**Computational Assignment 1**

Assigned Tuesday, 1-22-19, Due 1-28-19

**Justification**: Most modern physical chemistry requires some sort of computational calculation, simulation and analysis. Most problems are too complex to solve analytically and using a computer to arrive a numerical solution can give very useful physical insights into chemical problems.

**Overall Learning Objective**: The goal of these assignments is to teach you how to perform physical calculations and analysis using modern and versatile scientific computing tools. In these assignments, we will be using the python programming language and scientific libraries to perform our calculations. We will use a notebook document as the environment where we perform our calculations.

**Assignment:**

This first assignment will involve setting up the Jupyter notebook on your laptop and running your first line of code. Notebooks are documents that can include code, rich text, graphics, and equations. They code in these documents can be run in real time to perform calculations. You can think of it as a computational combination between a lab manual and a lab bench!

**Procedure:**

1. Navigate over to the Project Jupyter website (<https://jupyter.org/)> and explore the site to get an initial sense of the notebook
2. Go to the Jupyter installation page and follow the directions under the heading “**Installing Jupyter using Anaconda**”
3. After installing Anaconda, open the notebook program.
   1. If your machine is running windows open the command prompt (search for “cmd” or “command”) and type “jupyter notebook”
   2. If you have a Mac or Linux machine, open the terminal (search for terminal) and type “jupyter notebook”
4. Navigate to and open the file “comp\_assignment-1.ipynb” (downloaded from Blackboard).
5. Follow directions on notebook.