HL 99: Organic Semiconductors: Transport

Time: Friday 9:30–12:30 Location: EW 203

HL 99.1 Fri 9:30 EW 203

Theoretical Studies on the Dynamical Conductivity in Organic Crystals — •André Fischer[1], Frank Ortmann[2], Friedhelm Bechstedt[1], and Karsten Hannewald[1] — [1]European Theoretical Spectroscopy Facility and Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — [2]Institut Català de Nanotecnologia (ICN), Barcelona, Spain

The theoretical description of charge-transport and excitation properties of organic semiconductors is of crucial importance for the understanding and improvement of organic (opto)electronic devices. As an extension of our previous theories for the static conductivity [1,2], we present here a theory for the dynamical conductivity in organic crystals. Based on the Holstein Hamiltonian, we derive an analytical expression for the temperature-dependent intraband absorption of polarons. The methodological development is supplemented by numerical studies for a 1D model crystal [3] and predictions are made for the expected signatures in corresponding THz experiments.

[1] K. Hannewald et al., Phys. Rev. B **69**, 075211 (2004); Phys. Rev. B **69**, 075212 (2004); Appl. Phys. Lett. **85**, 1535 (2004)
[2] F. Ortmann et al., Phys. Rev. B **79**, 235206 (2009); New J. Phys. **12**, 023011 (2010); Phys. Stat. Sol. B **248**, 511 (2011)
[3] A. Fischer et al. (submitted)

HL 99.2 Fri 9:45 EW 203

Understanding charge and spin transport properties of $\pi-$conjugated polymers — •Sandip Bhattacharya, Mauro Ferreira, and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

An efficient spin polarized transport through Organic Spin Valves, which is quinessential for a high and stable MR, require a much broader understanding of how spins travel through an organic media. In this respect the general consensus among the Organic Spintronics community on the principal spin scattering mechanisms is often quite contentious. In the current work, we discuss our microscopic approach to this problem [1]. Organic π-conjugated polymers are represented by using a Hubbard-Peierls model that also includes Hyperfine (HF) and Spin Orbit interactions (SOC). The phononic degrees of freedom and the nuclear spins in the Hamiltonian are evolved in Monte Carlo simulations. The transport observables investigated are the spin-polarized conductance (Landauer-Buttiker formalism) and the charge carrier mobility (Kubo formula). We are able to extract the spin diffusion length and spin lifetimes of carriers from the observables and thereby compare them directly to experimental results. The problem at hand is quite an intriguing one involving a significant deal of complexity in terms of controlling the number of microscopic parameters. The strengths of the SOC constant and the HF integral are estimated from first-principle calculations. In this work we present our results on spin and charge transport properties calculated in the entire region of parameter space of the problem.

[1] S. Bhattacharya et al JPCM, 23, 316001 (2011).

HL 99.3 Fri 10:00 EW 203

Polaron Transport in Organic Crystals: Temperature Tuning of Disorder Effects — •Frank Ortmann[1,2] and Stephan Roche[2,3] — [1]CEA Grenoble, France — [2]CIN2 (ICN-CSIC), Universitat Autónoma de Barcelona, Catalan Institute of Nanotechnology, Spain — [3]ICREA, Spain

We explore charge transport in three-dimensional models of disordered organic crystals with strong coupling between electronic and vibrational degrees of freedom. [1] By studying the polaron dynamics in a static disorder environment, temperature-dependent mobilities are extracted and found to exhibit different fingerprints depending on the strength of the disorder potential. At low temperatures and for strong enough disorder, coherence effects induce weak localization of polarons. These effects are reduced with increasing temperature (thermal disorder), resulting in mobility increase. However, at a transition temperature, phonon-assisted contributions driven by polaron-phonon scattering prevail, provoking a downturn of the mobility. The results provide an alternative scenario to discuss controversial experimental features in molecular crystals.

[1] F. Ortmann and S. Roche, Phys. Rev. B **84**, 180302R (2011)

HL 99.4 Fri 10:15 EW 203

Multiscale simulations of the density of states, DC and terahertz mobility of charge carriers in disordered conjugated polymers — •Nenad Vukmirovic — Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Serbia

Understanding the relationship between the atomic structure of an organic material and its electrical properties is of utmost importance for the development of materials for organic electronic devices. In this work, recently developed simulation frameworks [1,2,3] were used to understand the factors that determine the density of states, the DC and the terahertz mobility of several materials.

It was found that the size of the torsion barrier between neighbouring polymer units strongly affects the density of electronic states and consequently all electrical properties. Next, it was shown that alkyl chains act not only as insulating barriers that impede the transport but their presence may also reduce the disorder caused by other chains and consequently enhance the transport. Finally, the simulations also give insight into the distribution of carrier energies and transport distances that are probed in measurements of the mobility at terahertz frequencies. Their fingerprint is much weaker dependence of the terahertz mobility on temperature in comparison to the DC case.

[1] N. Vukmirovic and L.-W. Wang, J. Phys. Chem. B 115, 1792 (2011). [2] N. Vukmirovic and L.-W. Wang, Nano Lett. 9, 3996 (2009). [3] N. Vukmirovic and L.-W. Wang, J. Phys. Chem. B 113, 409 (2009).

HL 99.5 Fri 10:30 EW 203

Positive feedback between Joule heating and current density in organic devices based on C_{60} — •Axel Fischer[1], Paul Pahner[1], Björn Lüssem[1], Karl Leo[1], Reinhard Scholz[1], Thomas Koprucki[2], Jürgen Fuhrmann[2], Annegret Glitzky[2], and Klaus Gärtner[2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden — [2]Weierstraß-Institut für Angewandte Analysis und Stochastik, Mohrenstraße 39, 10117 Berlin

We have studied the influence of heating effects on the device performance in an organic device containing a layer sequence of n-doped / intrinsic / n-doped C_{60} between crossbar metal electrodes. Due to the fact that C_{60} can withstand temperatures above 200°C, these devices give a perfect setting for studying the heat transport. At high current densities beyond 100 A cm^{-2}, a strong positive feedback between current and temperature is observed, as predicted by the extended Gaussian disorder model (EGDM) applicable to organic semiconductors [1]. Approximate analytical studies and detailed 3D numerical simulations for the stationary heat transport problem reveal the temperature distribution. The result is confirmed by thermal imaging of the device. Additionaly, strong heating at the edges of the device is obtained and cannot be understood quantitatively by assuming homogeneous Joule heating in the active volume. Instead, 3D effects have to be included even for the seemingly 1D electrical transport pathways between the two electrodes. [1] R. Coehoorn, W. F. Pasveer, P. A. Bobbert, and M. A. J. Michels, Phys. Rev. B **72**, 155206 (2005).

HL 99.6 Fri 10:45 EW 203

Bipolar organic semiconductors: application in thin film transistors and photovoltaic cells — •Andreas Opitz[1,2], Andreas Wilke[1], Norbert Koch[1], Mark Gruber[2], Ulrich Hörmann[2], Matthias Horlet[2], Michael Kraus[2], Julia Wagner[2], and Wolfgang Brütting[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institut für Physik, Universität Augsburg

Organic semiconductors used in thin-film devices have traditionally been reported as either electron or hole transporting materials. For this contribution the transport of electrons and holes in molecular semiconductors is analysed in organic field-effect transistors [1]. Additionally the ability of molecular semiconductors to act as donor or acceptor material was investigated [2,3]. Furthermore the device behaviour is compared to the energy levels of the semiconductors [2].

Our findings show that the classical distinction between hole and electron conducting organic semiconductors is mostly related to the suppression of electron transport due to electron traps at oxide surfaces for the former and the impossibility of hole injection into the deep lying HOMO level for the latter. By adjusting the energy levels for injection at the contacts and for exciton dissociation at the organic/organic in-

terface the same molecular semiconductors (e.g. diindenoperylene) can be used as active material in light-emitting transistors and as donor or acceptor material in solar cells with the appropriate counterpart.

[1] M. Horlet et al., Appl. Phys. Lett. 98 (2011) 233304.
[2] J. Wagner et al., Adv. Func. Mater. 20 (2010) 4295.
[3] U. Hörmann et al., phys. stat. sol. RRL 5 (2011) 241.

Coffee Break (15 min)

HL 99.7 Fri 11:15 EW 203

Charge carrier injection properties of the Au-P3HT interface — Shahidul Alam, •Torsten Balster, and Veit Wagner — School of Engineering and Science,Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The contact between the metal and the organic semiconductor is crucial for the device performance of an organic field effect transistors. To study the injection properties of the holes into the organic semiconductor vertical Au/rr-P3HT/Au structures on PET foil has been prepared and investigated in this study.
This structures with an area varying from 0.05 to 1.0 mm^2 and a P3HT film thickness of 270 nm were characterized using I-V-measurements. The devices showed asymmetric I-V curves, which are attributed to the exposure of the bottom Au contact to air during the processing of the sample in contrast to the top electrode, which was sputter coated on the P3HT film. Additional UV-Ozone treatment of the bottom electrode increased the current ratio between forward and reverse bias by a factor of two.
For lower bias voltages (<0.5V) the data were evaluated using thermionic emission and tunneling models. Whereas the latter gives barrier heights of $\approx$ 0.5 V and rather high ideality factors of more than 10, the tunneling model predicts a much smaller barrier. In the space charge limited region the curves were modelled using the mobility model of Vissenberg and Matters.

HL 99.8 Fri 11:30 EW 203

Transport properties of molecular thin films connected by strained nanomembranes — •Carlos Cesar Bof Bufon[1], Celine Vervacke[1], Dominic J. Thurmer[1], Michael Fronk[3], Georgeta Salvan[3], Dietrich R. T. Zahn[3], and Oliver G. Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany — [3]Institute of Physics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany

In this work, rolled-up metallic nanomembranes are used to contact thin film molecular layers (CuPc) with thickness (10nm) smaller than the interdiffusion length of metallic atoms. The fabrication process is based on a recently developed method where strained nanomembranes are used to create hybrid organic/inorganic heterojunctions[1]. The fabricated heterojunction allow us to precisely control and map the charge transport mechanisms in such devices over a wide range of temperatures and electric fields. The transport characteristics of CuPc thin films resembles what have been reported for molecular wires, namely, the transition from activated hopping to tunneling by changing temperature and voltage. In the Au/CuPc/Au heterojunctions the transport is dominated by impurities/defects states at high temperatures and by cooling down, the continuous transition from direct tunneling to resonant tunneling to field emission is obtained by sweeping the voltage bias up. Such a continuous transition has not been reported so far for this type of heterojunction. [1]Bufon,C.C.B., Nano Lett.11,3727 (2011)

HL 99.9 Fri 11:45 EW 203

Seebeck Measurements on Two Air-Stable n-Dopants for C60 — •Torben Menke[1], Peng Wei[2], Debdutta Ray[1], Zhenan Bao[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Department of Chemical Engineering, Stanford University, USA

Thin layers (30nm) of fullerene C60 are doped, using two different air-stable n-dopants with varying doping concentration. Conductivity and thermovoltage (Seebeck) measurements in vacuum are discussed and the influences of doping ratio and temperature are compared to investigate the nature of the doping process. The n-dopants investigated are the commonly used 3,6-bis(dimethylamino)acridine (acridine orange base, AOB) and a novel 1,3-dimethyl-2-phenyl-2,3-dihydro-1H-benzoimidazole derivate (R-DMBI). With increasing doping concentration the Seebeck coefficient is found to decrease, indicating a Fermi energy shift towards the transport state. For both dopants and different doping concentrations the energetic difference between the Fermi energy and the transport level is observed and compared to the thermal activation energy of the conductivity. Both energies show the same trend of a strong reduction with increasing doping concentration, confirming an increase of the free charge carrier density. Conductivity and Seebeck measurements are combined to estimate the mobility of the layers. These results show that R-DMBI is a promising and air-stable n-dopant for replacing AOB in the future.

HL 99.10 Fri 12:00 EW 203

Characterization of Codeposited Pentacene:Perfluoropentacene Thin-Films via Transmission Electron Microscopy — •Benedikt Haas, Katharina I. Gries, Tobias Breuer, Gregor Witte, and Kerstin Volz — Philipps-University Marburg, Faculty of Physics and Materials Science Center, 35032 Marburg, Germany

Organic semiconductors (OSC) are up-and-coming in research and industry. Perfluoropentacene (PFP) is the perfluorinated sibling of the well-known OSC pentacene (PEN), which exhibits high hole mobilities of up to 40 $\frac{cm^2}{(Vs)}$. The two materials are interesting in combination due to the fact that they have a very similar crystal structure but are p-type (PEN) and n-type (PFP) OSCs.

Samples of coevaporated PEN:PFP (grown by organic molecular beam deposition) on alkali halide substrates (KCl, NaF) were investigated using transmission electron microscopy (TEM). Beam damage is very critical for these materials but adequate sample preparation and microscope operation enables one to obtain invaluable information about the morphology and crystalline orientation.

TEM allows for a high spatial resolution of the occurring phase separation, including a 1:1 PEN:PFP mixed phase. The formation of different phases of the segregated PEN has also been evidenced, depending on the substrate used. First results concerning lattice spacings of the PEN:PFP mixed phase have been obtained and are of special interest because x-ray reflectivity analysis has been shown to be hindered due to the intricate phase separation.

HL 99.11 Fri 12:15 EW 203

Scanning Kelvin Probe Microscopy on FIB-milled crosssections in organic semiconductor devices — •Rebecca Saive[1,2], Florian Ullrich[1,2], Lars Müller[1,2], Michael Scherer[1,2], Dominik Daume[1,2], Michael Kröger[1,2,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

Scanning Kelvin Probe Microscopy (SKPM) offers the possibility to measure the surface potential in operating devices and thus revealing the charge carrier transport. We show that SKPM does not necessarily reflect the potential distribution in the region of charge transport but that measurement results are a superposition of all effects occuring in the bulk. Therefore we introduce a method to directly measure in the charge transport region. Via focused ion beam (FIB) we milled our samples and measure the device's crosssections with SKPM. With our combined SEM-FIB crossbeam and SPM microscope we prepare our devices in-situ which avoids surface degradation by water or oxygen.