

## Electronic Materials and Processing Room 309 - Session EM1-ThA

### Organic and Molecular Optoelectronics

Moderator: A.V. Walker, Washington University in St. Louis

#### 2:00pm EM1-ThA1 Quantum Dot Light Emitting Devices for Pixelated Full Color Displays, V. Bulovic, MIT INVITED

Quantum Dot Light Emitting Devices (QD-LEDs) developed over the past three years demonstrate high external quantum efficiencies, saturated visible color emission, narrow-band infra-red emission, and a scalable fabrication technique. This recent development is a result of advancements in the chemistry of colloidal quantum dot synthesis and demonstrations of new fabrication methods for generating thin films of QDs. The talk will present the recent technical and physical highlights, and chart the way to the next generation of the QD-LED technology.

#### 2:40pm EM1-ThA3 Organometallic Approaches to Achieving High Efficiency Monochromatic and White Electroluminescence from OLEDs, M.E. Thompson, University of Southern California INVITED

There has been a great deal of interest in developing new materials for the fabrication of light emitting diodes, built from molecular and polymeric materials. A significant motivation for this work has been their potential for use in future flat panel displays. Our work has been focused on developing new emissive and charge transporting materials for these devices. Our materials have led to marked improvements in the efficiencies of these devices. In particular, we have efficiencies for LEDs close to 100%, by using phosphorescence based emitters. The phosphorescent dopants in these devices are heavy metal containing complexes (i.e. Pt, and Ir compounds). I will discuss the basic mechanism of electroluminescence in OLEDs, and then elaborate on the use of phosphorescent complexes to achieve high EL efficiencies in monochromatic OLEDs. In the discussion of electrophosphorescence I will highlight specifically how we tune emission color in both Pt and Ir based emitters by careful design of both the metal complexes and ligands. We have also demonstrated white light emitting OLEDs, using many of the same emissive materials. These devices emit simultaneously from monomer and dimer/aggregate states of Ir and Pt dopants. The result is an emission spectrum that covers the entire visible spectrum, giving true white illumination. We have recently prepared binuclear Pt complexes and can show that the low energy emissive species in the white OLEDs is most likely a ground state dimer or aggregate. This aggregate state undergoes a structural change in the excited state, similar to an excimer. I will discuss the mechanism of electroluminescence in this system and describe our recent advances in achieving high efficiency white electroluminescence.

#### 3:20pm EM1-ThA5 Chemical Vapor Deposition of Thin Films of Electrically Conducting PEDOT, J.P. Lock, J.L. Lutkenhaus, N.S. Zacharia, P.T. Hammond, K.K. Gleason, MIT

Chemical vapor deposition (CVD) technology, vital to the fabrication of traditional semiconductor devices, is also desirable for next-generation organic devices, particularly for creating layers which are difficult to process by solution methods or for coating substrates which can not tolerate exposure to solvents. In this work, a CVD process has been demonstrated for the deposition of conducting poly-3,4-ethylenedioxythiophene (PEDOT). This CVD process eliminates the need for polystyrene sulfonate (PSS), which is used to disperse PEDOT in water, but has been identified as a possible source of corrosion in OLEDs leading to shortened device lifetimes. The CVD PEDOT films range from 50 nm to several microns in thickness. Fourier transform infrared spectroscopy confirms the similarity in chemical structure of PEDOT synthesized by CVD and solution techniques. An electrical conductivity as high as 4.37 S/cm has been achieved. The CVD process utilizes a modest stage temperature and results in conformal coatings of high surface area features like fibers and pores. This combination of characteristics has allowed PEDOT deposition onto paper and fabrics to be demonstrated. Conformal coating of microporous or fibrous materials by CVD PEDOT has the potential to lead to better efficiencies in organic devices with high effective surface areas including photovoltaics. Reversible electrochromic responses of CVD PEDOT have been observed as well. The light blue films in their as-deposited state turn darker blue upon electrochemical reduction. The maximum contrast to date is 16.5% with a switching speed of 27 msec for a film having a thickness of 50 nm.

#### 3:40pm EM1-ThA6 Molecular Level Alignment and the Role of the Charge Neutrality Level at Organic-Organic Heterojunctions, W. Zhao, Princeton University; H. Vazquez, F. Flores, Universidad Autonoma de Madrid, Spain; A. Kahn, Princeton University

The electronic structure of organic-organic (OO) interfaces is a key aspect of organic devices such as OLEDs and PV cells. Molecular level offsets at OO interfaces determine transport across devices, and directly affect their performance. This talk reports a recent investigation of the electronic structure of several OO interfaces between films of molecules such as tris(8-hydroxy-quinoline)aluminum (Alq<sub>3</sub>), 1,4,5,8-naphthalenetetracarboxylicdianhydride (NTCDA), iridium-bis(4,6-difluorophenyl-pyridinato-N,C<sup>+</sup>)-picolate (Flrpic) or copper phthalocyanine (CuPc). The filled and empty states of these materials, their ionization energy (IE) and electron affinity (EA), and the interface molecular level alignment are determined via ultra-violet and inverse photoemission spectroscopy (UPS, IPES). Unlike many previously investigated OO heterojunctions, these are found not to follow vacuum level alignment and exhibit significant interface dipoles ranging from 0.2 to 0.5 eV. The analysis of these and previous results on OO heterojunctions is performed using the extension of the concept of charge neutrality level (CNL), developed for metal/organic interfaces, to the OO heterojunction. The energy-level alignment is driven by the alignment of the CNLs of the two organic semiconductors. The initial offset between the CNLs gives rise to a charge transfer across the interface, which induces an interface dipole and tends to align the CNLs. The initial CNL difference is reduced according to the screening factor  $S$ , a quantity related to the dielectric functions of the organic materials. Good quantitative agreement with experiment is found. This allows, for the first time, a semi-quantitative prediction of the electronic structure of OO heterojunctions. I.G. Hill et al., Appl. Surf. Sci. 166, 354 (2000); H. Vazquez et al. EuroPhysics Lett. 65, 802 (2004); H. Vazquez et al. Phys. Rev B Rapid Comm. 71, 041306 (2005).

#### 4:00pm EM1-ThA7 New Device Functionalities and Materials, N. Tessler, Technion, Israel Institute of Technology INVITED

For certain device applications, semiconducting polymers can replace inorganic semiconductors at lower cost because they are more easily processed. Examples include the development of organic light emitting diodes (OLEDs), for full color screen applications, and of the development of field effect transistors (FETs) for smart circuit applications. These device applications make use of the semiconducting nature of conjugated polymer. However, by accounting for the organic (molecular) nature of these materials one can extend the material and device functionalities. In this contribution we highlight two approaches: a) the use of nano-composites b) the use of bio-inspired chemical modifications to produce libraries of functional materials. We will also address device properties and suitable methods for analysis.

#### 4:40pm EM1-ThA9 Photoelectron Spectroscopy of Phenylene Ethynylene versus Phenylene Vinylene Oligomers: a Search for Bond Alternation Effects, L.B. Picraux, C.D. Zangmeister, S.W. Robey, R.D. van Zee, NIST

Interest in factors controlling transport through conjugated molecular systems has lead to a significant experimental effort investigating conductivity in various configurations of metal-molecule junctions. One interesting result of these efforts was an investigation of the relative conductivity in junctions formed using crossed wire techniques containing phenylene ethynylene (OPE) or phenylene vinylene (OPV) oligomers. Vinylene-based oligomers were found to exhibit higher conductivity, a result that was attributed to an increased bandgap in phenylene ethynylene systems due to the larger impact of bond alternation effects in the triple bond containing system. We have used photoelectron spectroscopy to investigate the  $\pi$  electronic structure of these two systems, namely three-ring phenylene ethynylene oligomers with thiol bound to gold and the analogous three-ring OPV system, which were the compounds employed in the crossed-wire investigations. Spectra for the two oligomers are quite similar but the  $\pi$  levels in the OPV variant are approximately 0.2 eV closer to the Fermi level than in OPE, possibly consistent with the higher conductivity measured in crossed-wire junctions. While this could be construed as being consistent with a narrowing of the band gap in the OPV system, it appears to arise from a rigid shift of the levels. There is no evidence of increased dispersion within the  $\pi$  manifold as expected if reduced bond alternation were the cause. Finally, we will also discuss the potential impact of the self-assembled monolayer structure on transport measurements.

# Thursday Afternoon, November 3, 2005

@FootnoteText@@footnote 1@Kushmerick JG, Hold DB, Pollack SK, et al.,  
J. Am. Chem. Soc. 124(36): 10654-10655 2002.

5:00pm **EM1-ThA10 Monomolecular Insulator Film**, Y. Tai, H. Noda, A. Shaporenko, M. Grunze, M. Zharnikov, Universität Heidelberg, Germany  
Progress in fabricating smaller and more efficient structures in electronic and spintronic devices depends on better dielectric materials for nanofabrication. A perspective nanoinsulator is a molecular thin organic film - self-assembled monolayer (SAM), which provide an alternative to commonly used oxide dielectrics such as e.g. SiO<sub>2</sub> or Al<sub>2</sub>O<sub>3</sub>. A so far unresolved technological problem for applications of SAMs in microelectronics and spintronics is the difficulty of fabricating stable metal layers on their surfaces, i.e. at the SAM-ambient interface. Such a film is generally leaky for metal adsorbates, which makes it impossible to integrate it into a multilayer assembly (e.g. in a tunnel junction magnetic memory cell) or to fabricate metal electrodes on its surface (e.g. in an organic thin film transistor). Using nickel as a test metal adsorbate and several different substituted and non-substituted SAMs as test substrates, we show that this difficulty can be overcome by the combination of a special design of the SAM constituents and their extensive cross-linking by low-energy electron irradiation. The properties of the SAM insulator and the metal overlayer were monitored by several complementary experimental techniques, including X-ray absorption spectroscopy and electrochemical measurements. The approach represents an important step toward the technological applications of monomolecular dielectric layers.

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