CSCI699 Assignment 3 — Nonadiabatic Molecular Dynamics (NAQMD)

Due: Monday, March 19, 2018

Perform nonadiabatic quantum molecular dynamics (NAQMD) simulation for a 2×2 unit cell of $MoSe_2$ monolayer (3×2×2 = 12 atoms) using the QXMD software (https://github.com/USCCACS/QXMD_Course), following the do-it-yourself instruction (http://cacs.usc.edu/education/cs699/NAQMD-DIY.pdf).

***Procedure*:** Excite four electrons from 2 occupied bands—highest occupied molecular orbital (HOMO) and the next highest (HOME-1)—to two unoccupied bands—lowest unoccupied molecular orbital (LUMO) and the next lowest (LUMO+1), and perform NAQMD simulation in the canonical (NVT) ensemble at temperature 300 K for 100 steps with a unit time step of Δt = 20 a.u.

Submit: (a) plot of the time evolution of Kohn-Sham (KS) energies, using different colors for doubly occupied, singly occupied and unoccupied bands, and (b) visualization image of HOMO and LUMO wave functions at the first time-step.