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Fine screening of high-performance organic photovoltaics GIAN-MARCO RIGNANESE, NICOLAS DARDENNE, Univ Catholique de Louvain, STEVEN A. LOPEZ, ALAN ASPURU-GUZIK, Harvard University, XAVIER BLASE, CNRS and Grenoble-Alpes University, GEOFFROY HAUTIER, JEAN-CHRISTOPHE CHARLIER, Univ Catholique de Louvain — Organic photovoltaic (OPV) devices are a promising (cheap and versatile) technology for harvesting the solar energy. Their efficiency depends critically on the charge transfer (CT) effects taking place at the interface between electron donor and acceptor phases. In order to theoretically devise new OPV devices with high efficiency, it is thus important to describe these CT effects adequately. Tens of thousands of donor molecules have been already tested in a multiple-step screening within the Harvard Clean Energy Project (CEP), leading to a ranking of potential candidates. However, these calculations have been performed relying on density-functional theory. The latter is known to underestimate the band gap and not to describe electron-hole interaction and CT effects correctly. Here, we investigate the top 20 donor molecules from the CEP ranking using the GW/BSE formalism.

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