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RT-TDDFT simulation of the optical properties of a model organic photovoltaic device[1] F. VILA, J.J. REHR, U. of Washington — Organic solar cells are attracting much interest because of their potential as cost-effective photovoltaic devices. Prototypical cells consist of a bilayer of p- and n-type materials. The conversion of light into a current is initiated by the absorption of a photon in the p-type donor, mediated by the creation, diffusion and dissociation of an exciton, and finalized by a charge transfer to the n-type acceptor, with subsequent transport to the electrodes. To explore this issue, we simulate the optical response of a model bilayer cell composed of a polythiophene(pT)/C_{60} donor/acceptor pair using an efficient implementation of real-time TDDFT.[2] We find that the chain twist induced by the C_{60} on the pT shifts the absorption onset from 1.8 to 2.0 eV. This shift is larger and of opposite sign compared to that induced by the inclusion of either regioregular or random side-chains in pT, and by the interaction between two pT chains. Finally, we discuss extensions for the simulation of charge transport and exciton mobility.

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[2]Y. Takimoto *et al.*, J. Chem. Phys. **127**, 154114 (2007).

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