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First-Principles Studies of Single-Molecule Photovoltaics PETER DOAK, UC Berkeley Chemistry, R. A. SEGALMAN, UC Berkeley Chemical Engineering, T. D. TILLEY, UC Berkeley Chemistry, J. B. NEATON, LBNL Molecular Foundry — Organic photovoltaics consist of electron donor and acceptor polymers or molecules blended together, and are promising inexpensive, lightweight alternatives to conventional silicon solar cells. However, many of the physical processes responsible for their poor efficiencies are not well understood. Here, using first-principles calculations based on density functional theory, including self-energy corrections within the GW approximation and a discussion of excitonic effects, we examine the relationship between molecular structure and electronic level alignment at a covalent donor-acceptor interface. We consider small asymmetric molecules subdivided into discrete covalently linked moieties based on thiophene, tetrafluorobenzene, pyridine, and durene. Excited states of each of these moieties, as well as their covalently-linked combinations, are computed and discussed in the context of their ability to absorb photons and separate charge. Work supported in part by the DOE Helios SERC. Computational resources provided by NERSC.

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