CSCI699 Assignment 3 — Nonadiabatic Molecular Dynamics — Answer

We have performed nonadiabatic quantum molecular dynamics (NAQMD) simulation of $MoSe_2$ monolayer.

1. Time Evolution of Kohn-Sham (KS) Energies

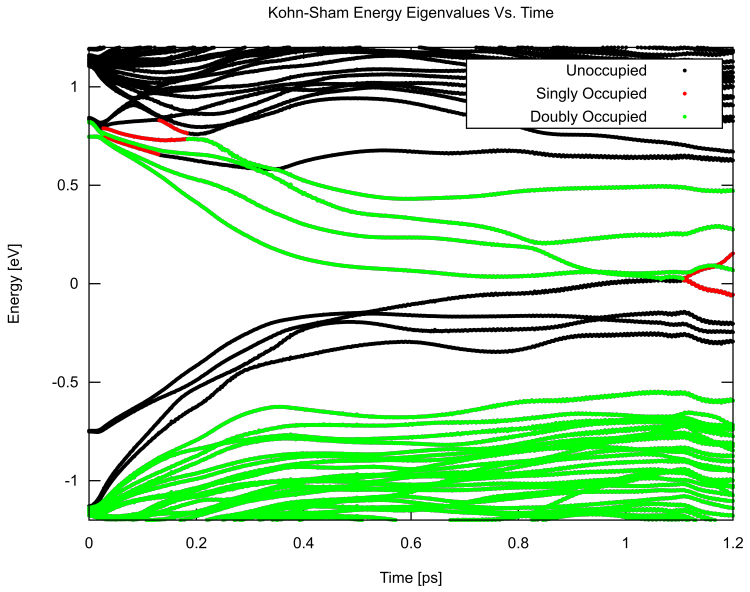

Fig. 1: Time evolution of KS energies, where green, red and black curves show doubly-, singly- and non-occupied states. The origin of energy is the Fermi level.

2. Visualization of the Wave Functions

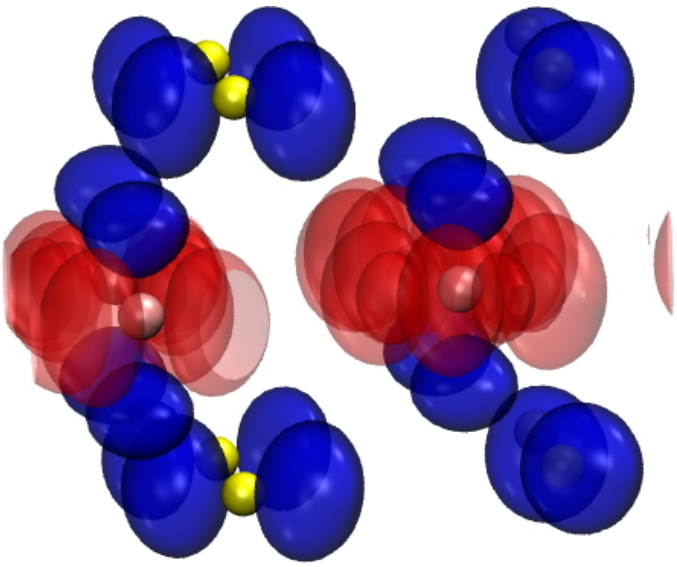

Fig. 2: Isosurfaces of the wave functions for the highest occupied molecular orbital (blue, HOMO) and lowest unoccupied molecular orbital (red, LUMO) at the first time-step.