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Gap renormalization of molecular crystals from density-functional theory SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel, SAHAR SHARIFZADEH, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, USA, MANISH JAIN, Department of Physics, Indian Institute of Science, Bangalore, India, ROI BAER, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, Hebrew University, Jerusalem, Israel, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, USA, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel — Fundamental gap renormalization due to electronic polarization is a basic phenomenon in molecular crystals. Despite its ubiquity and importance, all conventional approaches within density-functional theory completely fail to capture it, even qualitatively. Here, we present a new screened range-separated hybrid functional, which, through judicious introduction of the scalar dielectric constant, quantitatively captures polarization-induced gap renormalization, as demonstrated on the prototypical organic molecular crystals of benzene, pentacene, and C60. This functional is predictive, as it contains system-specific adjustable parameters that are determined from first principles, rather than from empirical considerations [Phys. Rev. B 88, 081204(R) (2013)].

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