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Electronic structure and carrier transport in disordered conjugated polymers¹ NENAD VUKMIROVIC, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Thin films of realistic conjugated polymer materials contain both crystalline and amorphous regions, where the latter ones are less understood. This study was therefore focused on electronic structure and carrier transport in amorphous regions of polythiophene (PT) and poly(3-hexylthiophene) (P3HT). Atomic structures were obtained from classical molecular dynamics using a simulating annealing procedure and the charge patching method [1] was used to calculate the electronic structure. It was found that disorder in the electronic structure of P3HT comes from disorder in the conformation of individual chains, while in the case of PT there is an additional contribution due to disorder in electronic coupling among the chains [2]. The electron-phonon coupling matrix elements in P3HT were also calculated and carrier mobility due to phonon-assisted hopping was estimated.

[1] N. Vukmirovic and L.W. Wang, J. Chem. Phys. 128 121102 (2008).

[2] N. Vukmirovic and L.W. Wang, J. Phys. Chem. B, submitted.

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