

**HL 117: Organic semiconductors: Material properties (with CPP/DS)**

Time: Friday 10:15–12:30

Location: POT 051

HL 117.1 Fri 10:15 POT 051

**Pressure dependent Electronic Structure from First Principles** — ●FRANZ KNUTH<sup>1</sup>, CHRISTIAN CARBOGNO<sup>1</sup>, VOLKER BLUM<sup>1,2</sup>, and MATTHIAS SCHEFFLER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — <sup>2</sup>MEMS Department, Duke University, Durham, NC, USA

The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress and pressure [1]. To clarify the role of these effects electronic-structure theory is uniquely suited. However, standard density-functional theory approaches that neglect van-der-Waals interactions and that treat exchange and correlation in a semi-local approximation often fail to describe organic materials properly. To overcome this limitation, we have extended our implementation of the analytical strain derivatives (stress tensor) to include the contributions that stem from (a) the van-der-Waals interaction [2] and (b) the Fock-exchange in hybrid functionals. We discuss the details of our implementation that is based on a local resolution of identity (LVI) of the Coulomb matrix [3]. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene, polyaniline, and anthracene under pressure. We show that the fraction of exact exchange included in the calculations is critical – and non-trivial to choose – for a correct description of these systems. [1] J. H. Kim, S. Seo, and H. H. Lee, *Appl. Phys. Lett.* **90**, 143521 (2007).

[2] A. Tkatchenko, and M. Scheffler, *PRL* **102**, 073005 (2009)[3] A. Sodt, and M. Head-Gordon, *J. Chem. Phys.* **128**, 104106 (2008)

HL 117.2 Fri 10:30 POT 051

**DFT study of vibronic properties of partially fluorinated nickel phthalocyanine** — ●DAVOUD POULADSAZ — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Since fluorinated phthalocyanines are shown to be sensitive to reducing gases due to the withdrawing effect of fluorine atoms, by means of density functional theory, we have investigated the effect of fluorination on the vibronic couplings and ionization potential in nickel phthalocyanine.

HL 117.3 Fri 10:45 POT 051

**Ab-initio investigation of Charge and Spin transport properties of Organic Semiconductors.** — ●SANDIP BHATTACHARYA and STEFANO SANVITO — School of Physics and CRANN, Trinity College Dublin, Ireland

In this talk I will describe in detail our procedure to explore the spin and charge transport properties of organic single-crystal semiconductors from first principles. Our technique involves representing the organic semiconductor with a tight-binding model, including coupling of the charge carrier to phonons and spin relaxation due to hyperfine and spin-orbit coupling interaction. The ab-initio Hamiltonian parameters are extracted from DFT and the maximally localized Wannier functions scheme. We evolve the classical fields in the Hamiltonian via Monte Carlo simulations, and then compute the mobility from Kubo formula and the spin-diffusion length from a Landauer-Buettiker approach. We shall demonstrate calculated charge carrier mobilities very close to those measured in single-crystal rubrene-based organic field effect transistors and spin-diffusion length quite close to that estimated in experiments on rubrene-based spin valves. In the second part of my talk, I shall discuss the use of a similar procedure to predict the ab-initio spin and charge transport characteristics of Triarylamine-based organic nanowires, recently synthesized. We obtain quite superior estimates for hole mobilities as well as spin-diffusion lengths in such organic nanowires, corroborating the experimental find of exceptional conductance through nanodevices made out of such nanowires.

HL 117.4 Fri 11:00 POT 051

**Growth control of AgTCNQ nanowire arrays by using template-assisted electro-deposition method** — ●CHENGLIANG WANG<sup>1</sup>, LIAOYONG WEN<sup>1</sup>, THOMAS KUPS<sup>2</sup>, RANJITH VELLACHERI<sup>1</sup>, YAOGUO FANG<sup>1</sup>, PETER SCHAAP<sup>2</sup>, HUAPING ZHAO<sup>1</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>Institute for Physics and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany — <sup>2</sup>Institute of Materials Engineering and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany

One dimensional (1D) organic semiconductor nanostructures, especially their aligned arrays, have attracted extensive attention due to their potential application in organic optoelectronics, and template-assisted methods have been proved to be one of the most powerful methods to achieve this kind of arrays. Due to the small size of the AAO nanopores, diffusion of the objects into the nanopores is one of the crucial issues to achieve nanowire arrays. Here, the growth control of AgTCNQ (TCNQ: 7,7,8,8-tetracyanoquinodimethane) nanowire arrays is achieved by using template-assisted electro-deposition methods. We find that the diffusion of the electrolyte into the nanopores takes an important role in the electro-deposition process and the equilibrium between the reduction and the diffusion is necessary to achieve continuous AgTCNQ nanowire arrays. We believed that the analysis of the equilibrium between the deposition and the diffusion and the controllable synthesis of organic semiconductor arrays will benefit the preparation of other semiconductor arrays.

HL 117.5 Fri 11:15 POT 051

**Energy-transfer in ZnO/ladder-type oligophenylenes hybrid structures** — ●FRANCESCO BIANCHI<sup>1</sup>, SYLKE BLUMSTENGEL<sup>1</sup>, FRITZ HENNEBERGER<sup>1</sup>, BJÖRN KOBIN<sup>2</sup>, STEFAN HECHT<sup>2</sup>, RAFAEL SCHLESINGER<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Institut für Physik Humboldt-Universität, Berlin, Germany — <sup>2</sup>Department of Chemistry Humboldt-Universität, Berlin, Germany

Inorganic/organic hybrid systems designed to inherit the advantageous properties of each of their constituents are of great interest both to basic science as well as for optoelectronic applications. In this regard it is required to find an organic material that exhibits specific properties like narrow transitions, large dipole moment, small emission-absorption Stokes shift and an optical gap that corresponds to the inorganic material. The design we use consists in a three spiro-bridged ladder-type quarter-phenyl (SP3-L4P) grown on ZnO-based single quantum wells (SQW) to obtain incoherent coupling. In such a setting, it should be possible to convert Wannier excitons of the SQW into Frenkel excitons of the organic layer via a Förster type energy transfer (FRET).

We investigate the FRET between SQW with different cap thickness and a 3Sp-L4P thin layer evaporated on top of them. With photoluminescence excitation and time-resolved spectroscopy we demonstrate that these hybrid structures exhibit energy transfer with an efficiency up to 65%. Despite the high efficiency, UPS measurements show a type II interface between ZnO and the molecules layer, leading to a charge separation process that limits the light emitted. Finally we investigate on the use of high gap material spacer to reduce this effect.

HL 117.6 Fri 11:30 POT 051

**Temperature dependent PL measurements of rubrene single crystals with  $\mu\text{m}$ -resolution** — ●T. SCHMEILER<sup>1</sup>, J. GABEL<sup>1</sup>, R. CLAESSEN<sup>1</sup>, and J. PFLAUM<sup>1,2</sup> — <sup>1</sup>Inst. Exp. Phys. VI/IV, University of Würzburg, 97074 Würzburg — <sup>2</sup>ZAE Bayern e.V., 97074 Würzburg

Our previous demonstration of spatial confinement effects on exciton dynamics in rubrene (rub) single crystals, microcrystals and amorphous films [1] has raised fundamental questions on excitonic processes occurring at surfaces and interfaces of molecular stacks. We address this topic by analyzing the temperature dependent PL characteristics of rub single crystals on  $\mu\text{m}$ -length scales and under various boundary condition by e.g. capping them with thin films of different polarizability such as Au or LaVO. At first, a pronounced enhancement of the total PL intensity of up to two orders of magnitudes was observed in case of the Au top layer which can be attributed to a resonant coupling of the excited rub states to the surface plasmon modes of the metal. This coupling phenomenon is further corroborated by relative intensity changes within the PL spectra of the Au covered rub upon cooling below 100K. In case of a LaVO capping layer, providing high polarizability without significant contributions by exciton quenching, a strong temperature dependent influence in the rub PL peaks at short wavelengths is observed. This behavior will be discussed in the context of temperature dependent changes of the LaVO layer itself as well as different coupling mechanism for the interfacial excitonic species. Financial support by the DFG research unit FOR 1809 (project PF385/6) is gratefully acknowledged. [1] B. Giesecking et al., arXiv:1309.1107

HL 117.7 Fri 11:45 POT 051

**Optical absorption and photoluminescence properties of perylene single-crystals** — ●ANDRE RINN, NIKLAS KRAUS, ANDRÉ PICK, GREGOR WITTE, and SANGAM CHATTERJEE — Phillips Universität Marburg, Marburg, Germany

Organic semiconductors are considered promising candidates for next-generation optical devices. However, a detailed systematic understanding of the electro-optical response is in a much less holistic state than for inorganic materials such as Si or GaAs. Therefore, we investigated the two crystalline phases of perylene as model organic semiconductors and gain further insight in their optical response. This system crystallizes in two different phases: the beta-phase has a monomeric herringbone structure with two molecules per primitive unit cell, whereas the alpha phase grows in a dimeric herringbone configuration with four molecules per unit cell. The single-crystalline samples have been grown in silicon oil, which results in microcrystals of excellent quality. Hence, we can investigate the consequences of the respective crystal orientation on the Davydov splitting of the excitons as well as excimer formation. Both configurations have been investigated with polarization resolved absorption spectroscopy and time resolved luminescence experiments. Absorption spectroscopy reveals results with significant deviations from the widespread Davydov picture. The data obtained by time resolved luminescence shows characteristic excimer behavior. Additionally, the optical spectra are compared to the response of perylene in solution and the vapour phase.

HL 117.8 Fri 12:00 POT 051

**Direct measurement of the charge carrier mobility in organic donor-acceptor blend in device geometry – including extreme stoichiometry** — ●JOHANNES WIDMER<sup>1</sup>, JANINE FISCHER<sup>1</sup>, CHRISTIAN KOERNER<sup>1</sup>, KARL LEO<sup>1</sup>, and MORITZ RIEDE<sup>1,2</sup> — <sup>1</sup>Institut für Angewandte Photophysik (IAPP), TU Dresden, Germany — <sup>2</sup>Current address: Clarendon Laboratory, UK

Blend layers of an organic donor (D) and a fullerene acceptor (A) are a key component of highly efficient organic solar cells. The charge carrier mobility in the blend sensibly affects the device efficiency concerning transport and recombination of charge carriers.

The applied method “POEM” – potential mapping by thickness variation – is a direct measurement giving model-free experimental access to the effective mobility  $\mu(F, n)$  as a function of the electric field  $F$  and

the charge carrier density  $n$ . It is based on a novel evaluation strategy for space-charge limited current (SCLC) in single carrier devices in a vertical device geometry.[Widmer et al., Org. El. (2013)]

Here, we apply POEM to characterize the hole transport in D:A blends of small molecules with different blend ratios. The measurements cover common ratios as well as strongly diluted blends with only  $\approx 1\%$  donor content, which are known to yield efficient solar cells. Beyond characterizing disorder and trap states, which influence  $\mu$ , the POEM measurements reveal that also in the diluted blend effective hole transport is possible, but takes place not only on the donor.

The obtained  $\mu(F, n)$  functions allow for an advanced understanding of charge transport in D:A blends – also in moderate blend ratios.

HL 117.9 Fri 12:15 POT 051

**Polymer aggregation control in polymer: PCBM bulk heterojunctions adapted from solution** — ●CHRISTIAN KÄSTNER<sup>1</sup>, DANIEL EGBE<sup>2</sup>, and HARALD HOPPE<sup>1</sup> — <sup>1</sup>Ilmenau University of Technology, Ilmenau, Germany — <sup>2</sup>Linz Institute for Organic Solar Cells, Linz, Austria

It is common knowledge that the polymer conformation and its phase separation with fullerene derivatives are delicate issues crucially impacting on the photovoltaic parameters of polymer based solar cells. Whereas strongly intermixed polymer:fullerene phases provide large interfacial area and consequently a high quantum efficiency of exciton dissociation, pristine and primarily ordered polymer and fullerene domains support efficient charge transport and percolation. To study the aggregation and phase separation in polymer solar cells we investigated counterbalancing influences of polymer solution concentration and PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) blending ratio on the basis of a semi-crystalline anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer statistically bearing either branched 2-ethylhexyloxy or linear octyloxy side-chains (AnE-PVstat). The polymer aggregation varied with both, solution and PCBM concentrations, yielding a specific maximum within the parameter range. We explicitly demonstrate the counterbalancing effect on charge generation and transport for increasing polymer aggregation. Furthermore the influence of polymer aggregation on fundamental optoelectronic properties is discussed, providing detailed understanding of resulting photovoltaic parameters.