

# UTAH STATE UNIVERSITY

## CHEMISTRY 6010

### FALL SEMESTER 2018

Instructor: Alexander I. Boldyrev

Office: ML 369

Email: a.i.boldyrev@usu.edu

Class times: MF 4:00 pm – 5:30 pm, ML 151

Office hours: ML369 MF TBA

I will be happy to make appointments with anyone who has unavoidable conflicts at these times. The best way to contact me outside office hours is by email.

The last day to add this class is the September 17. Attending this class beyond that date without being officially registered will not be approved by the Dean's Office.

**The last day to withdraw from the class is October 29, 2018.**

#### CHEMISTRY 6010 QUANTUM CHEMISTRY

##### Syllabus

Fall Semester 2018

In accordance with the Americans with Disabilities Act, reasonable accommodation will be provided for all persons with disabilities in order to ensure equal participation in this course.

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**Text:** Modern Quantum Chemistry (1996) by Attila Szabo and Neil S. Ostlund.

I will make reading assignments from the text. You are responsible for all material in these assignments even if it isn't covered in lecture.

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Course content: Approximately the first 3 weeks of Chemistry 6010 will be devoted to Molecular Symmetry. The following topics will be covered:

- Symmetry Elements and Operations
- Symmetry Point Groups
- Matrices as Group Representations
- Characters of Representations
- Reducible and Irreducible Representations
- Projector Operators: Symmetry Adapted Linear Combinations of Atomic Orbitals
- Electronic Configurations and Spectroscopic States
- Symmetry of Normal Vibrational Modes

The next 3 weeks will be devoted to Mathematical Review and Many Electron Wave Functions and Operators. The following topics will be covered:

- Linear Algebra
- Orthogonal Functions, Eigenfunctions, and Operators
- The Variation Method
- The electronic Problem
- Orbitals, Slater Determinants, and Basis Functions
- Operators and Matrix Elements
- Second Quantization
- Spin-Adapted Configurations

The next 3 weeks will be devoted to the Hartree-Fock Approximation. The following topics will be covered:

- The Hartree-Fock Equation
- Derivation of the Hartree-Fock Equations
- Implementation of Solutions to the Hartree-Fock Equations
- Restricted Closed-Shell Hartree-Fock: The Roothaan Equations
- Polyatomic Basis Sets
- Some Illustrative Closed-Shell Calculations
- Unrestricted Open-Shell Hartree-Fock: The Pople-Nesbet Equations

The next 3 weeks will be devoted to Configuration Interaction and Many-Body Perturbation Theory. The following topics will be covered:

- Configurational Interaction Methods
- Multi-Configurational Self-Consistent Field Methods
- Moller-Plesset Perturbation Theory
- Coupled-Cluster Methods

The last 3 weeks devoted to Density Functional Theory. The following topics will be covered:

- The Hohenberg-Kohn Theorem
- The Kohn-Sham Method
- The Local-Density Approximation (LDA)
- The  $X\alpha$  Method
- The Local-Spin-Density Approximation (LSDA)
- Gradient-Corrected and Hybrid Functionals

After every chapter there will be a test (50 pts.).

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Final grades will be computed with an A, A- >90%, a B+, B, B- > 80% and a C+, C, C- >70%. These cutoffs may be revised slightly downwards.

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