

CPP 85: Molecular films: Photovoltaics, electronics and morphology (joint session O/CPP)

Time: Friday 10:30–11:30

Location: MA 144

CPP 85.1 Fri 10:30 MA 144

Excitonic states in films of 1,3-diphenylisobenzofuran — ●JANEK RIEGER, DANIEL NIESNER, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, University of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Films of 1,3-diphenylisobenzofuran (DPIBF) show singlet fission (SF), a mechanism for multi-exciton generation that might be used to enhance the efficiency of organic photovoltaics [1]. The yield of singlet fission depends strongly on the structural polymorph of the film [2]. We use ultraviolet photoelectron spectroscopy, monochromatic two-photon photoelectron spectroscopy, photoluminescence (PL) spectroscopy and time-resolved PL to investigate the occupied molecular orbitals and excitonic behavior in different polymorphs of DPIBF on Cu(111). Preparations under ultra-high vacuum conditions provided well-defined samples, on which in-situ measurements were carried out. In disordered films an excimer trapping state with a lifetime of 50 ns was found with an energy ~ 0.5 eV below the first excited singlet state S_1 . For ordered films additional three vibrational progressions were found, which can be attributed to the S_1 excitons of two different polymorphs with energies of 2.62 eV and 2.66 eV and an emissive triplet pair species with an energy of 2.72 eV. The latter decays with two time constants in the subnanosecond regime. A relative PL yield < 0.12 was determined for the ordered films, which points towards a highly SF active film.

[1] M. C. Hanna, and A. J. Nozik, *J. Appl. Phys.* **100**, 074510 (2006).

[2] J. L. Ryerson et al., *J. Phys. Chem. C* **118**, 12121-12132 (2014).

CPP 85.2 Fri 10:45 MA 144

Polarized-Light Induced Contact Potential Differences in Small-Molecule Organic Aggregates and Thin Films —

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Crystalline organic thin films often exhibit linear dichroism and birefringence. Illumination with polarized light might therefore lead to polarization dependent changes of the electric surface potential. Here, we present results for birefringent and dichroic nanofibers from functionalized *para*-quaterphenylene molecules [1], and for thin films and thin film blends from an dihydroxy anilino squaraine (SQIB) [2]. Considerable differences in the light-induced changes of the surface potential are observed, probed by Kelvin probe force microscopy (KPFM). These changes are associated with the local molecule orientation within the samples.

[1] *J. Chem. Phys.* **146** (2017) 134704. [2] *Cryst. Growth Des.* (2017), doi: 10.1021/acs.cgd.7b01131.

CPP 85.3 Fri 11:00 MA 144

Work function variation due to electron induced conversion

of self-assembled monolayers into carbon nano-membranes — PAUL PENNER¹, ●SASCHA KOCH¹, MARCIN KIESIEL², THILO GLATZEL², EMANUEL MARCHEWSKI¹, XIANGHUI ZHANG¹, ERNST MEYER², and ARMIN GÖLZHÄUSER¹ — ¹Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany — ²Department of Physics, University of Basel, 4056 Basel, Switzerland

For the realization and improvement of molecular electronic devices as for instance nano capacitors, the determination and specific tuning of electrical properties of the build-in materials plays an important role [1]. Our main research is focused on Carbon nano-membranes (CNMs), made by e.g. electron irradiation induced cross-linking of self-assembled monolayers (SAMs) of aromatic, organic molecules. Using different precursor molecules for the SAM preparation allows us to tune various properties of the resulting CNM [2]. Here, we present a material study about the change in the work function of pristine SAMs and CNMs on a Au(111) substrate by means of Kelvin Probe Force Microscopy (KPFM) for different precursor molecules. For different samples, the morphology as well as the work function of partially cross-linked and pristine SAM areas were compared, showing only differences in the contact potential (CPD). This effect can be attributed to the dipole moment modification of the molecular layer as well as the molecule-substrate interface but also to influences of different head-group functionalizations. [1] X. Zhang et al., *J. Appl. Phys.* **2017**, 122, 055103. [2] A. Turchanin et al., *Adv. Mater.* **2016**, 28, 6075-6103.

CPP 85.4 Fri 11:15 MA 144

Local near-field spectroscopy of squaraine J-aggregates —

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Investigating the relationship between structure and function of organic molecular systems is of great interest for understanding their optical and electronic properties, inter- and intra-molecular coupling, and further applications such as solar cells, transistors, and photovoltaic devices. Optical microscopy on a nanometer length scale is one promising approach to obtain such insights. Here we employ scattering-type near-field scanning optical microscopy (NSOM) to probe the local spectrum of squaraine J-aggregates (R-ProSQ-C16). We model two resonances in the far-field spectrum of the molecules as transitions from the ground state to two excited states which originate from the energy level splitting caused by the coupling between two adjacent monomers. The splitting strength and hence the transition energy is determined by the tilt angle between the two coupled monomer dipoles. Near-field spectral measurements resolve local scattering spectra in 10-nm-radius domains. They reveal that the resonance energies measured in the individual domains vary from each other. These near-field spectral measurements, in combination with our theoretical modelling, reveal local variations in the tilt angle between the two monomer dipoles.