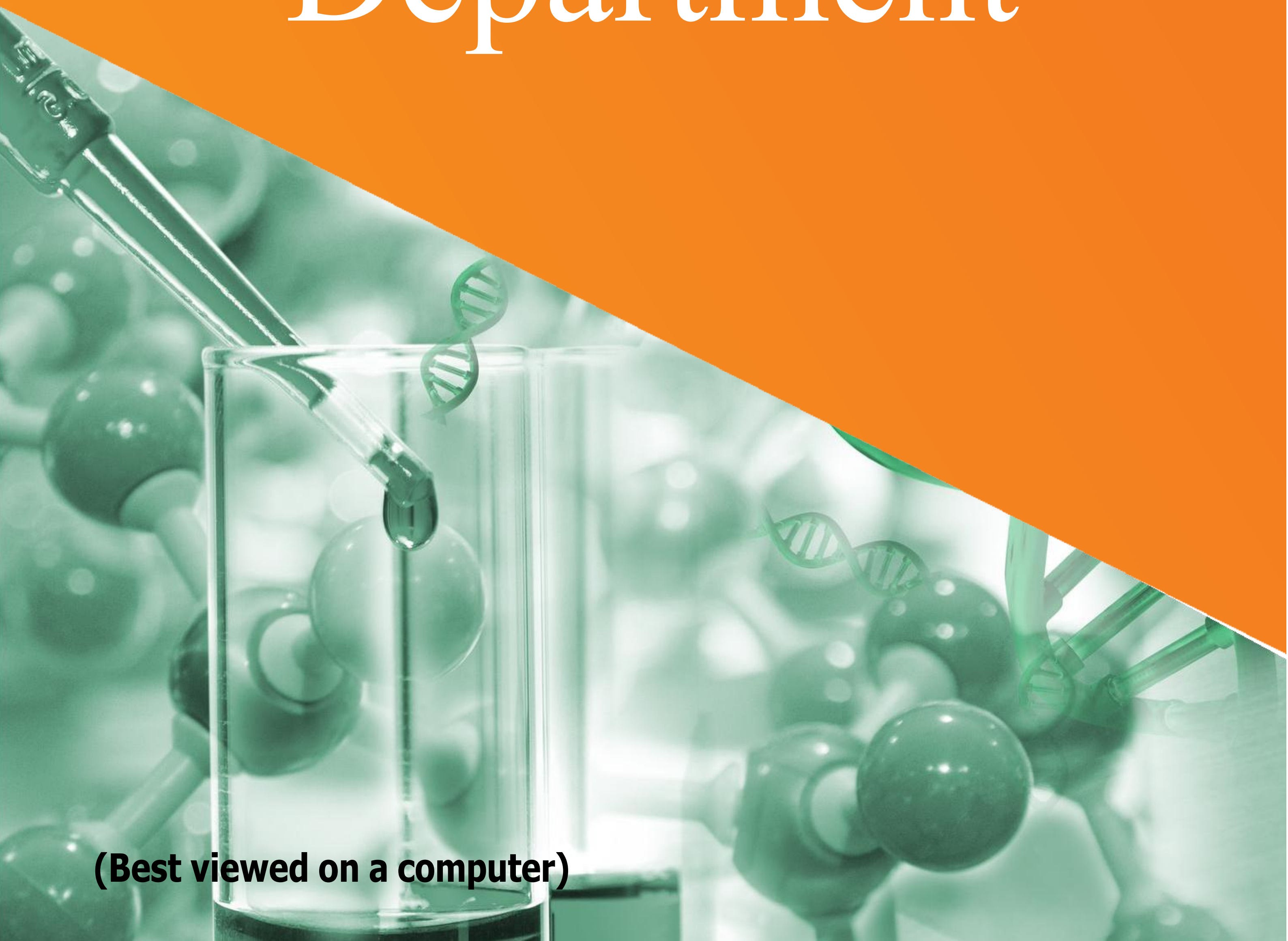
The Faculty of Natural Sciences
Ben-Gurion University of the Negev

The Chemistry Department



(Best viewed on a computer)

Prof. Barak Akabayov

Laboratory of Protein and Nucleic Acid Chemistry

Our overarching goal is to understand DNA replication and protein translation at the molecular level. Our research lab utilizes innovative tools and approaches to assess the structural nature and the biomolecular interactions in protein-protein and protein-nucleic acid complexes. In turn, we learn how these interactions determine and impact the biological catalysis. Our multidisciplinary approach, spanning chemistry, biology, and data science, employs both computational and experimental techniques. The need to develop new antibacterial drugs will lead us to discover inhibitors targeting components of central molecular biology pathways in bacterial cells.

Keywords: Antibiotics, Biochemistry, Cheminformatics, DNA replication, Translation

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Prof. Eyal Arbely

Synthetic Biology, Biochemistry, Chemical Biology

Expanding the chemical repertoire of living organisms

Synthetic Biology is a new and rapidly evolving interdisciplinary research field that aims to design and create new (synthetic) life forms with enhanced functionalities that do not exist in natural organisms. For example, genetic code engineering (also known as genetic code expansion technology) now enables the site-specific incorporation of non-proteinogenic (*i.e.*, non-natural) amino acids into ribosomally synthesized proteins. The incorporated non-natural amino acid may carry a chemical group that is not part of the engineered organism's chemical repertoire, thereby enable the expression of proteins with unique chemical and physical properties. Our group develops and utilizes genetic code expansion technology, with the aim of unraveling the role of lysine post-translational modifications in the regulation of enzymatic activity. Specifically, we conduct an interdisciplinary research at the interface of chemistry, biology, and engineering, to understand how metabolic processes are regulated by lysine acetylation, and how these regulatory mechanisms are modified in cancerous cells.

In addition, we devise and implement new technologies for site-specific chemical modification of proteins in living organisms. To this end, we explore new methodologies for expression of proteins with non-natural chemical groups and chemically synthesize new reagents for chemical reactions in living cells.

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Prof. Gonen Ashkenasy

Laboratory of Systems Chemistry

The Systems Chemistry of Peptide Networks

The main research effort in our lab is devoted to the design and synthesis of multi-component chemical systems, termed as Molecular Networks, and for analysis of their dynamic self-organization. This study within the new field of Systems Chemistry is inspired by the complexity in structure and function observed within natural cells. We use peptides and proteins as the active components in these studies, and thus the observed structure-function relationships are further interpreted for understanding fundamental processes, such as protein folding as well as protein interactions with small molecules and bio-macromolecules. Our findings can be used for understanding the organizational principles of biological systems, to shine light on plausible scenarios in early molecular evolution and the Origins of Life, and to develop devices of nanotechnology and biotechnology importance.

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Prof. Maya Bar Sadan

Advanced functional nano-materials

Chemistry at the atomic scale

My research is driven by fundamental questions on how to design materials that can carry out key energy-related reactions in an efficient, selective, and stable manner. We focuse on reactions such as water splitting for hydrogen production, the synthesis and utilization of alcohols as fuels, and the conversion of nitrate from industrial waste into valuable nitrogen-containing compounds. To address these challenges, we investigate how the precise local atomic and electronic structure in materials, such as 2D layered compounds, metal phosphides, and hybrid systems, governs catalytic activity and selectivity. In particular, we focus on identifying and controlling active sites, defects, and interfaces at the atomic scale. By combining atomic-resolution characterization with catalytic studies, we aim to establish direct correlations between specific atomic configurations and performance. This approach enables the development of design principles for next-generation catalysts and photocatalysts that convert simple, abundant molecules into sustainable fuels and chemicals.

Keywords: Atomic-scale materials design; Structure–property relationships; Nanoscale interfaces; Energy-related catalysis; Hydrogen and nitrogen conversion

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Prof. Joshua H. Baraban

Physical Chemistry, Spectroscopy

Research in the Baraban group focuses on understanding reactive species. We pursue this goal by exploring high temperature chemistry and developing spectroscopic tools to interrogate kinetics and dynamics. Novel homebuilt sources of reactive molecules, creative optical systems, and other innovative experimental strategies are key to these efforts, as is close coordination with high accuracy quantum chemistry.

Keywords: physical chemistry, spectroscopy, radicals, lasers

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Prof. Yonatan Dubi

Theoretical nano-science

Research in the Dubi group is devoted to the theoretical study of charge and energy transport in nano-scale systems such as single-molecule junctions, self-assembled monolayers, nano-particles, DNA-based structures, exciton networks and more. Such processes are relevant to a wide variety of physical and chemical phenomena, ranging from nanoscale photo-catalysis, through molecular magnetism to quantum biology. The group develops both models and theoretical tools needed to address the problems, including a wide variety of numerical and analytical methods.

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Prof. Leah Gheber

Biophysical chemistry, molecular nano-motors, cytoskeleton, mitosis

Mitosis is a process by which duplicated genomic information is transferred from mother to daughter cells. This essential process is accomplished by the spindle, a highly dynamic, microtubule-based structure, which in each mitotic cycle undergoes a well-programmed set of morphological changes. Compromised spindle integrity is one of the key factors for chromosome mis-segregation, which in turn may lead to genetic disease, cell death and cancer. Recent evidence indicates that molecular nano-motors from the Kinesin superfamily, which bind and move along microtubules, play central roles in mediating spindle dynamics.

Our research focuses on the Kinesin-5 mitotic motor proteins, whose function is essential for chromosome segregation during mitosis. Our objective is to explore the mechanisms by which Kinesin-5 motors perform their multiple mitotic functions. To achieve this goal, we combine biophysical, biochemical, cell biology and genetics approaches such as single-molecule fluorescence motility assays and live-cell and electronic microscopy.

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Prof. Idan Hod

Hybrid Materials for Sustainable Energy

In a world that is running out of natural resources, there is a growing need to design and develop sustainable and green energy resources. In that respect, photo-electrocatalytically driven reactions to produce alternative fuels (such as water splitting or CO_2 reduction) hold the potential to provide a route for future carbon neutral energy economy. Nevertheless, the slow kinetics of those catalytic reactions demands the development of efficient catalysts in order to drive it at lower overpotentials.

Our group utilizes Metal-Organic Frameworks (MOFs) as a platform for heterogenizing molecular electrocatalysts. Their unique properties (porosity and flexible chemical functionality) enable us to use MOFs for integrating all the different functional elements needed for efficient catalysts: 1) immobilization of molecular catalysts, 2) electron transport elements, 3) mass transport channels, and 4) modulation of catalyst secondary environment. Thus, in essence, MOFs could possess all of the functional ingredients of a catalytic enzyme.

GET IN TOUCH

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Prof. Raz Jelinek

Nanotechnology, Biophysical Chemistry, Two-dimensional nanostructures, Biomimetic cellular membranes

Research in the Jelinek laboratory is multidisciplinary and spans biological chemistry, nanotechnology, advanced sensors, and energy storage. The research activity in the laboratory has a certain applied-science emphasis, with several patents awarded/submitted. Current projects include *amyloid-mediated chemical catalysis; carbon dots for biological* and *chemical applications; chromatic polymers; porous matrixes for water purification; and advanced supercapacitors.*

Keywords: amyloids; carbon dots; chromatic polymers; gas sensors; bacterial sensors; photodetectors; supercapacitors; organic batteries

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Prof. Sebastian Kozuch

Computational Chemistry

Chemistry from a Computational Perspective

Computational chemistry is an increasingly powerful tool to understand chemical reactions. In our group we use quantum chemistry tools to understand and predict molecular effects mainly on three areas:

1. Homogeneous catalysis through mechanistic and kinetic modeling.
2. The nature of hole interactions and other novel types of chemical bonds.
3. Quantum mechanical tunneling reactions.

GET IN TOUCH

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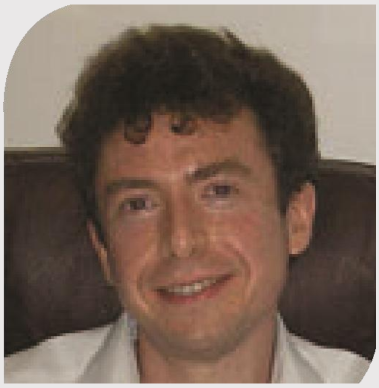
Prof. N. Gabriel Lemcoff

Organometallic Chemistry, Olefin Metathesis, Polymers, Organic Chemistry

Development of Novel Synthetic Methodologies, Catalysts, and Polymers

Modern polymer science drives innovation through the development of functional molecular architectures and advanced macromolecular catalysts—goals that continue to challenge and inspire the chemical community. Our research focuses on synthesizing, characterizing, and analyzing novel macromolecular compounds while developing new catalytic systems and reactions. We specialize in latent ruthenium-based catalysts, having pioneered the first thermoswitchable and photoswitchable olefin metathesis systems. Over the past five years, our achievements include: highly selective olefin metathesis reactions; "plasmomer" hybrid materials that generate heat under IR irradiation; innovative "solid solvent" methodologies for accessible latent catalysts in 3D-printing applications; and stereospecific alcohol halogenations using simple thiourea additives with halosuccinimide donors. These advances demonstrate our commitment to bridging fundamental polymer and organic chemistry with practical applications.



GET IN TOUCH

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Prof. David Lukatsky

Theoretical Biophysical Chemistry, Biophysics Design principles of protein-protein recognition, promiscuity and plasticity versus specificity

The main focus of the research activity of the Dr. Lukatsky’s laboratory is the problem of specificity and design principles of protein-protein and protein-DNA interactions, and principles of biomolecular recognition in general. The main finding of the last academic year was the discovery of the genetic code for nonspecific protein-DNA interactions. In particular, we predicted that genomic DNA of eukaryotic organisms encodes its intrinsic propensity for nonspecific binding to transcription factors (TFs), and other DNA-binding proteins. Using extensive bioinformatics analysis, we verified that the predicted effect is operational in the yeast *S. cerevisiae* genome. We showed that nonspecific protein-DNA binding significantly influences TF-DNA binding preferences and nucleosome occupancy in yeast. We are currently analyzing the consequences of the predicted effect in the worm and fly genomes.

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Prof. Michael M. Meijler

Synthetic Bioorganic Chemistry, Chemical Biology, Quorum Sensing

Bacterial Intra- and Interspecies Communication

Every living being on Earth talks – *chemically*; an important focus of our research is the study of bacterial intra- and interspecies signaling molecules. Cell-to-cell communication is used by all organisms to coordinate their behavior and function in such a way that they can adapt to changing environments and possibly compete with multicellular organisms. Chemical communication amongst bacteria has been termed "quorum sensing" (QS). Examples of QS-controlled behaviors are biofilm formation, virulence factor expression, antibiotic production and bioluminescence. These processes are beneficial to bacterial populations only when they are carried out in a coordinated fashion. Quorum sensing systems exist in both Gram-positive and -negative bacteria and a wide range of peptides, acylhomoserine lactones and other motifs have been identified as QS molecules. We aim to clarify the role of various QS molecules in bacterial signaling through synthesis and evaluation of QS molecules and potential antagonists and we develop methodologies to study a wide variety of newly discovered and undiscovered QS molecules.

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Prof. Yifat Miller

Computational Biophysical Chemistry, Computational Physical Chemistry

Our research activity mainly focuses in self-assembly of amyloids – proteins that are related to type 2 diabetes, Alzheimer's disease, and Parkinson's disease. Our computational laboratory conducts fundamental and applied research at the interface of computational structural biology, biomaterial, and bio-nanotechnology, with the goal to better understanding of biophysicochemical interactions in the self-assembly of peptides for practical applications in biomaterials and medicine.

Our main research interests:
1. Molecular mechanisms of amyloid plaques formations in Alzheimer's disease, Parkinson's disease and type 2 diabetes.
2. Link between type 2 diabetes and neurodegenerative diseases.
3. Effect of metals on type 2 diabetes and neurodegenerative diseases.
4. Investigating inhibitors for amyloid plaques: Prevention and treatment for neurodegenerative diseases.
5. *In silico* design of novel self-assembling peptides for nanotechnology applications.

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Prof. Anat Milo

Physical Organic Chemistry, Catalyst design, Selectivity, Stereochemistry

From energy conversion, through the production of polymers and materials, to the synthesis of natural products, pharmaceutics, and fine-chemicals – catalysts have been key to advancing our modern lifestyle. However, most industrial catalytic processes rely on toxic, expensive metals that have to be rigorously removed from the products. Organocatalysis offers a greener alternative, but often requires high catalyst loading, suffers from reproducibility issues, and is tailored for a limited range of substrates. To overcome these limitations and unlock organocatalysts' full potential, it is necessary to uncover the structural origin of their reactivity and selectivity, thereby providing a knowledge-driven approach to their design and optimization.

My research group synergistically integrates experimental, computational, and statistical methods to design and construct modular catalyst libraries and provide a powerful strategy for discovering and optimizing selective catalytic reactions. To this end, we experimentally introduce transient directing groups to diversify known organocatalysts *in situ* under reaction conditions by forming orthogonal bonds. These directing groups serve to control and tune the secondary-sphere interactions between the organocatalyst and substrates or intermediates in the rate- and product-determining transition state(s). Modifying a catalyst structure *in situ* is challenging due to the required orthogonality between the binding mode and catalytic activity. Nonetheless, this approach is appealing as it can uncover general molecular design principles for the facile introduction of highly modular selectivity- and reactivity-controlling handles into a variety of catalytic systems.

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Prof. Taleb Mokari

Nanochemistry, Nanomaterials, Photovoltaics, Renewable Energy

Synthesis, characterization and application of nanostructures

The primary focus of our research activity is development of novel nanostructures for optical, electrical, biological and energy application. Our Laboratory studies the science of optimally preparing and characterizing metal, semiconductor, magnetic, insulating inorganic nanostructures, and multi-component nanostructures with various interfaces, including nanocrystals, nanotubes and nanowires with controlled size, shape, and composition. The synthesis of 1-dimensional nanostructures is conducted by gas- and solution-phase, where we develop our own approaches to achieve new nanomaterails and a better control of the synthesis parameters. The research encompasses the design and synthesis of precursors, the study of microscopic elementary processes in nanostructure nucleation and growth, and the use of nanostructures in functional, multi-component devices.

The applications our group focuses on are catalysis and solar energy conversion USING nanomaterial composite systems. As catalysts, nanomaterials could improve product selectivity, thereby reducing chemical waste and produce cleaner fuels. As energy conversion materials, they could lower the final cost per kWh to the end user. From precursor design to impact on the environment, we examine the possible contributions nanomaterials could have on our world.

GET IN TOUCH

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Prof. Benjamin A. Palmer

Organic biomineralization and bio-inspired optical materials

Many animals use crystals of small organic molecules to manipulate light. For example, crystals of the nucleotide base guanine are used to produce the silvery reflectance of fish, the tunable iridescent colors of chameleons and crustaceans and image-forming mirrors in animal eyes (Fig. 1). These organisms exert exquisite control over the shape and size of the constituent crystals, utilizing crystallization strategies far beyond the capabilities of solid-state chemistry.

The Palmer lab sits at the interface between solid-state chemistry, photonics and cell biology. Our aim is to uncover the crystallization 'tricks' which organism use to produce biological optical materials, revealing new synthetic methods for the design of organic materials. We have three main research directions: (i) the discovery and characterization of new organic bio-crystals in animals, (ii) mechanisms of biologically controlled crystallization and (iii) bio-inspired crystallization of novel organic optical materials. We utilize a raft of physical characterization techniques to explore these problems including cryo-electron microscopy (Fig. 1), optical microscopy, X-ray and electron diffraction.

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Prof. Doron Pappo

Synthetic Organic Chemistry

Organisms Synthetic Methodologies

The research in the Pappo group focuses on the design and development of novel redox C–H functionalization catalytic systems based on earth abundant metals. Our main aim is to offer a strategy to synthesize a vast array of complex arene-based materials that exist in many pharmaceuticals and natural products and used in catalysis in a direct manner, starting from simple and available starting materials.

Number of iron, cobalt, manganese and copper catalysts that bring together two arene, arenol or aniline units in a single step were developed. By adopting a mechanistic oriented approach, the chemoselectivity, regioselectivity and stereoselectivity in these sustainable transformations were controlled. Therefore, by selecting one catalytic system over another, a given pair of substrates can lead to different coupling products and hence to unlimited possibilities.

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Prof. Menny Shalom

Materials Science, Supramolecular Chemistry, Photoelectrochemistry

One of the promising technologies for future alternative energy sources is the direct conversion of sunlight into chemical or electrical energy by using photocatalysis or photoelectrochemical cells (PEC), respectively. The greatest challenge in these fields is to develop new types of advanced materials with the desired electrical and optical properties that will replace the conventional raw materials that are currently used. Although in the last years a significant progress has been made, it is still an essential task to find efficient and low-cost materials as photoactive materials and co-catalysts. More importantly, it is necessary to gain a basic understanding of the physical properties and the fundamental operation mechanisms in this field.

Our group develops new methods to synthesize metal-free materials and earth-abundant metal-containing materials with welldefined structure and properties toward their utilization in energy-related applications such as photo- and electro-catalysis. Our focus is the synthesis of materials appropriate for utilization in solar-to-fuel conversion reactions.

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Prof. Amichay Vardi

Quantum Dynamics and Thermodynamics

We theoretically study the dynamics of many-body quantum systems, focusing on fundamental questions concerning the emergence of irreversible macroscopic thermodynamics from the reversible microscopic quantum dynamics of isolated systems. We aim to construct minimal models for demonstrating quantum ergodization, thermalization and many-body localization and to establish the role of dynamical chaos in mesoscopic thermodynamics and quantum control. Recent research achievements include the study of adiabatic passage through chaos and the discovery of quantum detours around it, the suggestion of probabilistic hysteresis in isolated Bose-Hubbard models, the observation of prethermalization in an array of subsystems exhibiting negative specific heat, and the development of semiclassical methods for characterization of many-body localization. Notable past results include the discovery of anisotropic solitons in Bose-Einstein condensates of dipolar particles, the stabilization of coherent matter-wave states in driven atom interferometers via a Kapitza inverted pendulum effect and a many-body quantum Zeno effect, the optimization of atom interferometry below the standard quantum limit, phase-space tomography via temporal fluctuations, the discovery of interferometric signatures of chaos in bosonic Josephson junctions, the discovery of incoherent matter-wave solitons, and the proposal of Bose-enhanced chemistry.

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Prof. Ira A. Weinstock

Metal-oxide cluster science

Numerous intellectually substantive phenomena and societally important issues can be addressed using metal-oxygen cluster anions (polyoxometalates, or POMs), and much of Weinstock's work involves their use as physicochemical probes of molecular processes, as molecular catalysts and photocatalysts of renewable-energy processes and organic transformations, as supramolecular capsules for exploring the effects of nanoconfinement on complex reaction systems, and as ligands and building blocks for the design of functional nano-scale assemblies of metal nanoparticles and metal-oxide nanocrystals.

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Prof. Yossi Weizmann

Laboratory of DNA Nanotechnology and Materials Science

Our research focuses on designing functional nanomaterials and nucleic acid nanostructures to address key challenges in chemistry, materials science, and biomedicine. We develop plasmonic and photothermal nanoparticles that use light to drive precise, energy-efficient chemical synthesis, catalysis, and environmental processes. In parallel, we engineer programmable DNA and RNA architectures that act as scaffolds, sensors, and dynamic molecular machines for probing biology and enabling advanced molecular diagnostics.

Central to our approach is building hybrid systems with emergent function by integrating biomolecules, synthetic components, and inorganic nanostructures through covalent and supramolecular interactions. This multidisciplinary strategy yields nanoscale platforms for selective polymerization, real-time biosensing, water harvesting, and light-triggered molecular transformations.

We also cultivate a collaborative, interdisciplinary research environment that empowers students and trainees to develop independence and creativity, training the next generation of innovators in nanoscale science and technology.