Wednesday Afternoon, November 11, 2009

Energy Frontiers Research Centers
Room: A8 - Session EN-WeA

Energy Frontiers Research Centers
Moderator: E.S. Aydil, University of Minnesota

2:00pm **EN-WeA1 "Nano" Solutions to "Macro" Energy Problems**, ***V.I. Klimov***, Los Alamos National Laboratory **INVITED**

In this presentation, I will review some of our work on novel nanostructured materials and new nanoscale physical phenomena related to the problem of high-efficiency conversion of solar light into electrical or chemical energy. Specifically, I will discuss topics such as carrier multiplication (multiple exciton generation by single photons), plasmonic and photonic effects for improved light harvesting, and exploratory device structures comprising nanocrystal quantum dots. I will also give a brief overview of our newly funded Energy Frontier Research Center (EFRC) for Advanced Solar Photophysics where some of these problems are being tackled.

2:40pm **EN-WeA3 Understanding Charge Separation and Transfer at Interfaces in Energy Materials and Devices**, ***P.F. Barbara***, University of Texas, Austin **INVITED**

This seminar focuses on our recently constructed research program, selected for funding by the U.S. Department of Energy as an Energy Frontier Research Center (EFRC), that is uniquely well-suited to critically advance the fundamental understanding of interfacial charge separation and transfer processes in nanostructured organic photovoltaic (OPV) and electrical energy storage (EES) materials. Current limitations in the basic scientific understanding of charge separation and transfer processes in these materials represent a major scientific roadblock to achieving U.S. energy security. The mechanistic understanding of these processes in nanomaterials is in its infancy, without a broadly accepted theoretical description. Moreover, existing experimental tools and theoretical models are insufficient to definitively address the many outstanding scientific issues for the complex nanomaterials in this field. Instead, completely new multidisciplinary approaches, featuring greater molecular-level precision and accuracy and closer coupling between theory and modeling, are necessary to drive the fundamental aspects of this field forward. Therefore, we have constructed an EFRC research program that is based on two critical strategies: (i) We will support a set of coordinated research projects that study unique and novel interfacial prototypes that climb the ladder of molecular complexity from well-defined epitaxial crystal/crystal interfaces, through isolated crystal/crystal interfaces, to model polymer/crystal interfaces and then to actual OPV and EES devices. (ii) We will use powerful, state-of-the-art imaging and sub-ensemble methods (e.g., single particle spectroscopy and imaging) to make correlated measurements of structure and charge separation/transfer processes on the molecular scale for each type of interfacial prototype. Experimental data obtained by means of these two strategies will be modeled and analyzed by advanced theoretical and computational methods, leading to new insights on the molecular-level mechanisms of charge separation and transfer functions of complex OPV and EES nanostructured materials. This seminar will introduce the three major research thrusts of our EFRC (interfacial charge separation, interfacial charge transfer and Li^+-coupled charge transfer) and describe ongoing research projects within these three thrusts. If successful, this EFRC will produce three important outcomes: (1) new OPV and EES materials that are rationally designed to be substantially more efficient than current state-of-the-art materials; (2) a new suite of molecular-level tools to be used both in academia and in industry to evaluate and optimize these new molecular materials; and (3) the education of a new generation of energy researchers who are trained to produce these materials and utilize these molecular tools.

4:00pm **EN-WeA7 The Center on Nanostructuring for Efficient Energy Conversion (CNEEC) at Stanford directed by Stacey Bent and Fritz Prinz**, ***F.B. Prinz***, Stanford University **INVITED**

The center will identify ways in which high gradients, high surface to volume ratios and and low dimensionality can improve materials properties such as light absorption, charge transport, and catalytic activity.

This talk will outline strategies and plans for tuning thermodynamics/kinetics, photon management, and optimizing transport at reduced dimensions that may lead to improved photovoltaic devices, fuel cells, and batteries.

4:40pm **EN-WeA9 Excitonics**, ***M.A. Baldo***, Massachusetts Institute of Technology **INVITED**

Conventional electronic devices can be difficult to manufacture; their constituent materials require very high levels of order and achieving such low entropy in a semiconductor requires expensive and energy intensive fabrication. For example, the energy payback time for a crystalline silicon solar cell is on the order of 2 years, and at current manufacturing growth rates, it is expected to take at least 20 years to produce enough silicon-based solar cells to make a significant impact on the world energy supply.[1] Similarly, epitaxial growth constraints are likely to limit solid state lighting sources to a small fraction of the overall demand for lighting. There is an alternate approach that is more suitable for large scale production. In the new Energy Focused Research Center (EFRC) for Excitonics, we address materials with only short-range order. Such nanostructured materials are compositions of nano-engineered elements such as organic molecules, polymers, or quantum dots and wires, in films bound together by weak van der Waals bonds. These materials are characterized by *excitons* that are *localized* within the ordered nanostructures. Excitons provide a unique means to transport energy and convert between photons and electrons. Due to localization of excitons, the optical properties of the films are relatively immune to longer-range structural defects and disorder in the bulk. And in contrast with the painstaking growth requirements of conventional semiconductors, weak van der Waals bonds allow excitonic materials to be readily deposited on a variety of materials at room temperature. We address two grand challenges in excitonics: (1) to understand, control and exploit exciton transport, and (2) to understand and exploit the energy conversion processes between excitons and electrons, and excitons and photons.

References 1. Lewis, N. S. & Crabtree, G. (eds.) *Basic Research Needs for Solar Energy Utilization* (U.S. Department of Energy, http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf, 2005).

5:20pm **EN-WeA11 Excitonic Charge Separation at Interfaces**, ***X. Zhu***, University of Texas, Austin **INVITED**

When a molecular or nano material is electronically excited by a photon, the Coulomb attraction between the excited electron and the hole gives rise to an atomic-H-like quasi-particle called an exciton. The bound electron-hole pair also forms across a material interface, such as the donor/acceptor (D/A) interface in an organic heterojunction solar cell; the results are charge-transfer (CT) excitons. In a conventional p-n junction cell, the exciton binding energy is very small and there is a built-in potential to ensure charge separation. In contrast, there is not a priori a built-in potential in an excitonic solar cell based on organic molecules, polymers, or inorganic quantum dots. In this talk, I will attempt to address key factors determining charge separation in two model systems: organic semiconductor interfaces and inorganic quantum dot/electron conductor interfaces. I will highlight the roles of excess electronic energy and strong electronic coupling in determining excitonic charge separation.

Muntwiler, M.; Yang, Q.; Tisdale, W. A.; Zhu, X.-Y. *Phys. Rev. Lett.* **2008**, *101*, 196403.

Zhu, X.-Y.; Yang, Q.; Muntwiler, M. *Acct. Chem. Res.* **2009**, *42*, published on web 04/21/09.

Williams, K. J.; Tisdale, W. A.; Leschkies, K.; Haugstad, G.; Norris, D. J.; Aydil, E. S.; Zhu, X.-Y. *ACS Nano* **2009**, 3, 1532-1538.

Tisdale, W. A.; Williams, K. J.; Timp, B. C.; Norris, D. J.; Aydil, E. S.; Zhu, X.-Y. *to be published.*

Authors Index

Bold page numbers indicate the presenter