

The Graduate Student Division

The 8th Graduate Students' Chemistry Symposium

December 8, 2016

Ben-Gurion University of the Negev

W.A. Minkoff Senate Hall, Samuel and Milada Ayrton

University Center (#71)

8:30 AM – 5:00 PM





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8:30 AM – 5:00 PM*

8:30-9:00	Coffee and registration	
Chair	Oren Meiron	
9:00-9:10		OPENING REMARKS
9:10-9:55	Itamar Willner	DNA – AN ACTIVE COMPONENT IN MEDICAL SCIENCE AND TECHNOLOGY
9:55-10:15	Maya Bar-Sadan	FROM STUDENTS TO PIS: WHAT TO PREPARE FOR
10:15-10:30	Ayelet Ofarim	A UNIQUE NEW TOOL BY CAS FOR SEARCHING AND COMPARING ANALYTICAL METHODS
10:40-11:00	Coffee Break	
Chair	Itay Pitussi	
11:00-11:15	Hanna Noa Barad	HOW TRANSPARENT METAL OXIDES GAIN SOME COLOR: UTILIZING COMBINATORIAL MATERIALS SCIENCE TO DISCOVER NEW PEROVSKITE OXIDES
11:15-11:30	Eran Aronovich	BIMETALIC CATALYSTS FOR HYDROGEN EVOLUTION
11:30-11:45	Kiran Kumar Tadi	ON THE ELECTROCHEMICAL PROPERTIES OF FUNCTIONAL MATERIALS: SENSING AND ELECTROCATALYSIS
11:45-12:00	Jesus Barrio Hermida	SUPRAMOLECULAR ORGANIZATION DIRECTED GROWTH OF C ₃ N ₄ MATERIALS WITH HIGH PHOTOCATALYTIC PERFORMANCE
Chair	Miran Liber	
12:00-12:15	Maya Miller	DECIPHERING MOLECULAR PATHWAYS AND CELLULAR INTERACTIONS INITIATED BY ANTICANCER TI(IV) PHENOLATO COMPLEXES
12:15-12:30	Partha Jyoti Das	SYN-(ME,ME)BIMANE AND ITS THIONATED ANALOGS: SYNTHESIS AND COORDINATION CHEMISTRY
12:30-12:45	Roi Rutenberg	NATURAL POLYMER BASED ENCAPSULATION SYSTEMS FOR ANTIMICROBIAL AGENTS CONTROLLED RELEASE
12:45-14:00	Lunch Break	
13:15-14:00	Poster session	
Chair	Daniel Aminov	
14:00-14:20	Elinor Zerah-Harush	LIGHT-HARVESTING IN MOLECULAR SYSTEMS: THE ROLE OF ENVIRONMENT IN OPTIMIZING THE EFFICIENCY OF ENERGY TRANSFER ON THE NANO-SCALE
14:20-14:40	Itay Pitussi	ADSORPTION OF CO ON THIN LAYERS OF PT ON SN
14:40-15:00	Inbal Oz	NANOTUBES MOTION ON LAYERED MATERIALS: A REGISTRY PERSPECTIVE
15:00-15:20	Yoav G. Pollack	FINDING FORCE-LAWS AND EMERGENT MANY-BODY INTERACTIONS IN AMORPHOUS SOLIDS
15:20-15:40	Coffee Break	
Chair	Maya Miller	
15:40-16:00	Miran Liber	TOWARDS ARTIFICIAL DNA MOLECULAR MOTORS THAT CAN WALK OVER MICROMETERS
16:00-16:20	Shifra Lansky	MULTIPLE CONFORMATIONAL STATES OF A UNIQUE EXTRACELLULAR ARABINANASE SUGGEST A "HARPOON" MECHANISM OF ACTION
16:20-16:40	Miri Krupkin	AVILAMYCIN INDUCES STRUCTURAL CHANGES IN RPROTEINS UL16 AND CTC THAT ENHANCE THE INHIBITION OF A-SITE TRNA BINDING
16:40-17:00	Rona Shaharabani	THE DEVELOPMENT OF MULTIPLE SCLEROSIS FROM A BIOPHYSICAL PERSPECTIVE



From the Chairman

The GSD was founded almost three years ago on the grounds that the graduate chemistry students currently have no official body to represent and support them.

Prof. Ehud Keinan, the president of the Israel Chemical Society, has identified the need for a body of graduate chemistry students to represent and support the graduate chemistry students of Israel. A representative was elected from each university and thus the first executive board of the GSD was founded.

During the past three years, the board has worked hard to identify needs that the graduate students might have and ways to help and support the students with different issues.

We have found several major areas where the GSD might benefit the graduate chemistry students:

1. Annual symposium – will create a platform for chemistry graduate students to present their work and to network.
2. Workshops – will create opportunities for students to learn about new analytical tools and techniques.
3. Connections with similar groups abroad – will improve collaborations between groups from Israel and other countries, as well as open study opportunities.
4. Expanding the education of chemistry – will promote programs in which graduate chemistry students will give short lectures to high school students.
5. Creating connections to the industry – will promote connections and collaborations with the chemical industry in Israel.

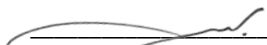
Being part of the GSD board for the past three years has been a privilege. We were fortunate to be the first to shape this unique division of the Israel Chemical Society and provide new and novel opportunities for chemistry graduate students.

I want to personally thank each and every board member for the wonderful work they have done in these three years and to Prof. Ehud Keinan and Dr. Rami Batrice for founding the GSD in the first place.

It is my personal hope that the GSD will continue to grow and support the chemistry graduate students in Israel and help them to concentrate on becoming the best scientists they can be.

If you wish to take part in the work we are doing, you can approach the GSD representative in your university for more information.

I hope you will enjoy the 8th students' symposium and our activities throughout the year.



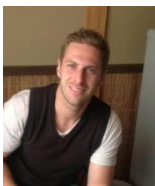
Oren Meiron
GSD chairman

GSD Board Members



Oren Meiron
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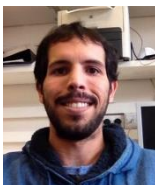
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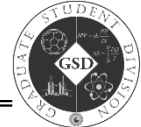
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DNA – An Active Component in Medical Science and Technology

Itamar Willner

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The base sequence in nucleic acids encodes functional and structural information into the biopolymer, and provides a rich “tool-box” to develop the area of DNA nanotechnology, and to design functional DNA-based materials.

The lecture will address recent advances in the areas of DNA nanotechnology and DNA materials. Topics that will be addressed include the use of DNA as a dynamic scaffold for operating DNA machines, the use of the dynamic properties of DNA nanostructures to organize nanoparticles, to generate chiroplasmonic nanostructures and to develop the area of “origami chemistry”.

The topic of DNA-based materials will be introduced by describing different stimuli-responsive materials. Stimuli-responsive DNA hydrogels exhibiting triggered stiffness properties will be introduced, and their application as shape-memory matrices and as signal-triggered dynamically modulated structures will be discussed. Also, the use of stimuli-responsive DNA-functionalized nano/micro-carriers (SiO₂ nanoparticles, MOFs, microcapsules) for controlled drug release will be introduced.

From students to PIs: what to prepare for

Maya Bar Sadan¹

¹Chemistry Department, Ben-Gurion University of the Negev, Beer Sheba, Israel



Cannabis; A changing approach - a need for new tools

“Nothing is more important than an idea whose time has come” (Victor Hugo)

Ayelet Ofarim¹

¹Arad-Ofir

Looking at the number of articles and patents published on the pharmaceutical development of cannabinoids, one can clearly see that this subject is now taking off.

Big pharmaceutical companies are trying to follow up on the unique healing evidence. The issue is discussed intensively in forums, Facebook and websites. Pharmaceutical commercial development, of course, should apply with regulations and validation demands and, as usual, needs updated and comprehensive tools to do that.

Accordingly, the need for analytical methods for extraction of Cannabinoids (the API in Cannabis) is increasing. Searching Cannabinoids on shows us a trend – **the number of patents has increased by over 4 times since 2000.** More specific, searching for analytical methods for the extraction in , gave a fully specified protocol, list of equipment, conditions etc of over 100 validated analytical methods.

This presentation will guide you through the development of the medicinal Cannabis and will get you familiar to a new one-of-a-kind tool for searching and comparing analytical methods – .



How transparent metal oxides gain some color: Utilizing combinatorial materials science to discover new perovskite oxides

Hannah Noa Barad^{*}, David A. Keller Kevin J. Rietwyk, Adam Ginsburg, Maayan Priel, , Ilya Grinberg, Assaf Y. Anderson^{*}, and Arie Zaban

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All-oxide photovoltaic devices are an emerging type of solar cells, due to their low-cost, high abundance, and easy fabrication methods. These characteristics allow the metal oxides to be potential absorbers as well as electron/hole conductors in solar cells. Perovskite metal-oxide structures have recently been studied as absorbers for solar cells since the perovskite structure has shown interesting characteristics, which allow, in part, better charge transport in photovoltaic devices. As such, development of new metal oxide perovskites, with lower bandgaps as absorbers for solar cells, is important.

In this work, combinatorial material science was used, to form CeNiO_3 , a new perovskite metal oxide. The CeNiO_3 was synthesized in a combinatorial library by sequential cycles of pulsed laser deposition (PLD) using targets of CeO_2 and NiO , which are wide bandgap transparent (3.3 eV and 3.5eV, respectively) semiconductors. The combinatorial library was fully characterized by x-ray diffraction (XRD) and energy dispersive x-ray spectroscopy (EDS) to detect the perovskite phase and determine the Ce-Ni-O ratios. Seebeck measurements and Kelvin probe analysis show a change in the conduction type (n- or p-type) with variation in the chemical composition throughout the library. Optical characterizations reveal that the obtained bandgaps for the CeNiO_3 range from 1.48-1.77 eV, which are much lower than those of the original starting materials. The low bandgaps and the energetics of the CeNiO_3 indicate its potential to be used as an absorber material in all-oxide photovoltaic devices.

Designing efficient bimetallic photocatalysts for hydrogen Production

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² Schulich Faculty of Chemistry, The Russell Berrie Nanotechnology Institute, and The Nancy and Stephen Grand Technion Energy Program; Technion – Israel Institute of Technology, Haifa 32000, Israel

³ Peter Grünberg Institut 5 and Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany.

The search for alternative clean and renewable energy source is a major pressing issue. One promising direction is the use of semiconductor nanoparticles as photocatalysts which absorb the solar radiation and produce hydrogen from water. Upon radiation, excited electrons and holes are created. They then migrate to the surface and react with the aqueous solution. Efficient photocatalysts should maintain charge separation of the holes and electrons and contain different sites for oxidation and reduction. Usually a small metallic particle is deposited on the semiconductor as a co-catalyst which acts as an electron sink and a reduction site for protons. Hybrid core-shell structures such as CdS@CdSe increase the charge separation and reduce the particle dissolution by confining the holes to the core and leaving the electrons delocalized over the entire structure. A bi-metallic co-catalyst composed of metals such as gold and palladium should improve the photocatalytic activity of the system. Such bimetallic particles possess the ability to attract electrons from the semiconductor and discharge them into the aqueous solution more efficiently than each of the metals on their own. Here we use the CdSe@CdS-Au@Pd system as a case study to explore the effect of the inner structure of the bimetallic tip on the photocatalytic performance. In addition we study the dynamic processes which occur during photocatalysis. For this aim we used high resolution energy dispersive spectroscopy (EDS) for the system characterization and an online GC equipped setup for the long duration photocatalytic hydrogen evolution measurements.

On the Electrochemical Properties of Functional Materials: Sensing and Electrocatalysis

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The constant search for new functional materials for electrochemical sensing and electrocatalysis has led to evolve new surface modification strategies and the pure/doped nanomaterials. In the present talk, electrochemical applications of two functional materials namely molecularly imprinted polymers (MIPs) and 2-dimensional nanomaterials will be focused. MIPs possess several advantages over biological counterparts such as low cost, ease of preparation and good physical and chemical stability over wide range of experimental conditions and solvents. Rational and fast method for searching optimal imprinting conditions using computer aided study to improve the recognition properties of MIP is discussed. The molecular modelling is followed by fabrications of highly sensitive and selective electrochemical sensor for pindolol and epinephrine. The electrochemical behavior of the analytes at MIP modified electrodes has been investigated employing various electroanalytical techniques. Graphene based biosensors are receiving tremendous scientific attention due to the engineering possibilities of graphene by bringing specificity and sensitivity in the device via doping and defects. Electrostatic interaction between the most electronegative element fluorine (F) and hydrogen (H) is one of the strong interactions in hydrogen bonding, and here we report the selective binding of ammonia/ammonium with F in fluorographene (FG) resulting to a change in the impedance of the system. Recently, 2D-metal dichalcogenides (especially XS_2 , where X = Mo, W etc) were highly explored for various applications. Here we report a bulk, single step method to synthesize metals modified MoS_2 quantum dots (QDs). Three elements, namely Fe, Mg and Li, are chosen for studying the effects of dopants in the catalytic activities of MoS_2 . Efficacy and tunability of these luminescent doped QDs towards various electrocatalytic activities (hydrogen evolution reaction, oxygen evolution reaction and oxygen reduction action) are reported.

Supramolecular organization directed growth of C_3N_4 materials with high photocatalytic performance

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Over the past few years, graphitic carbon nitride (g-CN) has attracted widespread attention due to its outstanding electronic properties, which have been exploited in various applications, including in photo- and electro-catalysis, heterogeneous catalysis, CO_2 reduction, water splitting, light-emitting diodes, and PV cells. g-CN comprises only carbon and nitrogen, and it can be synthesized by several routes. The synthesis of this material can be carried out by polymerization of C and N rich monomers, such like cyanamide, dicyanamide or melamine (1-3). Recently we showed that supramolecular preorganization of monomers (Melamine, cyanuric acid) using non-covalent bonds prior their calcinations at high temperatures yield highly efficient materials for photocatalytic [applicatons \(4-7\)](#) ([water splitting \(8\)](#)), or [degradation of Rhodamine B dye \(9\)](#).

In this work, we will show the effect of anion bridging between starting monomers (Melamine, cyanuric acid and barbituric acid) in supramolecular assemblies that are used as precursors for carbon nitride synthesis. The anion role on the materials growth and their final chemical, photophysical and catalytic properties will be discussed. The resulting carbon nitride exhibits a great enhancement either in Rhodamine B dye degradation and water splitting compared to the regular reference carbon nitrides mainly due to an increase in the porosity and surface area of the material. This work aims to open new opportunities for the rational design of carbon nitride based photocatalysts for environmental and energy-related applications.

Deciphering Molecular Pathways and Cellular Interactions Initiated by Anticancer Ti(IV) Phenolato Complexes

Maya Miller¹, Ori Braitbard², Jacob Hochman², Edit Y. Tshuva¹

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²*Alexander Silberman Institute of Life Science, The Hebrew University of Jerusalem, 9190401 Jerusalem, Israel.*

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Metal containing compounds have entered the field of anticancer research with the introduction of cisplatin in the early 70th, followed by titanium complexes a decade later. Unlike platinum, titanium is a biocompatible metal providing a clear advantage for the use in therapy. The first class of titanium containing drugs introduced suffered from rapid hydrolysis in biological environment, which hampered the identification of the active species and the study of its molecular mechanism, thus ultimately resulting in failure in clinical trials. Later titanium complexes based on phenolato ligands achieved enhanced resistance to hydrolysis;¹ these compounds have shown high anti-tumor activity toward various cancer cell lines, selectivity to cancer tissue, durability in aquatic solutions and effectiveness in *in vivo* models.

This work aims to promote our understanding of the molecular mechanism involved in the activity of Ti(IV) phenolato complexes. A leading phenolato Ti(IV) compound influenced the cell cycle, causing G1 arrest. Cytotoxicity measurements have shown significant decrease in cell viability only within 24 hours of incubation, supporting a programmed rather than instant cell death. Additionally, upregulation of p53 and caspase9 proteins imply on apoptotic pathways involved. Comparing cytotoxicity, cellular uptake, and protein levels in two cell lines imply that different mechanisms are plausible.² Additional experiments suggest that chromosomal DNA and/or mitochondria may serve as cellular targets for this class of complexes. Preliminary results with chiral complexes will also be presented. Altogether, the preliminary mechanistic insights gained should advance these promising Ti(IV) phenolato complexes for the use in cancer treatment.

1. Miller M; Tshuva E.Y.; Eur. J. Inorg. Chem. (2014) 9, 1485.

2. Miller M; Braitbard O.; Hochman J.; Tshuva E.Y.; J. Inorg. Biochem. (2016) 163, 250-257.

syn-(Me,Me)Bimane and its thionated analogs: synthesis and coordination chemistry

Partha Jyoti Das, Ankana Roy.

Department of Chemical Sciences, Ariel University, Ariel, Israel.

Corresponding authors. Dr. Michael Montag and Dr. Flavio Grynszpan.

syn-Bimanes (**1**) represent a class of fluorophores that have been widely used for labelling thiol bearing biomolecules due to their low toxicity, low molecular weight and high fluorescence. Recently we showed that the imide system present in *syn*-bimane can be used as a ligand in metal complexes. Thus, the first *syn*-bimane-Pd(II) complex (**2**) was prepared.

The strongly fluorescent *syn*-bimane chelates the Pd(II) center via its carbonyl oxygen atoms, affording a non-fluorescent complex. The X-ray structure of the complex shows that the coordinated bimane departs from planarity with its bicyclic framework bent about the N-N bond. Spectroscopic evidence demonstrates that bimane coordination is reversible in solution.

1. P.J. Das, Y. Diskin-Posner, M. Firer, M. Montag, F. Grynszpan, *Dalton Trans.* **2016**,

DOI: 10.1039/C6DT02141G.

2. M. J. Milewska, M. Gdaniec, T. Polonski, *J. Org. Chem.* **1997**, 62, 1860-1862.



Natural polymer Based Encapsulation Systems for Antimicrobial Agents Controlled Release

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A series of biodegradable active films based on various cellulose derivatives was prepared. Films were loaded with propionic acid (PA), a volatile antimicrobial agent used for grain storage. The effect of β -Cyclodextrin (β -CD) in the films' composition on the capacity and long term release of PA was studied. In addition, the influence of β -CD and PA on the biodegradable films' mechanical, physical and morphological properties was examined. It was found that by adding β -CD, the films' capacity was effectively enhanced up to a ten-fold. β -CD has also shown to yield a longer release of PA from the films, prolonging their applicative use. β -CD and PA were found to exert a synergistic effect on each other in the polymer matrix. The combination of the two allowed the formation of biodegradable active films that benefit good physical and mechanical properties as well as a high content and effective release of an antimicrobial component. This behavior was further investigated as the inclusion complex between the two was examined in a variety of spectroscopic, thermodynamic, crystallographic and computational methods. Despite being previously described in the literature as impossible to form, this inclusion complex, which embodies the system's core chemical feature, was found not only to form, but also to follow a previously unreported complexation mode.

Light-harvesting in molecular systems: the role of environment in optimizing the efficiency of energy transfer on the nano-scale

Zerah-Harush Elinor, Yonatan Dubi

Department of Chemistry and Ilse-Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

The striking efficiency of electronic energy transfer in natural photosynthetic systems and the recent evidence for long time quantum coherence in biological light harvesting complexes has triggered theoretical research aiming to resolve the underlying puzzles. The complexity of these systems is beyond the scope of reliable ab-initio calculations, and schematic models were suggested in order to support theoretical idea.

Our main concern is the effect of a molecular environment on the energy transfer efficiency. We propose to optimize the environment for complex chromophores networks, to compare computationally optimized structures to evolutionarily optimized ones in nature, and to propose criteria for educated design of artificial energy transfer molecular networks.



Adsorption of CO on thin layers of Pt on Sn

Itay Pitussi^a, Alex Schechter^a, Amir Natan^b and Haya Korenwitz^a

^a Department of Department of Chemical Sciences, Ariel University

^b Department of Physical Electronics, Tel-Aviv University

Fuel cells are electrochemical devices which convert chemical energy to electrical energy in a much more efficient and clean manner compared combustion engines. Typically, these devices utilize pure hydrogen and air that reacts on Pt based catalyst in the anode and the cathode respectively. Never the less the cost of Pt and its poisoning by CO in the ppm level in hydrogen prevents their commercialization market. Highly dispersed very thin layers of Pt on metallic Sn is being studied in our group. This approach may provide high utilization of Pt as well co-catalysis of adsorbed CO removal from Pt surface via a well-known Pt-Sn bi-functionality mechanism^{1,2}. PtSn alloys and their CO adsorption have been reported before. However, this research deals with tin coated by Pt and not with an alloy. The effect of various number of Pt(111) slabs on a well-defined core of Sn was studied. The effect of Pt layer number on the adsorption energy of CO was studied in comparison to the adsorption energy of CO over pure Pt.

The approach in this research was mainly computational. The calculations have been carried out using the Vienna Ab initio Simulation Program (VASP) using periodic boundaries, PAW PBE pseudopotentials and default cut off energies were used. According to the computational result, the coated Pt on a tin core changes the adsorption energy of CO on selected sites and geometrical configurations. Correlation between the number of Pt slabs and the adsorb CO adoption energy was found. Reducing the adsorption energy was demonstrated on a single atomic layer slab.

(1) Wang, K.; Gasteiger, H. a.; Markovic, N. M.; Ross, P. N. On the Reaction Pathway for Methanol and Carbon Monoxide Electrooxidation on Pt-Sn Alloy versus Pt-Ru Alloy Surfaces. *Electrochim. Acta* **1996**, *41* (16), 2587–2593.

(2) Mukerjee, S.; Urian, R. C. Bifunctionality in Pt Alloy Nanocluster Electrocatalysts for Enhanced Methanol Oxidation and CO Tolerance in PEM Fuel Cells: Electrochemical and in Situ Synchrotron Spectroscopy. *Electrochim. Acta* **2002**, *47* (19), 3219–3231.

Nanotubes Motion on Layered Materials: A Registry Perspective

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²The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv, IL 6997801

At dry and clean material junctions of rigid materials the corrugation of the energy landscape is dominated by variations of Pauli repulsions. These occur when electron clouds centered around atoms in adjacent layers overlap as they slide across each other. In such cases there exists a direct relation between interfacial surface (in)commensurability and superlubricity, a frictionless and wearless tribological state. The Registry Index is a purely geometrical parameter that quantifies the degree of interlayer commensurability, thus providing a simple and intuitive method for the prediction of sliding energy landscapes at rigid material interfaces. In the present study, the applicability of the Registry Index was extended to treat to non-parallel surfaces, using a model system of nanotubes motion on flat hexagonal materials. Our method successfully reproduces sliding energy landscapes of carbon nanotubes on Graphene calculated using a Lennard-Jones type and the Kolmogorov-Crespi interlayer potentials. Furthermore, it captures the sliding energy corrugation of a boron nitride nanotube on hexagonal boron nitride calculated using the *h*-BN ILP. Finally, we use the Registry Index to predict the sliding energy landscapes of the heterogeneous junctions of a carbon nanotubes on hexagonal boron nitride and of boron nitride nanotubes on graphene that are shown to exhibit a significantly reduced corrugation. For such rigid interfaces this is expected to be manifested by superlubric motion.

Finding Force-Laws and Emergent many-body interactions in Amorphous Solids

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Given an athermal and amorphous packing of particles (e.g. athermal glasses and colloids), force-balance equations are insufficient for directly determining the inter-particle forces, posing a difficulty for studying phenomena such as force chains and instabilities. We propose a solution of this long-standing problem by expanding the inter-particle normal force-law in a Laurent-Taylor series of the inter-particle distances. A visual providing the particle positions in addition to a measurement of the pressure is all that is required¹. The method is shown to accurately recover the force-law in simulation. When applied to thermal systems using the mean positions, this method can predict an effective force-law². This will allow us to analyze thermal systems using tools hitherto reserved for athermal ones (e.g. stability via Hessian eigenvalues).

I will also discuss my recent and still ongoing work where, quite remarkably, we see the emergence of many-body interactions in the effective force-law, even when the bare forces are purely 2-body.

Towards Artificial DNA Molecular Motors That Can Walk Over Micrometers

Miran Liber, Toma E. Tomov, Roman Tsukanov, Yaron Berger, and Eyal Nir*

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The manufacturing of high-performance well-functioning machines is a major challenge for the scientific community. DNA nanotechnology holds a very promising path towards the realization of this goal on the molecular level by mimicking biological machines such as Kinesin and Myosin. It's been demonstrated that DNA based devices and motors operating upon DNA Origami based tracks could potentially be used in a variety of applications and nano assembly lines. However, these motors and devices are only limited by the length of the track, which is, so far, embedded on a single origami platform. This dictates the size of the devices and their operational length to be several hundred nanometers. For the purpose of exceeding the size boundaries of a single origami unit, in order to induce large scale maneuvering of molecular motors, a larger track must be created. This can be done by increasing the size of the origami through biological means (i.e. creating larger ssDNA scaffold) or by binding together several origami units. The latter is preferable due to the easier nature of connecting origami units together and the increased flexibility and functionality given to the superstructure when connecting different-properties origami units.

We previously demonstrated the successful operation of a dynamic DNA device constructed from two different DNA origami building blocks combined with a DNA bipedal walker. The two different origami units were linked together in high yield to form a long range track using a binding approach in which the bridging strands hybridize to the scaffold of the adjacent origami unit (Weaving-Welding). In order to elongate the superstructure by linking many different units and operate the device at different condition, a stable and strong connection must hold the units together. Using Single Molecule Fluorescence (SMF) techniques we investigated the stability of the connection and the kinetics of the assembly and disassembly reactions of the two main binding approaches: (i) Weaving-Welding and (ii) Sticky Ends (in which binding occurs through external overhangs with sticky ends interactions)

Our work present the most comprehensive study about the conditions necessary for the stability of the connections between origami units and the kinetics of the assembly and disassembly reaction of the dimer origami structure. This is a major step towards the realization of large scale superstructures made of many origami units.

[1] Liber, et al. A Bipedal DNA Motor that Travels Back and Forth between Two DNA Origami Tiles *Small* 11 (2015): 568-575.

Multiple conformational states of a unique extracellular arabinanase suggest a "harpoon" mechanism of action

Shifra Lansky¹, Rachel Salama², Omer Shwartzhtien¹, Dina Schneidman³, Yuval Shoham² and Gil Shoham¹

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α -L-arabinanases are key bacterial enzymes in the breakdown of arabinan, one of the main polysaccharides constituting the plant cell-wall. Such enzymes present a wide range of important potential biotechnological applications, e.g. conversion of plant organic waste into bio-ethanol. **GsAbn43A** is an extracellular α -L-arabinanase from the thermophilic bacterium *Geobacillus stearothermophilus*-T6 that belongs to the GH43 family, containing 848 amino-acid residues and possessing low sequence identity to related arabinanases. The 3D structure of GsAbn43A has recently been determined by X-ray crystallography, revealing a unique and novel multi-domain architecture, the largest structure reported so far in the GH43 family. The enzyme is built of four different domains, arranged in a pincer-like structure. The catalytic domain (in red; left figure) corresponds to the typical five-bladed b-propeller fold commonly observed in GH43 enzymes. The second domain (green) has also been reported before in some homologous two-domain arabinanases, but the third (blue) and fourth (orange) domains are unique to GsAbn43A and present new protein folds. Three different crystallographic conformational states have been determined for the enzyme, two "closed" states and one "open" state, differentiated by approximately 13 Å movement in the relative location of the fourth domain. Normal mode analysis (NMA), small angle X-ray scattering (SAXS) and dynamic light scattering (DLS) experiments suggest additional conformational changes for GsAbn43A, involving up to 100 Å movement in the positions of the third and fourth domains (right figure). Substrate-binding structural experiments demonstrate, surprisingly, that an arabino-pentaose substrate binds to a dedicated site in the fourth domain in addition to the catalytic domain (left figure). These findings, together with complementary ITC, mutagenesis and kinetics experiments, suggest a novel "harpoon-like" catalytic mechanism for the arabinan degradation action of GsAbn43A.

Avilamycin Induces Structural Changes In rProteins uL16 And CTC That Enhance The Inhibition Of A-Site tRNA Binding

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Albeit many battles have been won in the war on nosocomial pathogens with the discovery of antibiotics, emergence of multi-drug-resistant (MDR) pathogenic strains of Enterococci, Staphylococci and Streptococci gram positive bacteria pose a serious threat on modern medicine .

The ribosomal antibiotic avilamycin possess inhibitory activity against these gram positive bacteria .

We have determined the crystal structures of avilamycin free and in complex with the eubacterial large ribosomal subunit, shedding light on their binding, inhibition, selectivity and resistance modes. These structures reveal novel binding site and mechanism for the orthosomycin family antibiotics, not shared with other antibiotics from other families .

This antibiotic family is extensively metabolized in vivo, thus reducing their ecological toxicity, and placing them at the frontline of drugs with reduced environmental footprint .

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The Development of Multiple Sclerosis from a Biophysical Perspective

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The myelin sheath, a repeating multilamellar stack of lipid-protein complex, acts as an electrical insulator, forming a capacitor surrounding the axon of the nervous system. The lipid and protein ratios found *in-vivo* are assumed to play a critical role in determining the structure of the myelin layers. In neurodegenerative diseases, such as multiple sclerosis (MS), demyelination is attributed to alterations in lipid composition and to decreased concentration of myelin basic protein (MBP), the key protein in myelin sheaths. Using synchrotron small X-ray scattering and direct cryogenic transmission electron microscopy we performed *in-vitro* structural measurements in model systems mimicking cytoplasmic myelin sheath complexes. Modifications in lipids composition, as in the MS diseased state, result with structural instabilities and pathological phase transition from lamellar to inverted hexagonal phase that involve enhanced local curvature. Similar enhanced local curvatures are also found in diseased *in-vivo* myelin sheaths¹. Since the etiology and recovery pathways of MS are currently unclear, these findings delineate novel functional roles to dominant constituents in cytoplasmic myelin sheaths, shed new light on mechanisms disrupting lipid-protein complexes, and suggest new courses for diagnosis and treatment for MS, a disease that more than 2.5 million worldwide are suffering from.

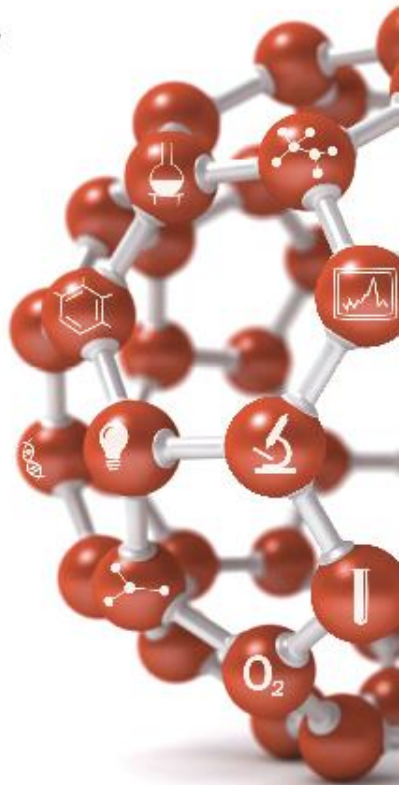
(1) *J. Am. Chem. Soc.* **2016**, *138* (37), 12159–12165.



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Poster session

1

Catalytic Decomposition of Hazardous Organophosphate Agents

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Organophosphates are organic esters of phosphoric acid, which are widely used for various industrial and household applications, e.g., as pesticides, plasticizers, flame retardants and solvents. Some organophosphates are also employed as chemical warfare agents. Those compounds that are utilized as pesticides or warfare agents are highly toxic, and may also be environmentally persistent. Their toxicity stems from potent inhibition of the enzyme acetylcholinesterase, which is crucial for the regulation of neural activity.

The adverse effects of organophosphate toxins on human health and the environment necessitate efficient decontamination strategies. This may be carried out by physical means (e.g., adsorption, flushing) or by chemical decomposition to more benign products. The latter is often done by hydrolysis, either stoichiometrically (e.g., alkaline solutions) or catalytically (e.g., enzymes, transition metal complexes). Contemporary examples of inorganic catalysts for organophosphate hydrolysis include polyoxoniobates, zirconium-based metal-organic frameworks, and zinc-based complexes.

We have recently begun efforts to develop new metal-complex-based catalysts for the decomposition of organophosphates, focusing on hydrolytic cleavage of P-O bonds. A combinatorial approach has been chosen for catalyst identification, based on a library of phage-displayed peptides that will be scanned for hydrolytic activity in the presence of various transition metal cations. Catalyst screening and isolation will be aided by activity-based probes (e.g., fluorescent tags), which are currently being designed and synthesized. Herein, we shall outline our general strategy for catalyst development, including some preliminary results pertaining to the synthesis of organophosphate toxin surrogates.

2

Synthesis of Core-Shell MoS₂ Fullerene-Like Incorporating Gold Nanoparticle Au@IF-MoS₂

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Nanoparticles and more specifically gold nanoparticles (AuNPs) attracted a great scientific and technological interest in the last few decades. Their popularity is attributed to their unique optical, electrical and magnetic properties when compared to the bulk. However, one of the main problems of AuNPs is their long-term stability. On the other hand, MoS₂ nanoparticles (NPs) and single layers show great chemical stability, and exhibit excellent mechanical and tribological properties as well as being biologically benign. Moreover, it is known that MoS₂ can form conformal coating on topologically complex surfaces. Finally, due to the MoS₂ NP unique optical properties, a hybrid AuNP core and MoS₂ shell would be a unique, stable and interesting hybrid nanomaterial. In this work we present a synthesis of AuNPs coated by MoS₂ single-layer. i.e. a core-shell nanostructure (Au@MoS₂).



Poster session

3 Allosteric conformational and topology changes in the *E. coli* membrane fusion CusB dimer

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Bacterial cells have developed sophisticated systems to deal with the toxicity of metal ions. The *E. coli* CusCFBA is a complex efflux system, located in the periplasm, involving four proteins: CusA, CusB, CusC, and CusF which is responsible for transferring Cu(I) and Ag(I) ions. The CusA, CusB and CusC are connected together in an oligomerization ratio of 3:6:3 CusA:CusB:CusC to form the CusCBA periplasm membrane transporter. CusB is an adaptor protein which connects the two membrane proteins CusA (inner membrane) and CusC (outer membrane). The CusF is a metallochaperone who transfers Cu(I) and Ag(I) to the CusCBA transporter from the periplasm. The crystal structures of CusB, CusC, CusF, and CusBA complex have been resolved, shedding some light on the efflux mechanism of this intriguing system. However, since CusB is an adaptor protein, its role in operating this system is significant, and should be understood in detail. Here, we utilize EPR spectroscopy to target the conformational changes of the full CusB protein upon binding Cu(I). We reveal that CusB is a dimer in solution, where the orientation of one molecule with respect to the other molecule is varies up on Cu(I) coordination, resulting in a more compact CusB structure. These structural and topology changes upon Cu(I) binding probably play the role of a switch for opening the channel and transferring metal ions from CusB to CusC and out of the cell.

4 Insight into the self-assembly of α -synuclein oligomers in Parkinson's disease

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α -Synuclein (AS) oligomers are toxic aggregate species and the major hallmarks of Parkinson's disease (PD). It is known that the central domain of the 140-residue AS protein (residues 61-95), known as the non-amyloid- β component (NAC), plays a crucial role in aggregation. The structure of the self-assembled NAC oligomers has been solved for the first time in our group.¹ A recent solid-state nuclear magnetic resonance (ssNMR) study has solved the self-assembly of AS(1-140),² and suggested that the N-termini and the C-termini of the self-assembled AS(1-140) are disordered domains. Our work presents a first study that shows that extensions of the NAC (residues 61-95) oligomers in the N-termini to residues 30-95 provide polymorphic well-organized self-assembled AS(30-95) oligomers. However, in the full-length self-assembled AS(1-140) only one state is preferred. Solving the structure of the self-assembly of AS oligomers provides a basis for understanding the structural difference and improving our knowledge on the mechanistic processes of the self-assembly AS in PD. Furthermore, our work may assist for developing imaging agents and drug candidates for the treatment of PD.

Atsmon-Raz Y. & Miller Y. J. Phys. Chem. B. **2015**, 119, 10005-10015.
Tuttle M.D. et al, Nature Structural & Molecular Biology **2016**, 23,409-415



5

Conformational Dynamics of the Carbohydrate-Binding Protein in the GanPST Bacterial Three-Component Sensing System

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Two-component sensing systems (TCSs) are crucial for bacteria to adapt to changes in their environment, regulated mainly *via* conjugation between an external stimulus and a cellular response. These systems usually consist of two proteins, typically a transmembrane histidine kinase (HK) that autophosphorylates upon receiving an extracellular input, and a response regulator (RR) that receives the phosphoryl group from the HK and leads to the appropriate cellular response. Recently, the existence of similar three-component sensing systems have been reported. These unique systems contain in addition a substrate-binding protein (SBP) that binds the signal molecule and interacts with the HK to initiate its autophosphorylation. GanP is the SBP of the newly discovered GanPST three-component system of the thermophilic bacterium *Geobacillus stearothermophilus*, putatively responsible for the binding of extracellular galactose and activation of the galactan utilization system of the bacterium. In order to study the structural basis of the GanP function, its 3D structure in complex with galactose has been recently determined by X-ray crystallography at 1.8 Å resolution. The GanP structure reveals the presence of two distinct domains (marked in blue and green in the figure below), connected by a three-stranded hinge, with a galactose molecule trapped in the interdomain interface (yellow). This atomic-resolution structure enables identification of the residues involved in the specific binding of galactose. The tight binding of galactose between the two domains raises the possibility of domain conformational changes upon ligand binding. Small-angle X-ray scattering (SAXS) measurements on GanP, conducted in the presence and absence of galactose, validate these global conformational changes, which are further supported by independent theoretical simulations.

6

Nickel Complexes as Potential Catalysts for Urea Conversion

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In order to meet the growing global demands for energy in the age of environmental awareness, alternative clean energy sources must be explored. Hydrogen gas is such a source of energy, with water being the only byproduct in its energy conversion process. Urea electrolysis is a promising new technology that has the capacity to produce high-purity hydrogen from sustainable sources, such as wastewater. Urea is a highly attractive hydrogen carrier, because it is abundant, stable, non-toxic and non-flammable, and can be stored and transported conveniently, since it is solid under ambient conditions.

Nickel metal and nickel oxides have been studied extensively as electrocatalysts for urea conversion, providing relatively high current densities and low overpotentials of oxidation to CO₂ and N₂. Moreover, nickel is intimately involved in urea hydrolysis within the active site of the enzyme urease, and this has inspired chemists to mimic the naturally-occurring bimetallic core of this enzyme. Simplified synthetic bimetallic model systems have been studied as part of the effort to probe the enzymatic mechanism, as well as examine other reactivity patterns.

To the best of our knowledge, no molecular nickel-based system has thus far been reported to promote the electrochemical conversion of urea. Herein, we present the synthesis and characterization of nickel complexes of phenol-based binucleating ligands. These are intended to mimic the active nickel-oxide surfaces previously shown to promote urea conversion, with the aim of developing catalysts for urea electrooxidation.



7

Quantum-trajectory Monte Carlo method for study of electron–crystal interaction in STEM

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A novel quantum-trajectory Monte Carlo simulation method is developed to study electron beam interaction with a crystalline solid for application to electron microscopy and spectroscopy. The method combines the Bohmian quantum trajectory method, which treats electron elastic scattering and diffraction in a crystal, with a Monte Carlo sampling of electron inelastic scattering events along quantum trajectory paths. We study in this work the electron scattering and secondary electron generation process in crystals for a focused incident electron beam, leading to understanding of the imaging mechanism behind the atomic resolution secondary electron image that has been recently achieved in experiment with a scanning transmission electron microscope. According to this method, the Bohmian quantum trajectories have been calculated at first through a wave function obtained via a numerical solution of the time-dependent Schrödinger equation with a multislice method. The impact parameter-dependent inner-shell excitation cross section then enables the Monte Carlo sampling of ionization events produced by incident electron trajectories travelling along atom columns for excitation of high energy knock-on secondary electrons. Following cascade production, transportation and emission processes of true secondary electrons of very low energies are traced by a conventional Monte Carlo simulation method to present image signals. Comparison of the simulated image for a Si(110) crystal with the experimental image indicates that the dominant mechanism of atomic resolution of secondary electron image is the inner-shell ionization events generated by a high-energy electron beam.

8

Specificity-determining DNA triplet code for positioning of human pre-initiation complex

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The notion that transcription factors bind DNA only through specific, consensus binding sites has been recently questioned. In a pioneering study by Pugh and Venter no specific consensus motif for the positioning of the human pre-initiation complex (PIC) has been identified. Here, we reveal that nonconsensus, statistical, DNA triplet code provides specificity for the positioning of the human PIC. In particular, we reveal a highly non-random, statistical pattern of repetitive nucleotide triplets that correlates with the genome-wide binding preferences of PIC measured by Chip-exo. We analyze the triplet enrichment and depletion near the transcription start site (TSS) and identify triplets that have the strongest effect on PIC-DNA nonconsensus binding. Our results constitute a proof-of-concept for a new design principle for protein-DNA recognition in the human genome, which can lead to a better mechanistic understanding of transcriptional regulation.

9 Polyoxometalates entrapped in sol-gel matrices for reducing electron exchange column applications

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Electron exchange columns are analogous to ion exchange columns and comprise entrapment of a strong redox reagent that performs oxidation/reduction cycles with the substrate passing through the columns. Such columns are reversible in nature and are more advantageous as the entrapped redox reagent do not contaminate the products. The electron exchange columns reported so far were designed for oxidation processes and have significant drawbacks, such as relatively small redox reagents that result in leaching, and some organic ligands are more procumbent to redox sensitivity and decomposed with time.¹⁻² Therefore to overcome these drawbacks, a redox active polyoxometalate was entrapped in silica sol-gel matrices for electron exchange column applications. Polyoxometalates (POMs) are the most suitable candidates for this purpose having the ability to accept/release several electrons without decomposing and changing their structure and moreover are expected to have stability for many redox cycles.³ The properties of the columns strongly depend on the composition of the precursors used to prepare the matrices.⁴ The columns exhibit good reversibility and are

The first reducing electron exchange columns ever prepared.

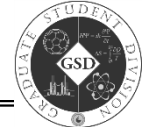
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10 Challenges in engineering phosphotriesterase from *Brevundimonas diminuta*

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Owing to the low catalytic efficiency (k_{cat}/K_M) for hydrolysis of organophosphate (OP) compounds, butyrylcholinesterase (BuChE) needs to be administered in stoichiometric amounts to detoxify OPs. Hence, evolving an enzyme capable of hydrolyzing OPs efficiently with $k_{cat}/K_M \sim 5 \cdot 10^7 \text{ M}^{-1}\text{min}^{-1}$ still remains a major challenge to the protein engineers and crystallographers. Recently, Cherny *et al.*, 2013 (1) reported directed evolution of phosphotriesterase (PTE) from *Brevundimonas diminuta* to detoxify VX (nerve agent) with k_{cat}/K_M to $5 \cdot 10^6 \text{ M}^{-1}\text{min}^{-1}$. Current study addresses various challenges that were overcome to improve k_{cat}/K_M of PTE $\sim 5 \cdot 10^7 \text{ M}^{-1}\text{min}^{-1}$ (2, 3). The results will be presented. The improved variant(s) with $k_{cat}/K_M \sim 5 \cdot 10^7 \text{ M}^{-1}\text{min}^{-1}$ are proposed to be used in animal models for *in vivo* detoxification of OPs.

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2. Goldsmith *et al.*, unpublished.
3. Dym *et al.*, unpublished.



11

Host:Guest complexes as 19F-CEST MRI Biosensors

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In recent years, water-soluble supramolecular systems are gaining interest due to their potential applicability in biological and biomedical research. The goal of this study to design, develop and implement an imaging platform in which host-guest molecular interactions are exploited to generate 19F-MRI signal from low concentration targets. Here we propose to use fluorinated guests as the imaging tracers that bind to water-soluble molecular cages (hosts). In the formed supramolecular complexes the bounded 19F-guest "pool" differs in its chemical environment than the "free" 19F-agent "pool" in the aqueous solution. Therefore, the two pools obtained for 19F-molecules (free vs. bound) should have, upon slow exchange process, different chemical shift ($\Delta\omega$) in 19F-NMR spectrum. Capitalizing on this phenomenon, the 19F-MRI signal will be manipulated for molecular and cellular imaging purposes.

12

Interlayer Potential for Graphene/*h*-BN Heterostructures

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The two dimensional heterostructure formed of graphene and hexagonal boron nitride (*h*-BN) exhibits rich physical properties and plays a central role in the field of nanotribology. In this study, a new interlayer force-field for layered graphene and *h*-BN based structures is presented. The force-field contains two terms representing the interlayer attraction due to dispersive interactions, and repulsion due to anisotropic overlaps of electron clouds. With appropriate parameterization against reference binding and sliding energy profiles obtained from density functional theory using a screened exchange hybrid functional augmented by a many-body dispersion treatment of long-range correlation, the potential is able to simultaneously capture well the binding and lateral sliding energies of planar *h*-BN and graphene based dimer systems. Furthermore, the transferability of the potential to multi-layered systems is demonstrated by considering the binding energy of bulk graphene/*h*-BN alternating stacks. The new developed force field thus enables the accurate and efficient modeling of the structural, mechanical, tribological, and dynamic properties of layered heterostructures based on graphene and *h*-BN.



13 Colloidal PbS Quantum Dot- AlPO_4 Nanoporous Glass Composites: Controllable Emission and Nonlinear Absorption

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In recent years, near-infrared (NIR) materials beyond the visible region (700–2500 nm) has emerged as a promising research field with applications toward telecommunications, photovoltaic, in-vivo imaging, etc. Such technologies will benefit greatly from the advantageous properties of NIR materials including broadband tunable emission, nonlinear optical properties, photostability, and simple chemical processing. Here, we report a facile approach to fabricate high stable and controllable luminescent NIR-emitting composites by confining PbS colloidal quantum dots (CQDs) in sol-gel nanoporous AlPO_4 glasses. The transmission electron microscopy images combined with X-ray photoelectron spectra in different depth of PbS- AlPO_4 composites (PACs) reveal the successful solidification of CQDs in nanoporous structure of glasses. The tunable and controllable luminescence of PACs is dependent on the size of PbS CQDs in solution and glass pore size. We show that the broadband (270 nm) and bimodal emission of PACs are tailored by designing different composited strategies on the incorporation of colloidal quantum dots in AlPO_4 nanoporous glasses. Ultrafast nonlinear optical properties of PACs were investigated using an open-aperture Z-scan technique with 515 nm 340 fs pulses. The PACs exhibited obvious reverse saturable absorption in our experiments, with a nonlinear absorption coefficient of 7.17×10^{-2} cm/GW. Furthermore, the stability of PACs is investigated by emission spectra from a few hours to 180 days. The results imply PACs has a better stability than other regular PbS-solid materials such as PbS- Al_2O_3 films and close-packed PbS-filter paper systems.

14 Structural insights into *Staphylococcus aureus* ribosome in complex with antibiotics, mRNA and tRNAs

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The ribosome translates the genetic code into proteins in all living cells. As the ribosomes are essential for cell life, inhibiting their function will damage cell's viability. In fact, about 40% of the antibiotics in clinical use target functional centers in the ribosome. With the increased use of antibiotics to treat bacterial infections, pathogenic strains have accumulated antibiotic resistance that is a major clinical threat.

Here we present the crystal structures of the large ribosomal subunit of *Staphylococcus aureus*, a Gram-positive versatile and aggressive pathogen, alongside its complex with a new potential high potency pleuromutilin derivative, called BC-3205 [1].

By analyzing these crystal structures we identified some internal and peripheral unique structural motifs that may be potential candidates for improving known antibiotics and for the design of selective antibiotic drugs against *Staphylococcus aureus*.

We also present here our single-particle cryo-electron microscopy studies on the structure of the entire 70S ribosome complex with two tRNA molecules, mRNA chain and two antibiotics drugs that bind the small ribosomal subunit in two distinct functional sites.

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15 Tuning the Catalytic Properties of Ternary Nano-Flowers of Layered Materials

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Tuning the properties of layered materials by modifying their chemical composition and electronic structure is important for nanoelectronic and optoelectronic device applications. Alloy of 2D layered materials by metal or nonmetal atom substitution is an effective way to tune bandgap and composition. Nanostructured MoS_2 and MoSe_2 were promising electrode materials for electrochemical hydrogen evolution reaction (HER) and Li-ion batteries. Here by employing the colloidal synthetic route, we obtained ternary $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ and $\text{Mo}(\text{S}_x\text{Se}_{1-x})_2$ alloy nanoflowers with different W concentration. The structure, composition and electrocatalytic HER activity of ternary nano-flowers were examined. X-ray diffraction (XRD) pattern revealed that the ternary $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ and $\text{Mo}(\text{S}_x\text{Se}_{1-x})_2$ alloy nanoflowers crystallized into 2H-hexagonal crystal structure. Flower-like structure in $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ and $\text{Mo}(\text{S}_x\text{Se}_{1-x})_2$ alloy was retained for different composition and the sizes were spanning in the range 300-500 nm. The $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ and $\text{Mo}(\text{S}_x\text{Se}_{1-x})_2$ alloy nanoflowers shows tunable electrocatalytic HER activity with composition. The electrochemical over potential and Tafel slope are increased with increasing x in $\text{Mo}(\text{S}_x\text{Se}_{1-x})_2$ nanoflowers. MoS_2 nanoflower for x=0 shows an over potential of 270 mV and Tafel slope of 32 mV/dec and these values reaches to 420mV and 46 mV/dec for MoSe_2 flower of x=1. $\text{Mo}_{1-x}\text{W}_x\text{Se}_2$ nanoflowers shows optimal minimum over potential of 320 mV and maximum Tafel slope of 56 mV/dec for x=0.5.

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