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Atomic and Electronic Structure of the P3HT/PCBM Interface From First-Principle Calculations[1] LONGHUA LI, OLEG KONTSEVOI, ARTHUR J. FREEMAN, Northwestern Universtiy — Fundamental research on donor/acceptor (D/A) interfaces of organic photovoltaics (OPV) have drawn immense interest because of their crucial roles in charge separation (CS), charge transfer (CT) and charge recombination (CR). The blend system consisting of regioregular poly(3-hexylthiophene) (rr-P3HT) and fullerene derivative [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) is a widely investigated binary system. Despite significant efforts that have been done to optimize the OPV, such as the D/A ratio, detailed information on their structure, interfaces, and morphology are far from complete. Additionally, fewer investigations have focused on the elementary charge transfer processes. In this work, such a hetero-interface was carried out by annealing simulation; and then interfacial electronic structure and charge transfer were studied by DFT calculations. The process of PCBM assembly on the P3HT surface were shown and the carrier mobilities could be tuned by PCBM orientations.Our calculations provide an important understanding on the assembly of PCBM and charge transfer at the binary interface.

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