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Quantum Mechanical Calculations of Free Energy and Open-Circuit Voltage in Lattice Modeled Organic Photovoltaic Devices. VLADIMIR LANKEVICH, ERIC BITTNER, Univ of Houston — In organic photovoltaic devices (OPVs), initially bound electron and hole can take many different paths to dissociate and become free charge carriers. This leads to the increase in their density of states and therefore increase in the entropy of the system.[1] Accurate description of the energy barriers that charges have to overcome, therefore requires calculation of the free energy.[2] Free energy of an OPV is directly related to its open-circuit voltage and depends only on few important parameters such as average life-time of a charge-transfer state, average energy of the charge-transfer state and energetic disorder in the system.[3] We extend these ideas to the quantum mechanical simulations of the dissociation in the lattice modeled bulk-heterojunction system. We observe average excitonic and free energies that agree with theoretical predictions and the number of experimental results from previous studies. We study effects of the energy disorder and importance of the dimensionality and morphology in materials such as polymer-fullerene blends.

[1]T. M. Clarke, J. R. Durrant, **Chem. Rev.**, 110, 11
[2]S. N. Hood, I. Kassal, **JPC Letters**, 7, 22
[3]T. M. Burke, S. Sweetnam, K. Vandewal, M. D. McGehee, **Adv. Energy Mat.**,5,11

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