

Abstract Submitted
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Hole Localization in Molecular Crystals From Hybrid Density Functional Theory¹ NA SAI, PAUL F. BARBARA, University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratory — Charge trapping in organic solids and interfaces plays an important role in organic photovoltaic efficiencies. Experimental confirmation of intrinsic charge trapping at the atomic scale and the tools to directly probe the trap energy landscape, however, remain lacking. We use first principles computational methods to examine hole trapping in organic molecular crystals. We present a computational scheme based on the tuning of the fraction of exact exchange in hybrid density functional theory to eliminate the many-electron self-interaction error [1]. With small organic molecules, we show that this scheme gives accurate descriptions of ionization and dimer dissociation. We demonstrate that the excess hole in perfect molecular crystals can form self-trapped hole polarons. The predicted absolute ionization potentials of both localized and delocalized holes are consistent with experimental values.

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