HL 16: Organic Semiconductors

Time: Tuesday 9:30–12:00 Location: H14

HL 16.1 Tue 9:30 H14

Modeling charge transport in organic semiconductors: why and when the conventional Miller-Abrahams rate is inappropriate

— •Magdalena Dörfler, Heinz Bässler, Andrey Kadashchuk, Harald Oberhofer, and Anna Köhler — Universität Bayreuth, 95447 Bayreuth

A widely applied expression to model charge transport in organic semiconductors is the Miller-Abrahams rate, which describes the probability for charge transfer from one site, e.g. a molecule, to a neighboring site. However, the expression that is conventionally referred to as Miller-Abrahams rate is an approximation of a more general term. This approximation is only valid when energy differences between neighboring sites are large compared to the thermal energy. Here, we show the differences that result when charge transport is modelled by kinetic Monte Carlo simulations (KMC) using either of the two expressions. The widely used, approximate, rate can lead to serious errors in the magnitude and, more importantly, in the trends obtained for the temperature and field dependence of charge transport. The implications for modelling work and the interpretation of experimental data are discussed.

HL 16.2 Tue 9:45 H14

Accurate ab-initio parametrization of electron-phonon coupling models with Gaussian and plane-wave basis sets

— •Konrad Merkel[1], Maximilian Dorfner[1], Manuel Engel[2], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, TU Munich, Germany — [2]VASP Software GmbH, Vienna, Austria

For the simultaneous treatment of electronic and vibrational degrees of freedom, the Holstein-Peierls model has become a cornerstone in various scientific communities due to its versatility and remarkable success in the accurate description of materials. To use it, one needs to calculate all model parameters for the electronic structure, phonons and electron-phonon coupling constants. In particular, the calculation of the electron-phonon coupling constants is a challenge as they involve both degrees of freedom. Although various approaches exist, comprehensive benchmarks comparing different methods and basis sets are still rare. In our study, we investigate two different methods to calculate the electron-phonon couplings. The first approach was developed by Engel et al. [1] and is based on the projector-argumented-wave formulation and maximally localized Wannier functions and is implemented in the VASP code. The second approach is based on a real-space description in terms of Gaussian basis functions and is implemented using cp2k. Both approaches use a finite-displacement and finite-difference scheme to calculate the coupling constants. We compare both methods using different molecules and discuss critical points for accurate calculations.

[1] Physical Review B 106, 094316 (2022)

HL 16.3 Tue 10:00 H14

Excitons in organic donor-acceptor cocrystals

— •Sebastian Anhäuser[1], Ana Maria Valencia[2], Caterina Cocchi[2], and Gregor Witte[1] — [1]Philipps-Universität Marburg, FB Physik — [2]Carl von Ossietzky Universität Oldenburg, Institut für Physik

Organic donor-acceptor heterostructures have gained significant attention due to their unique properties, such as low-bandgap semiconductivity and ambipolar transport, making them promising candidates for optoelectronic applications like organic photovoltaics. There, the formation of charge-transfer excitons is typically regarded as the precursor state for charge separation. However, the microscopic nature of these excitons is not yet well understood. In the presented study, we perform detailed polarization-resolved optical spectroscopy on high quality acene-perfluoroacene donor-acceptor single crystals in the optical and UV range. This approach allows us to investigate both the excitation energies and the transition dipole moments of various (charge-transfer-)excitons. Using complementary state-of-the-art first principles calculations based on density functional and many-body pertubation theory, we analyse the nature of different classes of excitons within the cocrystalline structure. Our findings provide a refined understanding of charge-transfer excitons in organic materials, paving the way for improved design strategies in organic optoelectronics.

HL 16.4 Tue 10:15 H14

Detecting charge patterns on a novel type of rubrene crystals by time-of-flight photoemission electron microscopy

— •Moha Naeimi[1,2], Ingo Barke[1,2], and Sylvia Speller[1,2] — [1]University of Rostock, Institute of physics, Rostock, Germany — [2]University of Rostock, Department of life, light and matter, Rostock, Germany

Organic molecules are increasingly drawing attention due to their broad applications, not only in organic field effect transistors and organic light emitting diodes [1], but also with respect to the exciton dynamics and charge transfer [2]. To this end, single crystalline domains with compact and stable molecular packing are beneficial. In this work, we focus on charge patterns and its dynamics for a recently discovered type of rubrene single crystals consisting of two distinct types of domains [3]. We show that both domains exhibit different charging properties, and that one of them can be controlled by photon exposure. This charge pattern can be *reset* by a second light source with lower photon energy, essentially neutralizing the charged sections. We tentatively attribute the behavior to the selective photo-injection of mobile excitons, resulting in spatially dependent conductivities.

[1] Wei-Cheng Su et al., Influence of Singlet and Charge-Transfer Excitons on the Open-Circuit Voltage of Rubrene/Fullerene Organic Photovoltaic Device ACS Appl. Mater. Interfaces, 8, 28757-28762 (2016) [2] Drew M. Finton et al., Routes to singlet exciton fission in rubrene crystals and amorphous films AIP Advances 9, 095027 (2019) [3] Moha Naeimi et al., Characteristics of zone-sectored tabular orthorhombic rubrene microcrystals in preparation.

HL 16.5 Tue 10:30 H14

Toward High Efficiency and Stable Blue OLEDs/Organic Light-Emitting Diodes with Lanthanide-Based Complexes: Host Material Impact

— •Mahmoud Soleimani[1,2], Paulius Imbrasas[2], Sebastian Schellhammer[1], Carsten Rothe[2], and Sebastian Reineke[1] — [1]Institute for Applied Physics (IAP), Technische Universität Dresden, Germany — [2]beeOLED GmbH, Dresden, Germany

Lanthanides offer a new approach for achieving blue emission in organic light-emitting diodes (OLEDs). Cerium (III) and Europium (II) complexes emit in the blue range via the 5d-4f transition, potentially enhancing the stability and efficiency of OLEDs, outperforming current emitters. However, precise ligand design around the lanthanide is required for a stable, blue-emissive complex. With the right ligands, emitters with near-unity photoluminescence quantum yield in solution have been demonstrated. In the transition to OLED-compatible thin-films, we found that the host material plays a key role in maintaining this luminescence efficiency and that it can also impair emission through quenching mechanisms caused by unfavorable energy level alignment and coordination of the metal-organic complex by the host. This study investigates the photoluminescence of Cerium (III) tris(pyrazolyl)borate complex blended with four common OLED emission layer hosts. These insights guide the development of efficient blue OLEDs with lanthanide complexes.

HL 16.6 Tue 10:45 H14

Modifying the density of states in dipolar organic semiconductors

— •Andrei Stankevich[1], Prakhar Sahay[3], Heinz Bässler[1], Wolfgang Brütting[3], Fabian Eller[2], Eva M. Herzig[2], Andrey Kadashchuk[1], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Dynamics and Structure Formation, University of Bayreuth — [3]Institute of Physics, University of Augsburg,

Charge transport properties of amorphous organic semiconductors are controlled by energetic disorder. Certain device properties, such as the energies of charge transfer states in organic light-emitting diodes, can be improved by using dipolar molecules as host. Such molecules, however, also introduce interactions between charge carriers and randomly aligned dipoles. A key consequence of this is that increases the energetic disorder, hence causing a broad distribution of localized states, which hinders charge transport. We combined thermally stimulated luminescence studies with grazing incidence wide angle X-ray scattering, to demonstrate how the density of states in dipolar materials can be tailored. We demonstrate that the DOS is highly sensitive to the deposition technique and, consequently, the resulting film morphology. Furthermore, we show that the energetic disorder is not only determined by the static dipole moment, but also by the polarizability of charged molecules. Through this insight we derive design rules for common OLED materials that exhibit a with high dipole moments while maintaining charge transport properties comparable to those of non-polar counterparts.

15 min. break

HL 16.7 Tue 11:15 H14

Electrical and Optical Processes in Blue TADF OLEDs Studied by Temperature-Dependent Spectroscopy — •Ahmed Mohamed, Felix Kübert, Klara-Maria Bögle, Tolga Durmus, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, German

This study explores the electrical and photophysical processes in Thermally-Activated Delayed Fluorescence (TADF) Organic Light-Emitting Diodes (OLEDs) using temperature-dependent spectroscopic techniques. Key aspects such as charge carrier transport, current loss mechanisms and recombination dynamics are examined to provide a comprehensive understanding of device performance. We analyze current density-voltage-luminance (JVL) with respect to leakage current, efficiency roll-off, and current density at 90% external quantum efficiency *90. Electroluminescence (EL)/photoluminescence (PL) microscopy is employed to analyze the photophysical processes in OLEDs. EL spectra of blue OLEDs with the multi-resonance emitter *-DABNA exhibit remarkable spectral stability at temperatures between 200-300 K. Analysis of transient EL with rate equations yields activation energy and the rates of triplet-singlet transitions in OLEDs, including reverse intersystem crossing (rISC), triplet-triplet annihilation (TTA), and triplet-polaron annihilation (TPA). Understanding the mechanisms of current loss and (non-)radiative transitions is the prerequisite for enhancing the efficiency and stability of blue OLEDs.

HL 16.8 Tue 11:30 H14

Low Invasive Deposition of Metal Films on Carbon Nanotubes — •Martin Ernst[1,2], Martin Hartmann[1,2,3], and Sascha Hermann[1,2,3,4] — [1]Center for Micro and Nano Technologies, Chemnitz University of Technology, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, Chemnitz University of Technology, Germany — [3]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz, Germany — [4]Center for Advancing Electronics Dresden, Dresden University of Technology, Germany

Carbon nanotubes (CNTs) are one of the most promising materials for the next generation of electronics. Their unique one-dimensional electronic structure and their remarkable optical, thermal and mechanical properties makes them ideal candidates for different application scenarios. These range from the integration in transistors for analog and digital applications, as well as their usage in CNT-based gas, bio and stress sensors. One of the key challenges is the realization of a proper CNT-metal contact, in order to effectively transport charge carriers trough an electronic device, such as the carbon nanotube field-effect transistor (CNTFET). In this study we investigated the effects of different deposition parameters on the amount of lattice defects in single-walled semiconducting CNTs by Raman spectroscopy. There, a clear dependency between the amount of introduced defects and the deposition parameters, like the kinetic energy of the incident target atoms, was observed. Moreover, these finding were correlated to electrical results of CNTFETs, that were fabricated with the same deposition parameters.

HL 16.9 Tue 11:45 H14

High-Frequency CNT-based FETs for Radio Frequency Communication — •Martin Hartmann[1,2,3], Simon Böttger[1,2,3], Martin Ernst[1,2], and Sascha Hermann[1,2,3,4] — [1]Center for Micro and Nanotechnologies, Chemnitz University of Technology, Germany — [2]Center for Materials Architecture and Integration of Nanomembranes, Chemnitz University of Technology, Germany — [3]Fraunhofer Institute for Electronic Nanosystems ENAS, Chemnitz, Germany — [4]Center for Advancing Electronics Dresden, Dresden University of Technology, Germany

High frequency carbon nanotube-based (CNT) field effect transistors (FETs) are a highly promising candidate for future communication electronics due to their high charge carrier mobility and low intrinsic capacitance. It has already been shown in 2019 that this technology surpassed comparable silicon-based radio frequency FETs e.g. in terms of their extrinsic current gain cut-off frequencies as well as maximum frequencies of oscillation [1]. Moreover, in recent years their performance was further enhanced approaching the THz region [2]. We report on the impact of the device geometry as well as the CNT layer properties of high frequency CNTFETs onto their operating speed, linearity and contact resistance. Therefore, the spacers between the gate and the source electrode and gate to drain electrode were varied resulting in extrinsic current gain cut-off frequencies up to 14 GHz. By manipulating the spacer region, the device electrostatics in the CNT-metal contact area are balanced. This impacts the charge carrier injection and reflection at the Schottky-like barriers.