

CPP 21: Organic Electronics and Photovoltaics III: Mobile and Trapped Charges (joint session CPP/DS/HL, organized by CPP)

Time: Tuesday 9:30–12:45

Location: ZEU 260

CPP 21.1 Tue 9:30 ZEU 260

A Kelvin-Probe study of the electrical transport in organic semiconductors — ●KARL-PHILIPP STRUNK¹, VALERIA MILOTTI¹, ALEXANDER ULLRICH², and CHRISTIAN MELZER¹ — ¹Centre for Advanced Materials, University of Heidelberg, Germany — ²Chemisches Institut, Universität of Heidelberg, Germany

DC current-voltage measurements on organic field-effect transistors (organic FET or OFET) are commonly used to characterize the planar electrical transport in organic semiconductors. In this study we report an alternative AC dark-injection method giving likewise access to in-plane transport parameters of organic semiconductor thin films. Exposing a macroscopic FET-like structure to a periodic bias leads to a periodic change in surface potential which can be tracked via a Kelvin-Probe giving direct insight into the movement of lateral charge-carrier waves along the organic film. Tracking the temporal evolution of the surface potential distribution allows for the determination of the charge-carrier mobility at low currents, a regime which is conventionally hardly accessible. It will be shown that this regime allows for a mobility determination at P3HT based devices fairly independent on contact properties. In order to elucidate the influences of electrical properties like doping concentration, traps states and injection barriers on the device response, time-dependent finite-element simulations have been carried out.

CPP 21.2 Tue 9:45 ZEU 260

Spin dynamics and spin current in a high-mobility polymer — ●THORSTEN ARNOLD¹, ANDREAS LÜCKE², UWE GERSTMANN², WOLF GERO SCHMIDT², and FRANK ORTMANN¹ — ¹Institute for Materials Science, Center for Advancing Electronics Dresden and Dresden Center for Computational Materials Science, Technische Universität Dresden, 01069 Dresden, Germany — ²Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Organic semiconductors are characterized by small spin-orbit coupling, which leads to a relatively long spin relaxation time. This makes them particularly interesting materials for spintronics. We describe spin transport in the thiophene-based polymer PBTTT using a recently developed generalization of the Kubo formalism to spin and an appropriate definition of the spin current operator in tight-binding form to investigate the spin conductivity tensor in PBTTT. The transfer integrals of the Hamiltonian and spin current operator are extracted from the DFT band structure with and without spin-orbit coupling. The spin propagation and spin conductivity for different spin-orbit transfer integral models are compared and the energy dependence and relaxation are analyzed.

CPP 21.3 Tue 10:00 ZEU 260

Virtual screening for high carrier mobility in organic semiconductors — ●CHRISTOPH SCHOBER, KARSTEN REUTER, and HARALD OBERHOFER — Technische Universität München

Low carrier mobilities still hamper the use of organic semiconductors in many applications. Using a staged virtual screening approach we compute the electronic couplings and intramolecular reorganization energies as two main descriptors for charge mobility for a set of 95445 molecular crystals extracted from the Cambridge Structural Database (CSD). Descriptor calculations are performed using efficient density functional theory methods developed in our group, together with a fully automated workflow system for data preparation and verification. As a final step, based on the calculated coupling values we identify materials with long-range charge percolation pathways. We readily find many acclaimed compounds, as well as a number of most promising materials that have not yet been considered for an application in organic electronics. Together with the unique meta-data provided in the CSD the large descriptor database allows to extract important trends and correlations that will further accelerate the theoretical design and discovery of high mobility organic semiconductors.

C. Schober, K. Reuter, H. Oberhofer, *J. Chem. Phys.* **2016**, *144*, 054103.

C. Schober, K. Reuter, H. Oberhofer, *J. Phys. Chem. Lett.* **2016**, *7*, 3973-3977.

CPP 21.4 Tue 10:15 ZEU 260

Utilizing Schottky barriers to suppress short channel effects in organic transistors — ●ANTÓN F. FERNÁNDEZ and KARIN ZOJER — Institute of Solid State Physics and NAWI Graz, Graz University of Technology, Graz, Austria

High switching speeds constitute one of the optimization targets for organic thin film transistors (OTFT). Reducing the channel length is a major handle to boost the switching speed of OTFTs. However, upon reducing the channel length one has to cope with undesired short-channel effects, i.e., a loss of saturation, a reduced ON-OFF ratio, and a disproportionately larger impact of the contact resistance. We demonstrate by virtue of device simulations that the ON-OFF-ratio of a short channel transistor is enhanced by orders of magnitude when a Schottky barrier at the injecting contact is intentionally introduced. The key effect is the efficient suppression of the OFF-current while trading in only a small loss in the ON current. We show that, in fact, it is possible to establish a minimal Schottky barrier such that the short channel transistors can be operated without premature turn-on while retaining an ON current as large as expected from Gradual Channel approximation. This strategy is suited for staggered and coplanar transistor architectures.

CPP 21.5 Tue 10:30 ZEU 260

Direct Au-C contacts based on biphenylene for single molecule transport — ●NARENDRA P. ARASU and HÉCTOR VÁZQUEZ — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10/112, Prague, Czech Republic

Metal-molecule contacts strongly influence the mechanical, electronic and conducting properties of molecular junctions [1]. Here we use Density-Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods to study biphenylene-based molecular circuits. We expect that at the Au surface the biphenylene molecule will break a weak intramolecular C-C bond and form covalent bonds to the substrate. Direct Au-C metal-molecule links were shown to be highly-conducting [2,3]. With these Au-C links to the substrate, we then consider several linker groups at the other end of the molecule, which is contacted by a Au tip. We calculate the mechanical properties of the junctions from tip approach trajectories and find that Au-C bonds are stable under the stress induced by the approaching tip. We then discuss the conductance of the junction focusing on the dependence of transport behaviour on linker chemistry.

[1] F. Schwarz et al., *J. Phys.: Condens. Matter* **26**, 474201 (2014).

[2] Z. L. Cheng et al., *Nat. Nanotechnol* **6**, 353-357 (2011).

[3] W. Chen et al., *J. Am. Chem. Soc* **133**, 17160 (2011).

CPP 21.6 Tue 10:45 ZEU 260

Controlling the transport in organic electronics via self-assembled Monolayers — ●ANJA FÖRSTER¹, SIBYLLE GEMMING^{2,3}, and GOTTHARD SEIFERT¹ — ¹TU Dresden, Center for Advancing Electronics Dresden (cfaed), 01062 Dresden, Germany — ²Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden Rossendorf, Center for Advancing Electronics Dresden (cfaed), Bautzner Landstr. 400, 01328 Dresden, Germany — ³Institute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Self-assembled monolayers (SAM) can be used to control the transport in organic field-effect transistors. The SAM creates a dipole moment induced electric field that is able to change the major transport type in organic materials.

In the case of fluoroalkyl SAMs, their strong dipole moment induces electric fields up to 10^9 V/m. These fields are strong enough to affect the underlying organic material up to a distance of 10-20 Å from the SAM. Due to the orientation of the dipole moments this leads to a hole dominated transport.

Amine-based SAMs, on the other hand, enhance the electron transport as their dipole moment is counter-directional to the one from fluoroalkyl SAMs. Due to their lower absolute dipole moment, their effect is not as strong as for fluoroalkyl SAMs.

Finally, we exemplarily show for pentacene how the SAM molecules connect to the organic material. The resulting distance of the SAM layer to the organic material determines the maximum strength of the dipole moment induced electric field.

15 min break

CPP 21.7 Tue 11:15 ZEU 260

Electronic components embedded in a single graphene nanoribbon — ●PETER JACOBSE^{1,2}, FABIAN SCHULZ³, ADRI VAN DEN HOOGENBAND², MARC-ETIENNE MORET², ROBERTUS KLEIN-GEUBINK², PETER LILJEROTH³, and INGMAR SWART¹ — ¹Debye Institute for Nanomaterials Science, Utrecht University, PO Box 80000, 3508 TA Utrecht, The Netherlands — ²Princetonplein 1 — ³Department of Applied Physics, Aalto University School of Science, PO Box 15100, 00076 Aalto, Finland

On-surface synthesis offers a convenient route to atomically well-defined graphene nanoribbons (GNRs) with a precisely controlled width and edge structure. In addition to monocomponent ribbons, GNR heterojunctions joining two semiconducting segments with different band gaps (through ribbon width) or different band-alignment (through nitrogen substitution) have been demonstrated. The driving force in this direction is to build more functionality into a single ribbon for applications in GNR-based electronics or photovoltaics. However, the GNR equivalents of a metal-semiconductor junction or a tunnel barrier have not yet been realized. We embed these junctions in a single GNR by joining armchair GNRs belonging to the metallic (5-atom wide) and semiconducting (7-atom wide) families through on-surface synthesis. We characterize the atomic scale geometry and electronic structure by combined atomic force microscopy (AFM), scanning tunneling microscopy (STM) and conductance measurements. The GNR equivalent of a tunnel barrier constitutes a first step towards complete electronic devices built into a single GNR.

CPP 21.8 Tue 11:30 ZEU 260

Thermoelectric thin films based on a polymer/nanoparticle nanocomposite — ●NITIN SAXENA^{1,2}, MIHAEL CORIC³, ANTON GREPPMAIR⁴, JAN WERNECKE⁵, MIKA PFLÜGER⁵, MICHAEL KRUMREY⁵, MARTIN S. BRANDT⁴, EVA M. HERZIG³, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Center for Nanoscience, LMU München, 80539 München, Germany — ³TU München, Munich School of Engineering, 85748 Garching, Germany — ⁴TU München, Walter-Schottky-Institut and Physik-Department, 85748 Garching, Germany — ⁵PTB, BESSY II Helmholtz-Zentrum Berlin, 12489 Berlin, Germany

Thermoelectric materials pose a compelling technology for power generation from renewable energies, since temperature gradients are transformed into voltages and thus electrical power. So far, highly efficient thermoelectrics comprise rare and/or toxic inorganic materials, and require cost- and energy-intensive fabrication. These points hinder their large-scale application. In order to overcome these limitations, we pursue a hybrid approach combining the semiconducting polymer blend PEDOT:PSS for its high electrical conductivity and inorganic nanoparticles in order to reduce thermal conductivity within the thin film. Beside the thermoelectric properties, we investigate the thermal conductivity of pristine PEDOT:PSS and of the hybrid film, in order to ultimately calculate the figure-of-merit ZT. Tender resonant x-ray scattering (T-ReXS) is used to derive a morphological model, and describe the influence of the nanoparticles on the thermoelectric properties.

CPP 21.9 Tue 11:45 ZEU 260

Modelling long-term isothermal charge decay in modified PTFE electrets — ●DMITRY RYCHKOV — University of Potsdam, Potsdam, Germany

Electret stability is usually best characterised by means of charge decay as a function of time. In highly stable electret materials, charge-decay measurements require very lengthy experiments even at elevated temperatures. Isothermal charge-decay curves, however, can be modelled if thermally-stimulated discharge data are known. Here, we attempt to deal with this problem for electrets made from chemically modified polytetrafluoroethylene (PTFE) films. PTFE films were treated with TiCl₄ vapor in a flow-type reactor and electrically charged in a positive corona discharge. Using the charge-transport theory by Simmons, frequency factors and energy spectra for the relevant surface traps have been extracted from thermally stimulated surface-potential decay curves. The data were then used to calculate isothermal charge-decay curves at different temperatures. A detailed comparison between the modelled and the experimental curves reveals good agreement at elevated temperatures. At lower temperatures, however, the modelled isothermal charge-decay curves deviate from the experimental ones and

show a slower decay, which indicates that additional mechanisms that are not covered in the theory may contribute to the electret-charge decay in this temperature range. We propose a simple phenomenological model to illustrate the effects of such mechanisms and to determine the applicability limits of our charge-decay modelling method.

CPP 21.10 Tue 12:00 ZEU 260

Large area three-dimensional polarization control in P(VDF-TrFE) polymer films on graphite — ●ROBERT ROTH¹, MARTIN KOCH¹, JAKOB SCHAAB², MARTIN LILIENBLUM², THOMAS THURN-ALBRECHT¹, and KATHRIN DÖRR¹ — ¹Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle, Germany — ²Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Ferroelectric polymers are attractive candidates for functional layers in electronic devices like non-volatile memories, piezo- and magnetoelectric sensors, and capacitor-based high speed energy storage devices. Unfortunately, such thin films often reveal low di- and piezoelectric responses due to reduced crystalline and electrical dipole order, leading to compensation effects and low effective electric performance. One of the best characterized and often applied ferroelectric polymers is poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)). We will present results on micron-sized domains with three dimensional ferroelectric polarization alignment in P(VDF-TrFE) films on graphite. The ferroelectric domains have been achieved by a combined procedure of electrical poling and mechanical annealing with an atomic force microscopy tip. They show strongly increased lateral and vertical piezoresponse compared to the as-prepared film and can be deliberately written and switched.

CPP 21.11 Tue 12:15 ZEU 260

Significantly enhanced charging efficiency for higher piezoelectricity in polymer ferroelectrets — ●XUNLIN QIU — Department of Physics and Astronomy, University of Potsdam, 14469 Potsdam, Germany

Ferroelectrets are internally charged polymer foams or cavity-containing polymer-film systems. They are charged through a series of dielectric barrier discharges (DBDs) inside the cavities which interact with the internal polymer surfaces [1]. The breakdown strength of the gas strongly influences the charging process. A gas with a lower breakdown strength has a lower charging voltage, but leads to a lower remanent polarization. Charging in gases with higher breakdown strength requires higher voltage but allows higher remanent polarization. Here, a charging scheme involving gas exchange during charging is proposed [2]. The cavities of a tubular-channel fluoroethylenepropylene (FEP) ferroelectret are first filled with helium (lower breakdown strength), so that DBDs can be easily triggered by applying a relatively low voltage. The charging voltage should not be turned off until the gas inside the cavities has been replaced with nitrogen or air (having higher breakdown strength), in order to achieve higher remanent polarization. With the proposed charging scheme, the charging efficiency and hence the resultant piezoelectricity of ferroelectrets can be significantly enhanced.

[1] X. Qiu, W. Wirges and R. Gerhard, J. Appl. Phys. 110, 024108 (2008).

[2] X. Qiu, Appl. Phys. Lett. 109, 222903 (2016).

CPP 21.12 Tue 12:30 ZEU 260

Tuning the Electronic Properties of 3D Covalent Organic Networks by Collective Electrostatic Design — ●VERONIKA OBERSTEINER, ANDREAS JEINDL, JOHANNES GÖTZ, AURELIE PERVEAUX, and EGBERT ZOJER — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Covalent organic frameworks have recently attracted substantial interest as materials for photovoltaics applications, as they can be synthesized mimicking donor-acceptor bulk heterojunctions.

On the basis of first-principle results we propose a novel design strategy for analogous 3D-organic networks, where a band offset between different semiconducting segments can be achieved by introducing periodic arrangements of dipolar elements into the material. Exploiting the resulting collective electrostatic effects, we are able to manipulate the electronic landscape of the 3D networks in a controlled way, thereby, achieving spatially confined pathways for electrons and holes. The distinct advantage of this approach over conventional strategies for achieving the band offset by using chemically distinct donor and acceptor units is that the magnitude of the band offset can be tuned continuously. The suggested electrostatic design strategy also enables

the realization of more complex structures like quantum-cascades and | 'quantum-checkerboards'.