CSCI699 Assignment 1—Born-Oppenheimer Molecular Dynamics—Answer

Born-Oppenheimer molecular dynamics (BOMD) simulation of a water molecule was performed in the canonical (NVT) ensemble at temperature 300 K for 500 steps, with a unit time step of $\Delta t = 20$ a.u.

1. Isosurfaces of Kohn-Sham (KS) Wave Functions

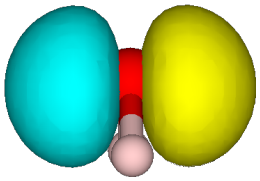

Fig. 1: Highest occupied molecular orbital (HOMO), where pink and red spheres are hydrogen and oxygen atoms, whereas cyan and yellow surfaces are positive- and negative-valued isosurfaces of the wave function.

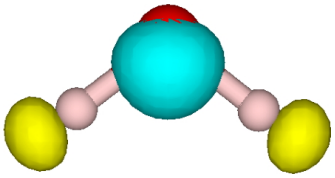

Fig. 2: Lowest unoccupied molecular orbital (LUMO), where the color schemes are the same as in Fig. 1.

2. Time Evolution of KS Energies

In the plot below, time has been converted from the atomic unit (1 t_{au} = 2.419×10^{-17} s) to femtosecond (1 fs = 10^{-15} s). The energies are in Rydberg unit (1 Ry = 13.6057 eV).

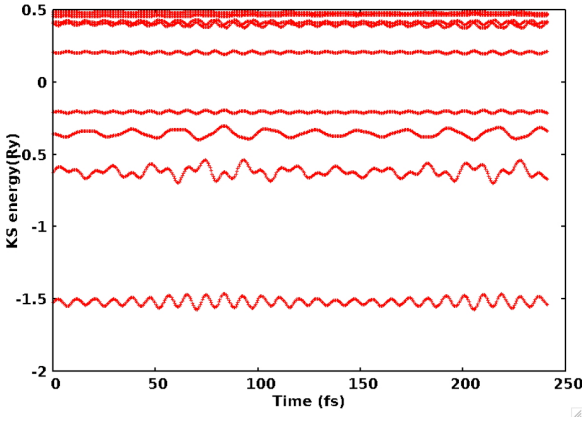

Fig. 3: KS energies as a function of time.

3. Movie

QuickTime movie, water-BOMD.mov, shows the trajectories of hydrogen (white) and oxygen (red) atoms.