There has been considerable debate in the literature on which mechanism is dominant [e.g. Adv. Mat. 25, 6801 (2013)]. Using a kinetic Monte Carlo (kMC) simulation of a 3D model of the complete device stack, we can now study these intrinsic processes on the molecular scale. By extending our electronic kMC model, as presented earlier [Nat. Mat. 12, 652 (2013)], with both radiative decay processes and non-radiative loss mechanisms, we can study the complex interplay of electrons and excitons in a complete multi-layer device. We have applied this methodology to two prototypical OLED stacks [Phys. Rev. B 77, 235215 (2008)] and show that we can describe both the experimental current-density versus voltage characteristics and the roll-off using only physical parameters as input for the simulation, i.e. without any fitting. Moreover, we can now study the role of the different molecular-scale mechanisms for different scenarios and determine which process is the dominant efficiency-limiting process.

add to my program **(close full abstract)**

14:30 **Break**

14:45 **Computational Prediction of Nanoscale Organic Solar Cell Performance from Morphology**
Authors : Geoffrey Hutchison
Affiliations : Department of Chemistry University of Pittsburgh
Resume : A key challenge is to create computational methods that can properly handle charge transport in organic electronics and particularly solar cells, bridging across multiple length and time scales, in the presence of defects, traps, impurities, disorder, and particularly variations in nanomorphology. Our research has focused particularly on developing high-performance Monte Carlo charge transport simulations that explicitly treat disorder and defects of various kinds. Charge transport parameters are, where possible, derived from first-principals calculations, particularly the charge delocalization length. Our simulations are validated against in-house and external experimental measurements and have reproduced several non-obvious effects, including a negative differential resistance (NDR) effect in organic semiconductor mixtures. We have also developed a delocalized charge model capable of classically treating accurate electrostatic interactions in organic solar cells. Currently, a new database of idealized, realistic, and intermediate two-phase morphologies are being generated to correlate between materials architecture and charge transport properties in organic solar cells. We find that "obviously optimal" designs suggested by many in the community may perform worse than conventional bulk heterojunction morphologies. Progress towards identifying important structure-property relationships for optimal solar cell efficiencies will be discussed. O.134

add to my program **(close full abstract)**

15:15 **Effects of dynamic disorder on the electronic structure of crystalline poly-3-hexylthiophene**
Authors : Marko Mladenovic, Nenad Vukmirovic
Affiliations : Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade
Resume : We have investigated the effects of dynamic disorder in side chains, main chains and both of them on the electronic structure of crystalline poly-3-hexylthiophene (P3HT). To obtain the atomic configurations of crystalline P3HT, we used Monte Carlo simulations. Electronic structure was found using the charge patching method [1], based on density functional theory, and overlapping fragments method [2]. From 100 different realizations for 2 different stable configurations of crystalline P3HT we calculated: electronic density of states and hole localization in the backbone direction (one chain) and in the π-π stacking direction (different chains). We found that effect of side chains disorder is more pronounced in the more stable configuration of P3HT than in the other one due to wider distribution of the torsion angle between thiophene ring and side chain. Disorder of main chains affects the electronic structure more than disorder of side chains. Finally, in the case of disorder of both main and side chains, effects of disorder on the electronic structure are most pronounced and they are similar to the effects of complete disorder of P3HT in the amorphous phase. [3] [1] N. Vukmirovic, L. Wang, J. Chem. Phys. 128, 121102 (2008) [2] N. Vukmirovic, L. Wang, J. Chem. Phys. 134, 094119 (2011) [3] N. Vukmirovic, L. Wang, J. Phys. Chem. B 115, 1792 (2011) O.135

add to my program **(close full abstract)**

15:30 **Massively parallel kinetic Monte Carlo simulations of charge carrier transport in organic semiconductors**
Authors : Niels J. van der Kaap, L. Jan Anton Koster
Affiliations : Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4 9747, AG, Groningen, The Netherlands
Resume : Kinetic Monte Carlo methods play an important role in organic semiconductor research. They allow the translation of nanoscale features into macroscopic properties like mobility and current density, by explicitly modeling phonon-activated hopping of O.136