CHEM 548 Molecular Electronic Structure
Spring 2023

Room:	157 Noyes Laboratory
Period:	January 17 – May 3, TR 9:30 – 10:50 AM
Instructor:	So Hirata Email: sohirata@illinois.edu Phone: 217-244-0629 Office: Noyes Laboratory 355F 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 17	Project #1: Finite-difference method, basis-set method, Lagrange's undetermined multiplier method	
19	Slater determinants, Dirac bra-ket notations, orthogonal functions, unitary transformation, diagonalization, delta function	
24	Electronic structure overview, Hartree-Fock theory, full configuration-interaction theory	
26	*Presentation: Quantum field theory for chemistry*	
31	Operators, molecular integrals, Slater-Condon rules	
Feb 2	Second quantization	
7	Normal ordering, Wick's theorem, Feynman diagrams	
9	Project #2: Gaussian functions, Fourier transform, real and reciprocal spaces, correlation function	
14	Project #2: Wave packet propagation, phase and group velocities, Ehrenfest theorem, convolution theorem, path integrals	#1 due
16	Hartree-Fock theory I	
21	Hartree-Fock theory II	
23	Molecular integrals over Gaussians	
28	*Presentation: Artificial intelligence for chemistry*	
Mar 2	Configuration-interaction theory	
7	Coupled-cluster theory	
9	Many-body perturbation theory	
21	Project #3: Hückel and Su-Schrieffer-Heeger band structure calculations of 1D and 2D solids	#2 due
23	*Presentation: Many-body Green's function theory*	
28	Density-functional theory	
30	*Presentation: Finite-temperature many-body perturbation theory*	
Apr 11	HF and DFT in density matrix form	
13	Time-dependent HF and DFT for excited states	
18	Coupled-cluster theory for excited states	
20	*Presentation: Why is energy extensive?*	
25	Crystal orbital theory	
27	Size consistency	
May 2	BCS theory of superconductivity	#3 due