



## 3<sup>nd</sup> Solar Fuels I-CORE Workshop

September 12th-15th, 2016 \* Nahsholim, Israel

## **ABSTRACTS**

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Day 1 – Monday, September 12<sup>th</sup> 2016

**Opening Session** 

## The Road Ahead for Solar and Bioenergy Technologies

## **Martin Keller**

National Renewable Energy Laboratory

Every day, we face fluctuating oil and gasoline prices. We hear reports on the rising level of carbon dioxide in the atmosphere and its impact on the climate. And we see a growing world population with increasing needs for energy. Solar and bioenergy technologies are at the forefront of renewable, sustainable energy options that are meeting these needs now. Although renewable technologies have gained much greater levels of cost parity with fossil energy sources, continued innovation is necessary to meet global de-carbonization targets.

Solar electricity can be generated by photovoltaic technologies. Scientific advances in this area continue to squeeze more power from the solar modules, but are also boosting efficiencies, reducing costs, and improving reliability of other photovoltaic devices such as thin films, multijunctions, and emerging technologies. In the area of solar fuels, research targets semiconductor devices that can efficiently and economically split water to produce hydrogen as an energy carrier.

Bioenergy technologies include biological and chemical approaches to create solid, liquid, and gaseous fuels for electricity, transportation, and chemicals for industrial uses. Solid biomass can be combusted directly for heat and power. Various energy crops are used to produce a range of fuels.

Significant new innovation in both solar and bioenergy area are pushing the boundaries for the science and deployment of renewables. This presentation will feature the latest scientific accomplishments and discuss the global imperative of continued investment in clean energy research.

## Sugar synthesis from CO<sub>2</sub> in E. coli

## Ron Milo

### Department and Plant & Environmental Sciences, Weizmann Institute, Israel

Can a heterotrophic organism be evolved to synthesize biomass directly from CO<sub>2</sub>? So far, non-native carbon fixation where biomass precursors are synthesized solely from CO<sub>2</sub> has remained an elusive grand challenge. In this talk, I demonstrate how a combination of rational metabolic rewiring, recombinant expression and laboratory evolution has led to the biosynthesis of sugars and other major biomass constituents, by a fully functional Calvin-Benson-Bassham cycle in E. coli.

Day 2 – Tuesday, September 13<sup>th</sup>, 2016

**Morning Session** 

## **Overcoming recalcitrance in BESC; how far have we come?**

Paul Gilna BioEnergy Science Center, Oak Ridge National Laboratory Oak Ridge, Tennessee, USA

The challenge of producing and converting sustainable cellulosic biomass into fuels presents the opportunity for science and technology to make an appreciable national and indeed global impact in the next 20 years. However, overcoming the inability to easily access the sugars and other monomers in order to make fuels or other products, that is, recalcitrance of biomass to conversion is one of the major challenges to cost-effective biofuel production. This has been a central theme of the BioEnergy Science Center (BESC, www.bioenergycenter.org). Transformative advances to understand biomass recalcitrance require detailed scientific knowledge of (1) the chemical and physical properties of biomass that influence recalcitrance, (2) how these properties can be altered by engineering plant biosynthetic pathways, and (3) how such changes affect biomass-biocatalyst interactions during deconstruction by enzymes and microorganisms. This talk will illustrate how the BESC Team has applied the knowledge gained from these activities to develop a set of approaches and outcome on both the plant and microbial components to improve generation of fuels from biomass resources.

## Implementation of metabolomics in biofuel research

## <u>Sergey Malitsky</u>, Carmit Ziv, Shuning Zheng, Assaf Vardi and Asaph Aharoni

Department of Plant and Environmental Sciences, The Weizmann Institute of Science, Rehovot, Israel

Metabolomics (the comprehensive, non-biased, qualitative and quantitative study of all the small molecules in an organism) as well as its branching approach lipidomics have emerged as a functional genomics methodology that contributes to our understanding of the complex molecular interactions in biological systems. As such, metabolomics represents the logical progression from large-scale analysis of RNA and proteins at the systems level. We present analytical approaches which were set up in our laboratory and can be extremely useful in biofuel research. Additionally we present LC/MS-based lipidomics which was applied to explore the modulation of lipids during interaction in this unique host-pathogen system. We show that lytic viral infection leads to massive remodeling of the cellular lipidome, predominantly inducing the biosynthesis of viral specific glycosphingolipids as well as the accumulation of highly saturated neutral lipids.

## Utilizing Metabolic Engineering in Plants to Enhance Pathways for Biosynthesis of Higher Alcohols as Potential Biofules

Moran Oliva<sup>1,2</sup>, Michal Oren-Shamir<sup>2</sup>, Avichai Perl<sup>2</sup>, Asaph Aharoni<sup>1</sup>, Ephraim Lewinsohn<sup>2</sup> and Gad Galili<sup>1</sup>.

<sup>1</sup>Departiment of Plant Science, The Weizmann institute of science, Israel

### <sup>2</sup>Agricultural Research Organization, Israel

Aromatic amino acids (AAA) are important precursors for multiple specialized metabolites of plants, including aromatic volatiles. Some aromatic volatiles, such as 2-phenylethanol (2-PE), are classified as higher alcohols, which have advantages over traditional biofuels. Though 2-PE has a new potential usage, in addition to its aroma character, it is not produced in plants in high enough yields to be considered a gasoline substitute. Our laboratory is testing the potential to improve higher alcohol as 2-PE production in plants by metabolic engineering. Our goals are: (a) to elucidate metabolic bottlenecks in the shikimate pathway, which converts primary metabolism into AAAs; (b) to enhance fluxes towards aromatic higher alcohols in plants.

We use a transgenic approach in the model plants petunia and tomato that naturally produce 2-PE. Feedback insensitive forms of bacterial enzymes of the shikimate pathway were separately expressed in the plants: (i) PheA\*, a chorismate mutase/prephenate dehydratase enzyme; (ii) AroG\*, a DAHPS enzyme, encoding for the first enzyme of the shikimate pathway. Transgenic petunia flowers and tomato fruits expressing either AroG\* or PheA\* showed increased accumulation of phenylalanine and various derived secondary metabolites. 2-PE levels were increased in up to 10 fold, suggesting that our approach improving the production of biofuel volatiles in plants.

## Theoretical Modeling of the Metal/Oxide Interface

## **Maytal Caspary Toroker**

### Department of Materials Science and Engineering, Technion – Israel Institute of Technology

Metal/metal-oxide interfaces appear in a wide variety of disciplines including electronics, corrosion, electrochemistry, and catalysis. Specifically, covering a metaloxide with a metal is often thought to enhance solar energy absorption and to improve photocatalytic activity. For example, the platinum/hematite ( $Pt/\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) interface has demonstrated improved functionality. In order to advance our understanding of how metal coverage over an oxide helps performance, we characterize the geometry and electronic structure of the  $Pt/\alpha$ -Fe<sub>2</sub>O<sub>3</sub> interface. We investigate the interface using density functional theory +U, and find a stable crystallographic orientation relationship that agrees with experiment. Furthermore, there are significant changes in the electronic structure of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> as a result of Pt coverage. We therefore suggest the concept of "judging" the electronic properties of an oxide only with its cover. Specifically, covering Fe<sub>2</sub>O<sub>3</sub> with Pt reduces carrier effective mass and creates a continuum of states in the band gap. The former could be beneficial for catalytic activity, while the latter may cause surface recombination. In order to circumvent this problem, we suggest putting metal coverage behind the oxide and far from the electrolyte in a photoelectrochemical device in order to quickly collect electron carriers and avoid recombination with vulnerable holes accumulating as a result of catalysis at the surface.

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## Using First-Principles Calculations to Design Efficient Catalysts for Solar Water Splitting: Metallic Doping of NiOOH Material

## Jeremie Zaffran and Maytal Caspary Toroker

### **Technion – Israel Institute of Technology**

Solar energy is one important challenge of the current century. However, energy storage remains a considerable issue. Photoelectrochemical cells are devices aiming to convert solar energy into hydrogen fuel by water splitting. The process requires solid catalysts, often based on noble metals. We propose here to study an earth-abundant element based material already known for its outstanding catalytic activity, nickel oxyhydroxide (NiOOH).

NiOOH properties are strongly dependent on doping, generally involving metallic elements. To this date, only Fe presents a significant interest, attested by several experimental studies. Using computational methods, and especially the density functional theory (DFT), we performed a complete scan of the first row of the transition metal (TM) block of the periodic table. We concluded that only middle and late TM may be relevant for NiOOH doping, whereas early TM have globally an inhibiting effect on the reaction. Moreover, we were able to correlate the reactivity of such elements to specific bulk properties of NiOOH material. We demonstrate in particular that high metal-oxygen bond ionicity is not suitable for efficient catalysts in water splitting process.

This theoretical work provides new insights in surface reactivity and hydrogen production. It also expects to give some guidelines to experimentalists and industrials to elaborate new materials for photoelectrochemical cells.

## **Modeling Hematite Water Splitting with Theoretical Methods**

## Natav Yatom and Maytal Caspary Toroker

### Department of Materials Science and Engineering, Technion – Israel Institute of Technology

World increasing energy demand calls for a renewable energy technology to replace the 80% fossil fuels portion of the total consumption. The PEC (photo-electrochemical cells) is a promising technology for this task. It can convert sunlight, our most abundant energy resource, into hydrogen fuel gas by splitting water. In the search for a photo-anode materials that provide a low price, efficient, and stable system, hematite ( $\alpha$  -Fe<sub>2</sub>O<sub>3</sub>) was found to be a leading candidate. Many components of the photo-catalytic mechanism of hematite operation are still not fully understood. Better understanding can be achieved by a first principle study, especially with DFT (density functional theory) that is appropriate for the solid state. In this work we aim to gain insights on the mechanisms dominating the overall efficiency of pure and doped hematite, and use our understanding to promote the PEC technology. For this goal we choose the Nb-doped hematite system because it was widely experimentally researched. We use DFT based calculation to investigate the electronic structure of the bulk and different surfaces of pure hematite, Nb-doped hematite, and the alloyed FeNbO4 which appears above ~2at.%Nb concentration.

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2. N. Yatom and M. Caspary Toroker, "Hazardous doping for photo-electrochemical conversion: The case of Nb-doped Fe2O3 from first principles", Molecules 20 (11) 19900 (2015).

3. N. Yatom and M. Caspary Toroker, "Manipulating electrochemical performance through doping beyond the solubility limit", Phys. Chem. Chem. Phys. 18, 16098 (2016).

## Photosynthetic efficiency Insights from whole organism studies

## Avihai Danon

#### Department of Plant & Environmental Sciences, Weizmann Institute of Science

The efficiency with which plants capture sunlight and convert it to biomass has been the target of intensive research over the years. Notably, the near optimal short term efficiency of isolated photosynthetic reactions in test tube-reactions stands in contrast to the accumulated biomass of crop plants in agricultural fields. It is typically reasoned that the low photosynthetic efficiencies of plants in agricultural fields are either an inadvertent inherent fault of the photosynthesis itself or inflicted by environmental stresses. We have been studying regulatory mechanisms that participate in the attenuation of photosynthesis in planta. We show that the attenuating mechanisms are highly dynamic, continuously responding to environmental changes throughout the day. Intriguingly, we found evidence for the function of these mechanisms in response to very small environmental changes, suggesting that these mechanisms overreact and decrease photosynthetic efficiency also under optimal growth conditions. In the presentation, I will discuss the latest findings of our Lab in which we examined the effect of a genetic manipulation of the attenuating photosynthetic mechanisms on the photosynthetic productivity of plants in controlled growth chamber and in the green house.

## Fast disulfide-based control of photosynthesis

## Bat Chen Wolf- Ratzkowski and Avihai Danon

### Department of Plant and Environmental Sciences, Weizmann Institute of Science

The diurnal night to day shift represent a major challenge for photosynthetic organisms. During that time period the chloroplast metabolism switches from heterotrophic to photoautotrophic metabolism and a critical discrepancy between the photosynthetic electron flow produced by the light capturing reactions and the rate of stromal reactions consuming the photosynthetic reducing equivalents could arise even under low light intensity. Thus, to avoid photodamage a tight regulation of the photosynthetic electron flow is required. Plants evolved several photoprotective mechanisms that attenuate the light capturing reactions by dissipating excess absorbed light as heat, assessed by the non-photochemical quenching (NPQ) of chlorophyll fluorescence. The very fast NPQ induction and relaxation during night to day shift suggested the existence of a rapid and reversible type of regulation. Plants use redox signals as rapid and dynamically reversible means of regulating multiple post-transcriptional events and alleviating photosynthetic damage. We studied PGRL1 protein which was previously designated as a NPQ-related protein and possess six conserved cysteines. The regulation of protein activity by redox state involves changes of a disulfide bond between two intrinsic cysteine residues. We established that PGRL1 participates in two intermolecular disulfide linked complexes in plants in the dark. We found that these complexes underwent rapid transient reduction within seconds of illumination, which was followed by reoxidation within minutes of light. These oxidation-reduction cycles occurred simultaneously with the transient NPQ induction and NPQ relaxation phases during the dark to light transition. In addition, cysteine mutation analysis confirmed that the disulfide exchange of PGRL1 is required for the transient regulation of NPQ. Our findings suggest that PGRL1 participates in fast disulfide-based control of NPQ during the night to day shift.

## Driving the future: Development of advanced biofuels at the Joint BioEnergy Institute

### **Blake Simmons**

#### Lawrence Berkeley National Laboratory, USA

Today, carbon-rich fossil fuels, primarily oil, coal and natural gas, provide 85% of the energy consumed in the United States. Fossil fuel use increases CO<sub>2</sub> emissions, increasing the concentration of greenhouse gases and raising the risk of global warming. The high energy content of liquid hydrocarbon fuels makes them the preferred energy source for all modes of transportation. In the US alone, transportation consumes around 13.8 million barrels of oil per day and generates over 0.5 gigatons of carbon per year. This has spurred intense research into alternative, non-fossil energy sources. The DOE-funded Joint BioEnergy Institute (JBEI) is a partnership between seven leading research institutions (Lawrence Berkeley Lab, Sandia Labs, Lawrence Livermore Lab, Pacific Northwest National Lab, UC-Berkeley, UC-Davis, and the Carnegie Institute for Science) that is focused on the production of infrastructure compatible biofuels derived from non-food lignocellulosic biomass. Biomass is a renewable resource that is potentially carbon-neutral. Plant-derived biomass contains cellulose, which is more difficult to convert to sugars. The development of cost-effective and energy-efficient processes to transform cellulose and hemicellulose in biomass into fuels is hampered by significant roadblocks, including the lack of specifically developed energy crops, the difficulty in separating biomass components, low activity of enzymes used to hydrolyze polysaccharides, and the inhibitory effect of fuels and processing byproducts on the organisms responsible for producing fuels from monomeric sugars. This presentation will highlight the research efforts underway at JBEI to overcome these obstacles, with a particular focus on the development of an ionic liquid pretreatment technology for the efficient production of monomeric sugars from bioenergy crops.

## **Sculpting Photocatalysts on the Nano Scale**

## Yifat Nakibli and Lilac Amirav

### Schulich Faculty of Chemistry, Technion – Israel Institute of Technology

The solar-driven photocatalytic splitting of water into hydrogen and oxygen is a potential source of clean and renewable fuels. However, four decades of global research have proven this multi-step reaction to be highly challenging. The design of effective artificial photo-catalytic systems will depend on our ability to correlate the photocatalyst structure, composition, and morphology with its activity.

I will present our strategies, and most recent results, in taking photocatalyst production to new and unexplored frontiers. I will focus on unique design of innovative nano scale particles, which harness nano phenomena for improved activity, and methodologies for the construction of sophisticated heterostructures. I will share our design rules and accumulated insights, which enabled us to obtain a perfect 100% photon-to-hydrogen production efficiency, under visible light illumination, for the photocatalytic water splitting reduction half reaction. Finally, I will describe our future designs of systems capable of overall water splitting and genuine solar-to-fuel energy conversion.

## Mechanistic studies of catalyst photodeposition

## Nathan Walton, Philip Kalisman, Yifat Nakibli and Lilac Amirav

### Schulich Faculty of Chemistry, Technion – Israel Institute of Technology

Photodeposition is a method that utilizes the charge transfer of photocatalytic semiconductors to modify their surfaces. This gives us a means to deposit metal and metal oxide cocatalysts that improve photocatalytic activity and lends itself as a probing tool to help us detect when and where the successful charge transfer occurs in solution. We will present our work on the photodeposition of iridium oxide on CdSe@CdS seeded nanorods, which is the first example of photochemical oxidation on colloidal quantum dots, and how we used photodeposition as a probe to determine that the deposition occurs through a mediated oxidative pathway. Furthermore, we used platinum photodeposition to determine the accessibly and availability of the nanorod surface for modification. By understanding the photodeposition mechanisms for the platinum and iridium oxide cocatalysts we hope to improve our control over CdSe@CdS seeded nanorod surface modification, which has been demonstrated to be essential for achieving improved photocatalytic water splitting by the nanorods.

## Natural stress tolerance in extremophyte relatives of *Arabidopsis thaliana*

Yana Kazachkova, Gil Eshel, Ruth Shaked, Aaron Fait and Simon Barak

French Associates Institute for Biotechnology and Agriculture of Drylands, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev

Most studies of molecular mechanisms of plant stress tolerance have focused on the model plant Arabidopsis thaliana due to its unsurpassed genetic and genomic resources. Yet, Arabidopsis is a stress-sensitive plant and is unlikely to possess many stress tolerance mechanisms found in stress-tolerant plants. One successful approach has been to study stress-tolerant Arabidopsis relatives (Brassicaceae), which have many of the advantages of model systems. We have therefore been investigating naturally stress-tolerant Arabidopsis relatives from different extreme habitats. Eutrema salsugineum from saline coastal areas of China is tolerant to a variety of stresses including high salt, and low nitrogen stresses, while Anastatica hierochuntica from the Negev desert in Israel is tolerant to salt, low nitrogen and heat stresses. Using a combination of systems biology and molecular biology tools, we have demonstrated both common and diverse stress tolerance strategies. A recurring motif is that stress tolerant Arabidopsis relatives appear to be primed for stress by constitutive expression of genes that are normally induced by stress in Arabidopsis. Furthermore, the observation that Eutrema maintains salt tolerance despite different metabolic responses when grown in vitro or on soil suggests a considerable degree of adaptive plasticity in extremophile plants.

## A systems biology analysis of multiple abiotic stress tolerance in *Anastatica hierochuntica* (True Rose of Jericho), a Negev Desert relative of *Arabidopsis thaliana*

<u>Gil Eshel</u><sup>1</sup>, Dong-Ha Oh<sup>2</sup>, Shirli Bar-David<sup>1</sup>, Aaron Fait<sup>1</sup>, Maheshi Dassanayake<sup>2</sup> and Simon Barak<sup>1</sup>

<sup>1</sup>French Associates Institute for Agriculture and Biotechnology of Drylands, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Israel

<sup>2</sup>Louisiana State University, USA

We present a complete transcriptome (the sequences of all the expressed genes) of Anastatica hierochuntica (Brassicaceae), a native of the Negev desert and the Dead Sea valley in Israel. This reference transcriptome will serve as a vital tool to study the molecular biology and evolution of adaptation to extreme environments. In this lecture, we focus on a molecular evolutionary study including a phylogenomic and genome-wide positive selection analyses that was carried out on 17 genome/transcriptome-sequenced species from the Brassicaceae family, and one outgroup species from the sister family *Cleomaceae*. Our phylogenomic tree structure shows that the Brassicaceae lineage III clade (to which A. hierochuntica belongs) is more evolutionary closely related to the lineage II and lineage EII combined clade, than to lineage I. Among these 17 species, are so-called "extremophytes" which naturally grow in extreme habitats such as highly saline soils, hot and dry deserts, and freezing environments. In our genome-wide positive selection analysis, we identified positively selected genes from three different extremophytes, and one stress-sensitive relative, Arabidopsis thaliana. A low overlap of positively selected genes was observed between the different species. However, GO enrichment analysis indicate a large overlap in the functionality of these genes, suggesting that adaptation and speciation are related to changes in a common set of functions, while different sets of genes may change due to selective pressure in each species uniquely. We will discuss the potential relation of a few positively selected genes to adaptation to stressful environments, and to the ability of A. hierochuntica to cope with the desert environment.

# Supercritical water gasification of carbonaceous waste materials for hydrogen production: Problems of heat recovery

## Efim Korytnyi and Boris Duvidson

### Ben-Gurion University of the Negev, Israel

In spite of the recent decrease in fossil fuel prices and the efforts made by developed countries to optimize fuel consumption in various spheres of economy, as well as the increasing use of renewable energy, the problem of recycling organic materials into valuable products or energy remains urgent.

At present there is a world-wide belief that owing to high energy capacity, operability, and ecological safety of energy conversion processes involving hydrogen, the latter holds the greatest promise as energy carrier. Supercritical water gasification (SCWG) may be regarded as one of the most preferable processes for converting organic waste into hydrogen-rich gas. Experiments in the conversion of glycerol, biomass and their mixtures at sub- and supercritical conditions have demonstrated the possibility of obtaining a gas with high hydrogen content (up to 70%). However, heat recovery remains one of the key factors affecting the overall efficiency of the process. We have obtained new results explaining the features of the heat recovery in SCWG and have determined the elements of the technological scheme which are critical for the process efficiency.

# The metabolism and recycling of secondary plant cell-wall polysaccharides in B. *subtilis* Biofilms

## Natalia Kemper, Yaara Oppenheimer-Shaanan and Ilana Kolodkin-Gal

### Department of Molecular Genetics, Weizmann Institute of Science

The natural habitat of Bacillus subtilis is the soil, where it forms complex multicellular communities termed biofilms on plant roots and resides within the root's rhizosphere. Bacillus biofilms play a beneficial role in maintaining the optimal rhizosphere environment, which supports plant growth and protects it from fungal and bacterial pathogens. One key question in the interaction between B. subtilis and plant roots is the mechanisms by which Bacillus subtilis adapts to its host. We suggest that the colonization leading to a successful interaction can be facilitated by plant cell wall polysaccharides. Thus, we study the possible metabolism of root polysaccharides inside the biofilm and their incorporation into the biofilm matrix. Our work demonstrates that plant polysaccharides can serve as a secondary carbon source during stationary phase as well as signals that activate specific biofilm signalling pathways. These bacterial responses then allow B. subtilis to metabolize various plant cell wall polysaccharides from neighbouring roots or roots of different ages, leading to a beneficial interaction between B. subtilis and plant roots. Understanding this metabolism process can help improve the field of polysaccharide degradation for energy production.

Day 2 – Tuesday, September 13<sup>th</sup>, 2016

**Evening Session** 

## Molecular Water Oxidation Catalysis within the Energy Context

## Antoni Llobet

## Institute of Chemical Research of Catalonia (ICIQ), Barcelona Institute of Science and Technology, Tarragona, Spain

The replacement of fossil fuels by a clean and renewable energy source is one of the most urgent and challenging issues our society is facing today, which is why intense research is devoted to this topic today. Nature has been using sunlight as the primary energy input to oxidize water and generate carbohydrates (a solar fuel) for over a billion years. Inspired, but not constrained, by nature, artificial systems[1] can be designed to carry out redox catalysis induced by light for instance to oxidize water and reduce protons or other organic compounds to generate useful chemical fuels. In this context this contribution will present a variety of molecular water oxidation and proton reduction catalysts[2] based on first row and second row transition metal complexes. Their capacity to carry out these reactions induced by light will be analyzed and discussed.[3]

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# A biomimetic approach for the design of water oxidation electrocatalysts

### Galia Maayan

#### Technion – Israel Institute of Technology, Haifa, Israel

The catalytic splitting of water into hydrogen and oxygen is a bio-inspired challenge for chemists seeking to find "green" alternatives for fuel. In natural photosynthesis, this process utilizes sunlight energy and a high oxidation state manganese cluster. Few synthetic high-valent manganese complexes have been applied to date as water oxidation catalysts in homogeneous and heterogeneous systems. The use of electrochemical energy for homogeneous water oxidation catalyzed by a manganese cluster, however, has not been demonstrated. Herein we present the synthesis and characterization of а polynuclear Mn unique cluster, [Mn12O12(O2CC6H3(OH)2)16(H2O)4], which has a Mn(IV)-oxo cubane core and is highly soluble and stable in water as indicated by spectroscopic studies. Electrochemical investigations in acetate buffer solutions revealed pH dependent catalytic currents at an oxidation potential as low as 1.2V (vs the NHE). O<sub>2</sub> evolution was clearly detected by a typical reduction peak observed in cyclic voltammograms. Controlled potential electrolysis indicates that this catalyst not only performs at pH 6 with high turnover number in low potential, but also functions in seawater. We further advocate that the high electrocatalytic performance is due to the hydroxyl groups, which play an important role as proton acceptors.

## **Got Energy? Marine Metagenomics to the Rescue**

## Béjà O., Pushkarev A., Feingersh, R., Alalouf, O., and Shoham Y.

### Technion – Israel Institute of Technology, Haifa, Israel

With the current globe 'Energy Crisis', many labs are now searching for different alternative energy sources. In this talk I will describe our efforts to use microbial energy hidden potential via functional metagenomics. I will talk about screening for new glycoside hydrolases to degrade poly-sugars and for new rhodopsins to directly harvest light energy.

## Eco-friendly catalytic processes for production of renewable and fungible liquid fuels and chemicals

## Moti Herskowitz and Miron Landau

### Blechner Center for Industrial Catalysis and Process Development Ben-Gurion University of the Negev, Beer-Sheva, Israel

Carbon dioxide and water are the most abundant and low-cost renewable feedstock for production of renewable, environmentally-acceptable fuels. Two main routes are currently being explored: (1) artificial photosynthesis through photocatalytic and photoelectrochemical processes and (2) splitting water into its components, hydrogen and oxygen, and using the hydrogen so obtained in the conversion of carbon dioxide to liquid fuels.

The Blechner Center (<u>http://www.bgu.ac.il/indcat/</u>) has developed, over the past two decades, infrastructure and expertise required to deal with a wide variety of challenging projects in the area of fuels in general and renewable fuels in particular. Specifically, it has developed a novel process for converting vegetable and algae oils to advanced green diesel and jet fuels. The Blechner Center is developing an integrated catalytic system for conversion of mixtures of CO<sub>2</sub>/CO/H<sub>2</sub> to hydrocarbons that are readily converted to liquid fuels and chemicals. The renewable hydrogen could be produced from water by various splitting technologies. Novel catalytic Febased materials combined with a novel design of the process yielded excellent, unprecedented performance. CO<sub>2</sub> conversions as high as 90% were obtained, reaching high selectivity to liquid (C5+ hydrocarbons), well-beyond reported results in the scientific and patent literature.

## Fundamentals of the Active Catalytic Phases of a Novel High-Performance Spinel Catalyst for Carbon Dioxide Conversion to Liquid Fuels through Hydrogenation

## Meital Amoyal, Miron Landau and Moti Herskowitz

### **Ben-Gurion University of Negev**

The production of alternative and renewable liquid fuels for transportation from feedstock other than crude oil is one of the scientific and technological challenges of the 21<sup>st</sup> century. An attractive and sustainable alternative of green energy is the production of transportation fuels from carbon dioxide and water, the most abundant and low-cost sources for carbon and hydrogen, via the CO<sub>2</sub> hydrogenation process. The performance of Fe-based catalysts depends significantly on the potassium content found to be the most efficient promoter and a key-ingredient for this process .The effect of potassium was tested with unpromoted and K-promoted Fe-Al-O oxide and Fe<sub>5</sub>C<sub>2</sub> carbide materials, formed during CO<sub>2</sub> hydrogenation from Fe-Al-O spinel. Each one of the tested catalysts contained a single phase (oxide or carbide). 2 wt% potassium enhanced the RWGS activity of the oxide phase tenfold compared with the unpromoted oxide. This correlated with increase of Fe<sub>2</sub>+ / Fe<sub>3</sub>+ ratio (XPS) determining oxygen vacancies as active sites for RWGS. Potassium suppressed sevenfold the methanation activity of the carbide catalyst and increased the CO conversion to C2+ hydrocarbons by a factor of 1.6. EFTEM images and elemental profiles of unpromoted carbide nanocrystals measured after testing in CO hydrogenation displayed an amorphous surface layer enriched with oxygen. Potassium stabilized the surface iron atoms in reduced form. The observed effects of potassium on carbide phase were explained by a mode

## The hemicellulolytic system in *Geobacillus* stearothermophilus

## Yuval Shoham

#### Faculty of Biotechnology and Food Engineering, Technion-IIT, Haifa, Israel

*Geobacillus stearothermophilus* is a gram-positive, thermophilic, aerobic soil bacterium that was isolated over 20 years ago due to its ability to produce alkaline tolerant hemicellulases. The extracellular xylanase of this bacterium was produced on a tonnage scale and proved to be an efficient component in a chlorine-free bleaching process of paper pulp. The hemicellulolytic genetic system in G. *stearothermophilus* is composed of over 40 genes making three complete systems for the utilization of xylan, arabinan, and galactan. The bacterium secretes only a limited number of endomain chain-degrading enzymes that hydrolyze the high molecular polymers into rather large oligosaccharides that enter the cell via specialized ABC sugar transporters. The regulation of the hemicellulolytic genes in *Geobacillus* involves many levels including repression, activation, transition state regulation, catabolite repression and quorum sensing. This highly sophisticated regulatory network allows the bacterium to successfully compete on the scare carbon sources in the soil.

Shulami et al., Multiple regulatory mechanisms control the expression of the *Geobacillus stearothermophilus* gene for extracellular xylanase. J. Biol. Chem: 289:25957-25975, 2014.

## Structure-function studies of an extracellular arabinanase

## suggests a unique "harpoon" mechanism of action

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 $\alpha$ -L-arabinanases are key bacterial enzymes in the breakdown of arabinan, one of the main polysaccharides constituting the plant cell-wall. Such enzymes hence present a wide range of important potential biotechnological applications, e.g. the conversion of plant organic waste into bio-ethanol. GsAbn43A is an extracellular 2-L-arabinanase from the thermophilic bacterium Geobacillus stearothermophilus-T6, shown to degrade efficiently both linear and naturally-branched arabinan polymers. The enzyme belongs to glycoside hydrolase family 43 (GH43), contains 848 amino-acid residues, and possesses 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 (shown in red in the figures below) corresponds to the typical five-bladed 2-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. Interestingly, two different conformational states have been determined for the enzyme, a "closed" state (right figure) and an "open" state (left), differentiated by about 12 Å movement in the relative location of the fourth domain. Substrate-binding structural experiments demonstrate, surprisingly, that an arabino-pentaose substrate binds to a dedicated site in the fourth domain, rather than to the expected catalytic domain and active site (central figure). These findings, together with complementary ITC, SAXS, DLS, molecular dynamics, domain deletion, mutagenesis and kinetics experiments, suggest a novel "harpoon-like" catalytic mechanism for the arabinan degradation action of GsAbn43A.

## Synthesis of mesoporous K/Fe-Al-O ceramic fibers catalyst

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Sub-micron sized fibers are of great interest in the field of heterogeneous catalysis. Such fibers can potentially provide superior transport properties between the catalytic sites and the bulk. Providing the fibers with internal porosity that allows for larger catalytic surface, better mass transport and catalyst efficiency and lower deactivation rates is a major objective in this research. In this work we focus on the synthesis of K/Fe-Al-O ceramic fibers with mesoporous structure.

Fibers mats were prepared by electrospinning a solution of metal acetylacetonates in an organic solvent. The specific metal precursors and controlled thermal treatment gave rise to a promising mesoporous structure with fibers diameter in the 100-800 nm range. The formation of this structure was investigated and explained in terms of shrinkage rate vs. weight loss rate and metal acetylacetonates phase transitions. The increased understanding in fiber morphological evolution is a step towards new possibilities in mesoporous fiber formation and heterogeneous catalysis.

## Membrane-free water splitting with separate oxygen and hydrogen cells for PEC hydrogen production

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Water electrolysis cells comprise a sealed vessel with two electrodes and a membrane (or porous diaphragm) that separates the H<sub>2</sub> and O<sub>2</sub> gas products. This architecture gives rise to critical challenges in photoelectrochemical (PEC) water splitting cells that directly convert water and solar energy to hydrogen fuel. The low power density of the sunlight necessitates a large number of PEC cells, giving rise to critical challenges for gas separation, collection and transport to a centralized hydrogen storage and distribution facility. These challenges, in addition to efficiency and stability challenges, render PEC hydrogen production economically questionable. The objective is to decouple the H<sub>2</sub> generation from the O<sub>2</sub> generation in the PEC solar cells. In this presentation, we will talk about the possibility of cell separation using a solid redox mediator, as well as the conditions and criteria which the redox mediator must meet. We present a two-cell system wherein the ion exchange between the H<sub>2</sub> and O<sub>2</sub> cells is mediated by nickel hydroxide (Ni(OH)<sub>2</sub>) auxiliary electrodes commonly used in rechargeable alkaline batteries, which can be cycled many times with high efficiency. The cells are connected to each other by metal wires, enabling centralized H<sub>2</sub> production far away from the solar plant.

Day 3 – Wednesday, September 14<sup>th</sup>, 2016

**Morning Session** 

## Catalytic conversion of biomass-derived oxygenates to olefins for fuel

## and chemical production

## Yong Wang

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The chemistry of Lewis acid-base pairs on (mixed) oxide surfaces plays important roles in many catalytic reactions such as aldolization. Fundamental understanding of the Lewis acid-base pairs have long been studied.1-5 For instance, aldolization is an important reaction for C-C bond formation, and studies reveal that the nature (i.e., density and strength) of Lewis acid-base pairs has significant effects on the reaction pathway and product distributions. We recently found that Zn could be used to modify the surface Lewis acid-base properties on ZrO2. As a result, highly selective acetone aldolization and self-deoxygenation cascade reactions can be realized to produce isobutene.4,5 By combining theoretical calculations and experimental studies, herein, we present fundamental understanding of the Lewis acid-base pairs for the cascade conversions of ethanol, acetic acid, propanoic acid, and acetone to olefins on the Zn doped ZrO2 catalysts.

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[3] Snell, R. W.; Combs, E.; Shanks, B. H. Top. Catal. 2010, 53, 1248-1253.

[4] Leon, M.; Faba, L.; Diaz, E.; Bennici, S.; Vega, A.; Ordonez, S.; Auroux, A. Appl. Catal. B-Environ. 2014, 147, 796-804.

[5] Krivtsov, I.; Faba, L.; Diaz, E.; Ordonez, S.; Aydin, V.; Khainakov, S.; Garcia, J. R. *Appl. Catal. A-Gen.* 2014, *477*, 26-33.be used as ligands for the anatase nanocrystals.

## New protein-based platforms for artificial photosynthesis

### Dror Noy

#### Migal – Galilee Research Institute

The design and construction of small protein functional analogs of photosynthetic proteins is an appealing route toward novel solar energy conversion devices for two important reasons. First, it provides simple models to the elaborate multi-protein multi-cofactor complexes that carry out natural photosynthesis, and thereby a way to study the fundamental engineering principles of biological solar energy conversion and learn how to implement these principles outside their biological context. Second, successful designs may be integrated with artificial and/or natural components into novel hybrid systems for the production of viable solar fuels. Our focus is on natural photosynthetic light-harvesting complexes in which dense arrays of pigments are held in place by specific binding proteins. The particular arrangement of chromophores and their specific interactions with the protein environment fine-tune their absorption and emission spectra. This enables regulating the photon fluxes throughout the light harvesting system and directing excitation energy toward its final destination-the reaction center. Achieving precise control on pigment organization and protein pigment interactions is thus our primary design challenge. Here we present new and promising templates for such designs that open new possibilities for accurately assembling chlorophyll-protein arrays, and may teach us important lessons on controlling photoexcitation dynamics in multi-pigment protein complexes.

# Pure hydrogen production from ethanol and glycerol in a membrane reactor

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This research is focused on understanding and developing scaled-down pure H<sub>2</sub> production schemes in Pd membrane reactors, through simulations and experimental campaign. Following studies of methane steam reforming (MSR) in a Pd membrane reactor packed with a catalytic-foam, which showed that high conversion and high hydrogen recovery can be achieved, we studied the process of ethanol SR in the same system. Full ethanol conversion is achieved with H<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub> and CO as products. Separating H2 directs the selectivity towards CO and CO<sub>2</sub>, resulting also in increased CO to CH<sub>4</sub> ratios. In general, increasing temperature, pressure, and introducing sweep flow on the permeate side leads to better separation and higher permeate flow rates. In the above configurations the heat is supplied by an external heat source (electrically).

A mathematical model predicts the reactor's performance well, when membrane permeance is adjusted, but the apparent value is significantly lower than values measured in pure  $H_2$ . This is attributed to co-adsorbates, Concentration polarization effects are negligible as evident from a 2D model.

The design of an on-board autothermal membrane reactor producing pure hydrogen at atmospheric pressure is studied experimentally, with either methane or ethanol or glycerol as  $H_2$  source. The design incorporates two reactors exchanging heat; an endothermic Pd-membrane-reformer, and an exothermic oxidation-reactor fed by the reforming effluents. The oxidation feed is distributed axially to avoid hotspots. The obtained performance of the 1.3L system, with all feeds, is 0.15 kW (LHV) equivalent H2 flow rate at efficiency of ~25%. The mathematical model, considering membrane permeance inhibition, is validated and used for optimization, showing that high efficiencies can be achieved in larger systems. This design serves as proof of concept for on-board pure  $H_2$  generators, with flexible fuel source type, feeding an adjacent fuel cell.

## Supplementation of sulfate to the growth medium enhances biomass and organic sulfur in the halophyte Salicornia, but not in *Sarcocornia*

### Assylay Kurmanbayeva and Moshe Sagi

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The annual halophyte Salicornia and perennial, almost identical, Sarcocornia are promising saline agriculture developing crops due to their high tolerance to salinity. Enhanced demand for sulfur nutrition may be expected among halophyte plants grown in the vicinity of soil and water containing relatively high sulfate level. Yet the knowledge about sulfur metabolism in plants supplied with high sulfate level is limited, especially for halophyte plants. In the current study, Salicornia and Sarcocornia plants grown in 0.5 MS medium supplemented with sulfate (0 or 10 mM) and sodium chloride (50 and 200 mM, as NaCl with and without Na2SO4), exhibited the enhancement of biomass accumulation and organic sulfur by sulfate supplementation to Salicornia but not when added to Sarcocornia. This can be explained by the folds enhanced L-cysteine desulfhydrase and sulfite oxidase activities in Sarcocornia as compared to Salicornia, indicating the higher cysteine degradation followed by the need to detoxify the resulting sulfite generated during the sulfate reduction and/or degradation of organic-S metabolites. In contrast, the significantly higher Adenosine-phosphosulfate-reductase and Cysteine desulfurase activities in Salicornia as compared to Sarcocornia is indicative for the higher sulfate reduction activities and higher production of organic S that is involved in the formation of Fe-S clusters and S containing organic compounds such as thiamine.

# Hydrogen evolution and water oxidation catalyzed by polyoxometalate complexes of metal-oxide nanocrystals

## Ira A. Weinstock

### **Ben-Gurion University of the Negev**

Polyoxometalate cluster anions (or POMs) serve as redox-active ligands in watersoluble polyanionic "complexes" of metal-oxide nanocrystals (NCs), giving isolable nanostructures uniquely positioned between molecular macroanions and traditional-electrostatically stabilized-colloidal metal oxides. In POM complexes of TiO2 NCs, an iso-structural series of TiIV-substituted POM capping ligands, "[ $\alpha$ -XW11O39Ti]–O–" (X = Al3+, Si4+, P5+) are covalently attached to ca. 6-nm anatase- $TiO_2$  cores. The POMs serve as tunable electron-acceptors, and in a model photochemically driven hydrogen-evolution reaction, are an order of magnitude more reactive that either TiO<sub>2</sub> or the molecular POMs alone, with reactivities increasing in the order, X = AI3 + < Si4 + < P5 +. The kinetic and thermodynamic basis for this order will be discussed, along with new results documenting the preparation of analogous hybrid materials containing nano-scale cores comprised of other transition- and maingroup metal oxides or oxy-hydroxides. Those include POM complexes of hematite (alpha-Fe<sub>2</sub>O<sub>3</sub>) NCs, featuring rates of water oxidation exceeding those previously reported for that material. More generally, just as traditional ligands control catalytically active metal centers in molecular complexes, covalently coordinated POM capping ligands with tunable redox chemistries, quantum yields and other physical properties, provide new options for rationally controlling electron-transfer mediated processes of metal-oxide cores.

# Facile synthesis of catalytic layered double hydroxides nanoparticles

## Anup Tathod and Oz Gazit

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Incessantly increasing energy demand of the world has attracted the attention of the scientific community. Intuitively in last few years many attempts have been made to find alternative energy source. In this scenario, conversion of methane to syngas via dry reforming of methane is an attractive direction. Layered double hydroxides (LDH) have been used as basic supports in many catalytic applications. For dry reforming LDH have the capacity to resist carbon formation, which is one of the main limiting factors of this reaction. In this work we synthesized nanoscale LDH materials with the aim to support them on a thermal resistant acidic support. Herein we demonstrate an efficient and highly reproducible method for LDH nanoparticles (NPs) synthesis, avoiding the use of organic structure directing agent and forgoing a lengthy aging process. It is shown that by varying the nucleation temperature between 60 and -55 °C in conjunction with the fast addition of metal precursor we can obtain narrowly distributed isolated LDH NPs in the range of 20-200 nm. Nucleation temperature significantly affects the nucleation rate and crystal growth. At optimized temperature maximum nucleation rate can be achieved which leads to the formation of higher number of crystals with smaller size. Smaller crystal size is favorable for catalytic activity as active sites are proved to be associated with edges of crystal. Materials are characterized by DLS, XRD, HR-TEM and Cryo-TEM.

## Polymer-assisted dispersion of Ni on Zirconia through nonhydrolytic sol-gel method

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Nickel-based catalysts have been identified as highly active catalysts for dry reforming of methane, to make synthesis gas (CO +H<sub>2</sub>). Unfortunately, the Ni catalytic sites deactivate due to carbon deposits during reaction (i.e. coke formation). It has been reported that smaller Ni particles (1-3 nm) are more resistant to coke formation. However, obtaining such small dimensions and moreover to keep them from sintering under the high temperatures of the reaction (>700°C) has proven to be a difficult task. Encapsulating the Ni nanoparticles in a 3D porous support can form a highly dispersed Ni catalyst with higher stability and better catalytic performance. In this work, we develop a general methodology to make Ni nanoparticles within a porous  $ZrO_2$ support. This is achieved by combining the self-assembly of a chitosan, a natural polymer, for dispersing the Ni precursor followed by encapsulation using a nonhydrolytic sol-gel route (NNSG). Our results show that the obtained Ni@ZrO<sub>2</sub> samples are highly porous, with tetragonal-stable phase at elevated temperatures up to 800°C, with Ni dispersions around 12%. Surface area is shown to increase up to 140m2/g with the increase in the polymer content during the sol-gel process.

## Wheat straw as a feedstock for biofuel

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Wheat straw is a feedstock for biofuel production that does not compete with food. We screened 48 lines of wild and domestic wheat. Straw was fractionated into watersoluble and nonsoluble fractions. In the soluble fraction we found a broad variation in free soluble sugars (FSS) concentration and a narrow variation in starch. There was a significant variation among wheat lines in enzymatic saccharification. This means that wheat lines can be developed in which a significant amount of free soluble sugars can be easily extracted without the need for costly pretreatment and enzymatic deconstruction. Moreover, the high FSS trait might be combined with the high saccharification trait to develop varieties with a straw composition better adapted for biofuel. In order to test how various sugar fractions correlate with yield and environmental factors, we analyzed straw from a commercial line grown in the field and harvested each year for 17 years. A dataset of environmental conditions and yield was monitored each year. We found a very limited variation in all fractions throughout the years and thus no correlation with yield or the environment. In addition, we analyzed field grown wheat straw from 53 accessions provided by Evogene. Only the nonsoluble fraction was slightly correlated with yield parameters in a way that suggests that it is possible to genetically modify straw sugar components, albeit to a limited extent, without compromising yield under field conditions.

# Hybrid vigor results from the perturbation of growth-limiting safeguard pathways

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#### \*Equal contribution

The merging of genomes in inter-specific hybrids can result in increased growth rate and can provide resistance under stress conditions. This phenomenon, known as heterosis, can be exploited for biofuel production via enhanced biomass production and for developing ethanol resistant strains for fermentation. We describe a budding yeast hybrid that grows faster than its diploid parents, and use it as a model to systematically screen for alleles contributing to hybrid growth under different conditions. Guided by the screen's result, we show that the hybrid's shorter doubling time and faster biomass accumulation correlate with the loss of programmed cellcycle delays and weakened repression of respiratory metabolism. Furthermore, while the parental diploids slow down their growth when presented with ethanol stress, the hybrid maintains stable growth, a phenotype that is easily recapitulated in the parent by reducing dosage of individual genes. Based on these findings, we propose a new model of heterosis, in which an apparent superior growth performance results from the perturbations of safeguard mechanisms that limit growth in the parental background. Within this model, the hybrids maintain the activity of conserved pathways such as primary metabolism, but dysregulate more divergent safeguard mechanisms such as respiration repression or cell cycle checkpoints, leading to its apparent superiority, but at the cost of long-term instability, like increased DNA damage. Our model unifies the phenomena of hybrid vigor and incompatibility by proposing that heterosis results from perturbation of safeguard mechanisms.

## Ray optics based light trapping beyond the lambertian limit

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Concentrating light from the sun has many benefits for solar cells. It comes, however, at the price of having to constantly track the sun's position, and the cumbersome tracking mechanism reduces much of the cost effectiveness of this otherwise affluent approach. A possible way around this limitation is to use devices that react to sunlight for facilitating passive tracking. This bio-inspired idea is by itself not new but all existing approaches suffer from low performance of their reactive optical components. Here we show a type of reactive optical device that is based on a composite soft material that is capped between two glass slides. The composite itself is made form a dense collection of micro-sized beads that are immersed in water. Each bead is made from glass and is covered with a thin layer of silver (200nm). As a result the dense collection of such beads forms a good reflector for moderate light intensity. Beyond some critical intensity level, however, micro-sized boiling events, lasting no more than few tens of microseconds, occur. These rapid liquid/vapor phase transition act with significant force on the nearby beads such that the beam-path is cleared and transparency is achieved. The intricate thermodynamics of this events would is analyzed based on high speed camera captures of the bubble formation. Also, the measured reflection and transmission are both in the 80% range for visible to near infrared light - well beyond anything achieved to date. We will also present our view for a solar power conversion system based on the proposed reactive-reflector, and evaluate its performance. This will allow us to compare it against existing approaches, not just passive tracking. Finally we will describe some of the routes we intend to explore in order to push the reflectivity beyond 90%, and also for tuning the spectral responsivity of the reactive-reflector.

## Novel bifunctional catalysts based on crystalline multi-oxide matrices containing iron ions for CO<sub>2</sub> hydrogenation to liquid fuels and chemicals

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### and Moti Hershkowitz

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Carbon dioxide hydrogenation is a viable catalytic process that converts the greenhouse gas and hydrogen potentially produced from water into renewable chemicals and fuels. A variety of catalysts used in this process have been studied, most of them based on iron. The catalytic process hydrogenating carbon dioxide into hydrocarbon fuels C5+ (CDHF) proceeds via reverse water gas shift (RWGS) reaction producing CO followed by the Fischer-Tropsch synthesis (FTS). The challenge is to prepare a catalytic material that balances properly the two catalytic functions thus reaching a high activity, selectivity and stability. In this work, we focused on the effects of catalyst factors, especially the chemical state of active components and the nature of promoters. The main idea is to use Fe-based catalysts represented by solid mixed oxide matrices where Fe(2+,3+) ions are distributed in different structural environments in order to control the relative contribution of oxide and carbide phases to the performance of activated bi-functional catalyst.

## Cytokinins improve biomass production under environmental stress by shutting down plant's "avoidance processes" that have been favored by evolution over millions years

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### and Shimon Gepstein

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In nature, annual plants activate a specific genetic program leading to an early flowering and accelerated aging and death in response to abiotic stresses. Although this "avoidance" phenomenon is advantageous for survival in nature under severe stresses, it may have negative agro-economic impacts on biomass and crop productivity. Overcoming this genetic programing by cytokinins (CKs) has been recently shown in transgenic plants over-producing the plant hormones cytokinins. These transgenic plants displayed a significant increase in biomass under drought stress conditions. Analysis of RNAseq data suggests that CKs trigger transcriptional reprograming affecting events leading to moderating the stressdependent inhibition of vegetative growth and delaying the premature plant aging and death under stress. Moreover, phosphorylation processes known to participate in the signal transduction pathway of plant stress responses were inhibited by the additions of CKs. These results suggest that CKs cause plant's desensitization of environmental stress clues and as a result maintain regular growth on one hand and delay premature plant aging and death. We have applied this generic technology to the biofuel plants Camelina The transgenic Camelina plants showed increased biomass and delayed plant aging under drought and salt stress, without yield losses.

## Cytokinins-induced transcriptional reprogramming under stress conditions leads to stress adaptation of Arabidopsis plants

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Annual plants respond to abiotic stresses by activating a specific genetic program leading to early flowering and accelerated senescence. This phenomenon supports survival under unfavorable environmental conditions, but have negative agroeconomic impacts on crop productivity. Overcoming this genetic programing by cytokinins (CK) has recently been shown in transgenic plants that over-produce CK. These transgenic plants displayed a significant increase in plant productivity under drought stress conditions. We investigated the role of CK in reverting the transcriptional program that is activated under abiotic stress conditions and allowing sustainable plant growth. We employed 2 complementary approaches: Ectopic overexpression of CK, and applying exogenous CK to detached Arabidopsis leaves. Transgenic Arabidopsis plants transformed with the isopentyltransferase (IPT) gene under the regulation of the senescence associated receptor kinase (SARK) promoter displayed a significant drought resistance. A transcriptomic analysis using RNA sequencing was performed to explore the response mechanisms under elevated CK levels during salinity stress. This analysis showed that under such stress, CK triggered transcriptional reprograming that resulted in attenuated stress-dependent inhibition of vegetative growth and delayed premature plant senescence. Our data suggest that elevated CK levels led to stress tolerance by retaining the expression of genes associated with plant growth and metabolism whose expression typically decrease under stress conditions. In conclusion, we hypothesize that CK allows sustainable plant growth under unfavorable environmental conditions by activating gene expression related to growth processes and by preventing the expression of genes related to the activation of premature senescence.

## Functional semiconductors and interfaces for generating fuels from sunlight

## Ian D. Sharp

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The capture of solar energy and its direct conversion to chemical fuel in artificial photosystems provides a promising route to sustainably meet global energy demands and to overcome our current reliance on fossil fuels. However, development of practical photosystems requires semiconductor light absorbers that are simultaneously efficient, durable, and scalable. In addition, these light harvesting elements must be coupled to catalysts for selectively driving chemical transformations in harsh reaction environments. Here, I will present recent research advances and discuss future opportunities for creating assemblies capable of efficient and stable solar energy conversion. In the quest for a next generation of stable thin film semiconductors, basic mechanisms underlying the competition between photocarrier recombination and chemical reaction in emerging transition metal oxide semiconductors are investigated. In parallel, interfaces between catalysts and high efficiency semiconductors are precisely engineered. These studies reveal that future progress in artificial photosynthesis will require coupling of advanced semiconductor characterization and deposition methods to control the landscape of disorder in complex multi-phase, multi-component assemblies.

## Photocatalytic routes towards alternative fuels

### Yaron Paz and Sagi Pasternak

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Photocatalysis, i.e. the use of light to induce catalytic chemical reactions, may be applied in a variety of complementary ways, aiming at the production of non-fossil fuels. Here we discuss two different examples, for such applications: photocatalysis as a means to assist biomass production and photoelectrochemical cells based on bismuth- containing oxides.

The first example takes from the need to separate between lignin and cellulose. Here, the basic concept was to selectively degrade the lignin while leaving the cellulose intact. The second example has to do with the developing of photoelectrochemical cells based on bismuth-containing oxides. Bismuth-containing oxides have been shown to have relatively narrow band gaps and therefore attract considerable attention. One such oxide is BiYWO<sub>6</sub>, previously synthesized by hightemperature solid state reaction method, shown to be active for overall water splitting in its powder form. Here, we present the fabrication of a range of Bi2-xYxWO6 photoanodes by a sol-gel route, enabling the synthesis of Bi<sub>2-x</sub>Y<sub>x</sub>WO<sub>6</sub> powders and films with high surface area and offering convenient control of composition and morphology. The prepared electrodes were characterized using HRSEM, XRD, diffuse reflectance UV-VIS spectroscopy and impedance spectroscopy. The absolute positions of the energy bands were estimated using Mott-Schottky analysis and Kelvin probe measurements. Photoelectrochemical water splitting experiments, conducted under simulated solar-light conditions, revealed a clear dependence on the composition in the  $Bi_{2-x}Y_{x}WO_{6}$  solid solution in the range of 0.3<x<1. The correlation between the optical and structural properties and the photoactivity is discussed.

# Selection on microbial communities at the level of a single grain

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Natural microbial communities are key in degradation of biomass in the soil. Members of the community are interacting with one-another by secretion of anti-microbial agents and other metabolites to their close proximity. To study those interactions we developed a set of tools aimed at investigate microbial communities in the soil at the single cell level. To study the effect of anti-microbial agents in-situ, in the soil, we use bacterial probes that enable us to measure selection for antibiotic resistance on single grains. To understand the influence of such bacterial interactions we study the soil bacterial ecology on the single grain level; to that end, we sequence metagenomic amplicons of 16S gene from single grains. While no selection for antibiotic resistance is seen in bulk soil, we do find such selection on single grains. We currently explore the metagenomics data for further ecological insights.

## Sustainable microalgae biomass production and biorefinery for fuels and chemicals

## Stefan Leu, Aliza Zarka, Inna Khozin-Goldberg and Sammy Boussiba

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We have investigated outdoors production of microalgae biomass for production of biofuels, feed and high value bio-products in 80 m<sup>2</sup> pond system. Algae have been cultivated continuously for months in open raceway ponds without significant contamination or other pathologies, in spite of strongly varying pond temperatures and changing weather. Average annual biomass productivity was >20 gm<sup>-2</sup>day<sup>-1</sup>. BGU has integrated cultivation with a low energy biological growth medium treatment system for full reuse. On-site carbon dioxide production and nutrient recovery from organic waste materials can provide all process energy, carbon and nutrient needs. Energy saving harvesting and advanced fractionation and biorefinery technologies have been tested, resulting in an organic high value products extract, and starch and/or protein rich residue useful for ethanolic fermentation or as high quality animal feed. In summary, current productivities allow for biomass production with net zero or negative associated GHG emissions, eutrophication and other associated impacts. The Ramat Negev area alone holds sufficient resources for the production of about 20000 tons of high value algae biomass per year worth about \$ 100000000 per year under enhancing environmental and economic benefits. Such technology applied at the global scale will reduce global farm related emissions, and solve the looming water, food and land crisis.

## Maximizing TAG production for biodiesel production in Nannochloropsis Oceanica

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## Microalgal Biotechnology Lab, The French Associates Institute for Agriculture and Biotechnology for Drylands, J. Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev

Microalgae accumulate storage lipids (triacylglycerols, TAG) in lipid droplets (LDs) in response to environmental cues. Nitrogen availability and high light are considered as the major parameters impacting oil production. Aiming to maximize lipid productivity for biodiesel production in algal cultures of *Nannochloropsis oceanica*, manipulation of cultivation regime was tested both in one and two stage cultivation method.

To optimize high lipid productivity in *N. oceanica* we have first investigated the nitrogen-starvation response of cultures (two stage method), raised from either exponentially growing or early stationary inocula. When exposed to N starvation and high light (350 2mol photons m<sup>-2</sup>·s<sup>-1</sup>), TAG productivity is 60% higher over a starvation phase of 3 days versus a starvation phase of seven days, as dry weight and TAG content accumulation rates decrease after 3 days of starvation. Biomass and lipid productivities were 50% higher when using exponentially growing inoculum compared to early stationary inoculum. Moreover, for both inocula, increasing culture density by a factor of two further increased lipid productivity by a factor of three to a maximum of 0.45 g TFA/L/day. To conclude, adequate understanding of starvation physiology in Nannochloropsis allows enhancing oil productivity by over 5-fold. Furthermore, it is essential to use exponentially growing inoculum and adequately dense cultures during nitrogen starvation to obtain high lipid productivity by two stage cultivation of *N. oceanica*. Moreover, while increasing salinity level enhanced lipid productivity in one stage cultivation method, in two stage cultivation method it had the opposite effect.

Day 4 – Thursday, September 15<sup>th</sup> 2016

**Morning Session** 

## Utilizing photosynthetic complexes for solar energy conversion: Building a Bio-generator

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Photosynthetic organisms, membranes and complexes are attractive starting materials for solar energy conversion (SEC). Our overall goal is to develop methods to perform SEC using these materials in simple, inexpensive and totally non-polluting fashion. We have previously shown (Larom et al., PNAS, 2010) that a mutation in PSII in the cyanobacterium Synechocystis sp. PCC 6803 (Syn), results in a strain that has the enhanced ability to transfer electrons from water to electron carriers or to modified gold electrodes (Larom et al. Photosyn. Res. 2015). Here we show how the remarkable photocatalytic activity of the photosynthetic apparatus leads to overall water splitting with oxygen and hydrogen production in Bio-Photo-Electro-Chemical (BPEC) cells via the simplest and cleanest of deposition processes and without the need for sacrificial electron sources. With plant thylakoids, electrons are shuttled by FeCN to a transparent electrode, yielding a photocurrent density of 0.5 mA·cm-2. Hydrogen evolution occurs at the cathode at a bias as low as 0.8 V. A tandem cell comprising the BPEC cell with the thylakoid membranes and a Si photovoltaic module achieves overall water splitting with solar to hydrogen conversion efficiency of 0.3% (Pinhassi et al. PLOS One 2015 and Pinhassi et al. Nature Communications 2016). With cyanobacterial cells, following a brief treatment that does not kill the cells, electrons are transferred directly to a graphite electrode, utilizing endogenous electron carriers. The current produced can be used for hydrogen production at low additional bias for significantly longer durations than the plant thylakoids.

## Hybrid Bio-Photo-Electro-Chemical Cells for Solar Water Splitting

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Photoelectrochemical water splitting uses solar power to decompose water to hydrogen and oxygen. We showed how the photocatalytic activity of thylakoid membranes leads to overall water splitting in a Bio-Photo-Electro-Chemical (BPEC) cell via a simple process. Thylakoids extracted from spinach are introduced into a BPEC cell containing buffer solution with ferricyanide. Upon solar-simulated illumination, water oxidation takes place and electrons are shuttled by the ferri/ferrocyanide redox couple from the thylakoids to a transparent electrode serving as the anode, yielding a photocurrent density of 0.5 mA·cm-2. Hydrogen evolution occurs at the cathode at a bias as low as 0.8 V. A tandem cell comprising the BPEC cell and a Si photovoltaic module achieves overall water splitting with solar to hydrogen efficiency of 0.3%. These results demonstrate the promise of combining natural photosynthetic membranes and man-made photovoltaic cells in order to convert solar power into hydrogen fuel.

## From metal atoms to metal tips on photo-catalysts for hydrogen production

## Maya Bar Sadan

### **Ben Gurion University**

Correlating structure and function is fundamental for the design of functional materials. Specifically, the atomic rearrangement within a nanoparticle has a direct effect on its properties and overall performance as a building block. While synthetic efforts have succeeded in producing diverse complex materials, the rational design of new materials is still a challenge.

Our approach is using atomic resolution transmission electron microscopy to unravel the atomic structure of the particle, therefore allowing the understanding of the growth process and the origin of the functionality of the structures. We believe that by doing so, design rules can be offered to optimize the available nanoparticles for their designated role as functional units.

The above-mentioned rationale was used for understanding the enhanced activity of Au-Pd metal tips on seeded rods of CdSe@CdS, by studying the effects of structure both on efficiency and stability. In addition, I will present the evolution of the structures through the synthesis stages, showing how that atomic re-construction of the particles during the initial synthesis of the structures might have detrimental consequence on their stability. I will also discuss single atom dopant sites on semiconducting nanoflowers.

# Plant water-uptake effects on salt distribution near the root-soil interface

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The paradigm today is that when salinity increases beyond a certain threshold it will result in reduced crop yield at a fixed rate. Thus, there is a great importance of predicting salinization impact on crops. Current models do not consider the impact of environmental conditions on salt tolerance in plants, despite the conditions effect on plants water uptake and salts accumulation around the roots. Better parametrization of a model can help to improve predicting the real effects of salinity on crop growth and yield. The aim of this research is to study Na<sup>+</sup> distribution around roots at different scales by investigating different non-invasive methods, and study how this distribution is being affected by transpiration rate and plant water uptake. Results from tomatoes growing on Rhizoslides (capillary paper growth system), show that Na<sup>+</sup> concentration is higher at the root interface compared with the bulk. Also, Na<sup>+</sup> accumulation around the roots decreased under low transpiration rate. Rhizoslides allows to study roots' growth rate and architecture under different salinity levels. To observe the correlation of root system architectures and Na<sup>+</sup> distribution in 3 dimensions, we used Magnetic resonance imaging (MRI). MRI provides fine resolution of Na<sup>+</sup> accumulation around a single root, without disturbing the root system. With time, Na<sup>+</sup> was accumulating only where roots were found and later on around specific roots. These data are being used for model calibration, which is expected to predict root water uptake in saline soils for different climatic conditions and soil water availabilities. More up scaling measurements are being done in order to better understand Na<sup>+</sup> distribution around the roots.

## Granting heat tolerance to photosynthetic cells; The impact of point mutations in photosystem II reaction center

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The overarching goal of this work package is to generate photosynthetic organism that grow under stress conditions in open ponds. In our earlier studies we found that specific residues at the crossing domain of D1 and D2 protein subunits of PSII in cyanobacteria regulate the rate and yield of photosynthetic electron transfer. We have capitulated on this findings in three avenues: (1) Developing strains with double mutants in this domains and exploring the mechanism behind their thermotolerance and biomass generation compared with the wild type; (2) Resolve the mechanism of temperature control; (3) develop double mutants of this domain in higher organisms as a first step to crops production. We specifically explored growth under different temperatures and temperature cycles, light periodicity and light intensity, diurnal light regimen, normal and increase CO<sub>2</sub> concentrations. Finally, we initiated a pilot plan for comparing growth of the new strains in an outside open pool device, that mimics to a certain extent growth conditions presented by the Brazilian habitat.

We found out that the thermotolerance of the cyanobacteria double mutant involves modifications of the whole cell including pigment composition, changes in the level of heat shock proteins expression, cell morphology and membrane structure.

## Hematite photoanodes for solar water splitting

## **Daniel Grave and Avner Rothschild**

### **Technion - Israel Institute of Technology**

Hematite is a leading candidate for use as a photoanode material in tandem photoelectrochemical-photovoltaic (PEC-PV) cells for solar powered water splitting due to its stability in aqueous solution, 2.1 eV band gap, vast abundance, and low cost. However, the short diffusion length (2 – 20 nm) of photogenerated minority carriers in hematite results in massive bulk recombination. As a result, state-of-the-art devices fall far short of the theoretical efficiency. We employ a multifaceted approach towards solving this problem, starting with the growth and characterization of high quality model heteroepitaxial thin films with precisely controlled microstructures and compositions in order to gain insight into the fundamental processes limiting charge separation and collection. Using a combination of advanced characterization techniques and modelling, we determine routes for enhanced performance and couple them with innovative new device architectures at a full PEC-PV system level.

## Designer cellulosome technology: Where were we, where are we, and where do we want to be?

## **Ed Bayer**

### Department of Biological Chemistry, Weizmann Institute of Science

During the course of the I-CORE program, our group has developed and progressed immensely in our saga to extend and improve the concept of designer cellulosomes for (i) enhanced performance of these artificial multienzyme complexes and (ii) better understanding of cellulosome action. During the 5-year period of this consortium, we have extended the numbers of enzymes and other components that can be incorporated into these cellulosomes, including (i) expanded numbers of cohesindockerin specificities for integration of increased numbers of enzymes, (ii) the use of adaptor scaffoldins for further extensions of their numbers, (iii) additional integration of non-natural enzymes, notably oxidative enzymes, (iv) continued analysis of novel native cellulosomal components from newly discovered cellulosome systems, (v) improved thermostability of enzymes, cohesins and dockerins (and scaffoldins), and (vi) incorporation of cellulosome-relevant genes into host bacteria and metabolic engineering of bacterial pathways for biofuel production (e.g., ethanol and butanol). These studies have significantly contributed to our long-term efforts within the context of our aspirations to convert lignocellulosic biomass to biofuels.

## Engineering hyperthermophilic designer cellulosomes

## Amaranta Kahn, Johanna Stern, Sarah Moraïs and Edward A. Bayer

### Department of Biological Chemistry, Weizmann Institute of Science

Enzymatic breakdown of cellulose is the major challenge in the conversion of cellulose to biofuel. The use of thermostable enzymes has many benefits, as they are better suited for processing conditions. Caldicellulosiruptor bescii is one of the most thermophilic anaerobic bacteria, known to break down and ferment cellulose. We hypothesized that a trivalent scaffoldin comprising three cohesins coming from thermophilic bacteria, complexed with chimaeric dockein-bearing *C. bescii* enzymes will function at very high temperatures. We expect further that the resulting designer cellulosomes could be employed for high temperature reactions. In this study we used a tetravalent scaffoldin, consisting of three cohesins and a cellulose-binding module of thermophilic origin. The scaffoldin was combined with three thermophilic chimaeric enzymes, each fused with a dockerin whose specificity matched one of the cohesins. We then investigated the stability and activity of the individual enzymes, each bound to a monovalent scaffoldin, and of the three enzymes bound together to the tetravalent scaffoldin. We verified that the specific cohesin-dockerin pairs were stable and all complexes were stable and active for 24 h at 75°C. Finally, under these conditions, on microcrystalline cellulose as substrate, the combined individual enzymes are more active than the wild type enzymes, but the enzymes bound to the chimaeric scaffoldin were not further improved. The results of this study demonstrated that we can produce a highly thermostable designer cellulosome, but future work will focus on improving the synergy by examining enzyme position and composition.

## Metal-free efficient Cdot-C<sub>3</sub>N<sub>4</sub> composite photocatalyst for stable visible water splitting<sup>+</sup>

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The use of solar energy to produce molecular hydrogen and oxygen (H<sub>2</sub> and O<sub>2</sub>) from overall water splitting is a promising means of renewable energy storage. In the past 40 years, various inorganic and organic systems have been developed as photocatalysts for water splitting driven by visible light. These photocatalysts, however, still suffer from low quantum efficiency and/or poor stability. We report the design and fabrication of a metal-free carbon nanodot–carbon nitride (C<sub>3</sub>N<sub>4</sub>) nanocomposite and demonstrate its impressive performance for photocatalytic solar water splitting. We measured quantum efficiencies of 16% for wavelength  $\lambda$ = 420±20 nm, 6.29% for  $\lambda$  = 580±15 nm, and 4.42% for  $\lambda$  = 600±10 nm, and determined an overall hydrogen to solar energy conversion efficiency of 2.0%. The catalyst comprises low-cost, Earth-abundant, environmentally friendly materials and shows excellent stability. It enables production of H<sub>2</sub> for close to 4\$/kg, within the DOE target price.

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