Abstract Submitted
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First-principle study of the interfacial rehybridization in organic-inorganic composite photovoltaic devices[1] GEORGY SAMSONIDZE, FILIPE J. RIBEIRO, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Composites of organic conjugated polymers and inorganic nanostructures offer cheap but at present inefficient photovoltaic materials. The efficiency of the photovoltaic device is critically dependent on charge transfer and orbital rehybridization at the donor-acceptor interface. In this work we investigate the P3HT/PCBM interface from density functional theory (DFT) based first-principles calculations. We find a strong rehybridization of the conduction band edge states suggesting an efficient route for exciton dissociation at the interface. Using many-body perturbation theory, we compute the quasiparticle corrections on top of the DFT results. These corrections are critical for accurate predictions and to reach agreement with experiment.

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