

CPP 9: Organic Electronics and Photovoltaics I - Charge Transport and Electronic Devices

Time: Monday 15:00–17:15

Location: H18

Invited Talk

CPP 9.1 Mon 15:00 H18
Bulk Amounts of (6,5) Carbon Nanotubes for (Opto)- Electronic Devices — ●JANA ZAUMSEIL — Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany

Large volumes of highly purified dispersions of semiconducting (6,5) single-walled carbon nanotubes are readily available through polymer-wrapping and shear-force mixing. They enable the deposition (e.g. by aerosol jet printing) of semiconducting nanotube layers of variable thickness from sparse networks to 300 nm thick films with large optical density. These layers can be applied in lateral and vertical field-effect transistors with excellent device performance, but also as electrochromic filters, for organic light-emitting diodes in the near-infrared and photovoltaic cells. Here, we present examples of such applications and investigate the impact of novel n-dopants on nanotube networks, temperature-dependent charge transport and their optical properties at different charge carrier densities.

CPP 9.2 Mon 15:30 H18
The impact of energy barriers at grain boundaries on charge carrier motion in a high-mobility, electron-conductive organic semiconductor — ILJA VLADIMIROV¹, MICHAEL KÜHN¹, THOMAS GESSNER¹, FALK MAY¹, and ●THOMAS WEITZ² — ¹BASF SE, Ludwigshafen, Germany — ²AG Physics of Nanosystems, Faculty of Physics, LMU München, Germany

Using high-surface tension solvents allowed us to grow 3 * 10 nm thin, highly-crystalline films of a N,N*-di((S)-1-methylpentyl)-1,7(6)-dicyano-perylene-3,4:9,10-bis(dicarboximide) (PDI1MPCN2) at the liquid/air interface of a drying droplet [1]. We find, that charge carrier mobilities in these electron conductive films is as high as 4 cm²/Vs even for an only 3 nm thin PDI1MPCN2 film. Changing the solvent composition used for crystallization of our organic semiconductor also has allowed us to systematically tune the crystallinity and consequently the grain boundary density in thin films. From the temperature-dependent charge carrier mobility, we have extracted the density of states and compared it to Kinetic Monte Carlo simulations [2]. This combined theoretical and experimental approach has allowed us to identify, that it is rather the energetic barriers at grain boundaries than the usually identified traps that limit charge carrier motion. We also have revealed that the dipole moment of the PDI1MPCN2 is the cause for the energetic disorder at grain boundaries serving as clear guideline for future design of organic semiconductors with potentially no energetic barriers present at the grain boundaries. [1] Nano Lett. 18, 9, (2018) [2] Sci. Rep. 8, 14868, (2018)

CPP 9.3 Mon 15:45 H18
Electronic couplings in molecular crystals: Tight-Binding fits vs. cluster-based approaches — ●FLORIAN MAYER, CHRISTIAN WINKLER, and EGBERT ZOJER — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

The ever-growing interest in electronic properties of new materials triggers the development of new methodologies for their reliable description. For modelling charge-transport properties, theories span the full range from band transport via dynamic-disorder models to hopping approaches. For all these methods the electronic coupling between neighboring molecules is a crucial input. This quantity can be calculated with various approaches most of them relying on simulations of molecular dimers and small clusters. In contrast, the fitting of extended Tight-Binding models to full band structures allow the evaluation of intermolecular coupling, treating the molecules in their actual crystalline environments. In the present contribution, for the prototypical examples of pentacene and quinacridone, applying the above-mentioned complementary approaches, we discuss issues like next-nearest neighbor coupling, interference between different coupling directions for coherent transport, and how to deal with off-Gamma point band extrema. For non-periodic calculations we also present a new variant of the fragment orbital and electronic splitting method. The obtained results provide insight into the strengths and limitations of the various approaches and help to better understand electronic coupling in organic semiconductors.

15 min. break

CPP 9.4 Mon 16:15 H18
Finding the right building blocks for molecular optimization - Mining a database of organic semiconductors — ●CHRISTIAN KUNDEL, CHRISTOPH SCHÖBER, JOHANNES T. MARGRAF, KARSTEN REUTER, and HARALD OBERHOFER — Chair for Theoretical Chemistry, Technical University Munich

Improving charge carrier mobilities of organic semiconductors is usually tackled by empirical structural tuning of a promising compound. Knowledge-based methods can greatly accelerate such local exploration by providing an overview of the problem-specific design space. Here, we provide such an overview for organic semiconductors, applying data mining strategies to an in-house database of >64.000 organic molecular crystals, annotated with charge-transport descriptors (electronic coupling and the reorganization energy) that are calculated from first principles. This database-screening recovers many known and well-performing materials, while also uncovering many more promising candidates, not yet considered for organic electronics applications. Analysing the design space regions in this dataset by a chemical space network hints at already explored or promising regions. We further derive general design principles by evaluating the performance of molecular scaffold and sidegroup clusters of compounds. For these, we find certain scaffolds (sidegroups) to consistently improve charge-transport properties. Functionalizing promising scaffolds with favorable sidegroups then results in molecular crystals with improved charge-transport properties, highlighting the usefulness of data-based approaches for a targeted design of organic electronics materials.

CPP 9.5 Mon 16:30 H18
Calculating electron - phonon coupling with density functional theory to describe polaron dynamics — ●OLIVER STAUFFERT¹, ROMAN KREMS², MONA BERCIU², and MICHAEL WALTER¹ — ¹Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany — ²University of British Columbia Faculty of Science

In order to investigate on novel materials, we describe electronic structures for organic molecules, with density functional theory (DFT). Hereby we are especially interested in coupling of electronic and nuclear degrees of freedom to investigate polaron phenomena. These have been proposed based on the Su-Schrieffer-Heeger (SSH) Hamiltonian and might lead to superconducting states. We use DFT calculations to obtain the SSH parameters of polyacetylene and its derivatives in order to explore a set of possible materials with strong electron-phonon coupling. Our results predict an increase of the coupling parameter through stretching of the chain or by substitution of the hydrogens by other side groups. With the new insight gained in the electron phonon coupling within these simple chains, one might improve the understanding of polarons in more complex materials and take a step towards the direction of high temperature superconductors.

CPP 9.6 Mon 16:45 H18
Why are charge-carrier mobilities in organic semiconductors typically low? The instructive case of quinacridone — ●CHRISTIAN WINKLER, FLORIAN MAYER, OLIVER T. HOFMANN, GERNOT J. KRABERGER, and EGBERT ZOJER — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz

In this contribution, using first principles approaches, we study the interplay between transport relevant parameters, total energy, and crystal structure by using the instructive example of quinacridone. For this material, one finds three polymorphs with fundamentally different packing motifs. Additionally, based on the α -polymorph, an artificial coplanar quinacridone crystal can be constructed. The latter allows correlating electronic properties like transfer integrals t and effective masses m^* with the total energy of the crystal. This yields a clear correlation between energetic minima and poor transport parameters suggesting that in π -stacked systems Pauli-exchange repulsion triggers a shift between neighboring molecules such that the inter-molecular electronic coupling is minimized. Possible strategies for overcoming this negative correlation can be derived from the properties of β - and γ -quinacridone, where larger transfer integrals result from modified van der Waals interactions and complex H-bonding networks.

CPP 9.7 Mon 17:00 H18

Hopping-approach in organic semiconductors: mode-resolved vibrations and improved time-consistency — ●SEBASTIAN HUTSCH and FRANK ORTMANN — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

The charge carrier mobilities of different organic semiconductor systems can span several orders of magnitude, making the precise description of different transport regimes necessary. When a localization of the charge carrier is expected, e.g. due to a strong electron-phonon

coupling, the transport is assumed to be hopping-like. This regime is usually treated within the Marcus theory or Levich-Jortner theory, which however approximate the rich vibrational spectrum of organic semiconductors, for example in the high-temperature limit. We are presenting a hopping-approach that overcomes these limitations by treating the intramolecular modes in a mode-resolved fashion. This refined approach further allows to individually treat each mode statically or dynamically in the calculation of the hopping-rate, i.e. ensure the time-consistency in the treatment of the vibrations.