

Tuesday Afternoon, November 10, 2009

Nanometer-scale Science and Technology

Room: A8 - Session NS1+PV-TuA

Organic Photovoltaics I

Moderator: P. Sharps, Emcore Corporation

2:00pm **NS1+PV-TuA1 Probing Polymer Photovoltaics: Imaging Photocurrents and Controlling Morphology in Organic Solar Cells.** *D.S. Ginger*, University of Washington **INVITED**

Organic solar cells are a potential low-cost alternative to conventional inorganic photovoltaics. The most successful organic solar cells rely on nanoscale phase separation between different components to achieve high efficiencies. Understanding and controlling nanoscale film structure has thus become the central challenge that affects every aspect of the field, from the optimization of new low-bandgap polymers to early efforts to scale up manufacturing of polymer solar cells. Our group has pioneered several scanning-probe methods, including time-resolved electrostatic force microscopy (trEFM) and photoconductive atomic force microscopy (pcAFM), as tools to characterize active organic solar cells. We discuss applications of these tools to study several model polymer systems, including the local origin of the photocurrent in polyfluorene blends, the effect of annealing on the formation of hole transport, electron transport and photocurrent collection networks in the archetypal polythiophene (P3HT) fullerene (PCBM) system, and the role that mesoscopic PCBM crystallites play in polyfluorene-copolymer/PCBM cells during solvent-vapor annealing. These data show the power of scanning-probe methods in correlating morphology with performance, and underscore the need to model these devices as fully 3D networks, rather than as uniform 2D semiconductor slabs.

2:40pm **NS1+PV-TuA3 Nanoscale Confinement Induced 3-D Chain Alignment of Poly (3-hexylthiophene) for Organic Solar Cells.** *M. Aryal, K. Trivedi, W. Hu*, University of Texas at Dallas

Organic semiconducting polymers are of wide interests for many applications in organic solar cells, field effect transistors, light emitting diodes, and biosensors. The optical and electrical properties of these polymers are anisotropic which largely depends on their nanoscale morphology, crystallinity and the direction of chain configuration. Furthermore, control over direction of chain orientation is essential as certain devices prefer chain alignment in certain directions as determined by device structures, e.g. vertical alignment for solar cells where vertical charge transport occurs, while for FETs, lateral orientation along the channel is preferred instead. Though the significant progress has been made by the development of varieties of techniques for control of nanoscale morphology, crystallinity and orientation of polymer chains for years, the perfect crystallization and preferred chain ordering in nanoscale regime still remains challenging. We report the fabrication of highly-ordered nanostructure arrays of nanopillars and nanogratings in poly (3-hexylthiophene) (P3HT) using nanoimprint lithography and show 3-D chain ordering by x-ray diffraction (XRD) analysis. We have proved for the first time that nanoscale confinement exerted by the mold can induce only one possible configuration of the chain network in the three dimensional P3HT nanostructures during thermal nanoimprint process. Such monodical 3-D chain configuration strongly depends on the geometry of the nanoconfinement. Interestingly the configuration is arranged in a favorable way for solar cell and FET applications, e.g. vertical chain alignment, and π -stacking along gratings.

In this report, uniform 80 nm thin films of regioregular P3HT were prepared on a Si substrate. The nanograting of 200 nm height, 65 nm wide gratings at a period of 200 nm while hexagonal array of nanopillars of 150 nm high nanopillars with 80 nm diameter were fabricated using nanoimprint lithography. The P3HT nanostructures were characterized by SEM and crystallization and chain orientation were studied by both in-plane, out-of-plane and in-plane grazing incident XRD. The chain ordering of thin film, nanopillar and nanograting structures are proved to be entirely different. The conjugated polythiophene backbones which are horizontal to the substrate in the thin film are reordered into vertical direction in the imprinted structures of P3HT. The interaction of hexyl side chains with hydrophobic mold surface in turn results π -stacking along nanogratings. We will present XRD results analysis and expect to present solar cell device results using these imprinted P3HT nanostructures.

3:00pm **NS1+PV-TuA4 Porphyrin-Gold Junctions in Molecular Optoelectronics.** *S.U. Nanayakkara*, University of Pennsylvania, *P. Banerjee*, University of Maryland, *D. Conklin*, University of Pennsylvania, *T.-H. Park*, University of Michigan, *M.J. Therien*, Duke University, *D.A. Bonnell*, University of Pennsylvania

Photo-conductance in novel multi-chromophoric molecules with porphyrin centers has been measured. This class of molecules is fully conjugated optical absorption properties that induce hole mediated conductivity with delocalization lengths on the order of 8 nm. Conjugated linker groups that terminate with a thiolate functionality (on one or both sides of the molecule) enable facile, co-valent attachment to a gold surface. We have attached these multi-chromophoric molecules between surface-bound Au nanoparticles and have measured transport as a function of varying laser excitation wavelengths. Additionally, we have measured spatially varying, charge transport in individual molecules within a tunneling junction utilizing a laser-coupled ultra-high vacuum scanning tunneling microscope. The wavelength dependent conductance will be discussed within the context of the molecule-Au junction.

4:00pm **NS1+PV-TuA7 Torsional Defects in Conjugated Polymers: Modeling and Nanostructured Photovoltaic Materials.** *S.B. Darling, M. Sternberg*, Argonne National Laboratory **INVITED**

Conjugated polymers represent a promising class of organic semiconductors with potential applications in a variety of molecular devices. Poly(3-alkylthiophene)s, in particular, are garnering interest due to their large charge carrier mobility and band gap in the visible region of the spectrum. Defects play a pivotal role in determining the performance of polymer electronics, and yet the function of specific types of defects is still largely unknown. Density functional theory calculations of alkyl-substituted oligothiophenes are used to isolate the effect of static inter-ring torsion defects on key parameters such as electronic coupling between rings and band gap. These polymers are often modeled with very short backbones and without their side chains. These results demonstrate the shortcomings of this approach for modeling torsional disorder and identify a minimal acceptable model.¹ Two experimental systems, one based on block copolymers and the other on a hybrid oxide nanotube-polymer system, with nanoscale morphology rationally designed to minimize torsional disorder will also be discussed. Results have potential implications both for the fundamental understanding of intramolecular charge transport and for improving processing in organic optoelectronic devices.

¹ Use of the Center for Nanoscale Materials was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract #DE-AC02-06CH11357.

5:00pm **NS1+PV-TuA10 Locally Probing the Efficacy of Photoinduced Charge-Generation and Trap Clearing in Pentacene-Based Thin-Film Heterojunctions and Transistors using Electric Force Microscopy.** *J. Luria*, Cornell University, *A. Gorodetsky*, *C. Nuckolls*, Columbia University, *J.A. Marohn*, Cornell University

Pentacene and its derivatives are leading candidates for many organic electronics applications including electron donors in organic photovoltaics. Charge trapping, which is associated with device degradation in both photovoltaics and transistors, remains poorly understood even in this comparatively well studied class of materials. Northrup and Chabincyn [1] have carried out ab initio studies showing that reactions of holes with hydrogenated and oxygenated pentacene is a plausible charge trapping mechanism. Jaquith et al. [2] demonstrated a dependence of trap formation rate on hole concentration in pentacene, which is consistent with traps forming by a defect-mediated chemical reaction, and showed that traps could be cleared by the application of light. Coffey and Ginger [3] have shown that the fastest charging rates under illumination in polymer/fullerene films do not occur at phase interfaces, as widely assumed. Charge generation at the donor-acceptor interface in organic heterojunctions also remains poorly understood.

To resolve such open questions, we have developed a general approach to illuminating samples (from above) in an electric force microscope. We will describe studies where variable-wavelength light is utilized to clear traps in polycrystalline pentacene transistors. We will also discuss investigations into image charge generation in bis(thienyl)-pentacene/PCBM bulk heterojunction thin films.

[1] J.E Northrup and M.L. Chabincyn, *Phys. Rev. B* **68**, 041202 (2003).

[2] M.J. Jaquith, E.M. Muller, and J.A. Marohn, *J. Phys. Chem. B* **111**, 7711 (2007).

[3] D.S. Ginger and D.C. Coffey, *Nat. Mater.* **5**, 735 (2006).

5:20pm **NS1+PV-TuA11 A New Look at Si Inversion-Layer Solar Cells, Meeting Ground for Inorganic, Molecular and Organic Electronics**, *R. Har-Lavan, O. Yaffe, D. Cahen*, Weizmann Institute of Science, Israel

We suggest a near-ambient temperature, simple and potentially low-cost approach to fabricate semiconductor solar cells. To this end we use a monolayer of organic molecules that self-assembles onto n-Si, to passivate and buffer the Si surface. The direct binding of the molecules to the oxide-free Si surface also provides a strong interface dipole and effectively reduces the semiconductor's electron affinity by as much as 0.7 eV. A thin layer of a conducting polymer with a high work function, that is spin-coated on top of the molecular layer plays a threefold role:

the high work function induces inversion in the Si and leads to an n-p⁺ homojunction in the Si;

with n~1.5 refractive index the polymer acts as an anti-reflective coating to the Si.

because it protects the molecular monolayer, subsequent metal deposition and encapsulation is now possible.

Good and stable interface passivation along with strong inversion allow minority carriers, generated by absorbed sun light, to move laterally within the inverted Si top layer and to be collected by a minimal area metal grid, deposited on the conducting polymer. For the same reason (lateral conductance) photo-current losses, due to polymer sheet resistance, are minimized. Not only are cells fabricated without high temperature steps, the use of small organic molecules appears to convey here a unique advantage over inorganic passivation or buffer layers. The approach, which includes no or minimal (for metal grid) high vacuum steps, should be applicable to other inorganic absorbers, amorphous materials and thin films to improve photovoltaic solar energy conversion.

5:40pm **NS1+PV-TuA12 Modification and Characterization of Transparent Conducting Oxides for Generation III Nanostructured Photovoltaics**, *D. Placencia, N. Armstrong*, University of Arizona

Indium-Tin oxide (ITO), Indium-Zinc oxide (IZO), and Antimony-doped tin oxide (ATO) substrates were modified with ca. 3-5 nm gold nanoparticles to characterize their effect on the performance of Generation III organic photovoltaics (OPVs). This talk will focus on the presumed mechanism for their deposition, their impact on rates of electron transfer (solution), and OPV device performance parameters. ITO, IZO, and ATO thin films were deposited via magnetron sputtering and modified through a deposition-precipitation protocol. X-ray, UV photoelectron, and polarization modulated infrared reflection absorption spectroscopies were used to characterize the interfacial composition, work function changes, and the molecular nature of Au NP nucleation and growth. Planar heterojunction OPVs were created to evaluate the efficacy of oxide modification with metal nanoparticles, as an intermediate step towards the improvement of charge collection at the organic/oxide interface in organic solar cells.

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