CHEM 548 Molecular Electronic Structure
Spring 2021

Room: Zoom
Period: January 26 – May 4, TR 9:30 – 10:50 AM

Instructor: So Hirata
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                    Office hours: on appointment

Required text: A. Szabo and N. S. Ostlund, "Modern Quantum Chemistry:
                    Introduction to Advanced Electronic Structure Theory"

Recommended texts: B. O. Roos, "Lecture Notes in Quantum Chemistry" I and II
                    T. Helgaker, P. Jørgensen, and J. Olsen, "Molecular Electronic
                    Structure Theory"
                    I. Shavitt and R. J. Bartlett, "Many-Body Methods in Chemistry and
                    Physics"
                    N. H. March, W. H. Young, and S. Sampanthar, "The Many-Body
                    Problem in Quantum Mechanics"
                    R. D. Mattuck, "A Guide to Feynman Diagram in the Many-Body
                    Problem"

Objectives: This course is intended for graduate students who specialize in
                    computational or theoretical quantum chemistry. Its goal is to have
                    students acquire skills essential for developing new computational
                    methodologies broadly applicable to atomic, molecular, solid-state
                    chemistry. This course does not teach how to run computational
                    chemistry programs. Instead, it teaches how to write computational
                    chemistry programs and to derive formulas of the underlying theories.
                    This course interleaves lectures on theories and computer
                    programming projects. The lectures encompass advanced electronic
                    structure methods, introductory band theory, and introductory
                    quantum dynamics. The programming projects are fun.

Exams: There will be no exams.

Programming reports: There will be three computer programming projects. One or two
                    lectures will introduce each project and students are asked to work on
                    them individually or in small groups. Students who are not familiar
                    with programming are strongly encouraged to take advantage of the
                    instructor's office hours to seek hands-on assistance. Each student
                    must write his/her own research-paper-style report and submit it to
                    the instructor by the due date. Each student must have an access to
                    a basic coding environment (a UNIX or LINUX computer or cluster
                    with a C or Fortran compiler) and will be given one if he/she does not.

Grades: Attendance and class participation 50%. Programming reports 50%.
                    In grading the reports, given diverse prior programming experiences

of the students, emphasis is not placed on the correctness or completeness of the programs written.

Tentative schedules:

Date	Lecture topics	Project due
Jan 26	Project #1: Finite-difference method, basis-set method, Lagrange's undetermined multiplier method	
28	Slater determinants, Dirac bra-ket notations, orthogonal functions, unitary transformation, diagonalization, delta function	
Feb 2	Electronic structure overview, Hartree-Fock theory, full configuration-interaction theory	
4	Operators, molecular integrals, Slater-Condon rules	
9	Second quantization	
11	Project #2: Time-dependent perturbation theory, transition dipole moment, Franck-Condon principle, spectroscopies	
16	Project #2: Gaussian functions, Fourier transform, real and reciprocal spaces, correlation function	
18	Project #2: Wave packet propagation, phase and group velocities, Ehrenfest theorem, convolution theorem, path integrals	#1 due
23	Normal ordering, Wick's theorem	
25	Diagrams	
Mar 2	Hartree-Fock theory I	
4	Hartree-Fock theory II	
9	Molecular integrals over Gaussians	
11	Configuration-interaction theory	
16	Coupled-cluster theory	
18	Many-body perturbation theory	
23	Density-functional theory	
25	Project #3: Hückel and Su-Schrieffer-Heeger band structure calculations of 1D and 2D solids	#2 due
30	HF and DFT in density matrix form	
Apr 1	Time-dependent HF and DFT for excited states	
6	Coupled-cluster theory for excited states	
8	HF analytical gradients	
15	Green's function theory	
20	Crystal orbital theory	
22	Size consistency	
27	BCS theory of superconductivity	
29	Special theory of relativity	
May 4	Relativistic quantum mechanics and QED	#3 due