CPP 28: Polymer Physics V

Time: Thursday 17:15–18:15 Location: H40

CPP 28.1 Thu 17:15 H40

Lifetimes of photoexcited states in P3HT:PCBM heterojunctions — •Johannes Sieger[1], Andreas Wörle[1], Andreas Sperlich[1], Moritz Liedtke[1,2], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland. D-97074 Würzburg — [2]Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, D-97074 Würzburg

The photoinduced charge transfer and the resulting charge carrier generation in polymer-fullerene bulk heterojunctions are essential for organic photovoltaics. We present our investigations on the efficiency of singlet exciton dissociation and polaron generation in poly(3-hexylthiophene) (P3HT) : [6,6] phenyl-C61-butyric acid methyl ester (PCBM) blends by performing photoluminescence measurements, photoinduced absorption spectroscopy (PIA) and light-induced electron spin resonance (LESR). Particularly, we focus on the temperature dependence of the lifetime of the photoinduced states. The PIA measurements were possible at room temperature due to a high sensitivity of the setup and are relevant for applications of organic semiconductors such as solar cells.

CPP 28.2 Thu 17:30 H40

Low temperature mobility of Frenkel excitons on ampi-PIPE J-Aggregates — •Christian Spitz, Antonio Saghati, and Ralf Menzel — Universität Potsdam

The mobility of optically excited excitons on J-aggregates can be demonstrated by the phenomena of exciton exciton annihilation. In this intensity dependent process the collision of two excitons results in their annihilation and hence in a shortening of the mean excitation lifetime. By measuring the intensity dependent fluorescent lifetime in contrast to the predicted immobilization of the excitons at low temperature we could prove the excellent mobility of the excitons on the ampi-PIPE J-aggregates of the octyl derivate of 5,5,6,6-tetrachloro-1,1-diethyl-3-3 bis(4-sulpho-n-butyl) benzimidacarbocyanine (TDBC) at a temperature (4 K), which is far below their expected freezing point. The high mobility is further approved by fluorescence depolarisation at low temperatures.

CPP 28.3 Thu 17:45 H40

Integrated spin-on barrier layers a reasonable idea? — •Mine Memesa[1], Ya-Jun Cheng[1], Jan Perlich[2], Peter Müller-Buschbaum[2], and Jochen Gutmann[1,3] — [1]Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany — [2]TU München, Physik-Department LS E13 James-Franck-Str. 1, 85747 Garching, Germany — [3]Institute of Physical Chemistry, University Mainz, D-55099, Mainz, Germany

Titanium dioxide (TiO2) nanoparticles were prepared by using polystyrene block poly (ethyleneoxide) (PS-b-PEO) copolymer as a template. As a preliminary study whether poly (dimethylsiloxane) (PDMS) is a suitable polymeric replacement for barrier layers PDMS was spin coated over the TiO2 nanoparticles and subsequently etched away by oxygen plasma cleaning. The surface characteristics of the particles were investigated using Scanning Electron Microscopy (SEM) and photoluminescence (PL). The PL measurements indicated the formation of exciton traps close to the particle surface after plasma treatment. The stability of the TiO2 nanoparticles upon sealing with PDMS followed by etching of the polymer overcoating was confirmed with microbeam grazing incidence small angle x-ray scattering (μGISAXS) measurements.

CPP 28.4 Thu 18:00 H40

Accurate forces in Quantum Monte Carlo calculations with non-local pseudopotentials — •Alexander Badinski and R. J. Needs — Cavendish Laboratory, Cambridge, United Kingdom

Calculating accurate inter-atomic forces within variational and diffusion Monte Carlo (VMC and DMC) methods is a challenging and long-standing problem [1-2]. VMC and DMC methods have become quite successful for calculating ground state total energies of many-electron systems. However the lack of an accurate and efficient method for calculating forces usually requires one to perform VMC and DMC calculations with geometries obtained from either density functional theory or conventional quantum chemistry methods. We present a novel approach to calculate Hellmann-Feynman forces within these two methods using non-local pseudopotentials. The use of pseudopotentials allows one to overcome the severe problem of infinite variance in the sampling distribution of the force estimator which is vital when using statistical methods. Equilibrium geometries and harmonic vibrational frequencies are derived from the forces and compared with those obtained from the energies at the Hartree-Fock, VMC and DMC levels. Results for five small molecules show that the equilibrium bond lengths obtained from the force and energy calculations are in excellent agreement.

[1] R. Assaraf, M. Caffarel, J. Chem. Phys. 119, 10536 (2003) [2] S. Chiesa, D. M. Ceperley, and S. Zhang, Phys. Rev. Lett. 94, 036404 (2005)