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Computational Analysis of Energy Pooling to Harvest Low-Energy Solar Energy in Organic Photovoltaic Devices MICHAEL LACOUNT, Colorado School of Mines, SEAN SHAHEEN, University of Colorado Boulder, GARRY RUMBLES, JAO VAN DE LAGEMAAT, National Renewable Energy Laboratory, NAN HU, University of Colorado Boulder, DAVE OSTROWSKI, National Renewable Energy Laboratory, MARK LUSK, Colorado School of Mines — Current photovoltaic energy conversions do not typically utilize low energy sunlight absorption, leaving large sections of the solar spectrum untapped. It is possible, though, to absorb such radiation, generating low-energy excitons, and then pool them to create higher energy excitons, which can result in an increase in efficiency. Calculation of the rates at which such upconversion processes occur requires an accounting of all possible molecular quantum electrodynamics (QED) pathways. There are two paths associated with the upconversion. The cooperative mechanism involves a three-body interaction in which low energy excitons are transferred sequentially onto an acceptor molecule. The accretive pathway, requires that an exciton transfer its energy to a second exciton that subsequently transfers its energy to the acceptor molecule. We have computationally modeled both types of molecular QED obtaining rates using a combination of DFT and many-body Green function theory. The simulation platform is exercised by considering upconversion events associated with material composed of a high energy absorbing core of hexabenzocoronene (HBC) and low energy absorbing arms of oligothiophene. In addition, we make estimates for all competing processes in order to judge the relative efficiencies of these two processes.

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