001), highest award in chemistry in the United States, the Leopold Mayer Prize (2002), highest award in biomedical sciences of the French Academy of Sciences, and the Nobel Prize in Chemistry (unshared, 2006). He is a member of national academies in the US and Europe and a recipient of honorary degrees from universities in Europe and Israel. His longest and closest collaborator has been his wife, Professor Yahli Lorch. They have three children, Guy, Maya, and Gil.

Ferenc Krausz

Ludwig Maximilian University, Munich; Max Planck Institute of Quantum Optics, Garching

Attosecond Science: From Basic Research to Real-World Applications

Born around the turn of the new millennium, attosecond metrology has provided real-time insight into atomic-scale electron motions and light field oscillation, previously inaccessible to human observation. Until recently, this capability has relied on attosecond extreme ultraviolet pulses, generated and measured in complex

vacuum systems. Next-generation attosecond metrology is now about to change this state of matters profoundly. Sub-femtosecond current injection into wide-gap materials can directly probe ultrafast electron phenomena in condensed matter systems and also be used for sampling the electric field of light up to ultraviolet frequencies. Petahertz field sampling draws on a robust solid-state circuitry and routine few-cycle laser technology, opening the door for complete characterization of electromagnetic fields all the way from the far infrared to the vacuum ultraviolet. These fields, with accurately measured temporal evolution, serve as a unique probe for the polarization response of matter. Field-resolved spectroscopy will access valence electronic as well as nuclear motions in all forms of matter and constitutes a generalization of pump-probe approaches. Its implementation with a solid-state instrumentation opens the door for real-world applications, such as early cancer detection by measuring miniscule changes of the molecular composition of blood (liquid biopsy) via field-resolved vibrational molecular fingerprinting.

Ferenc Krausz

1986 - Diploma in Electr. Engineering, Budapest Univ. Technology, Hungary; 1991 - Ph.D. in Physics, Vienna Univ. Technology, Austria; 1998-2004 - Professor, Vienna Univ. Technology, Austria; 2003 - Director, Max-Planck-Inst. Quantenoptik, Garching, Germany; 2004 - Professor, Ludwig-Maximilians-Universität München, Germany; 2015 - Director, Centre for Advanced Laser Applications, Munich, Germany; Current research foci - Development of ultrafast laser sources and techniques; their applications for (i) exploring solid-state electron phenomena for attosecond metrology, (ii) pushing the frontiers of electron-based signal processing, and (iii) field-resolved molecular fingerprinting for early detection of diseases, such as cancer.

Leeor Kronik

Weizmann Institute of Science

Progress and Challenges in the Formalism and Application of Density Functional Theory

Density-functional theory (DFT) is an approach to the many-electron problem in which the electron density, rather than the many-electron wave function, plays the central role. DFT has become the method of choice for electronic-structure calculations across an unusually wide variety of fields in chemistry, physics, and materials science. This is because its relative computational simplicity allows for fully quantum-mechanical calculations of realistic systems. Despite many successes, DFT has often been fraught with very difficult questions as to the extent to which many important properties can be obtained even in principle, followed by serious concerns as to the reliability of typical DFT approximations in practice. This talk will focus on new formal and practical approaches, which offer fresh answers to some of the above long-standing questions. In particular, it will focus on generalized Kohn-Sham approaches and parameter tuning as systematic strategies for progress in accuracy and applicability to practical chemical systems.

Leeor Kronik is the Chair of the Department of Materials and Interfaces at the Weizmann Institute of Science, Israel. He obtained a Ph.D. in Physical Electronics from Tel-Aviv University, Israel. He pursued post-doctoral studies as a Rothschild Fellow and Fulbright Scholar with the Department of Chemical Engineering and Materials Science at the University of Minnesota and as a Research Fellow with the Minnesota Supercomputing Institute. His current research interests are in understanding and predicting mechanical, electronic, optical, and magnetic properties of materials from first principles. His research emphasizes applications to real-world materials science problems, often in close collaboration with experimental groups. At the same time, his work focuses on methodological advances within the approaches that make such calculations possible, primarily density functional theory. Among other honors, he received the Young Investigator Krill prize of the Wolf Foundation for Excellence in Scientific Research, Krill Prize of the Wolf Foundation for Excellence in Scientific Research and the Outstanding Young Scientist Award of the Israel Chemical Society, was an inaugural member of Young Israel Academy, and is a Fellow of the American Physical Society.

Richard A. Lerner

The Scripps Research Institute

The Chemistry of Large Numbers

The advent of combinatorial libraries allows synthesis of an immune system in a test tube without the use of live animals. The system, by linking recognition and replication, uses many of the strategies of the natural immune system but also has distinct advantages. First, the size of the synthetic repertoire is nowadays at least three orders of magnitude larger than that of any animal including man. Most importantly the central issue of immune tolerance that forbids against generation of antibodies to self is overcome, thus, allowing one to generate antibodies to any self-protein. This is important because all but one therapeutic antibody in clinical use today is an antibody to self. Recently, new formats for using combinatorial antibody libraries has allowed for direct autocrine selection of agonist antibodies that regulate the fate of normal and cancer cells. These cellular selections can proceed at a rate of 20 million events an hour! Essentially, antibody libraries have converted immunochemistry from a stochastic process into one that can be precisely controlled by the experimenter. These methods are based on the principals of evolution. We can duplicate this process in a laboratory setting, except for the issue of time. Selection during evolution occurs over billions of years which is a time constant not compatible with laboratory experiments. Essentially an input diversity of very large numbers of molecules substitutes for time!

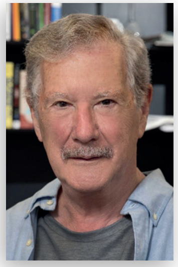
Richard A. Lerner's 40-year scientific career is significant not only for the broad scope of his scientific achievements, but for his leadership as President of The Scripps Research Institute (1986-2012), the country's largest private, non-profit biomedical research organization. The scientific accomplishments for which he is perhaps most well know are the groundbreaking work of converting antibodies into enzymes, permitting the catalysis of chemical reactions considered impossible to achieve by classical chemical procedures and his development of combinatorial antibody libraries (simultaneously with Greg Winter).

A member of the National Academy of Sciences and a foreign member of the Royal Swedish Academy of Sciences, Dr. Lerner graduated from Northwestern University and Stanford Medical School. He interned at Palo Alto Stanford Hospital and received postdoctoral training at Scripps Clinic and Research Foundation. Since 1970 he has held staff appointments at Wistar Institute in Philadelphia and at The Scripps Research Institute.

Dr. Lerner has received numerous honorary degrees, prizes and awards, Including, Parke Davis Award, San Marino Prize, Arthur C. Cope Scholar Award, CIBA-GEIGY Drew Award in Biomedical Research, Humboldt Research Award, Wolf Prize in Chemistry, California Scientist of the Year Award, Coley Award for Distinguished Research in Basic and Tumor Immunology, the Windaus-Medial/Award, President's Medal, University of California, Paul Ehrlich-and Ludwig Darmstaedter Prize, Frankfurt, Germany, AAAS Fellow, DART/NYU Biotechnology Achievement Award in Basic Biotechnology, New York, NY, Distinguished Visiting Scientist at IBM T.J. Watson Research Center, New York, Ulysses Medal, University College Dublin, Belfield, Dublin Ireland, Elected Associate Member of the Exeter Senior Common Room, Exeter College, Oxford University, Oxford, UK, Courage in Innovation Award, Oxbridge Biotech and Nature Biotech, London, UK, Prince of Asturias Award for Scientific and Technical Research, Spain; Honorary Doctorate of Medicine, Karolinska Institute, Honorary Doctorate Of Science Award, Technion-Israel Institute of Technology, Doctor of Science, Northwestern University, Evanston, IL, Honorary Doctorate Degree, Ben-Gurion University of the Negev, Beer-Sheva, Israel, Honorary Doctorate in Humane Letters from Florida Atlantic University, Boca Raton, Florida, Honorary Degree of Doctor of Science, honoris causa, Oxford University, Oxford, United Kingdom. Honorary Degree of Doctor of Science, *honoris causa*, University College Dublin, Belfield, Dublin Ireland and Honorary Degree of Doctor of Science, University of Warwick, Coventry, United Kingdom, Honorary Degree of Doctor of Science Honoris Causa, The Scripps Research Institute, La Jolla, CA.

Raphael D. Levine

The Hebrew University of Jerusalem



Raphael Levine 1968 - Professor of Theoretical Chemistry, HUJI; 1985 - Max Born Professor of Natural Philosophy, HUJI; 2007 - Emeritus; 2007 - Distinguished Professor of Molecular and Medical Pharmacology, David Geffen School of Medicine and of Chemistry and Biochemistry, The University of California, Los Angeles.

Current research topics: AttophotoChemistry; Molecular Logic; Surprisal Analysis; Systems Biology.

Recent biography: Addressing the Challenge of Molecular Change: An Interim Report. Ann Rev. Phys. Chem. 69:1-29, (2018).

Raphael Levine, known as Raphy to his friends, is a recipient of the Israel Prize, the Wolf Prize and the EMET prize. He is a member of the Israel Academy of Science and Humanities, Academia Europaea, The International Academy of Quantum Molecular Science, The Max Planck Society, The Royal Danish Academy of Sciences and Letters, The American Philosophical Society, The American Academy of Arts and Sciences and the US National Academy of Sciences.

Website: https://scholars.huji.ac.il/raphael.levine

Rudolph A. Marcus

1992 Nobel Laureate in Chemistry; Noyes Laboratory of Chemical Physics; California Institute of Technology

A Shot of Theory at a Biomolecular Machine

With the increasing use of single molecule experimental techniques to study biological and other systems, and the increasingly detailed structural studies becoming available, the theoretical study of these complex systems poses interesting questions in how to treat them at the molecular level.

One route for doing so is to divide the overall theoretical problem into component parts, use an analytical equation to treat the phenomenology of the rates of the various rate processes, when feasible, and then extract information such as rate constants of the individual reactions steps. In a favorable case, we will show, one can predict relations between different types of experiments on those steps, by developing expressions that permit the results from one type of experiment to make predictions of another. The individual components could then be treated using detailed computational methods, rather than computing the behavior of the entire system. Simple examples of relationships among reaction rates that permit predictions will be given, drawn from the fields of electron transfers and other chemical reactions.

A more complex example involves single molecule experiments on the F1 component of F0F1-ATP synthase, the rotary mechanical motor that uses an ion gradient across a membrane to synthesize an energy source, adenosine triphosphate (ATP), from ADP and inorganic phosphate. In this initial study we have focused on the F1 unit where there are extensive single molecule experimental data related to the reverse reaction, the conversion of ATP to ADP and inorganic phosphate.

The state of current results from the F1 component of the ATPase will be described when individual steps in the millisecond domain can be described by rate constants that depend on the angle of rotation. In the case of shorter time scales of microseconds a more complex approach, not described by simple rate constants, is needed to understand the experimental data on the F_1ATPase, and will be discussed.

A summary of some of our current findings on the F_1ATPase, in collaboration with Dr. Sandor Volkan-Kacso, is described in *Quarterly Reviews of Biophysics, 50*, 2017, no. 14, 1-13.

Rudolph A. Marcus, John G. Kirkwood and Arthur A. Noyes Professor of Chemistry at the California Institute of Technology, was born in Montreal, Canada in 1923. After receiving a B.Sc. (1943) and Ph.D. (1946) from McGill University (experiments on reaction rates in liquids), and post-doctoral research at the N.R.C. of Canada (experiments on rates in gases) and the University of North Carolina (reaction rate theory), he joined the faculty of the Polytechnic Institute of Brooklyn (1951-64), the University of Illinois (1964-78), and Caltech (1978-).

His research includes the "Marcus theory" of electron transfer processes, the RRKM theory of unimolecular reactions, and more recent theories in fields that include anomalous isotope effects in stratospheric ozone, catalysis of 'on water' organic reactions, and single molecule behavior of biological motors and of semiconductor nanoparticles.

A trademark of his research has been a strong interaction between theory and experiment. Marcus received the Wolf Prize in Chemistry in 1985, the U.S. National Medal of Science in 1989, and the Nobel Prize in Chemistry in 1992.

website: http://cce.caltech.edu/content/rudolph-rudy-marcus

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Todd Martínez

Stanford University

How Much Chemistry Can We Learn With Machine Learning?

Recent advances in machine learning, fueled by novel computational architectures developed for video gaming, promise to revolutionize diverse areas ranging from self-driving cars to image recognition to finance and commerce. I will discuss some of the ways in which these tools and ideas can be exploited for theoretical and computational chemistry. For example, insights gleaned from recommendation systems (such as those used by Netflix and Amazon) can lead to reduced scaling methods for electronic structure (solving the electronic Schrodinger equation to describe molecules) and electronic structure algorithms can be profitably adapted for commodity graphical processing units. These advances can be harnessed to progress from traditional "hypothesis-driven" methods for using electronic structure and first principles molecular dynamics to a "discovery-driven" mode where the computer is tasked with discovering chemical reaction networks. Can the computer learn how to efficiently discover new chemical reactions? If so, what will be the role of the human theoretical chemist? I will highlight some of the areas where ideas from machine learning remain to be exploited in theoretical chemistry and speculate about where these developments might lead.

Todd Martínez received his B.S. in Chemistry from Calvin College in 1989 and his Ph.D. in Chemistry from the University of California at Los Angeles in 1994. From 1994 to 1996, he was a Fulbright Junior Postdoctoral Researcher at Hebrew University in Jerusalem and a University of California President's Postdoctoral Fellow at UCLA. In 1996, he joined the faculty in the Department of Chemistry at the University of Illinois. He rose through the ranks to become the Gutgsell Chair in

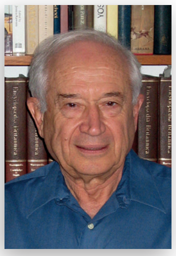
Chemistry. In 2009, he was recruited to join the faculty at Stanford University and the SLAC National Accelerator Laboratory, where he is currently David Mulvane Ehrsam and Edward Curtis Franklin Professor.

Professor Martínez' research lies in the area of theoretical chemistry, emphasizing the development and application of new methods which accurately and efficiently capture quantum mechanical effects of both electrons and nuclei. He pioneered the use of commodity videogame technology for computational chemistry and ab initio molecular dynamics. He has also developed new conceptual frameworks for understanding chemical reactivity induced by external force, i.e. "mechanochemistry."

Professor Martínez has received fellowships and/or awards from the Camille and Henry Dreyfus Foundation, the Alfred P. Sloan Foundation, the Arnold and Mabel Beckman Foundation, the David and Lucille Packard Foundation, and the John D. and Catherine T. MacArthur Foundation. Professor Martínez is an elected fellow of the American Physical Society, the American Association for the Advancement of Science and the American Academy of Arts and Sciences.

Raphael Mechoulam

The Hebrew University of Jerusalem



Raphael Mechoulam, Ph.D. is Professor Emeritus of the Department of Natural Products of the School of Pharmacy at the Faculty of Medicine of the Hebrew University of Jerusalem. Prof. Mechoulam received his M. Sc. degree in Biochemistry from the Hebrew University in 1952 and his Ph.D. from the Weizmann Institute in 1958 where he studied under Professor F. Sondheimer. He completed his postdoctoral research at the Rockefeller Institute. Prof. Mechoulam initiated his independent research at the Weizmann institute in 1960 and in 1966 moved to the Hebrew University in Jerusalem. He is best known for his work on the constituents of Cannabis sativa, including the isolation and structure elucidation of tetrahydocannabinol (THC) in 1964 and for his research on the endogenous cannabinoid system. The two major endogenous cannabinoids, anandamide and 2-AG, were first isolated and identified in his lab in 1992 and 1995. Over the last decade most of his research – in collaboration with numerous other laboratories in Israel and other countries - - has been on endogenous constituents, chemically related to anandamide, that act on brain trauma, on osteoporosis and on addiction.He is known as "The Father of Cannabis" and is an influential figure in the field of medical cannabis research.

Prof. Mechoulam was Rector of the Hebrew University in the early 1980's and is a member of the Israel Academy of Sciences. He serves on the Scientific Advisory Board of several pharmaceutical companies that are involved in cannabis. Prof. Mechoulam has received numerous scientific awards for his research, amongst them the Israel Prize in Exact Sciences, the Rothschild Prize, the German Heinrich Wieland Prize, the US National Institute of Drug Abuse (NIDA) Lifetime Achievement Award, the European College of Neuropsychopharmacology Lifetime Achievement Award, the Emet prize and others. He holds honorary doctorates from Universities in Spain, USA, Canada and Israel.

David Milstein

Weizmann Institute of Science

David Milstein is the Israel Matz Professor of Chemistry at the Weizmann Institute of Science in Israel. He received a Ph.D. degree at the Hebrew University in Israel in 1976 with Prof. Blum, and performed postdoctoral research at Colorado State University, with Prof. Stille. In 1979 he joined DuPont Company's Central Research & Development Department in Wilmington, USA as a Group Leader, and in 1986 he moved to the Weizmann Institute of Science in Israel, where he headed the Department of Organic Chemistry in 1996-2005 and the Kimmel Center for Molecular Design in 2000-2017. His research interests include fundamental organometallic chemistry, homogeneous catalysis, and the design and application of metal-catalyzed reactions for green chemistry and renewable energy. His recent Awards include The Israel Prize (Israel's highest honor, 2012), The ENI Award for protection of the environment (2016), the Gold Medal of the Israel Chemical Society (2017), and the European Prize for Organometallic Chemistry (2017). He is a member of the Israel Academy of Sciences and Humanities, the German National Academy of Sciences-Leopoldina, and this year he was elected as member of the US National Academy of Sciences.

Shaul Mukamel

University of California, Irvine

Novel Spectroscopic Probes of Photosynthetic Charge and Energy Transfer with Quantum and x-ray Light

Conventional nonlinear spectroscopy uses classical light to detect matter properties through the variation of its response with frequencies or time delays. Quantum light opens up new avenues for spectroscopy by utilizing parameters of the quantum state of light as novel control knobs and through the variation of photon statistics by coupling to matter. Entangled-photon pairs are not subjected to the classical Fourier limitations on their joint temporal and spectral resolution. Low intensity requirements for multi-photon processes make them ideally suited for minimizing damage in imaging applications.

We show how the unique temporal and spectral features of entangled light may be used to reveal properties of multiexcitons in photosynthetic aggregates. Simulations demonstrate that they provide unique control tools for two-exciton states in the bacterial reaction center of Blastochloris viridis. Population transport in the intermediate single-exciton manifold is suppressed by the absorption of photon pairs with short entanglement time, thus allowing the manipulation of the distribution of two-exciton states. The quantum nature of light is essential for achieving this degree of control, which cannot be reproduced by stochastic or chirped light. Classical light is fundamentally limited by the frequency-time uncertainty, whereas entangled photons have independent temporal and spectral characteristics not subjected to this uncertainty.

In another novel application of quantum light, the exciton relaxation dynamics of light-harvesting complex II (LHCII) in an optical cavity is manipulated and detected by multidimensional photon coincidence counting. This technique reveals the dynamics in both single and double excitation bands. We study how the cavity polariton dynamics are affected by coupling to photon modes and molecular vibrations described by a realistic spectral density at 77 K. Without the cavity, the energy transfer pathways are not resolved due to the line broadening caused by fast exciton dephasing. The strong coupling to cavity photons results in well-resolved polariton modes. The hybrid (matter and field) nature of polaritons slows down their energy transfer rates. Finally we show how Raman processes involving femtosecond X ray pulses can be used to monitor and coherently control long-range electron Transfer in Azurin.

(1) **F. Schlawin, K.E. Dorfman, B.P. Fingerhut, and S. Mukamel**. "Suppression of Population transport and Control of Exciton Distributions by Entangled Photons ", *Nature Communications, 4*:1782: DOI: 10.1038/ncomms2802 (2013).

(2) **Zhedong Zhang, Prasoon Saurabh, Konstantin E. Dorfman, Arunangshu Debnath, and Shaul Mukamel**. "Monitoring polaritons dynamics in the LHCII photosynthetic antenna in a microcavity by two-photon coincidence counting", *J.Chem. Phys, 148*, 074302 (2018)

(3) **Yu Zhang, J.D. Biggs, Niri Govind, and Shaul Mukamel**. "Monitoring Long-range Electron Transfer in Proteins by Stimulated Broadband X-Ray Raman Spectroscopy", *JPC Lett, 5*, 3656-3661 (2014)

(4) *Konstantin E. Dorfman, Yu Zhang, and Shaul Mukamel*. "Coherent control of long-range photoinduced electron transfer by stimulated X-ray Raman processes", *PNAS 2016 113* (36) 10001 10006

Shaul Mukamel B. Sc. - Tel-Aviv University, 1969, cum laude; M. Sc. - Tel-Aviv University, 1971, summa cum laude;
Ph.D. - Tel-Aviv University, 1976, summa cum laude
July 2013-present: Distinguished Professor of Chemistry, University of California at Irvine; 2003-June 2013: Chancellor Professor of Chemistry, University of California at Irvine; 2002-2003: Professor of Physics and Astronomy, University of Rochester, Rochester, New York; 2000-2003:C. E. Kenneth Mees Professor of Chemistry, University of Rochester, Rochester, New York; 1985-2000: Professor, Department of Chemistry, University of Rochester, Rochester, New York; 1982-85: Associate Professor, Department of Chemistry, University of Rochester, Rochester, New York

Research Interests: Design of novel ultrafast multidimensional coherent optical spectroscopies for probing and controlling electronic and vibrational dynamics in large molecules in the condensed phase; Attosecond nonlinear x-ray spectroscopy of molecules; Many-body theory of optical and photonic materials; a time dependent reduced density matrix framework for computing electronic excitations and nonlinear optical spectroscopy of conjugated polymers, molecular nanostructures, chromophore aggregates and semiconductor nanoparticles; Folding and dynamical fluctuations in proteins and DNA; Long range electron transfer, energy funneling, and collective nonlinear optical response of biological light harvesting complexes; Photon statistics in single molecule spectroscopy; Nonlinear dynamics and fluctuations in quantum and classical optical response.

Awards and Honors: 1971 Ben-Atar Rector Prize, Tel-Aviv University, 1976 Fulbright Hayes Fellow, 1976 Dr. Chaim Weizmann Fellow, 1980 Alfred P. Sloan Fellow , 1984

Camille and Henry Dreyfus Teacher-Scholar, 1987 Fellow of the American Physical Society, 1989 Fellow of the Optical Society of America, 1997 Guggenheim Fellow, 1997 Alexander von Humboldt Research Award for Senior US Scientists, 1998 Chair of Gordon Conference on Electronic Processes in Organic Materials, Newport, RI, 2000 General Co-Chair, Ultrafast Phenomena XII, Charleston, South Carolina, 2003 Lippincott Award, The Optical Society of America, 2005 JILA Distinguished Fellow, Award of The Time resolved Vibrational Spectroscopy (TRVS) Conference 2010, Earle K Plyler Prize for Molecular Spectroscopy, American Physical Society 2011, Hamburg Prize 2012, Lamb Award for Laser Science and Quantum Optics, Physics of Quantum Electronics (PQE), Elected Member of the American Academy of Arts & Sciences (AAAS), Mulliken Prize Medal, University of Chicago, Ahmed Zewail ACS Award in Ultrafast Science and Technology(2015), Elected Member of the National Academy of Sciences (2015). The Coblentz Society/ ABB Sponsored Bomem-Michelson Award (2016). The Optical Society (OSA) William F. Meggers Award (2017). Honorary Ph.D., University of Chicago (2017). Distinguished Scientist Award of the Chinese Academy of Science (2017).

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Edvardas Narevicius

Weizmann Institute of Science

Cold Chemistry with Cold Molecules

Understanding of the low temperature chemistry at the limit where de Broglie wavelength exceeds dimensions of atoms and molecules requires a change of intuition. In “warm” chemistry the knowledge about the transition state corresponding with the highest potential energy along the reaction path is sufficient and weak long-range interactions can be ignored. This picture changes in the cold regime where long range interaction start playing the central role in collision dynamics. Moreover, quantum phenomena such as tunneling and and quantum statistics become important in qualitative description of cold reactions. In our group we developed a method that enabled us to investigate cold chemistry with molecules demonstrating how molecular degrees of freedom fundamentally modify cold interactions. I will also present our latest efforts towards reaching quantum degeneracy with molecular ensembles.

Edvardas Narevicius Born in Vilnius, Lithuania, in 1973, Dr. Narevicius began his career in science by winning the first place in two all-Soviet Union Chemistry Olympiads for high school students, in 1989 and 1990. He then immigrated to Israel and did his undergraduate and graduate studies at the Technion – Israel Institute of Technology, earning a BSc summa cum laude in chemistry in 1995 and a PhD, also in chemistry, in 2002. From 2000 to 2005, he worked as a senior scientist for OpTun Inc., an optical telecommunications company, where he invented and patented an optical switching device that became the building block of many different functionality devices. From 2005 to 2008, he worked and studied as a postdoctoral fellow at the Center for Nonlinear Dynamics at the University of Texas at Austin. He joined the Weizmann Institute faculty as a senior scientist in 2008. Narevicius designs experimental methods for slowing down and cooling molecules to explore fundamental questions in chemistry and physics. He investigates chemical reactions at temperatures several fractions of a degree above absolute zero, when quantum effects become dominant. Narevicius received the Israel Chemical Society (ICS) Excellent Young Scientist Prize in 2014, Weizmann Institute Kimmel Award for Innovative Investigation in 2015 and Zehava and Zvi Friedenberg Prize from the Advancement of Education and Science from ISF in 2017.

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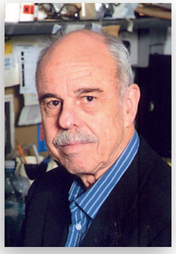
Nathan Nelson

Tel Aviv University

Photosynthetic Reaction Centers – The Engine of Life

The ability of photosynthetic organisms to use the sun’s light as a sole source of energy sustains life on our planet. Photosystems I (PSI) and II (PSII) are large, multi-subunit, pigment–protein complexes that enable photosynthesis, but this intriguing process remains to be fully explained. Crystal structure of photosynthetic reaction centers provided unprecedented insight into the architecture and mechanism of action of those intricate membrane complexes. The knowledge gained from these studies painted a detailed scenario for the evolution of life on our planet. An atomic-level structural model of higher plant PSI at 2.3 Å resolution has been constructed.

The structure includes 16 subunits and more than 200 prosthetic groups, the majority of which are light harvesting pigments.
Recently we solved the structure of trimeric PSI from *Synechocystis* at 2.5 Å resolutions. The structure of green and red algae PSI was solved at intermediary resolution. The structure of PSI supercomplex of the red algae *Cyanidioschyzon merolae* was solved to 4 Å resolutions. The perspective of robustness versus complexity of this highly important bioenergetic complex is discussed. From our studies, and several other laboratories, it has become apparent that advancements in evolution have resulted in increased complexity as well as increased sensitivity to structural alterations, without compromising on the robustness of the system.



Nathan Nelson was born in 1938 in Moshav Avihail and grew as a farmer cultivating citrus trees. He is married to Hannah and have three children Lee-Bath, Nirith and Ben. After the army he started his higher education in Tel Aviv University and received his PhD in 1970. After two years as a postdoctoral fellow in Cornell University he was recruited to the newly established biology department in the Technion where he promoted to full professor in 1980. In 1985 he joined Roche Institute of Molecular Biology till 1995 when he moved back to his Alma Metra, where he conducts active research up to date.
Nathan Nelson's achievements are in diverse areas of membrane protein studies: biochemistry, molecular biology, and structural biology. In the course of his career he has investigated proteins from plants, bacteria, yeast, flies, frogs, mice, cows and humans. His expertise is unraveling the subunit structure of membrane complexes and determining the structure of the purified proteins by X-ray crystallography. Nelson's most significant recent contribution is the crystal structure of plant Photosystem I (PSI) supercomplex, which was solved in his laboratory. The structure displays an ensemble of 16 different proteins, which comprise 45 transmembrane helices, 235 Prosthetic groups including 140 chlorophyll a, 16 chlorophyll b, 27 b-carotene, 7 Lutein, 2 Xanthophyll, 1 Zeaxanthin, 2 quinones, 3 Fe-S clusters and various lipid molecules. The determined structure of plant PSI, which is at the top of the evolutionary tree of this kind of complexes, provided the first high-resolution structural model of a supercomplex containing a reaction center and peripheral antenna complexes. This structure provides a framework for exploration not only of energy and electron transfer but also of the evolutionary forces that shaped the photosynthetic apparatus of terrestrial plants, following the divergence of chloroplasts from marine cyanobacteria over one billion years ago.

Hagai Netzer

Tel Aviv University

Abraham Nitzan

Tel Aviv University; University of Pennsylvania

Molecular Electronics and Plasmonics: Electrons, Light and Heat Transport at the Nanoscale

In molecular conductance spectroscopy, the current through a molecule (or molecules) connecting two metal or semiconductors electrodes is measured as a function of the applied voltage. With eye on potential technological applications, the main problems facing researchers in this field fall within the subjects of fabrication, characterization, stability, functionality and control. This talk will first review recent progress in understanding molecular conduction with particular emphasis on the role played by the molecular electronic structure and conformation, its coupling to the electrodes and its interaction with the underlying nuclear motion on one hand, and its interaction with the radiation field and the thermal environment on the other. The latter consideration brings into focus the need to study systems comprising molecules and metal nanostructures not only for their electrical transport properties but also for their optical and thermal response. These issues have been studied within different communities as separate fields, however their mutual effects are fully expressed in recent studies of molecular transport junctions. As a theoretical problem, one needs to deal with a non-equilibrium system open to electron and energy reservoirs, possibly under illumination. We will focus on relative timescales of different processes as a way to assess their importance in the overall conduction. Characterization, stability, functionality and control will be discussed in the framework of recent studies on inelastic tunneling spectroscopy, heating and heat conduction in molecular junctions and magnetic and optical response of such systems.

Abraham Nitzan was born in Israel in 1944, received B.Sc. and M.Sc. degrees from the Hebrew University, and Ph.D degree from Tel Aviv University (TAU) in 1972. Following post doctoral studies at MIT and the University of Chicago he has returned to Tel Aviv University in 1975 where he is a professor of Chemistry since 1982 (Emeritus since 2014). In summer 2015 he became a professor of Chemistry at the University of Pennsylvania. At TAU he has served as Chairman of the School of Chemistry in 1984-7, Dean of the Faculty of Sciences in 1995-8 and director of the Institute of Advanced Studies 2003-15. His research focuses on the interaction of light with molecular systems, chemical reactions in condensed phases and interfaces and charge transfer processes in such environments. He has published over 330 papers, a comprehensive text ("Chemical Dynamics in Condensed Phases", Oxford U. Press, 2006), was assigned one patent and has given invited talks in over 160 scientific meetings.
During 1992-2015 Nitzan was the incumbent of the Kodesh Chair of Chemical Dynamics at Tel Aviv University and since 2018 he holds the Donner Chair of Physical Sciences at the University of Pennsylvania. Among his main recognitions are the Humboldt Award, the Israel Chemical Society Prize (2004) and Medal (2015), the Emet Prize, the Israel Prize in Chemistry and the Hirschfelder Prize in Theoretical Chemistry. He is a Fellow of the American Physical Society and of the American Association for the Advancement of Science, a Foreign Honorary member of the American Academy of Arts and Sciences, a Foreign Associate of the US National Academy of Sciences and a member of the Israel Academy of Sciences and Humanities. In 2010 he has received an honorary doctorate (Dr. Honoris Causa) from the University of Konstanz.

Geraldine L. Richmond

University of Oregon

Understanding the Complex Liquid Interfaces of Environmental Importance

Although the special properties of water have been valued and appreciated for centuries, as scientists we continue to be perplexed by the molecular make-up of water in all its forms. Equally perplexing is the surface of water, a surface that is involved in some of most important reactions in our atmosphere, land waters and oceans. This presentation will discuss our recent studies to understand how molecules of environmental importance adsorb, bond and react at aqueous surfaces relevant to atmospheric aerosol surfaces. The studies are a combination of nonlinear optical spectroscopy and molecular dynamics simulations.

Geraldine (Geri) Richmond is the Presidential Chair in Science and Professor of Chemistry at the University of Oregon. Her research using laser spectroscopy and computational methods focusses on understanding environmentally and technologically important processes that occur at liquid surfaces. Richmond is a member of the National Academy of Sciences, the American Academy of Arts and Sciences. She has served in leadership roles on many international, national and state governing and advisory boards. She is currently serving as a member of the National Science Board, as the U.S. Science Envoy to the Lower Mekong River Countries and as Secretary of the American Academy of Arts and Sciences. Richmond is the founding director of COACh a grass-roots organization formed in 1998 that has helped over 20,000 women scientists and engineers in career advancement in the U.S. and countries in Asia, Africa and Latin America.
Awards for her scientific accomplishments include the 2018 Priestley Medal from the American Chemical Society (ACS), the National Medal of Science (2013), the American Phyical Society Davisson-Germer Prize (2013), the ACS Joel H. Hildebrand Award in the Theoretical and Experimental Studies of Liquids (2011) the Speirs Medal from the Royal Society of Chemistry (2004) and the ACS Olin-Garvan Medal (1996). Awards for her education, outreach and science capacity building efforts include the ACS Charles L. Parsons Award for Outstanding Public Service (2013), the ACS Award for Encouraging Women in the Chemical Sciences (2005), and the Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring (1997).
Website: http://richmondscience.uoregon.edu

William Schopf

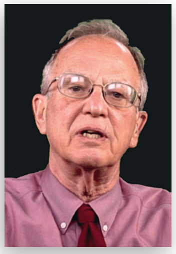
University of California, Los Angeles

Earth's Oldest Fossils: Primordial Life Evolved Early, Far and Fast

In 1859 Charles Darwin stated the problem: There was no known evidence of life before the oldest Cambrian-age fossils (dating from roughly 500 million years ago), no evidence of life's earlier evolutionary history. And these oldest fossils were lobster-like trilobites that were far too large and complex to be relevant to life's beginnings. Darwin realized, as did many of his contemporaries that if his theory were true there must have been an enormous amount of evolution – from simple to complex, from single-celled to many-celled – during pre-Cambrian pre-trilobite "deep time."

To Darwin this posed an "inexplicable" gapping void in his all-embracing theory, a void that remained unfilled – the "missing" fossil record of primordial life remaining unknown and assumed unknowable – for the following century. Indeed, it was not until the breakthrough discoveries of 1965 that a solution to "this greatest of unsolved problems in Natural Science" came into focus with more recent finds showing that the record of life extends to 3,500 million years ago, a seven-fold increase since Darwin's day.

How and why did this sea-change finally occur? This presentation by the last living participant in the initial handful of workers involved in these Paradigm-Changing discoveries outlines both the development of this science and the latest discoveries showing that the oldest fossils now known include primitive photosynthesizers and both methane-producers and methane-consumers, members of microbial lineages situated near the base of the rRNA "Tree of Life." The evidence is firm: Primordial life evolved early, far and fast.



William Schopf Distinguished Professor of Paleobiology and Director of the Center for the Study of Evolution and the Origin of Life at the University of California, Los Angeles, J. William Schopf received his undergraduate training in geology at Oberlin College, Ohio, and his Ph.D. degree, in biology, from Harvard University. Schopf's research focuses on the early evolution of living systems, microscopic organisms of the Precambrian Eon that spans 85% of the planet's 4,500 million-year-long history. He was first to discover such fossils in Precambrian rocks of Australia, China, India, South Africa, Soviet Russia and the USA including threadlike cellular microbes nearly 3,500 million years in age that are among the oldest fossils known. His current work focuses on the use of Raman spectroscopy, fluorescence spectroscopy, confocal laser scanning microscopy, and secondary ion mass spectrometry to characterize the morphology, molecular-structural chemistry, and metabolism-indicative isotopic composition of fossil microbes entirely entombed within rocks -- techniques he has pioneered to be used also in the search for evidence of past life in Mars rocks.

A member of the UCLA faculty since 1968, Schopf has received all of his university's campus-wide faculty awards: for teaching, research, and academic excellence. He is a member of the National Academy of Sciences, the American Philosophical Society, the American Academy of Arts and Sciences, and the American Academy of Microbiology. He is recipient of an honorary doctorate degree, three national book prizes, and of seven medals from national and international scholarly organizations. Twice he has received medals from the US National Academy of Sciences and twice he has been awarded Guggenheim Fellowships.

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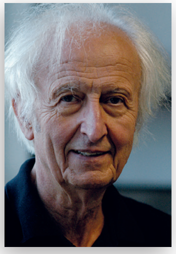
Helmut Schwarz

Alexander von Humboldt Foundation



Helmut Schwarz read chemistry at the Technische Universität Berlin (TUB) where, in 1972, he received his PhD and completed his habilitation in 1974. After having spent some time at the ETH Zürich, MIT, and Cambridge University, in 1978 he accepted a faculty position at TUB.

Helmut Schwarz has occupied numerous visiting professorships on all continents; he has authored > 1000 peer-reviewed articles and delivered an even larger number of (invited and named) lectures all over the globe. For his work on gas-phase chemistry and physics, Schwarz has received more than 50 distinctions and honors. After having served as Vice President of the German Research Foundation from 2001 – 2008, in January 2008 Dr. Schwarz was elected President of the Alexander von Humboldt Foundation.

Mordechai (Moti) Segev

Technion – Israel Institute of Technology

Moti Segev is the Robert J. Shillman Distinguished Professor of Physics, at the Technion, Israel. He received his BSc and PhD from the Technion in 1985 and 1990. After postdoc at Caltech, he joined Princeton as Assistant Professor (1994), becoming Associate Professor in 1997, and Professor in 1999. Subsequently, Moti went back to Israel, and in 2009 was appointed as Distinguished Professor.

Moti's interests are mainly in nonlinear optics, photonics, solitons, sub-wavelength imaging, lasers, quantum simulators and quantum electronics, although he finds entertainment in more demanding fields such as basketball and hiking. He has won numerous international awards, among them the 2007 Quantum Electronics Prize of the European Physics Society, the 2009 Max Born Award of the Optical Society of America, and the 2014 Arthur Schawlow Prize of the American Physical Society, which are the highest professional awards of the three scientific societies. In 2011, he was elected to the Israel Academy of Sciences and Humanities, and in 2015 he was elected to the National Academy of Science (NAS) of the United States of America. In 2014 Moti Segev won the Israel Prize in Physics and Chemistry (highest honor in Israel).

However, above all his personal achievements, he takes pride in the success of his graduate students and postdocs, among them are currently 21 professors in the USA, Germany, Taiwan, Croatia, Italy, India and Israel, and many holding senior R&D positions in the industry.

Michael Sela

Weizmann Institute of Science

Michael Sela was born in 1924 in Poland. The most important awards, prizes and academy memberships include: Israel Prize in Natural Sciences (1959); Rothschild Prize in Chemistry (1968); Otto Warburg Medal, German Society of Biological Chemistry (1968); Emil von Behring Prize of the Phillips University (1973); Gairdner Foundation International Award, Toronto (1980); The Prize of the Institut de la Vie, Fondation Electricite de France (1984); Commander's Cross of the Order of Merit of the Federal Republic of Germany (1986); Officer of l'Ordre de la Legion d'Honneur France (1987); Commandeur, (2011), Albert Einstein Golden Medal (UNESCO) (1995); Harnack Medal of Max-Planck Society (1996); Interbrew-Latour Health Prize, Belgium (1997); Caballero, Order de San Carlos, Colombia (1997); Wolf Prize in Medicine (1998), Commandeur l'Ordre de le Legion d'Honneur, France (2011). Gran uficiale of Decoration of the Italian Solidarity star (2007).

Honorary Doctorates: Universite de Bordeaux II (1985); National Autonomous University of Mexico (1985); Tufts University, Medford MA (1989); Colby College, Maine (1989); Universite Louis Pasteur, Strasbourg (1990); Hebrew University, Jerusalem (1995); Tel Aviv University (1999); Ben-Gurion University of the Negev (2001) Honorary Fellow, the Open University of Israel (2004),. Honorary Degree from the College of Management Academic Studies, Rishon Le Zion. (2009); Open University of Israel (2004); Interdisciplinary Center Herzlia (2014).

Membership in: Israel Academy of Sciences and Humanities; American Academy of Arts and Sciences; Pontifical Academy of Sciences; U.S. National Academy of Sciences; Deutsche Akademie der Naturforscher Leopoldina; Russian Academy of Sciences; French Academy of Sciences; Italian Academy of Sciences; American Philosophical Society; Romanian Academy; Polish Academy of Arts and Sciences. Honorary Member: American Society of Immunologists; Gesellschaft fur Immunologie; Scandinavian, French, Chilean and Colombian Societies of Immunology.

Activities: Michael Sela obtained his Ph.D. from the Hebrew University in Jerusalem for research carried out at the Weizmann Institute of Science. He continues until this day at this Institute, as a Professor from 1963, as Head of the newly created Department of Chemical Immunology from 1963 to 1975, as Dean of the Faculty of

Biology from 1970 to 1973, as Vice-President in 1970-71, as President from 1975 to 1985 and since then until now, as Institute Professor and Deputy Chairman of the Board of Governors. He has been a visiting scientist or professor at the NIH (1960-61, 1973-74), University of California in Berkeley (1967-68), College de France in 1973 and in 1986-87 he was at the Tufts University, MIT and Harvard University. Since 1967 he has been a Foreign Member of the Max-Planck-Institute for Immunobiology in Freiburg. Between 1970 and 1974 he served as Vice-Chairman and Chairman of the Basel Institute of Immunology, between 1975 and 1979 as Chairman of the EMBO Council, between 1978 and 1981 as Chairman of the Scientific Advisory Committee of EMBL, between 1977 and 1980 as President of the International Union of Immunological Societies, from 1989-1996 as President of the Pasteur-Weizmann Scientific Council, and from 1998 Honorary President, Pasteur-Weizmann Council.
Served in various capacities as a consultant to the World Health Organization, including between 1979 and 1982 as a Member of its Global Advisory Committee. Served between 1984 and 1993 as a Member of the Executive Committee of the International Council of Scientific Unions. In 1996 he became the first President of the newly created FISEB (Federation of Israeli Societies of Experimental Biology). Published more than 800 articles, chapters, books, in the fields of immunology, biochemistry and molecular biology.
Among his many activities outside of science can be mentioned that he serves as Honorary President of the Public Council of the Batsheva Company for Modern Dance, Honorary Vice-Chairman of the Arthur Rubinstein International Master Piano Competition, Chairman of the Committee of the Marcus Sieff Prize for Outstanding Initiative in Improving Relations between Jews and Arabs, Chairman of the Presidium of the Movement for Quality Government in Israel, and Founding Member of the Itzhak Rabin Memorial Center for Israeli Studies.

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Dan Shechtman

2011 Nobel Laureate in Chemistry; Technion – Israel Institute of Technology

Quasi-Periodic Materials Discovery – The Role of TEM

Crystallography has been one of the mature sciences. Over the years, the modern science of crystallography that started by experimenting with x-ray diffraction from crystals in 1912, has developed a major paradigm – that all crystals are ordered and periodic. Indeed, this was the basis for the definition of "crystal" in textbooks of crystallography and x-ray diffraction. Based upon a vast number of experimental data, constantly improving research tools, and deepening theoretical understanding of the structure of crystalline materials no revolution was anticipated in our understanding the atomic order of solids. However, such revolution did happen with the discovery of the Icosahedral phase, the first quasi-periodic crystal (QC) in 1982, and its announcement in 1984 [1, 2]. QCs are ordered materials, but their atomic order is quasiperiodic rather than periodic, enabling formation of crystal symmetries, such as icosahedral symmetry, which cannot exist in periodic materials. QCs are quite abundant - hundreds of quasi-periodic crystals have been discovered by now. They are easy to make – practically all the techniques for metallic alloy making can produce QCs, and are made of simple frequently use elements – aluminum, iron, chromium and manganese to name a few. However it took 70 years, from 1912 to 1982 to discover the first QC.
The reason is TEM. The tool of choice in crystal structural analysis was x-ray diffraction. Indeed, the science was names "X-Ray Crystallography". Although TEM is a powerful tool for the study of crystal structure, it was not recognized as such by the community of x-ray crystallographers. QCs had to be discovered by TEM, for the first QCs made by rapid solidification were small – a few microns in size at the most. It took the QC community 3 years to grow large enough QCs for x-ray diffraction to be performed on a single QC. This came only in 1987.
The versatility of TEM that provided detailed contrast analysis as well as lattice imaging made the difference and enabled the discovery. This talk will outline the discovery of QCs and describe the important role of electron microscopy as a prime discovery tool.

(1) **D. Shechtman, I. Blech**, *Met. Trans. 16A* (June 1985) 1005-1012.
(2) **D. Shechtman, I. Blech, D. Gratias, J.W. Cahn**, Phys. Rev. *Letters, Vol 53*, No. 20 (1984) 1951-1953.

Dan Shechtman After completing his doctorate studies at the Technion in Haifa, Israel, Danny Shechtman was an NRC fellow at the Aerospace Research Laboratories of Wright Patterson AFB, Ohio, where he performed research for three years. In 1975 he joined the Department of Materials Engineering at the Technion where he is currently a Distinguished Professor. During 1981-2004 he was several times on Sabbatical at the Johns Hopkins University, (joint program with NBS-NIST). During this period he discovered by TEM the Icosahedral Phase which opened the new science of quasiperiodic crystals and performed research on other subjects. As of 2004 he is also a Professor at MSE and Ames Lab, Iowa State University. His current research efforts center on developing strong and ductile magnesium alloys for a variety of applications. Shechtman is a member of several Academies of Science, including the US NAE, AAAS, The Russian Academy of Science and the Israel National Academy of Sciences. He is an Honorary Member of professional societies around the globe and was awarded many prizes including the Wolf Prize in Physics, the Gregori Aminoff Prize of the Royal Swedish Academy of Sciences, the EMRS award and the Nobel Prize in Chemistry 2011.
Dan Shechtman has twelve grandchildren, four children and one wife, Professor Zipora Shechtman of Haifa University.

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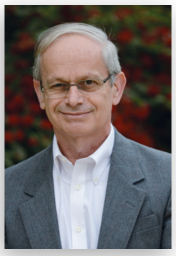
Yaron Silberberg

Weizmann Institute of Science



Yaron Silberberg is a Professor at the Department of Physics of Complex Systems at the Weizmann Institute of Science where he holds the Harry Weinrebe Chair of Laser Physics. He also serves as Head of the Crown Photonics Centre, which promotes the study of light and its applications. From 2002–2008, he served as Dean of the Faculty of Physics. His research on the properties of light and its interaction with matter encompasses the fields of nonlinear, ultrafast and quantum optics and contributed to important applications, particularly in optical microscopy. Professor Silberberg received a PhD in Physics in 1984 from the Weizmann Institute. He then carried out postdoctoral work at Bell Laboratories, Holmdel, NJ and subsequently spent almost a decade on the Technical Staff of Bell Communications Research, Bellcore, NJ. He holds 16 patents. His recent scientific honours include the Rothschild Prize in Physical and Chemical Science in 2018, the Weizmann Prize in Science in 2015, the Max Born Award from the Optical Society of America in 2013, and the Landau Prize in Exact Sciences in 2011. He was elected to the Israel Academy of Sciences and Humanities in 2013.

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Gabor A. Somorjai

University of California, Berkeley

Interface Materials on the Nanoscale. Dominant Media of Chemical Change and Evolution

The discoveries of the unique chemical properties of defects and low coordination sites of metals and the electronic properties of semiconductor transistors started the development of nanomaterials to optimize their utility as catalysts in energy conversion and chemical technologies and information storage using integrated circuits. The size and shape of nanoparticles maintained, altered, and improved their chemical activity and selectivity and the size as transistors became exponentially smaller from micron size to nanometer sizes as their numbers in the integrated circuits increased from thousands to billions.
The metal nanoparticles had to be supported by oxides or polymers that contributed to their chemical behavior including the rate and selectivity of the reaction making interfaces between the support and the nanoparticles part of the chemistry of the nanocatalyst. The catalysts became interface materials with complexity that often matched the formation of complex molecules, which was the purpose of the research. In the past four decades the instruments that characterize the size, composition and bonding of the interface materials on the atomic and molecular scales developed to permit the fabrication of these complex interfaces' reproducibly and develop protocols for their regeneration if they are deactivated. Transistor-based devices were converted to integrated circuits by connecting them to develop their use to information storage technology. Similar development converted the lithium battery

composed of an anode (silicon, graphite, and others) that can store and release lithium into an electrolyte to produce the electron flow as the lithium ions transported to the cathode where it is deposited and again released to make its way back to the anode to recharge the battery. This interface technology provides the energy storage that drives automobiles and other instruments that need charge to function.

The interface device we call catalyst produced by nanoparticle and mesoporous oxide synthesis, subjected to atomic level characterization under reaction conditions. The metal nanoparticles exhibit size dependent covalent bond catalysis. The oxide-metal interfaces are active sites for acid-base catalysis. The changing oxidation states of nanoparticles with decreasing size permits their conversion from homogenous to heterogeneous catalysts. Enzymes deposited to immobilize onto glass create hybrid systems that retain remarkably high selectivity towards their substrates with high catalytic rates. Integration of the three fields of catalysis (heterogeneous, homogenous, and enzyme) becomes a future promise along with biocatalysis as the human body is an interface system of great complexity and success.

Gabor A. Somorjai has been a leader in the fields of Surface Science and Catalysis for more than 50 years. He has published 1200 papers and 4 books. Somorjai received his Ph.D. in Chemistry from the University of California, Berkeley in 1960, and was appointed to the faculty there in 1964. Since then, he has won just about every honor in his fields, the most recent ones are the Theodore William Richards Medal from the Northeastern ACS Section (2017) and the William H. Nichols Medal of the New York ACS Section (2015). Previous major awards are the National Academy of Sciences Award in Chemical Sciences (2013), the Honda Prize, the ENI New Frontiers of Hydrocarbons Prize and the BBVA Foundation Frontiers of Knowledge Award (all in 2011); the Priestley Medal (2008); the Langmuir Prize from the American Physical Society (2007); the National Medal of Science (2002), the Wolf Prize (1998), the Von Hippel Award from Materials Research Society (1997), and several awards from the American Chemical Society, among them the Peter Debye Award in Physical Chemistry (1989). Somorjai is the recipient of eleven honorary doctorates from international institutions. He became a member of the National Academy of Sciences in 1979 and the American Academy of Arts and Sciences in 1983.

Amiel Sternberg

Tel Aviv University; Max Planck Institute for Extraterrestrial Physics Munich; Center for Computational Astrophysics Flatiron Institute Simons Foundation, New York City

Cosmic Chemistry: From Simplicity to Complexity

I will present an overview of chemistry in the cosmos, from the formation of the first stars in the early Universe, to present-day galaxies and the stellar and planetary systems they contain. The molecular composition of the interstellar medium in galaxies, including the Milky Way, plays an essential role in the thermal and dynamical evolution of the star-forming molecular clouds, the gravitational collapse of mutprotostellar cores, and the formation of protoplanetary disks and systems. A rich interstellar inventory, from simple diatomics to an array of multi-atom organic molecules, traces the growth of complexity in the Universe, including the habitable planetary zones required for the emergence of life.

Amiel Sternberg is a theoretical astrophysicist working in the fields of galaxy evolution, star formation, cosmic structure, black holes and active galaxies, intergalactic and interstellar medium, astrochemistry and plasma astrophysics, dynamics, spectroscopy and radiative transfer, computational methods and theory of fundamental processes. Sternberg is Yuval Ne'eman Professor of Theoretical Physics at Tel Aviv University, where he is a faculty member in the School of Physics and Astronomy, and serves as director of the Raymond and Beverly Sackler TAU-Harvard/ITC Astronomy Program. Sternberg is also senior associate scientist in the Infrared Group at the Max-Planck-Institute for Extraterrestrial Physics in Munich Germany, and research scientist in the Center for Computational Astrophysics at the Flatiron Institute Simons Foundation in New York City, USA.

Sir Fraser Stoddart

2016 Nobel Laureate in Chemistry; Northwestern University

The Rise and Promise of Artificial Molecular Machines Based on the Mechanical Bond

I will start my lecture by referring to engines through the ages – for example, steam, electric, internal combustion, diesel, jet, rocket and biological. The mechanical bond will be introduced as a means of employing chemistry in the pursuit of large amplitude motions between the component parts of mechanically interlocked molecules (MIMs) – for example, catenanes and rotaxanes.[1] The importance of template-directed synthesis in the construction of molecular shuttles, switches and machines will be stressed. The design and synthesis of a first generation molecular pump will set the stage for describing recent efforts[2] directed towards the development of a second generation (more efficient) molecular pump – a wholly synthetic compound which operates to compartmentalize highly charged rings in a high-energy state on an oligomethylene chain. The optimized artificial molecular pump operates rapidly thanks to well-tuned steric and electronic interactions, paving the way to address enthalpically and entropically demanding polymers that would be difficult to obtain with the available repertoire of synthetic methods.

(1) **J. F. Stoddart**, Mechanically Interlocked Molecules (MIMs) – Molecular Shuttles, Switches and Machines (Nobel Lecture), *Angew. Chem. Int. Ed. 2017, 56*, 11094–11125.

(2) **C. Pezzato, M. T. Nguyen, C. Cheng, D. J. Kim, M. T. Otley, J. F. Stoddart**, An Efficient Artificial Molecular Pump, *Tetrahedron 2017*, 73, 4849–4857.

Sir Fraser Stoddart, presently a Board of Trustees Professor of Chemistry at Northwestern University, was previously (1997–2002) the Saul Winstein Professor of Chemistry at the University of California, Los Angeles (UCLA) before holding the Fred Kavli Chair of NanoSystems Sciences at UCLA while he was the Director of the California NanoSystems Institute (CNSI) from 2002–2007. Stoddart has pioneered the development of the use of molecular recognition and self-assembly processes in template-directed protocols for the synthesis of mechanically interlocked molecules (MIMs), such as catenanes and rotaxanes. These MIMs led to the design and syntheses of molecular shuttles, switches, and machines, such as artificial molecular pumps. Sir Fraser obtained all his degrees (BSc, PhD, DSc) from Edinburgh University and has spent time (1967–1970) at Queen's University in Canada, Imperial Chemical Industries' Corporate Laboratory (1978–1981), as well as at the Universities of Sheffield (1970–1990) and Birmingham (1990–1997) in the UK before moving to the US in 1997. He was made a Knight Bachelor by Her Majesty Queen Elizabeth II in her 2007 New Year's Honors List for his services to chemistry and molecular nanotechnology. He is a Fellow of the Royal Society of London, the German Academy (Leopoldina) of Natural Sciences, and the Royal Netherlands Academy of Arts and Sciences, as well as an Honorary Fellow of the Royal Society of Edinburgh and the Royal Society of Chemistry. His many awards include the King Faisal International Prize in Science (2007), the Albert Einstein World Prize in Nanotechnology (2007), the Feynman Prize in Nanotechnology (2007), the Royal Medal (2010), and the Nobel Prize in Chemistry (2016). He was elected a Member of the American Academy of Arts and Sciences in 2012, the National Academy of Sciences in 2014, the EU Academy of Science in 2017 and a Foreign Member of the Chinese Academy of Sciences in 2018.

Albert Stolow

University of Ottawa; National Research Council Canada

Transition States in the Excited State: Dynamics at Conical Intersections

Chemistry, the making and breaking of chemical bonds, could be argued to be a rare event, given that bond energies greatly exceed collision energies under normal conditions. Fortunately, this is wrong: the old bonds need not be broken before the new bonds form. Instead, Chemistry is a concerted rearrangement, a dance involving both atoms and electrons on their way from reactant to product. As a configuration between reactant and product, the Transition State plays a central role in our understanding of chemical reactivity. In electronically excited states, the Conical Intersection (CI) plays the role of Transition State. A general electronic degeneracy, the CI impels non-adiabatic processes such as internal conversion. Dynamics at CIs underlie much of Photochemistry and many important biological processes, including Vision. Over the past 70 years much progress has been made in understanding how dynamics at transition states governs the likelihood and outcome of ground state reactions. Simple notions such as the Polanyi Rules may guide our thinking. Unfortunately, we have no such rules for excited state processes. Using a combination of ultrafast time-resolved spectroscopies and ab initio simulations, we have embarked on a phenomenological approach to the discovery of dynamical rules for excited state reactivity.

Albert Stolow is the Canada Research Chair in Molecular Photonics and Professor of Chemistry & Physics at the University of Ottawa. He founded the Molecular Photonics Group within the National Research Council Canada where he is a current member and maintains an ongoing collaborative research program. He is Adjunct Professor of Chemistry and of Physics at Queen's University in Kingston, and a Graduate Faculty Scholar in the Department of Physics, University of Central Florida. He is also a Fellow of the Max-Planck-uOttawa Centre for Extreme and Quantum Photonics. His research interests include ultrafast molecular excited state dynamics and quantum control, strong field physics of polyatomic molecules, and coherent non-linear optical microscopy with applications to Biophotonics and Geophotonics.

Albert Stolow studied Chemistry and Physics at Queen's University and then obtained his Ph.D. degree in Chemical Physics from the University of Toronto in 1988, studying under Nobel Laureate John C. Polanyi. Stolow was an NSERC post-doctoral fellow at the University of California, Berkeley from 1989-1992 where he worked with Nobel Laureate Yuan T. Lee. In fall 1992, Stolow joined the National Research Council in Ottawa and in 2014, he assumed the Canada Research Chair in Molecular Photonics at the University of Ottawa. Stolow is a Fellow of both the American Physical Society and the Optical Society of America. He has won several national prizes including the American Physical Society's 2017 Earle K. Plyler Prize, the 2018 Polanyi Award and the 2008 Laidler Award of the Canadian Society of Chemistry and the 2001 Barringer Award of the Spectroscopy Society of Canada. Stolow sits on the editorial boards of numerous international journals and on the Advisory Boards of several international research institutions. Stolow is a Member of the Executive Committee of the American Physical Society's Division of Laser Science and is Chair-Elect (2018) of its Division of Chemical Physics.

Zehev Tadmor

Technion - Israel Institute of Technology

Zehev Tadmor President Emeritus of the Technion - Israel Institute of Technology, is Distinguished Institute Professor at the Department of Chemical Engineering at the Technion. He also chairs the S. Neaman Institute for National Policy Research at the Technion. He is member of the Israel Academy of Sciences and Humanities and the USA Academy of Engineering. His professional specialty is polymer engineering and plastics processing and among his other interests are national policies in science, technology and higher education; university management, organization and history; and social issues relating to education and science.

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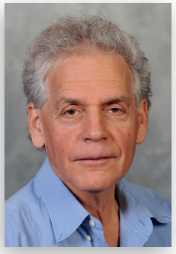
Reshef Tenne

Weizmann Institute of Science



Reshef Tenne's research interests focus on the synthesis, characterization and applications of novel inorganic nanomaterials nicknamed Inorganic Fullerene-like structures-IF and inorganic nanotubes (INT). These nanostructures were discovered in his laboratory in 1992 and form a new and ever expanding class of materials. Recently, new synthetic strategies allowed his group to synthesize nanotubes from many ternary and quaternary "misfit" layered compounds with many intriguing physical properties, like quasi-1D superconductivity. The diverse nano-chemistry that he developed is manifested by the fact that IF/INT are synthesized from chemical elements encompassing much of the periodic table. His research into these materials was published in a large number of publications most notably in *Nature and Science and first tier* journals in chemistry and physics. His studies demonstrated that IF-WS_2 (IF-MoS_2) provide superior lubrication when added to different lubricating fluids and self-lubricating coatings. Further research by him and by other groups showed that when added in small amounts, INT-WS_2

are very suitable for reinforcement of numerous matrices, including variety of polymers, concrete and metal alloys. Being non-toxic and robust, WS_2 nanotubes were also shown to be a preferable scaffolds for stem cell engineering and various other medical technologies.

To concur with the large number of applications of these materials he co-founded "NanoMaterials" (2002- www.apnano.com). This technology of this company was expanded recently to the US- "NIS" (www.nisusacorp.com) and "UTA" (www.utausa.com). Manufacturing and sales of lubricating products based on this technology (nicknamed "Nanolub") are expanding.

Prof. Tenne studied in the Hebrew University and was a post-doc in Battelle Institute in Geneva. He joined the Weizmann Institute in 1979 and was promoted to a full professor at 1995. He published more than 340 original papers and about 80 invited chapters in books and review articles. He is a well sought after speaker in international and national conferences and meetings. He was the head of the Department of Materials and Interfaces of the Weizmann Institute and the Director of the Gerhard M.J. Schmidt Minerva Center for Supramolecular Architecture (2001-2007), the Director of the Helen and Martin Kimmel Center for Nanoscale Science (2003-) and held the Drake Family Chair of Nanotechnolgy (2005- up to his retirement in 2014). He is a member of numerous boards of international journals devoted to materials science and nanotechnology. He was recognized by numerous awards and received many other accolades, the main ones being the *Materials Research Society (MRS) Medal (2005); the Landau Prize for Nanotechnology* by the Israeli Lottery (2006). He was elected as MRS (inaugural) class of *Fellows* (2008); received the *Israel Chemical Society Excellence in Research Award* (2008). He became a *Fellow of the Royal Society of Chemistry (FRSC)*, was elected to the *Israel Academy of Sciences and Academia Europaea* in 2011. He recently received the *Rothschild Prize for Physical and Chemical Sciences* for 2016 and the *Israel Chemical Society Gold Medal Award* (2015), which is the highest distinction of this society. He became a *Honorary Fellow of the Israel Society of Microscopy* (2017) and gave the 8th *Annual Chemistry Lecture* of the JNCASR research center in Bangalore, India (2018).

Home Page: http://www.weizmann.ac.il/materials/tenne/

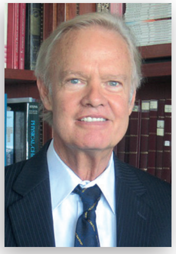
Mark H. Thiemens

University California, San Diego

The Use of Isotope Effects to Understand Atmospheres and Climates Present and Past and Track the Origin of Life

Stable isotopes historically have added in fundamental ways to studies physical and chemical processes. The discovery of an isotope of oxygen in atmospheric oxygen in 1929 by Giauque and Johnston was regarded as a successful test of quantum theory. Isotope spikes early in the 1930s were used to study chemical and biological processes. In 1947 Urey wrote a paper on the thermodynamic substances and Nier developed the isotope ratio mass spectrometer allowing minuscule changes in isotope ratios and application of Urey's calculations to measurements of various samples to study processes at a detail not possible any other way. Examples include paleo thermometry, which allows determination of oceanic temperature to 0.1 degree C sensitivity on hundreds of million year time scales. Geological processes, atmospheric carbon dioxide change and photosynthesis, stellar evolution from meteorites were all early application that continue today. To date, the only mechanism to study temperature change over time is from stable isotope measurements.

The discovery of anomalous variations of stable isotopes facilitated new studies of chemical reactions and photodissociattion and are under investigation. The selection rules and dynamics of photodissociattion and the physical chemistry of reactions are resolved in unique ways by following the changes at the isotopic record and complement theoretical and experimental techniques will be discussed. New results from seemingly unrelated topics have used anomalous isotope measurements coupled with new physical chemical studies allowing deeper penetration into understanding major natural phenomena. Reaction theory of isotope effects and synchrotron work is deepens understanding of solar system origin and planetary formation. Measurements of present day atmospheric species and samples stored in South pole, Greenland and Tibetan Himalayan ice are used to study climate change and glacial melting while simultaneously allowing new insight into the oldest geologic record of the earth geologic billions of years ago tracking the origin and evolution of life.



Mark Thiemens is a Distinguished Professor of Chemistry and Biochemistry in the Department of Chemistry and Biochemistry at the University California San Diego. His work combined studies of the basic physical chemistry of photochemical (photodissociattion) and chemical reactions in the production of mass independent isotope effects and their observations. The work in physical chemistry studies use a range of experimental techniques, ranging from chemical vapor deposition, laser photolysis to synchrotron-based UV photodissociattion studies. The measured samples range across space and time: from before 4.57 billion years ago to present and from Mars to earth, asteroids and moon to the sun.

Samples measured include Mars meteorites, moon rocks, and upper atmosphere of earth from rocket and balloon sampling, and rock samples across the earliest oldest rocks for the resolution of the origin of life. Chemical processes in the global oxygen and sulfur cycles are studied from global collections of air and aerosols from around the world, and the upper atmosphere from rocket and balloon sampling. The origin of the solar system and evolution is examined from the meteorite record, which possesses the chemical history prior to planetary formation and evolution of water on Mars over billion year times from Martian meteorites. Returned solar wind from a 2-year sampling at L1 is under investigation. Climate and global studies, including glacial melting is done from ice collected from the South Pole, Greenland summit and the Tibetan Himalayas, including Mt Everest.

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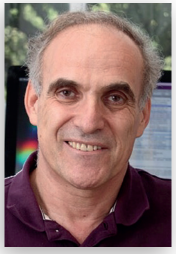
Naftali Tishby

The Hebrew University of Jerusalem

The Machine & Deep learning Revolution: How does it Change our Understating of Chemical Sciences?

In the past 30 years a new scientific discipline, called today: Machine Learning and Data Science emerged, has emerged. This discipline, which emerged from statistics and computer science, has a major impact not only on the way we collect and analyse scientific data, but on the very nature of our discovering and understating natural phenomena. It is recognised today as part of natural sciences and many theoretical physics and chemistry institutes open groups and programs in data science and machine learning. The most dramatic advance in these areas happened in the past 10 years with the surprising success of Deep Neural Networks, also known as Deep Learning, in solving many hard problems in various aspects of large scale pattern recognition, such as vision, speech recognition, natural language understanding, robotics, computational biology, etc. The reasons why these networks work so well on so many different problems remained a major scientific puzzle.

In this short talk I will briefly describe our novel theory of large scale learning with Deep Neural Networks, which is based on the correspondence between Deep Learning and the Information Bottleneck framework. The theory provide a new understating of the computational power of Deep Neural Networks and how they relate to statistical physics and can affect the way we should do natural science from now on.



Naftali Tishby is a professor of Computer Science and the incumbent of the Ruth and Stan Flinkman Chair for Brain Research at the Edmond and Lily Safra Center for Brain Science (ELSC) at the Hebrew University of Jerusalem. He is one of the leaders in machine learning research and computational neuroscience in Israel, and his numerous former students serve in key academic and industrial research positions all over the world. Tishby was the founding chair of the new computer-engineering program, and a director of the Leibnitz Center for Research in Computer Science at Hebrew University. Tishby received his PhD in theoretical physics from Hebrew University in 1985, and was a research staff member at MIT and Bell Labs from 1985 to 1991. Tishby has been a visiting professor at Princeton NECI, the University of Pennsylvania, UCSB, and IBM Research. Tishby recived several awards, including he Landau prize in computer science in 2015.

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Knut Wolf Urban

Helmholtz Research Center Juelich

Aberration-Corrected Electron Microscopy – Probing Physics and Chemistry of Matter in Atomic Dimensions

Electron microscopy is today in its most exciting state in its more than eighty years long history. The reason for this lies in the fact that during the nineteen nineties it became at last possible to construct aberration-corrected electron lenses. This formed the basis for an entirely new generation of transmission electron microscopes now offering genuine atomic resolution to physics, chemistry and materials science. Electron microscopy has become a tool for high-precision measurements.

Modern electron microscopes offer two basic modes of operation, the "conventional" directly imaging mode (CTEM) and the scanning transmission mode (STEM). For these the following key features can be noted: (i) Measurements down to the picometer scale, i.e. the range where physics and chemistry happen. (ii) In addition to structural investigations modern aberration-corrected instruments are offering unique analytical features. Equipped with high-resolution electron-energy loss or X-ray spectrometers not only atomically resolved elemental analyses are possible but also identification and measurement of chemically active electronic states. (iii) Electron holography and special electron-detector arrangements allow to measure magnetic and electric fields down to the atomic level. (iv) Aberration-corrected electron optics has also enabled the field of advanced in-situ experiments inside the electron microscope under direct observation. Ultraminiaturized experimental chambers are available in which, e.g., samples can be subjected to chemical reactions in gas environments of up to atmospheric pressure and to high temperatures. Furthermore microscale devices can be studied in operando.

The quantitative output of modern aberration-corrected electron microscopy benefits substantially from the progress in the theory of condensed matter: *ab-initio* calculations and DFT based modelling allow to validate and interpret the atomic-scale results.

Knut W. Urban studied physics at University of Stuttgart where he received his doctor degree in 1972. He then joined Max Planck Institute for Metals Research, and he spent extended research stays at CEN Saclay/Paris, at Bhabha Center Mumbai, and as a professor at Tohoku University, Sendai. In 1984 he was appointed Professor for Materials Science at University of Erlangen, and in 1987 he became Chair of Experimental Physics at RWTH Aachen University and Director of Institute for Solid State Research, Research Center Juelich. In 2004 he was co-founder of Ernst Ruska Center for Microscopy and Spectroscopy with Electrons. Since 2009 he is Distinguished Professor at Juelich-Aachen Research Alliance (JARA). He is also Adjunct Professor, Materials Science Faculty, Xi'an Jiaotong University. He worked in many fields of experimental solid-state physics. Currently his main interest is in structural and physical properties of oxide materials. He was President of the German Physical Society. For the co-development, 1997, of the first aberration-corrected electron optics in use in electron microscopes throughout the world today he received a number of awards. Among these are the MRS von Hipel Award, the HONDA Prize for Ecotechnology, the BBVA Award in Basic Sciences, and the WOLF Prize in Physics. He has an honorary degree of Tel Aviv University, and he is honorary member of many national and international materials societies.

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Arieh Warshel

2013 Nobel Laureate in Chemistry; University of Southern California

Progress and Challenges in Rational Computer Aided Enzyme Design

Enzymes were optimized by evolution to reach a maximum overall efficiency. However, the available structural, spectroscopical, and biochemical information does not allow one to determine what are the most important catalytic contributions. Apparently, in many cases it is crucial to use computer simulation approaches in order to find out the actual contribution from different proposed catalytic factors. After a brief description of reliable methods for simulations of enzymatic reactions, we will point out that all consistent simulation studies have concluded that enzymes work by using their preorganized polar environment to stabilize the transition state of the reacting substrates. This means that enzyme catalysis is due to enzyme-enzyme interactions and not to enzyme-substrate interactions. Considering the progress in computational analysis of enzyme catalysis, it is important to examine what can be accomplished with computer aided enzyme design. Thus, we describe our progress on these fronts, starting with a demonstration that we can reproduce the observed effect of mutations, including those generated by directed evolution. We also point out that such an ability is not shared by most current approaches of enzyme design and that the current successes are actually due to directed evolution. Significantly, when we tried to move between directed evolution steps, that already have the correct active site residues, it is found that the directed evolution paths must incudes residues that are not in the active site. Predicting the corresponding mutations is a combinatorial challenge that we are currently addressing. Related challenges in fighting drug resistance are also outlined.

Arieh Warshel, distinguished Professor of Chemistry at the University of Southern California's Dornsife College of Letters, Arts and Sciences, was awarded a Nobel Prize in 2013 for his groundbreaking research in theoretical chemistry. Dr. Warshel holds the Dana and David Dornsife Chair in Chemistry at USC, where he has served on the faculty since 1976. In 2016, he was appointed Distinguished Professor at Large, on the faculty of The Chinese University of Hong Kong, Shenzhen, China where he is also the director of the Warshel Institute.

Dr. Warshel has pioneered the field of computational enzymology, helping develop computer simulations of the functions of biological systems that have allowed scientists to understand how life processes operate on the protein level. Marrying classical and quantum mechanics, he and colleagues Martin Karplus and Michael Levitt received the Nobel Prize for developing powerful computer models that researchers use to understand complex chemical interactions and create new drugs.

Warshel holds a B.Sc. in chemistry, *summa cum laude*, from Technion–Israel Institute of Technology in Haifa, Israel, and both a M.Sc. and Ph.D. in chemical physics from Israel's Weizmann Institute of Science. Prior to joining USC, he was a postdoctoral scholar at Harvard University and a senior scientist and associate professor at the Weizmann Institute. In parallel he was also a European Molecular Biology Organization fellow at the MRC Laboratory of Molecular Biology in Cambridge, England.

He is a member of the National Academy of Science, an Honorary Fellow of the Royal Society of Chemistry, and a Fellow of the American Association for the Advancement of Science and is the recipient of numerous honorary degrees notably from Technicon, Bar Ilan University, the University of Uppsala, Lodz University, and the Chinese University of Hong Kong.

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Ira A. Weinstock

Ben-Gurion University of the Negev

Structure and Reactivity at the Interface between Molecules and Solid-State Materials

Colloid science, and its more recent iteration as a branch of nanoscience, lies at the conceptual interface between molecular systems and functional solid-state materials. Unlike molecules, most colloidal structures are not amenable to characterization by single-crystal X-ray crystallography, while characterization of their surface features (such as protecting-ligand domains) lies outside the scope of the crystallographic methods used to define bulk phases of solid-state materials. However challenging, progress in this area nevertheless requires a determined focus on structure and reactivity.

One approach, demonstrated in the present talk, is to use cryogenic transmission electron spectroscopy (cryo-TEM) to investigate soluble nanostructures stabilized by readily imaged (highly electron dense) polytungstate (POM) cluster-anion ligands. The POM ligands simultaneously serve as "leaving groups" for controlling the transformations of the metal-nanoparticle ligand shells, and guiding their self-assembly into supra-structures capable of host-guest chemistry. A related topic is the use of POMs as covalently attached ligands for reactive metal-oxide nanocrystals, giving a new class of nanostructures uniquely positioned between molecular macroanions and traditional colloids. As soluble "complexes" of metal-oxide cores, reactions of these nanostructures can be investigated using the toolbox of solution-state methods traditionally reserved for studies of molecular catalysts. In both cases – the self-assembly of metal nanoparticles into nanoscale analogs of supramolecular cages and containers, and the "harnessing" of reactive metal-oxides as the reactive cores of soluble inorganic complexes – the use of POM ligands, in combination with cryo-TEM imaging, provides new options for investigating structure and reactivity at the challenging interface between molecular and solid-state science.

Ira A. Weinstock obtained his Ph.D. in 1990 from the Massachusetts Institute of Technology (MIT), where he worked on alkyne metathesis with Richard R. Schrock. After one year at the Sandia National Laboratory, Albuquerque, New Mexico, he served as Team Leader at the U.S. Department of Agriculture, Madison, Wisconsin, where he initiated the use of redox-active metal-oxide cluster-anions (polyoxometalates) as green catalysts for aerobic oxidations of biomass in water. In 2006, he joined the Ben-Gurion University of the Negev, where his research concerns the use of polyoxometalates in molecular and supramolecular chemistry, and as versatile ligands for investigating the solution-state self-assembly, structures and reactions of metal and metal-oxide nanostructures.

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Paul Weiss

University of California, Los Angeles

Paul S. Weiss graduated from MIT with S.B. and S.M. degrees in chemistry in 1980 and from the University of California at Berkeley with a Ph.D. in chemistry in 1986. He is a nanoscientist and holds a UC Presidential Chair and a distinguished professor of chemistry & biochemistry and materials science & engineering at UCLA, where he was previously director of the California NanoSystems Institute. He also currently holds visiting appointments at Nanyang Technological University, Harvard's Wyss Institute, and several universities in Australia and China. He studies the ultimate limits of miniaturization, developing and applying new tools and methods for atomic-resolution and spectroscopic imaging and patterning of chemical functionality. He and his group apply these advances in other areas including neuroscience, and microbiome studies, and high-throughput stem cell transfection.

He led, coauthored, and published the technology roadmaps for the BRAIN Initiative and the U. S. Microbiome Initiative. He has won a number of awards, in science, engineering, teaching, and publishing. He is a fellow of the American Academy of Arts and Sciences, the American Association for the Advancement of Science, the American Chemical Society, the American Institute for Medical and Biological Engineering, the American Physical Society, the American Vacuum Society, the Canadian Academy of Engineering, and an honorary fellow of the Chinese Chemical Society. He is the founding and current editor-in-chief of *ACS* Nano.

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Shimon Weiss

Bar-Ilan University

Dynamic Structural Biology: Two Decades of smFRET Applied to Transcription Initiation

Classical structural biology can only provide static snapshots of bio-macromolecules. Single-molecule Förster resonance energy transfer (smFRET) paved the way for studying dynamics in macromolecular structures under biologically relevant conditions. Since its first implementation in 1996, smFRET experiments have confirmed previously hypothesized mechanisms and provided new insights into many fundamental biological processes, such as DNA maintenance and repair, transcription, translation, and membrane transport. Here we review two decades contributions of smFRET to our understanding of transcription initiation. Transcription by bacterial DNA-dependent RNA polymerase is a multistep process that uses genomic DNA to synthesize complementary RNA molecules. Transcription initiation is a highly regulated step in E. coli, but it has been challenging to study its mechanism because of its stochasticity and complexity. We describe how single molecule approaches have contributed to our understanding of transcription and have uncovered mechanistic details that were not observed in conventional assays because of ensemble averaging.

Shimon Weiss received his PhD from the Technion in Electrical Engineering in 1989. After a one year post doctorate at AT&T Bell Laboratories, where he worked on ultrafast phenomena in semiconducting devices, he joined Lawrence Berkeley National Laboratory as a staff scientist in 1990, where he continued to work on solid state spectroscopy. In 1994 he re-directed his interest to single molecule biophysics. In 2001 he joined the UCLA Chemistry & Biochemistry and the Physiology departments. In 2016 he also joined the Physics department at Bar Ilan University, Israel (part time).

The Weiss lab has been working on ultrasensitive single molecule spectroscopy methods for over two decades. They were the first to introduce the single molecule FRET method and together with the Alivisatos group the first to introduced quantum dots to biological imaging. They have also developed a variety of single molecule spectroscopy methods, a variety of novel detectors for advanced imaging and spectroscopy, a superresolution imaging method dubbed SOFI, and novel optical imaging tools for single cell physiology. Currently they are developing single inorganic nanoparticle voltage sensors for probing neural networks.

Dr. Weiss has published 166 peer-reviewed papers, and holds 32 issued and 35 published patents. He was awarded the Humboldt Research Award, the Rank Prize in opto-electronics, and the Michael and Kate Barany Biophysical Society Award. He holds the Dean Willard Chair in Chemistry and Biochemistry and he is a Fellow of the Optical Society of America.

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George M. Whitesides

Harvard University

Molecular Recognition in Water is *Different*. The Hydrophobic Effect, and Enthalpy/Entropy Compensation

Life occurs in water, and many of the most important processes in the cell involve molecular recognition: the structure-specific, non-covalent association of one molecule with another. Water plays a central role in molecular recognition, and the hydrophobic effect is central to molecular recognition, but exactly what it does is still a subject of debate. This talk outlines some of the issues and evidence

concerning the surprising mechanism of the hydrophobic effect and related phenomena contributing to molecular recognition.

George M. Whitesides received his AB degree from Harvard University in 1960, and his PhD from the California Institute of Technology in 1964 (with J.D Roberts). He began his independent career at M.I.T., and is now the Woodford L. and Ann A. Flowers University Professor at Harvard Univestiy. His current research interests include physical and organic chemistry, materials science, biophysics, water, self-assembly, complexity and simplicity, origin of life, dissipative systems, affordable diagnostics, and soft robotics.

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Itamar Willner

Itamar Willner completed his Ph.D. (Chemistry) at the Hebrew University of Jerusalem in 1978. After his postdoctoral research (1978-1981) at U.C. Berkeley, he joined the Institute of Chemistry at the Hebrew University of Jerusalem, where he has been a Professor since 1986. His research interests include bioelectronics and molecular electronics, nanobiotechnology, DNA-based nanotechnology, supramolecular chemistry, nanoparticle research, stimuli-responsive materials and their use as drug carriers, artificial photosynthesis and the development of sensor and biosensor devices. Prof. Willner is an author of over 770 research articles and holds 30 patents. He was listed by Thompson Reuters in the *World's Most Influential Scientific Minds* (2014, 2015, 2016, 2017), and holds an h-index of 126 (ISI), 141 (Goople Scholar). He received The Israel Chemical Society Award (2001), The Israel Prize in Chemistry (2002), the Rothschild Prize (2008), the EMET Prize in Chemistry (2008), and the Gold Medal of the Israel Chemical Society (2016).

Prof. Willner is a member of the Israel Academy of Science, and acts as the Chairman of the Sciences Division. He is a member of the German National Academy of Sciences - Leopoldina, the European Academy of Sciences and Arts, and is a Fellow of the Royal Society of Chemistry.

Xiaoliang Sunney Xie

Harvard University ; Peking University, China

Single Cell Genomics: When Stochasticity Meets Precision

DNA exists as single molecules in individual cells. Consequently, genomic variations such as copy-number variations (CNVs) and single nucleotide variations (SNVs) in a single-cell occur in a stochastic way, necessitating single-cell and single-molecule measurements to be identified. However, existing single-cell whole genome amplification (WGA) methods are limited by low accuracy of CNV and SNV detection. We have developed transposase-based methods for single-cell WGA, which have superseded previous methods. With the improved genome coverage of our new WGA method, we have also developed a high-resolution single-cell chromatin conformation capture method, which allows for the first 3D genome map of a human diploid cell.

Gene expression is also stochastic due to the fact that the DNA exists as single-molecules in individual cells. The correlations among different mRNAs in a single-cell are masked within the stochastic gene expression noise. We have developed a method for single-cell transcriptome with improved detection efficiency and accuracy, revealing intrinsic correlations among all detected mRNAs in a single-cell. For a particular human cell type, we uncovered ~120 transcriptionally correlated modules (TCMs) from the gene expression data of ~700 individual cells under a steady state condition. We found that the TCMs are cell type dependent.

Xiaoliang Sunney Xie received a B.S. from Peking University (1984), and a Ph.D. from the University of California San Diego (1990), did a brief post doctorate at the University of Chicago. In 1992, joined Pacific Northwest National Laboratory, where he became Chief Scientist. In 1999, he was appointed Professor of Chemistry at Harvard University. He is currently the Mallinckrodt Professor of Chemistry and Chemical Biology at Harvard and the Lee Shau-kee Professor at Peking University. Xie is also the Director of the Beijing Innovation Center for Genomics (ICG), and the Director of the Biomedical Pioneering Innovation Center (BIOPIC), both at Peking University.

Xie and his group have been developing tools for biology and medicine for more than 20 years. In doing so, he became a world leader in utilizing these tools to make fundamental discoveries in biochemistry and molecular biology. Xie has made groundbreaking contributions in three areas: single-molecule enzymology, singe-molecule gene expression in live cells, and single-cell genomics. His transformative innovations in single-cell genomics have direct impact in human health and provide a clear example of precision medicine at the single-molecule level.

His honors include Albany Prize in Medicine and Biomedical Research, U. S. Department of Energy Lawrence Award, Biophysical Society's Founders Award, National Institute of Health Director's Pioneer Award, Sackler Prize for Physical Sciences, American Chemical Society's Peter Debye Award, fellow of the American Academy of Arts and Sciences, member of the National Academies of Sciences and Medicine.

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Omar M. Yaghi

University of California, Berkeley

Reticular Chemistry

From a historical perspective, the covalent bond has occupied a central role in building up organic molecules leading to polymers and pharmaceuticals, while the M-L bond has extended our control of matter to metal complexes leading to homogenous catalysts. Accordingly, chemistry has been largely dominated by discrete molecules and complexes, with very little known on how to extend the exquisite control we now have on these bonds to extended structures. The advent of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), made by linking organic molecules (COFs) or poly-nuclear clusters with organic linkers (MOFs), using strong bonds, has extended the chemistry of precisely controlling bonds and structures to 2D and 3D solids. This new chemistry, termed reticular chemistry, has opened the way to carrying out reactions on frameworks while maintaining their porosity and crystallinity. This presentation will discuss the future of reticular chemistry in the context of introducing: (1) molecular weaving using COFs capable of flexibility and dynamics, yet are resilient, as in the familiar woven cloth materials, (2) sequences of functionalities within MOFs and COFs capable of coding for highly selective carbon dioxide capture and enzyme-like catalysis, (3) ideal porosity for harvesting water from air, and (4) designed apportionments of functionality within structures to allow compartments to be linked, yet perform diverse function.

Omar M. Yaghi received his B.S. from State University of New York at Albany (1985) and Ph.D. in Inorganic Chemistry from University of Illinois at Urbana-Champaign (1990). He was an NSF Postdoctoral Fellow at Harvard University (1990-92). He started his independent career as an assistant professor in 1992 at Arizona State University, moved to University of Michigan at Ann Arbor as Robert W. Parry Professor of Chemistry in 1999, and then UCLA in 2006 as Christopher S. Foote Professor of Chemistry and Irving and Jean Stone Chair Professor in Physical Sciences. Since 2012 he has been the James and Neeltje Tretter Chair Professor of Chemistry at University of California, Berkeley, and a Senior Faculty Scientist at Lawrence Berkeley National Laboratory. He is the Founding Director of the Berkeley Global Science Institute, and the Co-Director of the Kavli Energy NanoSciences Institute, as well as the California Research Alliance by BASF.

His work encompasses the synthesis, structure and properties of inorganic and organic compounds and the design and construction of new crystalline materials. He is widely known for pioneering the discovery and development of several extensive classes of new materials: Metal-Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), and Zeolitic Imidazolate Frameworks (ZIFs). These materials have the highest surface areas known to date, making them useful in many clean energy applications. The building block approach he developed has led to an exponential growth in the creation of new materials having a diversity and multiplicity previously unknown in chemistry. He termed this field 'Reticular Chemistry'. Yaghi has received many awards for his scientific accomplishment, including the Sacconi Medal of the Italian Chemical Society (2004), Materials Research Society Medal (2007), AAAS Newcomb Cleveland Prize (2007), American Chemical Society Chemistry of Materials Award (2009), Izatt-Christensen International Award (2009), Royal Society of Chemistry Centenary Prize (2010), China Nano Award (2013), King Faisal International Prize in Science (2015), Mustafa Prize in Nanoscience and Nanotechnology (2015), Turkish TÜBA Academy Prize (2016), Royal Society of Chemistry Spiers Memorial Award (2017), King Abdullah II Order of Distinction of the First Class (2017), Japan Society of Coordination Chemistry International Award (2017), Kuwait Prize (2017), and Albert Einstein World Award of Science by World Cultural Council (2017). He published over 250 articles, which have received an average of over 350 citations per paper. He is listed among the top five most highly cited and impactful chemists worldwide (Thomson Reuters 2011).

Ada Yonath

2009 Nobel Laureate in Chemistry; Weizmann Institute of Science

The Origin of Life, or: What was first the Genetic Code or its Products?

Ribosomes, the universal cellular machines for translation of the genetic code into proteins, possess spectacular architecture accompanied by inherent mobility, allowing for their smooth performance as polymerases that translate the genetic code into proteins. The site for peptide bond formation is located within an almost fully conserved internal semi-symmetrical pocket composed exclusively of RNA. The high conservation of this region implies its existence irrespective of environmental conditions and indicates that it may represent an ancient RNA machine, which could be the kernel around which life originated. Hence, called by us the "proto ribosome", Indeed, recently, for the first time, the validity of this suggestion was verified, by the formation of a peptide bond by a synthetic "proto ribosome", thus demonstrating the validity of the above statement, and indicating that the vestige of a molecular prebiotic bonding entity is still functioning in all living cells of all organisms. As the initially newly born dipeptide could be elongated by the proto ribosome to oligopeptides, those fulfilling crucial tasks in the probiotic world or stabilizing the proto ribosome survived and led to the creation of a genetic code, which evolved together with the pocket, which evolved together with its products, the proteins, and their creator, the ribosome.

Ada Yonath focuses on protein biosynthesis, on antibiotics paralyzing this process, on global problems relating to antibiotic resistance, and on the origin of life.

She graduated from Hebrew University (1964), earned her PhD from Weizmann Institute (1968) and completed postdoctoral studies at Mellon-Institute and MIT, USA. In 1971 she established the first biological-crystallography laboratory in Israel, which was the only lab of this kind in the country for almost a decade. Since then, she has been a faculty member at the Weizmann Institute, were she is also the Director of Kimmelman Center for Biomolecular Structures. In parallel, in 1978 she spent a Sabbatical year in the University of Chicago, and during 1980-2004 she headed the Max-Planck-Research-Unit for Ribosome Structure in Hamburg while collaborating with Max-Planck-Institute for Molecular Genetics in Berlin.

Among others, she is a member of the US-National-Academy-of-Sciences; Israel Academy of Sciences-and-Humanities; German Academy for Sciences (Leopoldina); European Molecular Biology Organization; Pontifical (Vatican) Academy of Sciences; Korean Academy of Sciences and Technology. She holds honorary doctorates from over 20 universities worldwide, in USA, Latin America, Europe and the Far East.
Her awards include the Israel Prize; Linus Pauling Gold Medal; Albert Einstein World Award for excellence; UNESCO-L'Oréal Award for Woman in science; Wolf Prize; the Louisa Gross Horwitz Prize; Erice Peace Prize; Indian Prime-minister medal; Nobel Prize for Chemistry.

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