Chem3208 Lecture 0
General Introduction

Megan O'Mara, Andrew Gilbert, and Pierre-François (Titou) Loos

Research School of Chemistry
Australian National University
Canberra, Australia

2nd Semester 2016

Content of the lectures

1. **Hückel theory** (Titou, 4 lectures)
2. **Hartree-Fock (HF) theory** (Titou, 4 lectures)
3. **Electronic correlation methods** (Titou, 4 methods)
   1. Configuration Interaction (CI)
   2. Møller-Plesset (MP) perturbation theory
   3. Coupled Cluster (CC)
4. **Density-functional theory (DFT)** (Andrew, 4 lectures)
5. **Illustrating the concepts** (Andrew, 4 lectures)
   1. Basis sets, solvent models, etc.
   2. Atomic charges, localised orbitals, etc.
   3. Geometry optimisation, transition state, etc.
   4. IR and UV/Vis spectra and NMR shift
6. **Excited states** (Titou, 2 lectures)
7. **Molecular modelling** (Megan, 6 lectures)
   1. Classical force fields (FF)
   2. Molecular dynamic (MD)
   3. Monte Carlo (MC) approaches
   4. Free energy, thermostats, etc.

Computational Labs

- Labs will be held on Monday afternoons between 2-5pm in Rm. 113 of the Gould Building (Bldg 116, RSB):
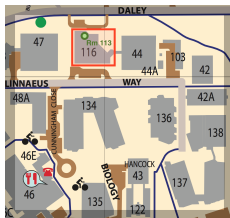
- Lab instructions will be distributed beforehand, and a short report will be due at the following lab session (1 week later).
- The laboratory exercises are designed to give hands-on experience with the theories covered in the lectures.
- The first lab will be an introduction to the IQmol and Q-Chem programs that will be used in subsequent labs.

Good books

- Introduction to Computational Chemistry (Jensen)
      = the one you probably should read...

- Essentials of Computational Chemistry (Cramer)
      = similar to Jensen...

- Modern Quantum Chemistry (Szabo & Ostlund)
      = the holy book of quantum chemistry!

- Molecular Electronic Structure (Helgaker & Friends)
      = for experts

- Molecular modeling and simulation: an interdisciplinary guide (Schlick)
      = for Megan's stuff

Assessement

Exams

- Lab Reports 30%
- Written Exams 70% (mid-term and end-of-term exam will be 35% each)
    - Mid-term exam = 100% Titou
    - End-of-term exam = 15% Titou + 50% Andrew + 35% Megan
- I can make a mock exam before the mid-term exam...
- Class reps?

To pass the course, you must

- complete all laboratory work
- submit all laboratory reports
- complete all in-class activities (for example, on-line quizzes and assignments)