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Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory[1] SIVAN REFAELY-ABRAMSON, Molecular Foundry, LBNL and Dept. of Physics, UC-Berkeley, MANISH JAIN, Dept. of Physics, IISc, Bangalore, India, SAHAR SHARIFZADEH, Dept. of Electrical and Computer Engineering and Physics Division of MSE, Boston University, JEFFREY B. NEATON, Molecular Foundry, LBNL, Dept. of Physics, UC-Berkeley and Kavli ESNI at Berkeley, LEEOR KRONIK, Dept. of Materials and Interfaces, Weizmann Institute — We present a framework for obtaining solid-state charge and optical excitations and spectra from optimally tuned range-separated hybrid density functional theory, which allows for the accurate prediction of exciton binding energies. We demonstrate our approach through calculations of one- and two-particle excitations in pentacene, a molecular semiconducting crystal, where we find excellent agreement with experiments and prior computations. We show that with one adjustable parameter, our method accurately predicts band structures and optical spectra of Si and LiF, prototypical covalent and ionic solids. For a range of extended bulk systems, this method may provide a computationally inexpensive alternative to many-body perturbation theory, opening the door to studies of materials of increasing size and complexity [Phys. Rev. B 92, 081204(R), 2015].

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