**Project assignment 1 CHM 673, Spring 2020**

*Due: Tuesday, February 17*

The class project is your chance to gain practical experience with the tools of computational chemistry. If possible, select a project related to your research interests, since this will provide you with a direct experience of how computational chemistry methods can assist your own work. However, if you study something like denaturation of DNA, be prepared to come up with a simplified model system that would be computationally feasible. Or you might decide to challenge yourself and develop a computer code for a new (or well forgotten) quantum chemistry model.

Typically, your final report will be structured as following:

1. Introduction

* here is a great chemical problem (briefly describe why it is important)
* we already know something about this problem (BRIEFLY refer to your research)
* however, not everything is clear; it would be great to obtain some additional information from electronic structure computations. Specify which information you want/need/expect to gain from calculations (Write this part in as much detail as you can)

2. Computational details

* here is a plan of action: specify the calculations you will perform

3. Results

- summary of your results in tables and figures (publication quality, please!)

4. Discussion

- what did you learn? Do the observed trends make sense? Any interesting observations related to computational methods? Any interesting observations that help/explain/contradict your findings from experiment?

5. Conclusions

- summary of what you did and what you learned

*In the first assignment you should sketch the idea of your project. Think of it as a mini-proposal, with Prof. Slipchenko being a (friendly) funding agency. In other words, you try to sell your idea of what computational work should be done. At this point, you do not need to worry about anything but part 1: introduction.*

*I will review the proposed projects and provide a feedback regarding their computational feasibility as well as soundness of specific goals. You will have a chance to refine your ideas in assignment 2.*

Some suggestions for possible projects are given below:

* Structures and relative energies of different conformations of a molecule or molecular cluster.
* Binding energies of a molecule in a protein pocket or on surface.
* Effects of solvent or surface on structure and other properties of a molecule.
* Energetics of a reaction and reaction pathways (reaction enthalpy and activation barriers: energies of reactants, products, and transition states).
* Thermodynamic properties of a molecule (including heat of formation).
* Absorption and/or emission spectra of a molecule.
* Charge density of a molecule and its implications for reactions governed by electrostatic effects.
* Substituent effects on structures and/or energetics.
* Vibrational frequency predictions to explain IR/Raman spectra.
* Rotational constant predictions to explain rotational spectra.
* Candidate molecules for unusual bonding, etc.