C343: Physical Chemistry Lab II

2 March 2021

2. Simulation of Electronic Spectra of Molecules

In this lab, we simulate the electronic spectra of a series of dienes using density functional theoretical (DFT) models. The vertical excitation energies are calculated using the time-dependent DFT (TDDFT) method for the minimum energy geometries of the molecules in their ground electronic state.

Consider the molecules, butadiene, hexatriene, and octatetraene.

1. Compare the energetics of the different forms of the three molecules.
2. What is the most stable form of the isomers for the three molecules?
3. Take all trans of the three molecules and compute the HOMO-LUMO energy gaps.
4. Compare the HOMO-LUMO energy gaps from the ab inito calculations with that computed with a 1-D particle in a box model.
5. Calculate the vertical transition energies of the three linear forms of the molecules using TDDFT method and 6-31g* basis set. What type of transitions do they correspond to?

Keywords for TDDFT Calculations:
td=(50-50,nstates=3) B3LYP/6-31G*