LITESOPH

Layer Integrated Toolkit and Engine for Simulations of Photo-induced Phenomena

Tutorial Day 1

LITESOPH is a comprehensive toolkit to launch, monitor, manage and analyse large-scale simulations of photo-induced phenomena. On day 1 of this workshop, we will do some simple tasks.

1. Free electron dynamics
2. Calculate photo-absorption spectrum of WSe_2 flake (n=4), coumarin, BODIPY and Silver cluster (Ag55).

Free electron dynamics:

When running a RT-TDDFT calculation, a variety of choices need to be made, such as the form of the applied field, the size of the time step, and what properties are of interest for analysis. These are in addition to the standard requirements of choice of density functional and basis set.

The calculation generally proceeds in three steps:

(1) prepare the reference state,

(2) choose the applied field and propagate the density in time,

(3) analyse the time-dependent observables of interest (dipole, population), with a possible Fourier transform into the frequency domain.

For our example RT-TDDFT calculations on the coumarin molecules,

(1) we will start from a converged ground state density,

(2) apply a perturbation in the form of a delta pulse,

(3) show the resulting time-dependent dipole moment, as well as the absorption spectra obtained from Fourier transform of the dipole moment.

Let's take an example of **coumarin molecule**.

First let's do the Ground state calculation,

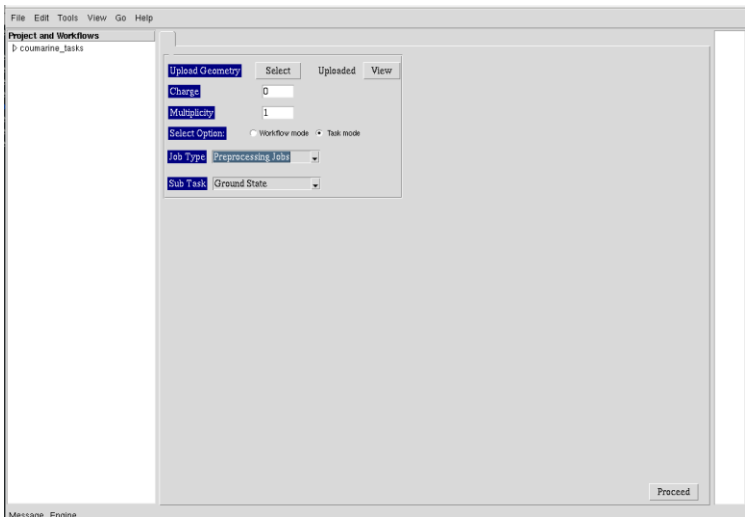
To do that, first we need to launch LITESOPH GUI using command (in the environment where LITESOPH is installed),

$ litesoph gui

Now, create a new project and unload the geometry (.xyz file)

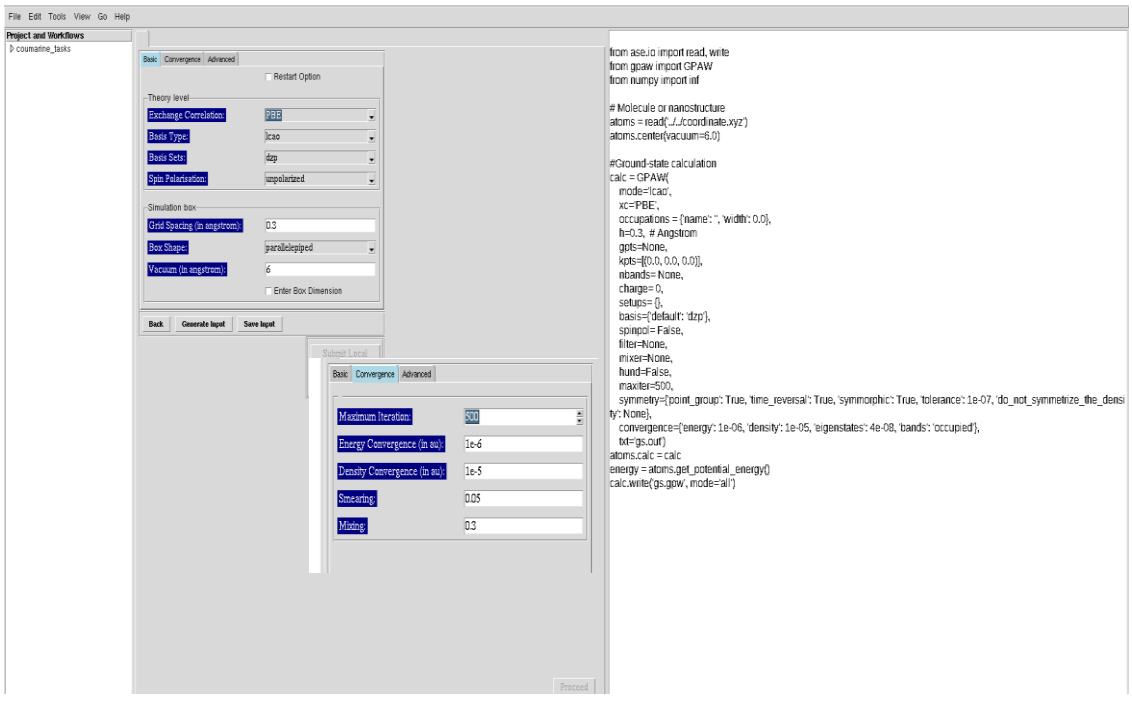
Then select Task mode in options, and Ground state as sub task in preprocessing jobs.

Ground State Calculation:



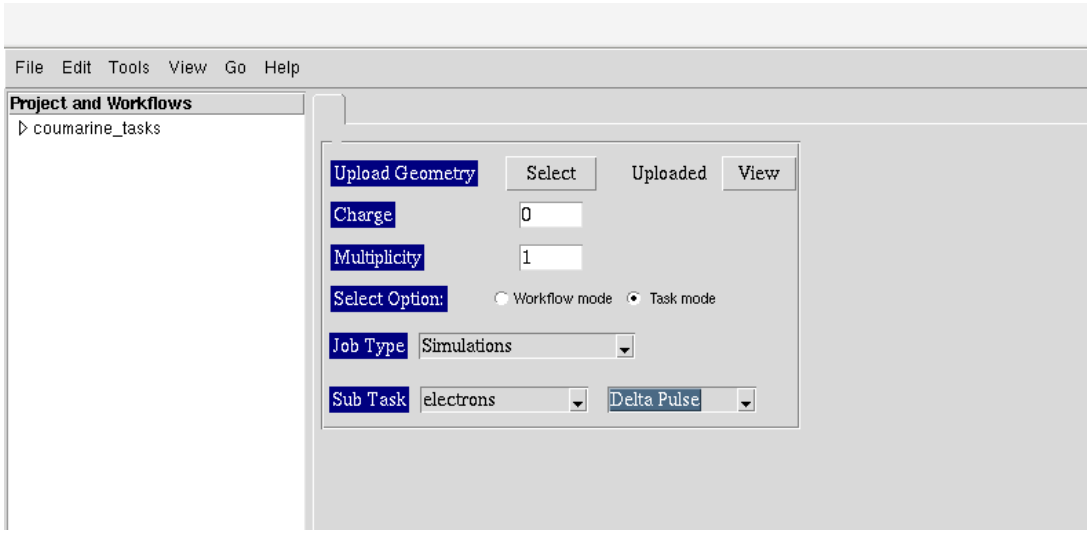
Here selects the exchange correlation functional, basis sets, and then in the convergence option we have to provide the values of density convergence and energy convergence thresholds.

Then generate and submit the input.

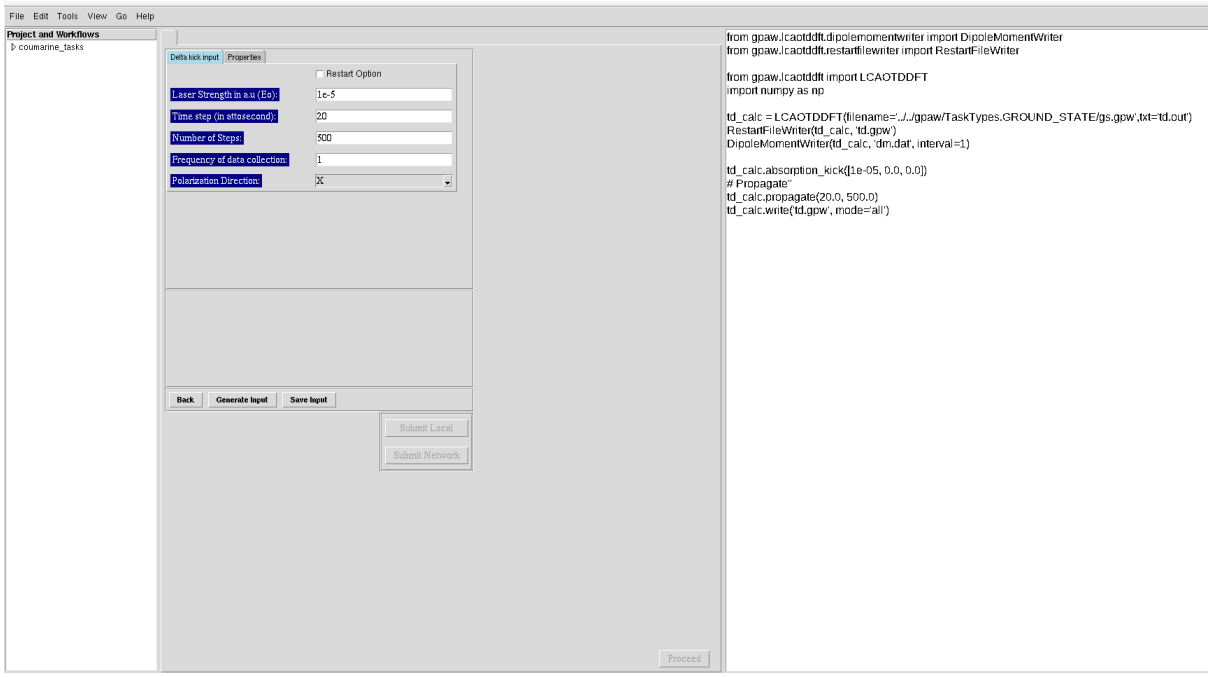


TDDFT calculation

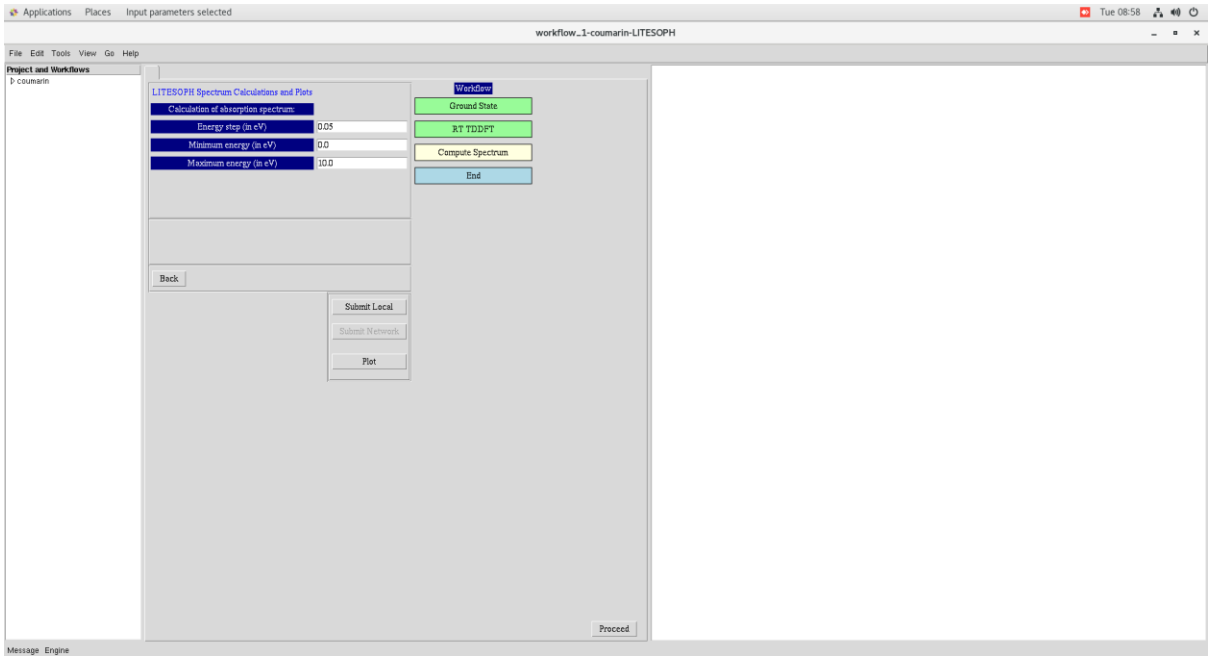
After the completion of the ground state calculation, we will select the job type- simulations and subtask- electrons and we will provide a weak perturbation using a delta pulse.



Here after providing suitable values in all then generate and submit the job script for TDDFT calculations.



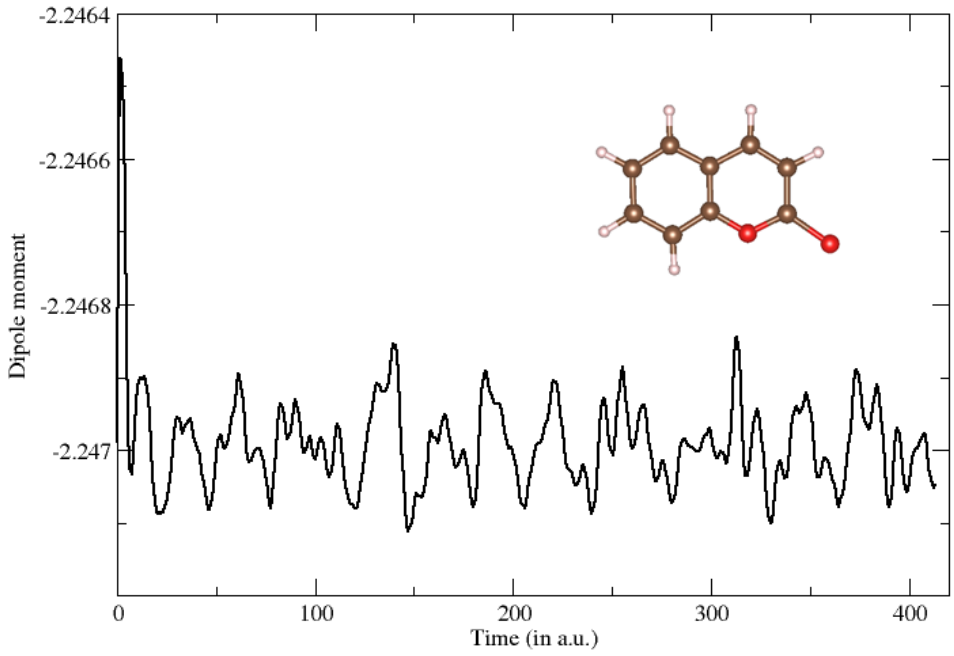
Then we plot spectrum



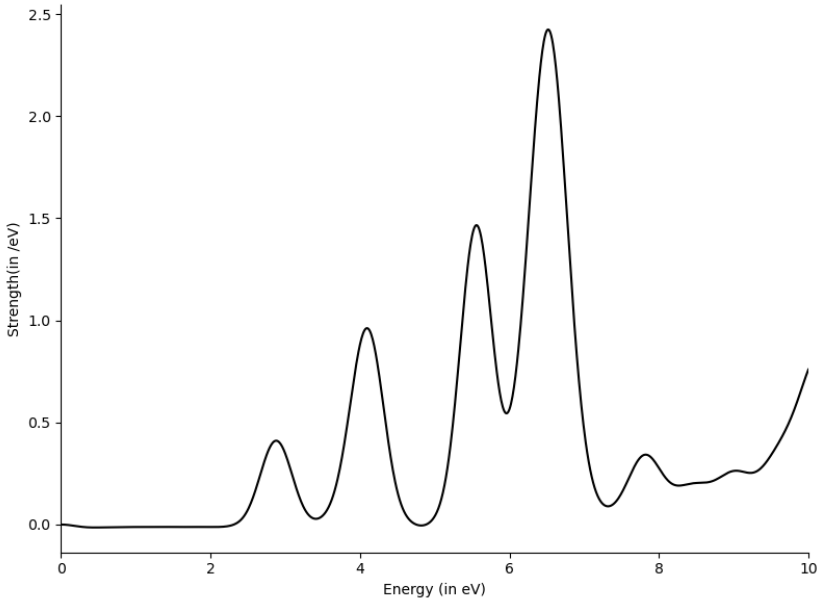
After the TDDFT calculation, from the .dat file dipole moment vs time plot can be extracted.

Coumarin

Time dependent dipole moment of coumarin molecule

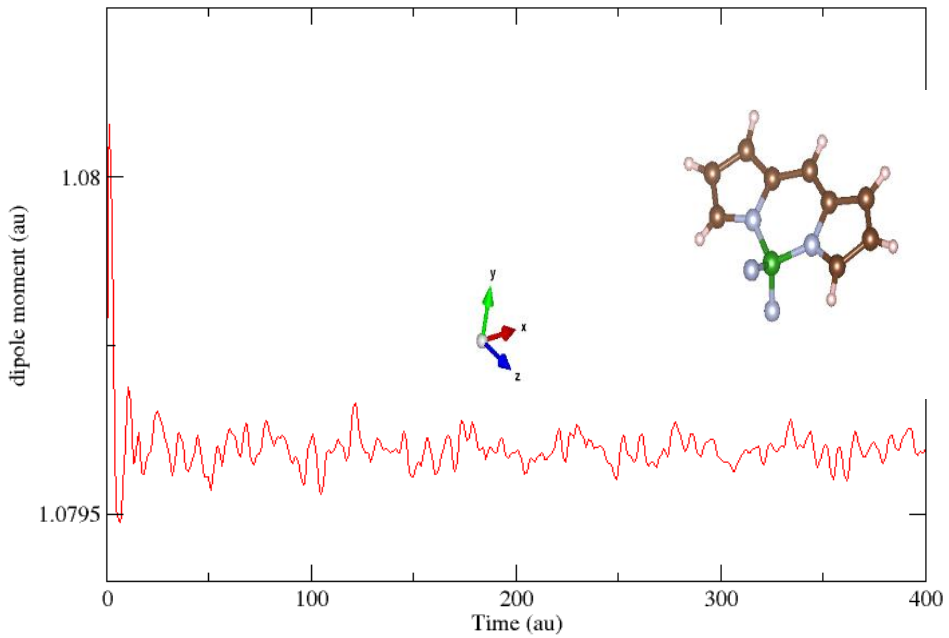


Absorption spectra the coumarin can be calculated by fourier transformation of the dipole moments.

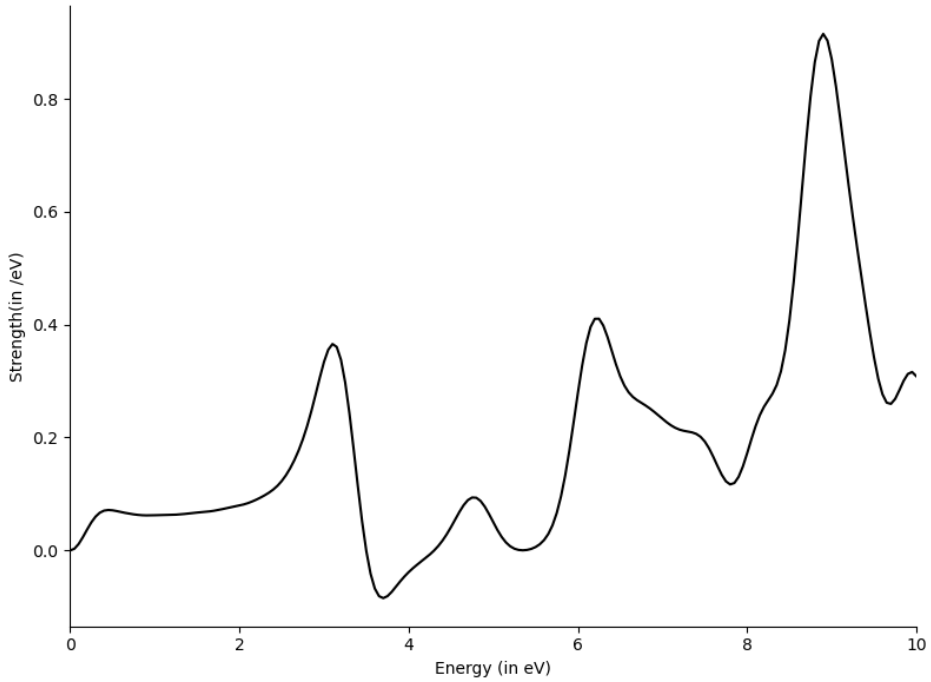


Bodipy

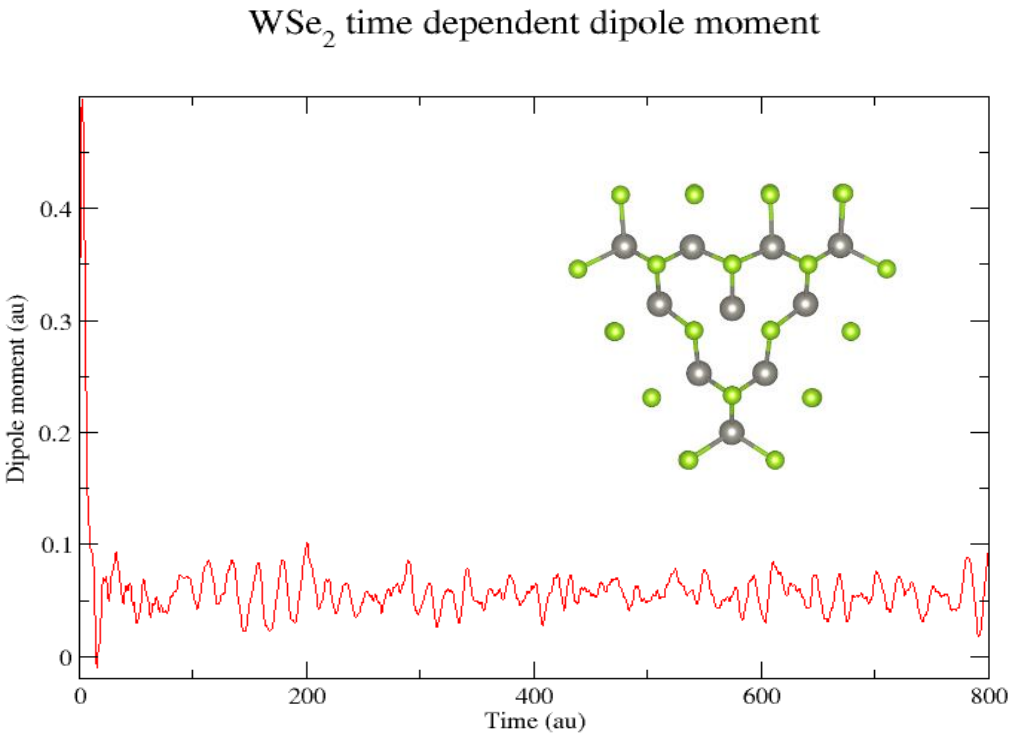
Bodipy time dependent dipole moment plot



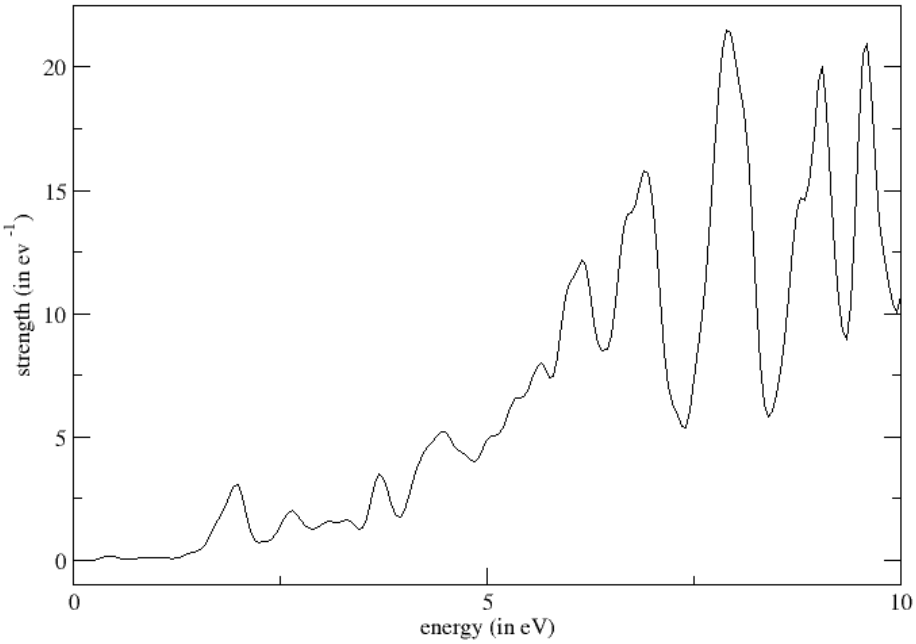
Absorption spectra



WSe_2

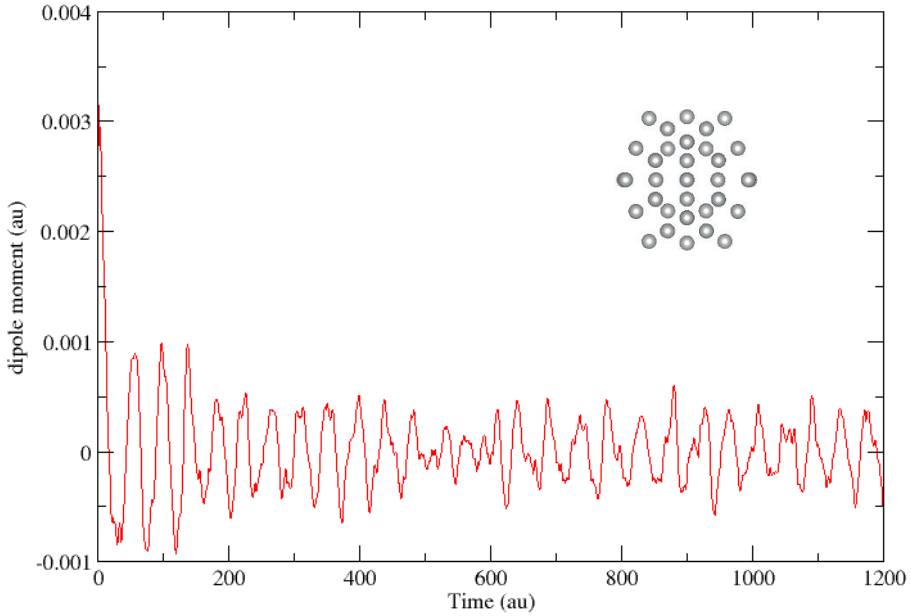


Absorption spectra



Ag_{55}

Time dependent dipole moment



Absorption spectra