CSCI699 Assignment 4 — Linear-Response Time-Dependent Density Functional Theory (LR-TDDFT) — Answer

We have computed the optical absorption spectrum of α-tellurene (a monolayer of tellurium) based on the linear-response time-dependent density functional theory (LR-TDDFT), with and without long-range exact-exchange correction.

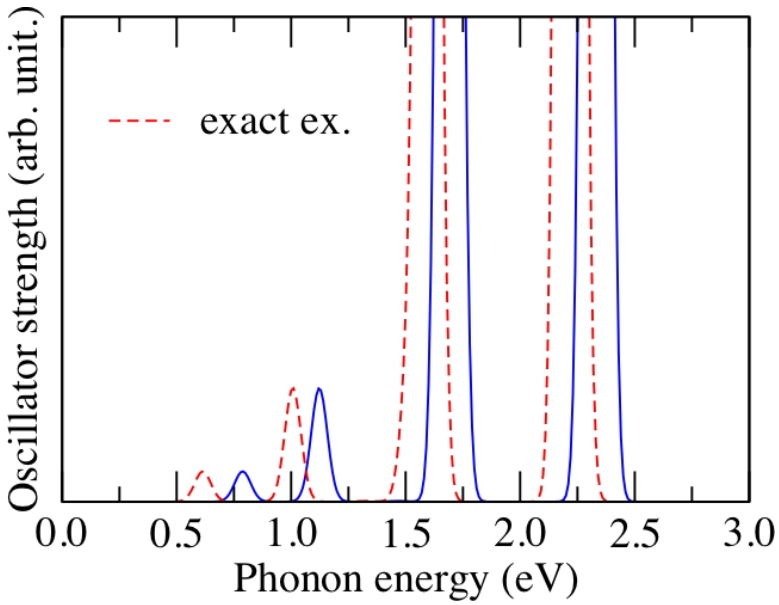

Fig. 1: Calculated optical absorption spectrum of α-tellurene with (red dashed line) and without (blue solid line) long-range exact-exchange correction.

Incorporating exact exchange has been shown to be indispensable for LR-TDDFT to describe the binding of an electron-hole pair (*i.e.*, exciton) [Dreuw *et al.*, *J. Chem. Phys*. **119**, 2943 (2003)]. Accordingly, the calculated excitation-energy peaks shift downward with inclusion of exact exchange, reflecting exciton binding energy.