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First-principles simulations of exciton diffusion in organic semiconductors XU ZHANG, ZI LI, GANG LU, Department of Physics and Astronomy, California State University Northridge — Exciton diffusion is of great importance to the performance of organic optoelectronic devices, including organic photovoltaics and solid-state lighting. The ability to control exciton diffusion in organic semiconductors is crucial to the design of efficient optoelectronic devices. However, such ability can only be achieved through a fundamental understanding of exciton diffusion mechanism. We have proposed a first-principles based frame work that can predict exciton dynamics in organic semiconductors.The framework is based on time-dependent density functional theory to provide the energy and many-body wave functions of excitons. Nonadiabatic *ab initio* molecular dynamics is used to calculate phonon-assisted transition rates between localized exciton states. Using Monte Carlo simulations, we determine exciton diffusion length, lifetime, diffusivity, and harvesting efficiency in poly(3-hexylthiophene) polymers at different temperatures, and the results agree very well with corresponding experimental values. We find that exciton diffusion is primarily determined by the density of states of low-energy excitons; a widely speculated diffusion mechanism has been confirmed and elucidatedby the simulations. Some general guidelines for designing more efficient organic solar cells can be gleaned from the simulation results

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