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

Due: Monday, April 9, 2018

Compute the optical absorption spectrum a 2×2 unit cell of α-tellurene (a monolayer of tellurium, 3×2×2 = 12 atoms) based on the linear-response time-dependent density functional theory (LR-TDDFT), with and without long-range exact-exchange correction:

$$\alpha(\omega) = \sum_I \frac{f_I}{\omega - \omega_I}$$

where ω_I is the I-th excitation energy and f_I is the oscillator strength

$$f_I = \frac{2\omega_I}{3} \sum_{\alpha=x,y,z} |\langle 0|\hat{\alpha}|I\rangle|^2$$

Here, $|I\rangle$ is the I-th excited-state wave function, with $|0\rangle$ being the ground state.

Use the QXMD software (https://github.com/USCCACS/QXMD_Course), following the do-it-yourself instruction (http://cacs.usc.edu/education/cs699/LRTDDFT-DIY.pdf).

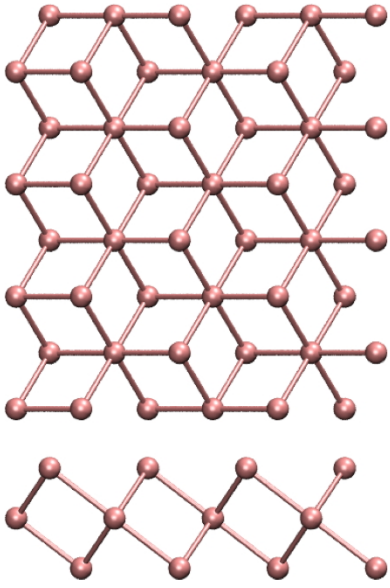

Figure: Top (top panel) and side (bottom panel) view of α-tellurene.

Submit a plot of the oscillator strength as a function of photon energy, both with and without long-range exact-exchange correction.