CHE 525 - Theoretical Chemistry
Draft 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: 9-9:50 AM, MWF
Instructors: Thomas Allison <thomas.allison@stonybrook.edu> Benjamin Levine <ben.levine@stonybrook.edu>.

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 Textbooks: *Modern Quantum Chemistry*, by Szabo and Ostlund. *A Chemist's Guide to Density Functional Theory* by Koch and Holthausen.

Other Useful Books: *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. We are still settling on the precise software package students will use, but we are leaning towards open-source options where students will have greater interaction with the underlying computer code.

With the emphasis more on the physical basis of electronic structure calculations, and less on computation, we anticipate that most calculations can be performed in reasonable time on the student's home computers. However, we will also make available computing resources in the Chemistry department as needed.

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%
Final Exam: 10%

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.