Track 1: Resnick Sustainability Institute Abstracts

I. **Research in Sustainability at Caltech**
II. **Overview of Sustainable Energy Research Centers at Caltech**
III. **Research in Renewable Power and Fuel Generation at Caltech**

1. Research in Sustainability at Caltech:

Speakers discussed research efforts broadly in the realm of sustainability and sustainable energy use. Topics included H2 storage, battery and fuel cell technologies, water purification, materials for carbon sequestration, and studies of the effects of renewable energy use on the existing energy grid.

Materials for Fuel Cells: Creating a Sustainable Energy Future

Professor Sossina M. Haile

Fuel cells, with their high efficiencies and zero (regulated) emissions, have emerged as important technologies that may ensure a sustainable energy future. We describe here recent breakthroughs in the materials for fuel cells, particularly for intermediate temperature operation at which catalysis is rapid and hydrogen fuel is not required. We focus in particular on fuel cells based on solid acid electrolytes that offer the potential for Pt-free operation. New materials development efforts have led to the discovery of new proton conducting materials such as Ba3-xKxHx(PO4)2 whereas nanostructured electrodes of known materials (i.e. CsH2PO4) have been obtained using electrohydrodynamic atomization

Beyond plug-in hybrids: Fuel cell vehicles and onboard hydrogen storage

Dr. Channing Ahn

In the 2003 State of the Union address, the Freedom Fuel Initiative was launched so that "America can lead the world in developing clean, hydrogen-powered automobiles." Since the time of that Address, research and development into hydrogen production and distribution have taken a back seat to the on-board storage problem. Marketing demands of auto manufacturers dictate a 300-mile range for hydrogen powered fuel cell vehicles with a refueling process that mimics your present service station experience. Test vehicles that are presently on the road use high-pressure tanks to store hydrogen that are made of expensive carbon fiber composites. The goal of the Department of Energy's hydrogen storage program is to find alternatives to high-pressure tanks, in the form of chemical or metal hydride storage. These hydrides can store hydrogen at densities greater than liquid hydrogen avoiding some of the volumetric penalties that accompany compressed gas storage technology. Given the challenges of attaining both high gravimetric and volumetric hydrogen density storage and the thermodynamic limitations that effect refueling times, we will discuss some of the recent hydrogen sorbent developments, and strategies that are being considered for hydrogen storage for the transportation sector

Novel Metal-Air Batteries with Soluble Anodes Powering Electrical Vehicles
Dr. Kumar Bugga
This paper describes a collaborative proposal from Caltech/JPL and Quallion to ARPA-E to develop a novel high-energy rechargeable battery, well beyond the current versions of Li-ion batteries. Our proposed battery technology is based on the innovative concept of employing a solvated electron solution of an alkali metal as the liquid phase anode in an air-battery system. We have validated feasibility of this novel battery technology by demonstration cells with Li SE anodes, ceramic glass membrane electrolyte and air electrodes, attaining an operation voltage of ~ 3V. We propose to optimize chemical, structural and energetic aspects of metal-SE anodes and ceramic membranes using first-principles-based full-chemistry modeling and simulation to guide materials selection and configurations, followed by experimental applications of the most promising designs to develop optimized prototypes. This battery technology is expected to provide several advantages such as high energy density, fast electrode kinetics and good reversibility, high current rates, enhanced safety, and reduced cost that meets the DOE targets. This paper will describe some of the proposed approaches to meet these goals.

Multiscale modeling of geomaterials and its impact on sustainable energy and infrastructure
Asst. Professor Jose Andrade
Our research objective is to develop a fundamental understanding of the multiscale and multiphysical behavior of porous media, with especial application to geologic materials (e.g., soils, rocks) and engineered infrastructure materials (e.g., cements). With this objective in mind, the aim is to establish frameworks by which the microstructural features of porous materials affect macroscopic material properties. The main tools are mechanics, physics, computational mechanics, and advanced experimentation. In this talk, I will present current applications dealing with reactive flow in deformable porous media for sustainable energy (e.g., CO_2 sequestration), mechanics and physics granular materials for resilient infrastructure (e.g., liquefaction, landslides), and nanoscale modeling of calcium silicate hydrate (CSH) for sustainable construction materials (cements).

Solar-Driven Electrochemical and Electromechanical Approaches to Sustainable Water Treatment
Professor Michael R. Hoffmann
The need for alternative energy sources with reduced carbon footprints is growing. Solar-powered electrochemical or photo-catalytic systems, which produce hydrogen via water splitting using organic pollutants as sacrificial electron-donors, provide a possible solution to achieve two objectives. Hybridization of a BiO_x-TiO_2/Ti anodes with stainless steel or functionalized metal cathodes, powered by photo-voltaic (PV) arrays, have been shown to

achieve simultaneous water purification coupled with H2 generation. Hydrogen generation can be suppressed by purging the reactor system with air. A variety of other hetero-junction, mixed-metal oxide semiconductors have also been shown to be highly efficient electro-chemical catalysts for both anodic and cathodic electron transfer. The electrochemical degradation kinetics of a variety of organic substrates has been investigated as a function of the background electrolytes. Observed substrate degradation kinetics are found to correlate well with the cell current and the H2 production energy efficiencies in the presence of NaCl as the background electrolyte. In the case of Na2SO4, no correlation is observed and the degradation rates are reduced in comparison to NaCl even though hydroxyl radical production is increased. This suggests the primary oxidant is electrolyte-dependent. Observed rate constants are found to be proportional to previously-determined bimolecular rate constants of chlorine radical anion with a variety of substrates. Additional active chlorine species such as chlorine atom and hypochlorite, act as electron shuttles, which compete with H2 production for cathodic or conduction-band electrons. In the presence of the organic substrates, the active chlorine species are quenched increasing the fraction of electrons utilized for the H2 production. In the presence of sufficient oxygen, the primary electron acceptor is dioxygen with the subsequent formation of superoxide and hydrogen peroxide. Peroxide reacts with an additional electron to produce hydroxyl radial and hydroxide at the cathode. Water is oxidized to hydroxyl radical and hydrogen peroxide at the anode. Solar-powered ultrasonic irradiation can also be employed as an advanced oxidation/reduction process for water purification via acoustic cavitation.

On load-shedding probabilities of power systems with renewable power generation and energy storage

Dr. Ufuk Topcu

The integration of renewable energy resources, such as solar and wind power, into the electric grid is made difficult due to source intermittency and physical distances between generation sites and users. These difficulties may be alleviated by effectively utilizing energy storage. We consider, as a case study, the integration of renewable resources into the electric power generation portfolio of an island off the coast of Southern California, Santa Catalina Island, and investigate the feasibility of replacing diesel generation entirely with solar photovoltaics (PV) and wind turbines, supplemented with energy storage. We use a simple storage model alongside a combination of renewables and varying load-shedding characterizations to determine the appropriate number of PV cells, wind turbines, and energy storage capacity to remain below a certain threshold probability for load-shedding over a pre-specified period of time.

2. Overview of Sustainable Energy Research Centers at Caltech:

This session gave an overview of several centers for renewable and sustainable energy research currently established on campus. This includes the Resnick Institute, Powering the Planet Center for Chemical Innovation (CCISolar), the Energy Frontier Research Center on light-matter interactions, and the newly awarded DOE solar fuels hub, the Joint Center for Artificial Photosynthesis.

Keynote:

The Joint Center for Artificial Photosynthesis

Professor Nate Lewis, Director

On July 22, the U.S. Department of Energy (DOE) announced an award of up to $122 million over 5 years to a multidisciplinary team of scientists to establish an Energy Innovation Hub with the goal of generating fuels directly from sunlight. The Joint Center for Artificial Photosynthesis, led by Caltech in partnership with the DOE's Lawrence Berkeley National Laboratory, will bring researchers together in an effort to simulate nature's photosynthetic apparatus for practical energy production. The goal is to develop an integrated solar energy-to-chemical fuel conversion system and move that system from the bench-top discovery phase to commercial scale.

The Resnick Institute: Science + Energy + Sustainability

Dr. Neil Fromer, Executive Director

The mission of the Resnick Institute is to foster transformational advances in energy science and technology through research, education and communication. The Resnick Institute strives to identify and address the most important outstanding challenges and issues in the generation, storage, transmission, conversion and conservation of energy.

The Light-Material Interactions in Energy Conversion EFRC

Professor Harry Atwater, Director

The "Light-Material Interactions in Energy Conversion" Energy Frontier Research Center (LMI-EFRC) is a national resource for fundamental optical principles and phenomena relevant to solar energy conversion, and for design of the optical properties of materials and devices used for energy conversion. The LMI-EFRC features a team that spans the campuses of Caltech, Berkeley and Illinois, and creates a foundational partnership between scientific leaders in optical properties of matter with experts in solar photovoltaic and photochemical energy conversion and innovators in the design and fabrication of novel electronic and photonic materials.

The Powering the Planet Center for Chemical Innovation

Dr. Siddharth Dasgupta, Managing Director

The Powering the Planet Center for Chemical Innovation (CCI Solar) focuses on one of the outstanding problems in 21st Century science – the efficient and economical conversion of solar energy into stored chemical fuels. Through this CCI, the NSF has established a partnership with the scientific community to develop the fundamental enabling chemistry that will ultimately deliver clean fuels produced from the sun.

The Caltech-KAIST collaboration on energy environment water sustainability

Dr. Andres Jaramillo-Botero

The Materials and Process Simulation Center at Caltech (MSC) directed by Prof. Goddard has established a research collaboration with KAIST (Korea Advanced Institute of Science and Technology) to use first principles based simulations to develop new materials for new generations of batteries, fuel cells, and photovoltaics and new catalysts for CH4 conversion, CO2 reduction, and new materials for storage and transport of H2, CH4, and CO2. In addition the MSC is collaborating with the Caltech-KAIST global water initiative developing new materials for water treatment (removal of toxic anions and cations, desalination)

3. Research in Renewable Power and Fuel Generation at Caltech:

Speakers discussed research efforts at Caltech on a range of different technologies related to the renewable generation of electricity or fuel. Topics included improvements to silicon PV efficiency, generation of power from thermoelectric devices and wave power, and generation of fuels directly from sunlight and from biological systems.

Pushing the Limits of Fundamental Energy-Relevant Materials Properties via Nanoscale Design

Professor Jim Heath

There are several cases in which a fundamental limit to a physical property is well-defined by physical laws, but extremely difficult to achieve through materials design. In this talk, I discussed two such limits, and how architectural control over the structure of a simple material can be harnessed to reach those limits. The first involves the theoretical limit on the maximum electrical current that can be passed through a superconductor. This is the depairing limit, and is defined as the point at which the kinetic energy of the charge carriers exceeds the superconducting condensation energy. This limit has been previously achieved only for transient currents, or in superconductors very near the transition temperature. I described a nanostructured Nb thin film that achieves the depairing current limit robustly, continuously, and over a broad temperature range. I also described the rationale for the design of that film. A second limit involves the lower limit on the thermal conductivity of a single component system. This is typically referred to as the amorphous limit. I discussed how single crystal Si thin films, designed as phononic materials with precise architectural features at the nanoscale, can be designed to reach, and, in a way, beat this amorphous limit, without detrimentally influencing other parameters, such as the electrical conductivity. Implications for thermoelectric-based energy conversion will be discussed.

Thermoelectric Materials Engineering at Caltech for Sustainable Waste Heat Recovery and HVAC

Dr. Jeff Snyder

A thermoelectric generator directly converts heat into electricity with no moving parts. Thermoelectrics could provide a substantial amount of electrical power from residential cogeneration and waste heat recovery from sources such as automotive exhaust. When connected to an external power supply, a thermoelectric generator becomes a solid-state refrigerator, cooling one end and heating the other. Such systems can be used to cool only when and where needed instead of traditional environment cooling thereby greatly improving overall efficiency. Materials research at Caltech focuses on improving the thermoelectric efficiency of the material using crystal chemistry, band structure engineering and nanostructured composites.

Si Microwire-Array Solar Cells

Dr. Morgan Putnam

Vertically aligned arrays of crystalline-Si (c-Si) microwires provide a promising pathway for the development of efficient, crystalline Si photovoltaics with thin-film fabrication costs. These Si wire arrays can be grown using thin-film deposition techniques and require only 1/100th the Si of a traditional Si-wafer-based solar cell. Here we will report on recent developments that have allowed for the fabrication of photovoltaic devices with Voc of 500 mV, Jsc of 24. mA/cm2, and FF > 65%, yielding photovoltaic efficiencies of 7.9%. Detailed analysis of these devices suggests that photovoltaic efficiencies > 15% should be possible with improved fabrication techniques.

Si Microwires for photoelectrochemical water splitting

Emily Warren, Professor Nate Lewis

Silicon wire arrays grown by the vapor-liquid-solid (VLS) mechanism are a promising material for the creation of low cost and efficient photovoltaic and photoelectrochemical devices. Our goal is to use silicon microwires as the photocathode material in a photoelectrochemical water splitting system that will use sunlight and water as the inputs to produce renewable hydrogen with oxygen as a by-product. The high aspect-ratio semiconductor rod electrode architecture allows for the use of low cost, earth abundant materials without sacrificing energy conversion efficiency due to the orthogonalization of light absorption and charge-carrier collection. Additionally, the high surface-area design of the rod-based semiconductor array inherently lowers the flux of charge carriers over the rod array surface relative to the projected geometric surface of the photoelectrode, thus lowering the photocurrent density at the solid/liquid junction and thereby relaxing the demands on the activity (and cost) of any electrocatalysts needed to drive chemical reactions. This talk will discuss progress that has been made towards the fabrication of silicon microwire photocathodes decorated with hydrogen evolution catalysts.

From Enzymes to Small Multimetallic Complexes in the Context of Energy Conversion

Asst. Professor Theodor Agapie

Increase in global energy consumption coupled with environmental challenges related to increased amounts of carbon dioxide in the atmosphere drive the need for carbon neutral energy production and energy efficient chemical transformations. In this context, catalysis is the basis for the development of technologies for renewable energy conversion and energy efficient chemistry. The conversion of energy in biological systems involves reactions at multimetallic enzyme active sites. With the biological systems as source of inspiration, small multimetallic molecular catalysts are designed and prepared. Our progress in the synthesis and characterization of these species will be presented.

Structure-guided recombination generates highly stable families of synthetic cellulases

Dr. Christopher Snow

The economic viability of enzymatic biomass-to-biofuel conversion processes is limited by the short lifetimes of industrial cellulases at the high temperatures preferred for biomass conversion. Accordingly, we employ protein recombination as a method of engineering more thermostable synthetic cellulase enzymes. The recombined protein segments make reasonably independent contributions to stability. As a result, we can predict the most stable recombinants after measuring the stability of a small fraction of the chimeric library. This approach is being used to generate dozens of new, highly stable cellulases including both cellobiohydrolases and endoglucanases.

Wave Rectifying Water Channel: A Novel Approach to Ocean Wave Energy Conversion

John Meier, Professor Mory Gharib

Extracting useful energy from oscillatory flows, such as ocean waves, is an important engineering challenge in fluid dynamics. Massive amounts of energy travel in the form of ocean waves and terminate on shorelines across the world, but the energy does not exist in a form we are familiar with extracting. In this study, we investigate an entirely new mechanism in the form of a wave rectifying channel that converts a periodic disturbance normal to the free surface to unidirectional flow around a suspended plate. The technique was inspired by a resonance based pumping phenomenon known as impedance pumping. A bench top experiment was carried out in a long, narrow channel with a total liquid volume of 3.3 L. The free surface was excited at frequencies of 1 Hz to 2.8 Hz and flow behavior was investigated using dye visualization and DPIV. We discuss system parameters such as channel geometry and excitation profile as they relate to wave reflections, wave interactions, and overall system performance. A simple scaling argument estimates a 100 m beach or breakwater installation could produce on the order of 1 MW of power.