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Modeling charge and energy transports in π-conjugated systems YONGWOO SHIN, XI LIN, Boston University — A generic 3D model Hamiltonian is developed to simulate the charge and energy transports in π-conjugated composite materials. The intrachain interactions are described by our recently developed adapted Su-Schrieffer-Heeger Hamiltonian and the interchain $\pi\pi$ interactions are modeled using distance-dependent hopping integrals. Excellent agreements in their binding energetics and geometries with post-Hartree-Fock ab initio methods and experiments are found in the cases of a benzene dimer, graphene bi-layer, and poly-(*p*-phenylene vinylene) (PPV) crystal. The computed photoinduced charge separated states and associated adsorption spectra of the PPV-C_{60} and PPV-C_{60}-graphene agree perfectly with experimental measurements.

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