CSCI699 Assignment 1 — Born-Oppenheimer Molecular Dynamics (BOMD)

Due: Wednesday, February 21, 2018

Perform Born-Oppenheimer molecular dynamics (BOMD) simulation of a water molecule using the QXMD software (https://github.com/USCCACS/QXMD_Course), following the do-it-yourself instruction (http://cacs.usc.edu/education/cs699/QXMD-DIY1-Tiwari.pdf).

Specifically,

1. Perform structural optimization (*i.e.*, minimize the energy with respect to both electronic wave functions and nuclei positions), then plot the isosurfaces of both highest-occupied molecular orbital (HOMO) and lowest-occupied molecular orbital (LUMO). ***Submit HOMO and LUMO images***.
2. Starting with the structurally optimized configuration in 1, perform BOMD simulation in the canonical (NVT) ensemble at temperature 300 K. ***Submit: (a) plot of the time evolution of Kohn-Sham (KS) energies, and (b) movie of the atomic trajectories***.
3. While using QXMD for your assignment and final project, it is required that you contribute to the completion of the QXMD readme file, QXMD_Manual_VS.md (https://github.com/USCCACS/QXMD_Course/blob/master/QXMD_Manual_VS.md). To lean about the markdown language, please refer to the markdown cheatsheet (https://github.com/adam-p/markdown-here/wiki/Markdown-Cheatsheet). ***Your contribution to the readme file will be checked at the end of the semester***.

Submit (1) a single PDF file containing your name, wave-function images for part 1 and KS-energy plot for part 2a, along with (2) a movie file for part 2b.