**Project assignment 2 CHM 673, Spring 2020**

*Due: Tuesday, March 24*

1. **Develop specific details of the project.**

Now it is time to think and develop a more specific outline of your project. Finalize your model system(s) and questions you intend to address. Discuss what type of calculations you will perform, and what quantities would be of most interest for you and why. Add these details to the *Introduction* and *Computational details* sections.

1. **Perform and analyze Hartree-Fock calculations.**

The first step in almost every ab initio study is the Hartree-Fock calculations along with a detailed analysis of the results. (You can use a simple DFT functional such as B3LYP or PBE0 instead).

What would we like to learn from these calculations?

* Prepare an input for your system. Perform single-point HF/6-31G\* calculations and analyze the orbitals (both occupied and some of virtuals), electronic configuration, symmetry, bonding picture/Lewis structure, etc. If you consider several molecules in your project, perform a detailed analysis for one of them and provide the most important details for the others. However, if you are interested in a reaction, provide detailed characteristics of both reactants and products.
* Perform HF/6-31G\* geometry optimization. Analyze the resulting structure as well as other properties (Koopmans IP, dipole moment, etc).
* Do you expect Hartree-Fock to be a good zero-order model in your case? How large is HOMO-LUMO gap?
* Increase the basis set. How fast do Hartree-Fock calculations converge with respect to the basis set? Are the polarization/diffuse functions important? How does basis set affect geometries, HOMO-LUMO gap, charge distribution?

**General guidelines for the final project**

* Start *Results and Discussion* section with presenting and explaining qualitative molecular orbital framework, electronic configuration and bonding picture of the ground and, if relevant, lowest excited states. If relevant, analyze symmetry (MOs, electronic states, vibrations).
* Characterize structures (and frequencies, if relevant) using the Hartree-Fock (or DFT) model. What did you learn from these calculations?
* If relevant, describe lowest excited states (using CIS and Koopmans’ theorem).
* Now, when you understand the system, proceed to your project question. Explain what calculations you perform to answer your question, what results did you obtain, and how you interpret them, i.e., what does it all mean.
* Make sure you clearly describe type of calculations performed. Ask yourself if you provide sufficient details for someone else to reproduce your results.
* Summarize the relevant data in tables and/or graphs. Pay attention to significant digits: total energies are typically reported in Hartrees with 6 decimal digits; excitation energies in eV with 3 decimal digits; binding energies and relative energy changes in chemical reactions in kcal/mol or kJ/mol with 2 decimal digits; geometries in Angstroms with 3 decimal digits. Discuss which trends you observed and what does it mean.
* In *Conclusions*, summarize your main findings. Additionally, critically assess the quality and reliability of your results, and suggest which calculations should be taken in the future work.