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A coarse-gained model of exciton dynamics on long-chain conjugated polymer system[1] ELIZABETH LEE, WILLIAM TISDALE, ADAM WILLARD, Massachusetts Inst of Tech-MIT — A comprehensive understanding of exciton dynamics in conjugated polymers is challenging, given the effects of electron-electron interactions , electron-nuclear coupling, and disorder at the molecular level up to the device scale has on electronic and optical properties. We present a new phenomenological model for simulating the dynamics of excitons in long-chain organic conjugated molecules. In our model, the polymer is described as a time-dependent array of ring-ring torsion angles mapped on a three-dimensional coarse-grained beads. Exciton dynamics arise in direct response to the evolution of this torsional landscape along its excited state potential energy surface, which includes exciton-induced forces (such as those that lead to self-trapping). The framework for generating an accurate description of these heterogeneous excited state forces was developed based on the analysis of QCFF/PI, a type of mixed QM/MM simulations. We show that this model can reproduce transient pump-probe experiments; we remark on the importance on the excited state force field when describing these systems. Then we go on to present molecular-level physical insights into exciton dynamics in these polymer materials, which have been previously speculative, to help better engineer organic solar cells.

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