CHEM 571A - Quantum Chemistry
Syllabus, Fall 2019

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Office Hours: by appointment

Class Time and Location: Mondays, Wednesday, Fridays 11:00am-11:50am
10 weeks: August 26th through November 3rd
Chemistry B102

Textbook: *Quantum Chemistry*, Donald A. McQuarrie, 2nd edition

Course Objective: to teach the concepts, methods, motivtations and approximations currently used in quantum chemical calculations.

Learning Objectives: Students successfully completing this course should be able to

1. Solve the standard quantum mechnical problem "harmonic oscillator";
2. Describe the connection between the "harmonic oscillator" solutions and vibrational spectroscopy of molecules;
3. Solve the standard quantum mechnical problem "rigid rotator";
4. Describe the connection between the "rigid rotator" solutions and rotational spectroscopy of molecules;
5. Solve the Schrodinger equation for the hydrogen atom;
6. Approximate the Schrodinger equation for the helium atom using basis functions;
7. Solve a spin Hamiltonian;
8. Relate a spin Hamiltonian to NMR spectroscopy;

Course Topics (subject to change):

Week 1: History of quantum mechanics and introduction to Jupyter notebooks
Week 2: Postulates of QM and Vibrtational spectroscopy and the "harmonic oscillator"
Week 3: Vibrational Spectroscopy continued
Week 4: Moving beyond the "harmonic oscillator"
Week 5: Rotational spectroscopy and the "rigid rotator"
Week 6: The hydrogen and helium atoms
Week 7: The hydrogen and helium atoms continued
Week 8: Electronic spectroscopy
Week 9: Spin and NMR spectroscopy
Week 10: Spin and NMR spectroscopy

Homework: There will be weekly homework assignments worth 40% of your grade.

Exams: There will be a midterm exam (week 5 or 6) worth 20% of your grade and a final exam worth 40% of your grade.

Academic Integrity: This course will adhere to the CSU Academic Integrity Policy as found in the General Catalog (URL given below) and the Student Conduct Code (URL given below). At a minimum, violations will result in a grading penalty in this course and a report to the Office of Conflict Resolution and Student Conduct Services.
General Catalog - 1.6, pages 7-9:
http://www.catalog.colostate.edu/Content/files/2012/FrontPDF/1.6POLICIES.pdf
Student Conduct Code:
http://www.conflictresolution.colostate.edu/conduct-code