We have performed nonadiabatic quantum molecular dynamics (NAQMD) simulation of MoSe$_2$ monolayer.

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

   ![Kohn-Sham Energy Eigenvalues Vs. Time](image)

   **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**

   ![Wave Functions](image)

   **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.