appearing in the dilute GaN:P alloy. We treat both the perfectly random case as well as the non-random microstructures formation, and investigate how their appearance is reflected in the EBS. It turns out that the EBS is extremely sensitive in determining the critical disorder level for which delocalised states start to appear in the intermediate band. In addition, the EBS allows us to identify the role played by atomic relaxation in the positioning of the impurity levels.

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