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**Correlating First-Principles Electronic Structure with Device Performance of Organic Photovoltaic Cells** ERIC B. ISAACS, SAHAR SHAR-IFZADEH, BIWU MA, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Organic photovoltaic cells (OPVs) are promising candidates for low-cost solar energy conversion. Here, we employ static and time-dependent density functional theory calculations to predict the excitation energy of the donor-acceptor charge transfer state ( $E_{CT}$ ) at the interface between  $C_{60}$  and several boron(subphthalocyanine)- and azadipyrrromethene-based donor moieties, comparing to measured open-circuit voltage ( $V_{OC}$ ) in bilayer heterojunction OPVs [1]. When  $E_{CT}$  is approximated as the difference between the ionization potential and electron affinity of the isolated donor and acceptor molecules, respectively, we observe no apparent correlation between  $E_{CT}$  and  $V_{OC}$ . Both bulk polarization and excitonic effects at the interface are found to influence the energetics significantly, the latter being strongly morphology dependent. We demonstrate that a linear relationship between  $V_{OC}$  and  $E_{CT}$  may be obtained once the interface morphology is considered. We acknowledge support from DOE, NSF-NCN, and NERSC.

[1] C. E. Mauldin *et al.*, ACS Appl. Mater. Interfaces **2**, 2833 (2010).

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