Truncated TDDFT Approach for the Calculation of Exciton Binding Energies in Solids

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The calculation of the excitonic effects in solids is a crucial step towards the prediction of the optical properties of new materials. The Bethe-Salpeter equation (BSE) is the standard method to compute excitations in solids, but its computational cost limits its applicability. In the last years, Time Dependent Density Functional Theory (TDDFT) has shown to be a low-cost alternative to the BSE that yields reasonable excitations[1]. By solving the Casida equation with exchange-correlation kernels that include the long-range Coulomb interaction, some excitonic features can be obtained. However, these results are critically dependent on the transition dipole moment, which is an ill-defined magnitude in solids[2] (see Fig. 1). Recently, a promising hybrid approach has been proposed by Sun et al.[3], which includes a fraction of the screened exact exchange (SXX) in conjunction with TDDFT.
In this work, we explicitly treat the singularity of the SXX kernel by truncating the Coulomb interaction in the Wigner-Seitz supercells of the compounds under analysis[4]. This way, we get a well defined, material dependent term that can be related with the exciton radius. Our preliminary results show that this approach can be used to get exciton binding energies in good agreement with experiments at the computational cost of TDDFT, which could be crucial for future investigations.

References

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Figures

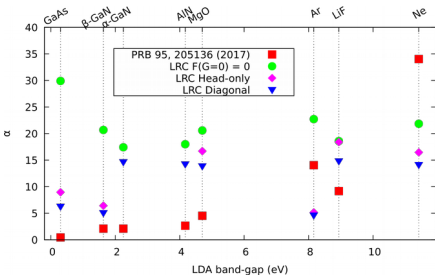

Figure 1: Scaling parameter of the Coulomb interaction needed to reproduce the experimental exciton binding energy with different TDDFT kernels.