

## HL 10: Organic semiconductors

Time: Monday 14:45–16:00

Location: H14

HL 10.1 Mon 14:45 H14

**Temperature dependence and anisotropy of charge-carrier mobilities in crystalline durene** — ●FRANK ORTMANN, KARSTEN HANNEWALD, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena

We report on the theoretical analysis of charge-carrier mobilities in durene crystals. The crystal is studied with DFT methods to examine structural, vibrational, and electronic properties. On that basis we employ a Holstein-Peierls model (see Hannewald et al. PRB **69**, 075211 (2004); PRB **69**, 075212 (2004)) to simulate the temperature dependence of the mobilities. The relation between the anisotropy of electron/hole mobilities and the band structure as well as lattice vibrations is discussed.

HL 10.2 Mon 15:00 H14

**Electronic transport in polypyrrole thin films** — ●THOMAS HEINZEL and CESAR BOF BUFON — Institut für Physik der kondensierten Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf

We demonstrate that polypyrrole (PPy) films can be prepared in lithographically defined patterns by vapor-phase polymerization. This technique allows the preparation of the PPy thin films (thicknesses between 6 nm and 170 nm) with low roughness onto a processed silicon substrate.[1]

The PPy thin films form granular systems, where the grains are separated by barriers which contain a certain level of dopants. The system shows an electronic transport strongly influenced by Coulomb interactions. The temperature dependence of the differential conductance exhibit an Efros-Shklovskii like hopping. The localization length was observed to depend on the applied electric field.

The PPy films can be used as an oxygen detectors. In addition, the operation of a PPy thin-film field-effect transistor at room temperature is demonstrated. Transport measurements indicate that the device works as Schottky barrier-type field-effect transistor.[1]

[1] C. Bof Bufon and T. heinzel, Appl. Phys. Lett. **89**, 012104 (2006).

HL 10.3 Mon 15:15 H14

**The colours of perylene pigments: Interference between Frenkel excitons and charge transfer (CT) states** — ●L. GISSELEN and R. SCHOLZ — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching

The oscillator strength of optical transitions in molecular crystals arises mainly from neutral excitations of the molecules, resulting in Bloch waves known as Frenkel excitons. However, if the underlying transitions are close to resonant with CT states, both types of crystal excitations are mixed via electron and hole transfer, resulting in complex absorption lineshapes. As a basis for our exciton model including Frenkel and CT states, we determine the deformation patterns in the relaxed excited state and in anionic or cationic molecules with density functional methods. The electron and hole transfer parameters are deduced from the splitting of the Kohn-Sham orbitals in a stacked dimer. The sign and size of these transfer parameters depend on the geometric arrangement of the stack neighbours, so that the interference of Frenkel and CT transitions may result in a strong modulation of the absorption lineshape. As the relative energetic arrangement of Frenkel and CT states is difficult to calculate with high precision, we treat

the difference  $E_F - E_{CT}$  as the only free fit parameter of the model. From an analysis of five perylene derivatives [PTCDI, PTCDA, DiMe-PTCDI, N,N'-bis(3,5-xylyl)perylene-3,4:9,10-bis(dicarboximide), and N,N'-bis(2-phenylpropyl)perylene-3,4:9,10-bis(dicarboximide)] we derive a monotonous dependence of the energetic difference between Frenkel and CT states on the length of the stacking vector.

HL 10.4 Mon 15:30 H14

**Temperature Dependence of the Trap State Distribution in C<sub>60</sub> Crystals** — ●A. OHLINGER<sup>1</sup>, A. BIEBERSDORF<sup>1</sup>, R. DIETMÜLLER<sup>1</sup>, T.A. KLAR<sup>1</sup>, J. FELDMANN<sup>1</sup>, D.V. TALAPIN<sup>2</sup>, and H. WELLER<sup>2</sup> — <sup>1</sup>Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Germany — <sup>2</sup>Institute of Physical Chemistry, University of Hamburg, Germany

Materials comprising C<sub>60</sub> are of great interest and are used in optoelectronic devices such as FETs, photoconductors or photovoltaic devices. Charge transport in C<sub>60</sub> crystals is dominated by trap states. The density of these trap states is commonly assumed to decay exponentially with the energetic depth from the conductivity edge.

In this contribution, we quantitatively determine the parameters of the trap state distribution by photodoping C<sub>60</sub> microcrystals. We find the characteristic trap depth to decrease by nearly 40% during the phase transition of the C<sub>60</sub> crystals from the fcc to the sc phase between 250 K and 200 K and the activation energy drops by approximately 50%. The conductivity below 200 K is predominately governed by trap states which are introduced by oxygen. In contrast, at room temperature trap states are dominantly related to the rotation of the C<sub>60</sub> molecules. Calculations based on our data show that the number of trap states at room temperature is about 100 times larger than below 200 K.

For the future we expect that photodoping will be used to determine characteristic parameters of trap states in other amorphous organic or inorganic semiconductors, as well.

HL 10.5 Mon 15:45 H14

**Resonant Raman spectra of pentacene in the UV range** — ●L. GISSELEN<sup>1</sup>, C. HIMCINSCHI<sup>2</sup>, J. PFLAUM<sup>3</sup>, and R. SCHOLZ<sup>1</sup> — <sup>1</sup>Walter Schottky Institut, Technische Universität München, Germany — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — <sup>3</sup>Physikalisches Institut, Universität Stuttgart, Germany

Pentacene has two prominent absorption bands, one in the visible and one in the near UV, the first being based on the HOMO-LUMO transition, the second on an interference between the transitions HOMO→LUMO+2 and HOMO-2→LUMO. In order to investigate the deformation in the relaxed excited state related to the transition in the UV, we have performed resonant Raman spectroscopy in that region. The experimental observation of the Raman spectra from a pentacene crystal was realised using a LabRam HR800 UV spectrometer in a micro-configuration. Light from a He-Cd laser at a wavelength of 325 nm was focused with the microscope, resulting in a beam diameter of  $\approx 1.5 \mu\text{m}$  on the sample, with a laser power of  $\approx 0.5 \text{ mW}$  measured under the objective of the microscope. Resonant Raman spectra were recorded in the Stokes region between  $200 \text{ cm}^{-1}$  and  $2000 \text{ cm}^{-1}$ . The intensity distribution differs strongly from Raman data obtained in resonance with the HOMO-LUMO transition, revealing different deformation patterns. The latter are determined by geometry optimisation of the excited states with time-dependent density function theory (DFT). For both transitions, the measured intensity distributions are well reproduced by the calculations.