Electronic Materials and Photonics Division
Room A214 - Session EM+2D+NS+TF-WeA

THEME Session: Electronics and Photonics for a Low-Carbon Future

Moderators: Michael A. Filler, Georgia Institute of Technology, Stephen McDonnell, University of Virginia

2:20pm **EM+2D+NS+TF-WeA-1 Uncovering the Materials Paradigm for Solar Absorbers through In situ Imaging and Characterization***, Mariana Bertoni,* Arizona State University **INVITED**

The behavior of solar cells is very often limited by inhomogeneously distributed nanoscale defects. This is the case throughout the entire lifecycle of the solar cell, from the distribution of elements and defects during solar cell growth as well as the charge-collection and recombination during operation, to degradation and failure mechanisms due to impurity diffusion, crack formation, and irradiation- and heat-induced cell damage This has been known for a while in the field of crystalline silicon, but inhomogeneities are far more abundant in polycrystalline materials, and are the limiting factor in thin-film solar cells where grain sizes are often on the order of the diffusion length.

We will show that the high penetration of hard X-rays combined with the high sensitivity to elemental distribution, structure, and spatial resolution offers a unique avenue for highly correlative studies at the nanoscale. We will present results on CdTe and Cu(In,Ga)Se_2 where carrier collection is directly correlated to the compositional and structural properties of the material under a large variety of synthesis and operating conditions. The segregation of copper at the grain boundaries of both solar absorbers will be discussed in detail as well as the defects impact to carrier collection efficiency. Furthermore, the kinetics of copper segregation during growth and processing will be presented.

3:00pm **EM+2D+NS+TF-WeA-3 Atomic Layer Deposition's Potential in Sustainability***, Karen Buechler,* ALD NanoSolutions **INVITED**

Atomic layer deposition (ALD) is an exciting thin film deposition technique which holds the promise to permit enormous material innovations. These material innovations are currently enabling advanced catalysts, high capacity energy storage, advanced manufacturing technologies and many other products. Many of these products work towards reducing energy needs. This talk will highlight several examples of advanced material development through ALD which lead to advanced products which in turn are reducing the carbon footprint of consumers and manufacturers.

4:20pm **EM+2D+NS+TF-WeA-7 Challenges in Materials and Processing to Implementation of Energy Efficient SiC Technology***, Mei-Chien Lu,* Monte Rosa Technology

Energy and sustainability have been the main driving forces for the implementation of silicon carbide technology for efficient energy conversion in recent applications in electrical vehicles, hybrid electrical vehicles, data center power management, and photovoltaic and wind power. The decades-long research and development efforts are attributed to the complexity of polytypes of crystal structures of silicon carbide. Reducing these inherent defects from crystal growth and epitaxial layer growth are crucial and continuing tasks. Device architectures are found to be more efficient along selected crystal planes. Innovative processing technologies have to be developed to make these devices built by compound semiconductors with strong covalent bonding manufacturable. Fundamental challenges in materials, devices, and processing technologies will first be briefed. A patent landscape analysis is then conducted herein to reveal the past trends to pave the paths for future research and development. Implementations of silicon carbide devices are in its infancy with some full SiC inverter adopted by a commercial electrical vehicle manufacturer. Market shares and momentum of silicon carbide power electronics as well as the expectations from perspectives of department of energy and industry major players will be discussed. The continuous efforts to address the challenges in materials and processing are encouraged to support the full scale implementation of energy efficient silicon carbide technology.

4:40pm **EM+2D+NS+TF-WeA-8 High Efficiency of Hot Electron Transfer at a Metal-Insulator-Semiconductor to Electrolyte Interface***, Hyun Uk Chae, R Ahsan, Q Lin, R Kapadia,* University of Southern California

Hot electrons generated from metal has drawn considerable interest in recent years due to the potential for lowering the high-barrier chemical reactions. The majority of hot electron controlling strategy at present have been plasmonic devices using localized surface plasmon resonance (LSPR). Several works have been done using plasmons to induce the hot electron generation to use as catalysts for chemical reactions like hydrogen evolution reaction (HER). However, the efficiency of those devices is extremely low and the mechanism behind it is quite complicated and remain unclear until now. To take advantage of hot electrons efficiently, properly and simply designed devices are required. Here, we demonstrate the different mechanisms of hot electron transfer in a thin gold film in an Au-Al_2O_3-Si metal-insulator-semiconductor (MIS) junction by modulating Au film thickness, the applied voltage between Au-Si junction. Hot electron injection contributes to modifying the electron distribution inside the Au electrode, which enables HER to be driven more at same overpotential in solution. This work present that the injection of non-equilibrium electrons can shift the onset voltage of HER by ~0.6 V on the gold film in a 0.5 M H_2SO_4 solution. The efficiency of hot electron density efficiency shows ~85% at 2V of MIS junction bias and solution bias of -1.5 V vs Ag/AgCl is also presented. In addition to experimental results, we carried out the 2-D Monte Carlo simulation to track the injected hot electrons to study for the detail behaviors of thermalization mechanism inside the Au region which indicates the rate of HER. Since electrons quickly lose their energy within femtosecond by electron-electron or electron-phonon scattering, it is significant to see how they behave inside the injected medium to understand the reactions more precisely. The high-efficiency of hot electron usage reported here can be an opening towards the creation of practical hot-electron devices, which could be widely applied to the various fields.

5:00pm **EM+2D+NS+TF-WeA-9 Integrated Photocathodes for Solar Driven Conversion of Carbon Dioxide to value-added Products***, Joel Ager,* Lawrence Berkeley Lab, University of California, Berkeley **INVITED**

If renewable power sources such as solar and wind could be used to produce chemical precursors and/or fuels, it would provide an alternative to mankind's unsustainable use of fossil fuels and slow the rate of CO_2 emission into the atmosphere [1,2]. Solar to chemical energy conversion by photoelectrochemical processes is a promising approach to address this challenge. Analogous to photovoltaics [3], driving the uphill redox reactions required for net solar to chemical energy conversion necessitates directional charge transport [4]. Additionally, in order to convert carbon dioxide to hydrocarbons, one must manage multi-electron transfer reactions (e.g. 12 in the case of ethylene and ethanol), and minimize potential losses in all parts of the system [5].

Charge selective contacts can be used to steer direct photo-generated carriers to catalytic sites that perform CO_2 reduction in an integrated photocathode. In contrast to conventional photocathode designs which employ p-type absorbers, we used a back illumination geometry with an n-type Si absorber to permit the use of absorbing metallic catalysts which would otherwise block the light. Back and front interfaces were configured by ion implantation and by surface passivation to achieve carrier selectivity. Surface texturing of the Si was used optimize light absorption on the illuminated side and increase the surface area available for catalysis on the electrolyte side. Selectivity to C-C coupled products was achieved by using hierarchical Au- Ag-Cu nanostructures as electrocatalysts [6].

The photovoltage, 550- 600 mV under simulated 1-sun illumination, confirms the carrier selectivity and passivation of the front and back interfaces. Compared to planar controls, textured photocathodes generate higher current densities, exceeding 30 mA cm^{-2}. Under simulated diurnal illumination conditions, over 60% faradaic efficiency to C_{2+} hydrocarbon and oxygenate products (mainly ethylene, ethanol, propanol) is maintained for several days. By coupling photocathodes to series-connected semi-transparent halide perovskite solar cells, we demonstrated stand-alone, CO_2 reduction with a 1.5% conversion efficiency to hydrocarbons and oxygenates [7].

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2. Chu, S.; Cui, Y.; Liu, N. *Nat. Mater.***2016**, *16*, 16–22.

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5:40pm **EM+2D+NS+TF-WeA-11 Modeling of Optical Scattering in White Beetle Scales**, ***Seung Ho Lee***, *S Han, S Han,* University of New Mexico

Keywords: Light Scattering; Diffusion Approximation

Abstract: Extremely thin “super-white” coatings that reject solar spectrum but radiate through the transparent atmospheric window in mid-infrared have broad implications in heat management and energy savings for diverse sectors, including building construction, ship manufacturing, and space vehicle operation. In our previous work, we were able to create paint-format “super-white” coatings from microsphere-based materials.[1,2] In this work, however, we borrow our inspiration from white beetles in nature that reveal structural ingenuity at the nanometer scale to achieve such white film. White beetle scales display exceptionally strong light scattering power from a thin anisotropic random biopolymer network. While previous studies have revealed that the anisotropy plays an important role in strong light scattering, the physics of anisotropic light propagation remains less than fully understood. In particular, the studies have shown that light scattering in anisotropic random media may deviate significantly from the anisotropic diffusion approximation. This uncertainty in diffusion approximation led to a study interrogating the scale structures by fully solving Maxwell’s equations. These calculations yet left questions on their accuracy, as the structural dimensions in perpendicular direction to the incident light were significantly greater than optical wavelengths. In this work, we systematically reduce the structural size in our simulations, using Fourier analysis of the white beetle scale structures. The size reduction enables fast, accurate calculations of light scattering in the biological structures. From these simulations, we find that the diffusion approximation is valid in describing light propagation in the white beetle scales. Further, we derive a light diffusion equation for anisotropic media from the radiative transfer equation and show that the equation for anisotropic diffusion derived in the past studies is inaccurate. We discuss how our newly derived equation can be used for accurate numerical calculations of light scattering and characterizing anisotropic light diffusion.

[1] S. Atiganyanun, J. Plumley, S. J. Han, K. Hsu, J. Cytrynbaum, T. L. Peng, S. M. Han, and S. E. Han, "Effective Radiative Cooling by Paint-Format Microsphere-Based Photonic Random Media," *ACS Photon.***5,** 1181-1187 (2018).

[2] J. D. Alden, S. Atiganyanun, R. Vanderburg, S. H. Lee, J. B. Plumley, O. K. Abudayyeh, S. M. Han, and S. E. Han, "Radiative Cooling by Silicone-Based Coating with Randomly Distributed Microbubble Inclusions," *J. Photon. Energy***9,** 032705-1:10 (2019).

6:00pm **EM+2D+NS+TF-WeA-12 Boosting the Performance of WO_3/n-Si for Photo-electrochemical Water Splitting: From the Role of Si to Interface Engineering**, ***Yihui Zhao***, Electrochemical Materials and Interfaces (EMI), Dutch Institute for Fundamental Energy Research (DIFFER), The Netherlands*; A Bieberle-Hütter,* Electrochemical Materials and Interfaces (EMI), Dutch Institute for Fundamental Energy Research (DIFFER),The Netherlands, The Netherlands*; G Brocks,* Center for Computational Energy Research, Department of Applied Physics, Eindhoven University of Technology; Computational Materials Science, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, The Netherla, The Netherlands*; H Genuit,* Dutch Institute for Fundamental Energy Research (DIFFER), The Netherlands*; R Lavrijsen,* Physics of Nanostructures and Center for NanoMaterials (cNM), Department of Applied Physics, Eindhoven University of Technology, The Netherlands

Metal oxide/Si is a promising model for designing high performing electrodes for photo-electrochemical (PEC) water splitting applications. This research provides a fundamental understanding of how and how much the Si contributes to the PEC process in a metal oxide/Si electrode. Applying separated monochromatic UV and IR illumination as well as an Ag interface layer in a WO_3/n-Si heterostructure, we find that the band bending depth in Si, which determines the photovoltage, plays a dominant role. This discovery breaks through the existing design ideas, which focused on facilitating charge transport via interface layers within the Z-scheme, but ignored the resulting changes in the band structure of Si. Based on this discovery, we use a Pt interface layer to enlarge the extent of the n-Si band bending. The resulting WO_3/Pt/n-Si photoelectrodes exhibit a 2 times higher photocurrent density at 1.23 V vs RHE and a 10 times enhancement at 1.6 V vs RHE compared to WO_3/n-Si. In addition, we found that the native SiO_2 layer at the interface prevents Fermi level pinning in the Schottky contact between the Si and the metal. These discoveries should guide future design of metal oxide/Si electrodes for PEC applications.

Author Index

Bold page numbers indicate presenter