Excitonic effects from real-time parameter-free hybrid functions

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Hybrid functionals are know to provide excellent band-gap of semiconductors compared to local and semi-local functional. Because hybrid functionals can be constructed to include the long-range part of the screened Coulomb interaction, they contains the basic ingredients that can produce the bound excitons in optical spectra of semiconductors and insulators. So far, the construction of such parameter-free functional requires complex procedures such that optimally-tune parameters [], or fitting of the band-gap on GW calculations []. This hampers the predictive power of such a functional and ancors it to the realm of optical properties of materials at equilibrium.
Because real-time time-dependent density functional theory (TDDFT) does not rely on perturbation theory, it has the capability to study materials out of their equilibrium or perturbed by strong fields. It is therefore of tremendous importance to find hybrid functionals that do not requires auxiliaryt calculations to adjust parameters, in order to bring their predictive power to nonlinear and out-of-equilibrium optical properties.

[1] Refaely-Abramson et al., Phys. Rev. B 92, 081204(R) (2015)
[2] Wing et al., Phys. Rev. Materials 3, 064603 (2019)