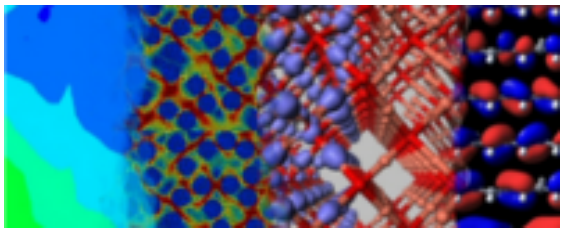

Contribution ID: **21** Type: **Poster**

Efficient scheme for modeling of disordered morphologies in organic semiconductors

Thursday, November 8, 2012 5:15 PM (10 minutes)

Organic light emitting diodes (OLEDs) are typically fabricated by vapor deposition or solution processing of organic charge-transport and emitter materials. The typical resulting morphology of the material is an amorphous film. Because of localization, charge transport in the disordered materials takes place by hopping of charge carriers from one molecule to another. As a consequence, the charge transport properties of organic semiconductors are extremely sensitive to the morphology of the material. Therefore, development of efficient simulation approaches for predictive characterization and optimization of the disordered morphologies in organic materials is very important in engineering of new efficient OLED devices. In this work we present a Monte Carlo based approach which generates disordered morphologies using method that simulates vapor physical deposition of molecular films: a single molecule deposition protocol. On a very rugged potential energy surface, such as those induced here by the roughness of the partially deposited film, the simulations can be trapped for long times in metastable conformations. To reduce the trapping of the system in metastable conformations, for each molecule we performed basin-hopping cycles, each of which consisted of a simulated annealing run. The individual steps in the simulated annealing run are standard Metropolis Monte Carlo moves. To increase the computational efficiency, a grid representations for electrostatic and for van der Waals interactions is used. This method leads to linear O(N) dependence of the computational time on the system size N in contrast to O(N^2) scaling for direct full atom-atom evaluation of the interatomic potentials.

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Session Classification: Poster Session