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Exploring mechanisms in excitonic photovoltaics from first principles PETER DOAK, Molecular Foundry, LBNL; Department of Chemistry, UC-Berkeley, PIERRE DARANCET, JEFF NEATON, Molecular Foundry, LBNL — Organic-based photovoltaics (OPV) are being explored as an alternative to inorganic PVs due to their potential for low cost and more flexible form factors. Single-molecule heterojunctions, containing donor and acceptor moieties linked by covalent bonds, provide an interesting model system for understanding processes fundamental to OPVs, such as light absorption and charge separation. In this work, the necessity of type II heterojunction electronic structure is critically examined for a series of small asymmetric molecules containing covalently-linked aromatic moieties. We present density functional theory and many body perturbation theory calculations of both single electron addition and removal energies using the GW approximation, and the neutral excitations using a Bethe-Salpeter equation approach. Implications for charge separation in these systems in the presence of metal contacts is also discussed. This work supported by DOE via Helios Solar Energy Research Center. Computational support provided by NERSC.

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