

Abstract Submitted
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First-principles study of the electronic structure of organic semiconductors SAHAR SHARIFZADEH, Molecular Foundry, LBNL, ARIEL J. BILLER, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, JEFFREY B. NEATON, Molecular Foundry, LBNL — Organic semiconductors are promising materials for next generation organic photovoltaics, with the characterization of their spectroscopic properties vital to improving the potential of such technologies. Here, we use density functional theory and many-body perturbation theory within the GW approximation to explore quantitatively the electronic structure of prototypical organic semiconductor crystals and compare directly with valence-band photoemission data. For pentacene and PTCDA, computed gas-phase ionization energies and electron affinities are compared with calculated crystal-phase quasiparticle band structures, and relationships between shifts in orbital energy with change of phase and static polarization of the bulk are discussed and compared with experiment. We acknowledge DOE, NSF, BASF, and ISF for financial support, and NERSC for computational resources.

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