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Tuesday, March 11, 2008 2:30PM - 5:30PM – Session L6 COM: Minorities in Condensed Matter Physics Morial Convention Center R04

2:30PM L6.00001 Multi-Scale Modeling of Conductive Polymers PEDRO DEROSA, Louisiana Tech University/Grambling State University — In spite of the tremendous impact of conductive polymers in a number of technological applications, molecular engineering of these materials has not been accomplished yet. One of the main reasons is the lack or limited understanding of the connection between changes occurring at the molecular level and the resulting polymer conductivity. Understanding the influence that local changes to the polymer's structure and chemical composition have on polymer properties, is the key to reach the stage where polymer-based materials and devices can be molecularly engineered with optimum properties. A multiscale model able to predict and accurately describe such a connection is thus a much needed tool to achieve this goal. The main aspect of this project is the bridging between scales in such a way that properties of the polymer at the molecular level are reflected in the observed and measured macroscopic properties. However, to achieve that integration, adapting and improving models at each of the involved scales must be done first. The progress towards improved models at the atomic and at the macroscopic level will be described. The atomic level is dealt with by using quantum mechanics calculations including semiempirical and ab initio methods. A semi-empirical/DFT study of oligomers will be described where extrapolation of electronic properties to an essentially infinite chain show excellent agreement with experimental results. The macroscopic level is addressed with probabilistic models, based on the Monte Carlo Technique, to study the charge transport process. The efforts toward the improvement and implementation of an existing transport algorithm, based on the hopping model, will be described. Existing models consider polymer and polymer devices as a cubic arrangement of sites and incorporate disorder as an ad-hoc parameter, in our model, the use of realistic configurations allows the distinction of intra- vs. inter-molecular conduction and the modeling of polymer devices. In addition, the model is reformulated to incorporate parameters calculated at the atomic level, thus the effect of on macroscopic properties produced by changes at the atomic level can be studied. Plans for the integration across scales, the final step to achieve multiscale modeling, will also be discussed.

3:06PM L6.00002 Characterization of Hybrid Electronic Materials for Molecular Based Device Electronics, THEDA DANIELS-RACE, Louisiana State University — Nanoscale device development, as an exercise in electronic materials fabrication, comes down to essentially one of two approaches—"top-down" or "bottom-up." In the former, the drive is to retain the macroscopic properties of the materials involved while shrinking toward ever diminishing device geometries. The latter approach attempts to control individual molecules and/or quantum-level structures, during the course of fabrication, in order to ultimately realize device functionality. This bottom-up design and control of molecular assemblies has united device engineers and scientists in testing new combinations of materials, both organic and inorganic. As a result, an entirely new class of nanoscale electronic structures and devices has emerged to create the field of hybrid electronic materials or HEMs¹. HEMs have shown promise as the basis for exciting device applications ranging from quantum computing to unique drug delivery methods. Although theoretical proposals of unimolecular transport began as early as the 1970s, it has been within the last decade in particular that research has yielded significant results in terms of nanoscale electronic applications for HEMs². However, many unresolved fundamental issues of electronic materials remain in this field. It is for this reason that in this talk, I will discuss a selection of HEM components (e.g.-self-assembled monolayers of n-alkanethiols, porphyrin molecules), their characterization, and their propensity for future nanoelectronic device development. 1. James R. Heath and Mark A. Ratner, *Physics Today*, May 2003; 43-49. 2. Mark A. Reed and Takhee Lee (Eds.), "Molecular Nanoelectronics," American Scientific Publishers, Stevenson Ranch, CA, 2003.

3:42PM L6.00003 Use of X-ray absorption spectroscopy in the search for the best LIGO mirror coatings¹, STEPHEN C. MCGUIRE, Southern University and A&M College — The Laser Interferometer Gravitational-wave Observatory (LIGO) seeks to improve its sensitivity for gravity-wave detection by a factor of ten during its next phase of operation, Advanced LIGO. In order to achieve this goal it is necessary to design and fabricate test mass mirrors that help minimize the noise in the interferometers and in doing so maximize gravity-wave detection capability. In this talk we will present recent results from our program of X-ray absorption spectroscopy measurements to obtain detailed chemical composition and structure of titania (TiO₂)-doped tantala (Ta₂O₅) multilayers fabricated via ion beam sputtering on SiO₂ substrates. Our investigations focus on how the microscopic features of the coatings influence their macroscopic mechanical loss properties. Our goal is to obtain correlations between chemical impurities and/or dopants and the optical absorption and mechanical loss characteristics of these multilayer coatings. To examine our samples we use synchrotron-based X-ray absorption Spectroscopy (XAS) techniques including Extended X-ray Absorption Fine Structure (EXAFS), X-ray Absorption Near Edge Structure (XANES) and X-ray Fluorescence (XRF). We present chemical and structural data obtained at the titanium K-edge and tantalum L_{III}-edge as well as relative elemental distribution information (Ti/Ta, Fe/Ta, and Cr/Ta) obtained via XRF. Following a brief description of the LIGO experiment, our program of research in optical materials for use in advanced versions of the interferometer will be described.

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4:18PM L6.00004 A Mathematical Solution to the Theoretical Band Gap Underestimation: Predictive Calculations of Properties of Semiconductors¹, DIOLA BAGAYOKO, Southern University and A&M College — Most density functional theory (DFT) calculations find band gaps that are 30-50 percent smaller than the experimental ones, as illustrated in this presentation that recalls some popular explanations of this band gap problem, i.e., self-interaction effects and derivative discontinuities of the exchange correlation energy. A survey of the increasingly numerous approaches aimed at resolving the theoretical underestimation follows these explanations. These approaches include the Green function and screened Coulomb approximation (GWA), time dependent density functional theory (TDDFT), the exact exchange and screened exchange methods, and the use of local density approximation (LDA) potentials plus additional potentials located at atomic sites. Using the Rayleigh theorem, we describe a basis set and variational effect inherently associated with calculations that employ a linear combination of atomic orbitals (LCAO) in a variational approach of the Rayleigh-Ritz type. This description concomitantly shows a source of large underestimation errors in calculated band gaps, i.e., an often dramatic lowering of some *unoccupied energies* on account of the Rayleigh theorem as opposed to the Hamiltonian. We present the Bagayoko, Zhao, and Williams (BZW) method [Phys. Rev. B 60, 1563 (1999); PRB 74, 245214 (2006); and PRB 76, 037101 (2007)] that follows from the description of the aforementioned effect and that leads (a) to DFT and LDA calculated band gaps of semiconductors in agreement with experiment and (b) theoretical predictions of band gaps that are confirmed by experiment. Unlike most calculations, BZW computations solve, self-consistently, a system of two coupled equations. DFT-BZW calculated effective masses and optical properties (dielectric functions) also agree with measurements. We illustrate ten years of success of the BZW method with its results for GaN, C, Si, 3C-SiC, 4H-SiC, ZnO, AlAs, Ge, ZnSe, w-InN, InAs, and AlN. We conclude with a request to revisit beliefs relative to actual limitations of DFT and of schemes purporting to correct it or to go beyond it.

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4:54PM L6.00005 New Possibilities for Understanding Complex Metal Hydrides via Synchrotron X-ray Studies¹, TABBETHA DOBBINS, Grambling State University and Louisiana Tech University — Ultrasmall-angle x-ray scattering (USAXS) and X-ray absorption spectroscopy (XAS) are used for the study of chemical and morphological changes in metal hydride powder (e.g. NaAlH₄) both before and after transition metal salt catalytic dopant additions by high energy ball milling. The variation in surface fractal dimension and particle size with milling time and dopant content were tracked. These studies show that dopant content level (e.g. 2 mol % and 4 mol %) and dopant type (i.e. TiCl₂, TiCl₃, VCl₃, and ZrCl₄) markedly affects NaAlH₄ powder particle surface area (determined using USAXS surface fractal dimension). As well, the chemical reaction between the catalyst and hydride powder was further elucidated using XAS. Ti-metal reacts with the Al desorption product (from NaAlH₄) to form TiAl_x product phases. These studies were able to link powder particle surface area to catalytic doping and were able to link dopant chemical state with dehydrogenation reactant and product phases.

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