significant. However, at lower absorbed pump powers, the transients were mono-exponential and independent of stirring. Moreover, the probability of a single QD absorbing more than one photon was found to be negligible at low pump powers and the transient spectra were free of the photo-induced absorption features characteristic of surface-trapped charges. The sub-nanosecond dynamics were thus attributed to the decay of bi-excitons created by MEG, with a quantum yield of 160% for a photon energy 2.9 times the band gap.

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17:45 **A computational comparative study of electrical properties of disordered conjugated polymers** PI 30

Authors : Nenad Vukmirovic
Affiliations : Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Serbia

Resume : The comparison of hole density of states (DOS) and hole mobilities of several organic polymer based systems was performed to gain insight into the main factors that determine the electrical properties of conjugated polymers. The DOS and the mobility of the systems under investigation were calculated using an atomistic multiscale procedure [1, 2]. The results suggest that the irregularities in the shape of the polymer chains increase the diagonal disorder, while alkyl side chains act as spacers that reduce the diagonal disorder which originates from long range electrostatic interactions. Intrachain electronic coupling in relatively ordered polymers narrows the tail of the DOS, while in less ordered polymers it represents the additional component of disorder and widens the tail of the DOS. The width of the DOS tail was confirmed to be an important factor that determines the activation energy for charge carrier transport. However, it is not the only factor since the system with smaller width of the DOS tail can have a larger activation energy due to, for example, smaller wave function overlap between transport states [3]. [1] N. Vukmirovic and L.-W. Wang, Nano Lett. 9, 3996 (2009). [2] N. Vukmirovic and L.-W. Wang, J. Chem. Phys. 134, 094119 (2011). [3] N. Vukmirovic, Phys. Chem. Chem. Phys, in press (2013).

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17:45 **Modelling Charge Transfer States in Organic Photovoltaics** PI 31

Authors : Sheridan Few, James Kirkpatrick, Jenny Nelson
Affiliations : Centre for Plastic Electronics, Department of Physics, Imperial College London, London SW7 2AZ, UK

Resume : Recently, much attention has been paid to the formation of charge transfer (CT) states at the donor : acceptor interface in organic photovoltaic materials, and to their role in charge pair generation.1 However, until now few theoretical studies have addressed the electronic properties of CT states in detail. In this work, we use density functional theory (DFT) methods to study the energies and properties of CT states of a complex consisting of an oligomer of a donor polymer (poly-3-hexyl-thiophene (P3HT), Poly((9,9-dioctylfluorenyl-2,7-diyl)-alt-5,5-(40,70-di-2-thienyl-20,10,30-benzothiadiazole)) (PFODTBT), and the thiophene-isoindigo based polymer, P3TI) and an acceptor molecule (fullerene derivatives phenyl C61 butyric acid methyl ester (PCBM), phenyl C71 butyric acid methyl ester (PC71BM), and bis-indenofullerene ICBA). The effects of position, relative orientation, and specific chemical structure of the molecules on charge distribution, absorption and emission spectra, and overlap of electronic states between the molecules are studied. Results are analysed in comparison with electroluminescence data on polymer:fullerene blends containing different fullerene derivatives. We discuss how studies on this model system help to elucidate the role of charge transfer states in charge generation and so help develop design rules for better photovoltaic materials.

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17:45 **The Role of the Oxygen and Triplet states in the PCPDTBT:PCBM organic solar cells: Investigation on the Photo-Induced Dynamics.** PI 32

Authors : Michele De Bastiani, Giulia Grancini, Annamaria Petrozza, Nicola Martino, Maria Rosa Antognazza, Daniele Fazzi, Mario Caironi, Hans-J Egelhaaf, Lorenzo Franco, Moreno Meneghetti and Guglielmo Lanzani
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