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Electronic structure properties as signatures of morphological motifs in organic photovoltaics MATTHEW GOLDEY, GIULIA GALLI, University of Chicago — The effect of polymer morphologies upon the efficiency of organic solar cells is difficult to determine experimentally; however, theoretical models may directly probe how structural changes affect electronic properties, such as band locations and band gaps and hence provide key insight into solar energy conversion processes. Using density functional and many body perturbation theory (G0W0) calculations, we investigated the dependence of the electronic states on order parameters such as backbone dihedrals of organic donor polymers. We focused on the donor polymers PTB7 and PID2 and the acceptor PC71BM for which recent experiments[1] reported promising photoconversion efficiencies of 8.22% for ternary blend cells. Our results suggest that accurate predictions of the device performance must include a description of local disorder in the active layer. In particular, we found multiple possible configurations of the donor polymer with relative energies 0.06-0.3 eV/monomer above the lowest energy conformer whose electronic structure differ significantly. Using the lowest energy conformations found at zero T, calculated electronic energy levels are in good agreement with experimental values, with errors within 0.2 eV. [1] Lu, L., et. al. Nature Photon, 8(9), 716722 (2014).

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