Solid-State Excitations from Density-Functional Theory

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The development of a non-empirical theory for quantitative electronic structure calculations, which combines predictive power with computational simplicity, is a long-standing challenge for computational studies in materials science, solid-state physics, and chemistry. In this talk I will present a new framework for obtaining reliable solid-state charge and optical excitations and spectra from an optimally tuned screened range-separated hybrid density functional, which allows for an accurate prediction of exciton binding energies. I will demonstrate this approach through first principles calculations of one- and two-particle excitations in organic semiconductors, fully from first-principles. I will further show that with one adjustable parameter, this method accurately predicts band structures and optical spectra of silicon and lithium fluoride, prototypical covalent and ionic solids. These findings indicate that for a broad 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 [1].

[1] S. Refaely-Abramson, M. Jain, S. Sharifzadeh, J. B. Neaton, and L. Kronik, *Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory,* Phys. Rev. B **92**, 081204(R) (2015).

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