CHE 525 - Theoretical Chemistry
Syllabus

Bulletin Course Description: (3 credits). This course stresses the physical theory underlying chemical phenomena. Special emphasis is given to advanced topics in electronic structure theory, molecular dynamics, condensed matter and surfaces, many-body and quantum ensemble theory, and the interaction of light and molecules.

Lecture: 9:15-10:10 AM, MWF

Instructors: Thomas Allison <thomas.allison@stonybrook.edu> Benjamin Levine <ben.levine@stonybrook.edu>.

Office Hours: Zoom links to be provided on Blackboard.

Allison: Wednesday, 1-3pm
Levine: Tuesday, 9:30-11:30am

Proposed Course Objectives: Students will acquire knowledge of the core aspects of advanced electronic structure methods and learn how to wisely operate Quantum Chemistry software packages. Students will also learn the basics of light-matter interactions and *ab initio* calculations of spectroscopic observables.

Course Textbook: *Modern Quantum Chemistry*, by Szabo and Ostlund.

Other Useful Books: *A Chemist's Guide to Density Functional Theory* by Koch and Holthausen. *Elements of Computational Chemistry*, by Cramer. *Methods of Molecular Quantum Mechanics*, by McWeeny. *Elements of Quantum Mechanics*, by Fayer.

Ambitious Summary of Contents

A Brief Review of Fundamentals. The Schrödinger equation for a collection of electrons and nuclei. The Born-Oppenheimer approximation and potential energy surfaces. The representation of a wave function as a superposition of basis functions. The variational principle, the linear variation method and the resulting finite-matrix representation of the time-independent Schrödinger equation.

Mean field theory. The Hartree-Fock approximation. Meaning of Hartree-Fock orbitals and Hartree-Fock energies. Koopman's correlation. Definition of electron correlation.

Wave function-based approaches to electron correlation. Variational vs perturbation theory approaches. Configuration interaction. Condon-Slater rules. Møller-Plesset perturbation theory. Coupled Cluster methods. Why excited states are hard.

Basis Sets. Understanding the optimization and limitations of basis sets for various problems. Basis set superposition error.

Density functional theory. The wave function has more information than necessary to calculate most observables. The Hohnenberg-Kohn thereoms. Kohn-Sham formalism. The local-density approximation. Hybrid functionals. Generalized gradient approximation.

Light interaction with matter fundamentals. Resonantly-driven two-level system. Dipole matrix elements. Selection rules. The rotating wave approximation. Rabi Flopping. Density matrices and the optical Bloch equations. Fermi's golden rule. Spontaneous emission.

Excited States. Multi-reference methods. Time-dependent density functional theory. Calculation of spectroscopic observables.

Electronic Structure Laboratory

Homework will involve extensive use of modern quantum chemistry software packages, comprising a virtual "laboratory" for the students to experiment with electronic structure calculations. Although using "canned" software, these laboratory exercises will focus on exploring the physical basis of the approximations and algorithms underlying practical electronic structure calculations, the circumstances in which they work well, and the circumstances under which they fail.

The open-source Psi4 package will be used for hands on exercises. Calculations will be performed on the SeaWulf cluster, thus also familiarizing students with how to operate in a real high-performance computing environment.

Assignments will be posted and announced via the blackboard system. Laboratory exercises will be written up in the form of lab reports in the format of short scientific articles, and submitted using SafeAssign.

Approximate Grade Weighting
Laboratory Exercises: 60%
Final Project: 30%
Take-Home Final Exam: 10%

Attendance/Participation: Attendance and participation in lectures is highly encouraged, but will not be required. All classes will be recorded and linked from the course Blackboard page.

Schedule of Course Assignments: Assignments and due dates will be communicated via the course Blackboard page and announced in class.

Schedule of Lectures: A schedule of upcoming lectures will be communicated via the course Blackboard page and announced in class.

Hardware and Software Requirements: Lectures will take place online via Zoom. The Zoom client application can be downloaded from https://stonybrook.zoom.us. In order to participate in discussions in synchronous lectures, students should have a camera and microphone on the device they use to participate in lectures. Lab exercises will utilize Stony Brook's SeaWulf computer cluster. All software needed to access it is available on the Virtual SINC Site, which can itself be accessed via standard web browsers (see https://it.stonybrook.edu/services/virtual-sinc-site). Lab exercises must be typed and figures included and reference in the text. This can be done with LaTeX or any word processor. Data analysis and figure preparation should also be done using computer software packages, and it is recommended that students use a software package geared towards scientific computing that allows easy plotting, curve fitting, statistical analysis, numerics, and comparison between data and analytic formulae. Occasionally, homework problems may also ask you to plot results. Learning how to do these tasks on a computer is an essential component of being a modern scientist or engineer.

Student Accessibility and Support Center (SASC): If you have a physical, psychological, medical, or learning disability that may impact your course work, please contact the Student Accessibility Support Center, 128 ECC Building, (631) 632-6748, or at sasc@stonybrook.edu. They will determine with you what accommodations are necessary and appropriate. All information and documentation is confidential. Students who require assistance during emergency evacuation are encouraged to discuss their needs with their professors and SASC. For procedures and information go to the following website: https://ehs.stonybrook.edu/programs/fire-safety/emergency-evacuation/evacuation-guide-people-physical-disabilities

Academic Integrity: Each student must pursue his or her academic goals honestly and be personally accountable for all submitted work. Representing another person's work as your own is always wrong. Faculty are required to report any suspected instance of academic dishonesty to the Academic Judiciary. For more comprehensive information on academic integrity, including categories of academic dishonesty, please refer to the academic judiciary website at https://www.stonybrook.edu/commcms/academic_integrity/

Critical Incident Management: Stony Brook University expects students to respect the rights, privileges, and property of other people. Faculty are required to report to the Office of Judicial Affairs any disruptive behavior that interrupts their ability to teach, compromises the safety of the learning environment, and/or inhibits students' ability to learn

Electronic Communication Email to your University email account is an important way of communicating with you for this course. For most students the email address is firstname.lastname@stonybrook.edu, and the account can be accessed here: http://www.stonybrook.edu/mycloud. *It is your responsibility to read your email received at this account.* For instructions about how to verify your University email address see this: http://it.stonybrook.edu/help/kb/checking-or-changing-your-mail-forwarding-address-in-the-epo .

Religious Observances: See the policy statement regarding religious holidays at

http://www.stonybrook.edu/commcms/provost/resources/rel.html

Students are expected to notify the course professor by email of their intention to take time out for religious observance. This should be done as soon as possible but definitely before the end of the add/drop period. At that time they can discuss with the instructor(s) how they will be able to make up the work covered.