

SYSA 1: Bandalignment in Organic Materials

Time: Tuesday 9:30–10:45

Location: H 0105

Invited Talk

SYSA 1.1 Tue 9:30 H 0105

Level alignment at metal/organic interfaces — ●FERNANDO FLORES — Universidad Autónoma de Madrid, Madrid, Spain

A unified model, embodying the Induced Density of Interface States (IDIS), Pauli repulsion and intrinsic molecular dipoles is presented for describing the level alignment at a metal/organic interface. The IDIS model takes into account how charge is transferred between the metal and the organic material [1]: in particular, charge transfer is determined by the relative position of the metal workfunction and the organic Charge Neutrality Level (CNL), as well as by an interface parameter, S , which measures how this potential difference is screened. The Pauli repulsion dipole originates from the orthogonalization of the metal and organic wavefunctions; this dipole is calculated using a many-body LCAO hamiltonian [2], resulting in an effective reduction of the metal workfunction. Intrinsic molecular dipoles are also introduced in this unified model, in such a way that the level alignment at the metal/organic interface is obtained from a calculation that combines all these effects in a selfconsistent way. As a first example, organic materials with no intrinsic molecular dipole are considered (PTCDA, PTCBI, CBP and CuPc). For these cases it will be shown that the IDIS-dipole represents most of the realignment induced at the metal/organic interface, with the Pauli repulsion dipole yielding minor corrections to the IDIS model. In a second example, the Cu/benzenethiolate/pentacene heterostructure is analyzed including IDIS, Pauli repulsion and intrinsic molecular dipoles [3]. The Cu/benzenethiolate interface realignment can be understood in these terms as a function of the benzenethiolate coverage: this also enables us to determine, using the metal workfunction evolution, the molecule orientation as a function of coverage. An extension of this model to heterostructures allows us to analyze in similar terms the benzenethiolate/pentacene interface.

[1] H.Vazquez et al, Europhys. Lett. 65, 802 (2004) [2] H.Vazquez et al, J. Chem. Phys. 126, 144703 (2007) [3] M.G.Betti et al, Phys. Rev. Lett., in press.

SYSA 1.2 Tue 10:00 H 0105

Consistent experimental determination of the charge neutrality level and the pillow effect at metal/organic interfaces — ●MANDY GROBOSCH¹, OLGA V. MOLODTSOVA¹, VICTOR YU. ARISTOV^{1,2}, and MARTIN KNUPFER¹ — ¹IFW Dresden, D-01069 Dresden, Germany — ²Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr., 142432, Russia

Experimental results of combined X-ray and ultraviolet photoemission spectroscopy studies for the interface dipoles at metal/organic and organic/organic heterointerfaces have been analyzed on the basis of the induced density of interfaces states model(1,2). For the estimation of the interface dipole as well as the metal work function we have analyzed the following interfaces: Au/CuPc, Ag/CuPc, Au/CuPcF4, Ag/CuPcF4, and the respective heterointerfaces between copper phthalocyanine (CuPc) and its fluorinated relative (CuPcF4). We demonstrate that a consistent analysis of a selected set of interfaces is possible, which allows the determination off all microscopic parameters of the model, and moreover enables the prediction of the electronic properties of further, yet unknown interfaces. This additionally represents a starting point for the experimental determination of further important material dependent parameters such as the charge neutrality level of organic semiconductors.

1 H. Vazquez, F. Flores, and A. Kahn, Organic Electronics 8, 241

(2007).

2 H. Vazquez, Y.J. Dappe, J. Ortega, and F. Flores, J. Chem. Phys. 126, 144703 (2007).

SYSA 1.3 Tue 10:15 H 0105

Measuring the energy level alignment at all interfaces in a complete OLED — SELINA OLTGHOF, RICO MEERHEIM, KARSTEN WALZER, and ●KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

As the number of layers used for typical organic semiconductor devices is increasing in the course of optimization, interfaces between those layers become increasingly important for device performance. These interfaces are governed by the relative HOMO and LUMO positions as well as by interface dipoles originating from effects like polarization, chemical reactions and bond formation. As our charge injection layers are electrically doped, band bending and the resulting depletion layers play a significant role as well. To be able to perform simulations of the full device for further optimization it is necessary to measure the energy alignment at all metal/organic and organic/organic interfaces. This can be done by ultraviolet photoelectron spectroscopy (UPS) and x-ray photoelectron spectroscopy (XPS). We performed such interface resolved studies of a complete OLED by UPS and XPS. As an example, we chose the structure of a long living red OLED: ITO - MeO-TPD:F4-TCNQ - α -NPD - α -NPD:Ir(MDQ)2acac - BA1q - BPhen:Cs - Ag.[1] For photoelectron spectroscopy, the OLED was built stepwise measuring for each interface the thickness dependent photoelectron spectra. The measurements show that the doped layers strongly influence the energetic positions of the intrinsic layers, and that the commonly assumed vacuum level alignment is not fulfilled. [1] R. Meerheim et al., Appl. Phys. Lett. 89, 061111 (2006)

SYSA 1.4 Tue 10:30 H 0105

Intramolecular band structure and disorder effects in monolayers of linear molecules — ●M. HÄMING¹, J. ZIROFF¹, M. WIESSNER¹, O. SEITZ², E. SALOMON³, A. KAHN³, D. CAHEN², A. SCHÖLL¹, F. REINERT¹, and E. UMBACH¹ — ¹Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg — ²Weizmann Institute of Science, Department of Materials and Interfaces, Israel — ³Princeton University, Department of Electrical Engineering, USA

For a detailed understanding of charge transport on a molecular level a comprehensive understanding of the molecular electronic structure is mandatory. Self assembled alkyl monolayers (SAM) are appropriate model systems due to interesting charge transport properties and their relatively simple molecular structure. We have investigated the intramolecular band structure of alkyl/Si(111) SAMs with high resolution photoemission spectroscopy (HR-PES) using variable photon energy. There are significant changes in the valence band spectra for photon energies between 30 eV and 190 eV indeed, but the electronic dispersion is blurred due to a strong DOS effect. This is very unlikely a property of the intramolecular band structure, but rather the consequence of disorder in the molecular layer. In reverse, this effect can provide structural information. A comparison between the PES data and projections of the total DOS onto the free electron final state for different distributions of alkyl orientations allows to estimate the spread in the molecular orientation angle and thus the degree of disorder. Consequently, this needs to be taken into account for a proper description of the intramolecular electronic structure.