Computational Inorganic Chemistry
Lecture Implementation Notes

Purpose
To present a brief yet adequate introduction to computational chemistry with a focus on applications to inorganic systems.

Timing
I typically present this lecture at the end of the second semester advanced inorganic chemistry class. In the first semester, the students have studied atomic structure and geometries, pigments, molecular orbitals, symmetry, acid-base chemistry, photographic chemistry and basic coordination chemistry. In the second semester, we study group theory and applications to vibrational spectroscopy, advanced coordination chemistry and electronic spectroscopy, bioinorganic and organometallic chemistry, and computational chemistry. Although I have chosen to present this material at the end of a year-long course sequences, I believe the majority of this lecture could be presented at the end of a 1 semester introductory class.

Computational Methods Overview
- There are many different methods of modeling molecules in a computer
- Each method has strengths and weaknesses depending upon the system you are interested in studying
- Computational Methods
    - Ab initio (quantum methods)
    - Semi-empirical
    - DFT
    - Molecular mechanics
    - QM/MM

Why do I give this lecture?
One of the goals of the lecture is to give students an appreciation for computational "expense". There are always trade-offs in computational chemistry and this is especially true of inorganic systems with unpaired electrons. It is important to help the class gain perspective on the many different variables so they can appreciate the choices made by researchers in the field. I also want the class to have an understanding of the advantages and disadvantages of each method.

Evaluation
Exam questions I have used over this material have been posted as a Problem Set.