CHEM/QSE 245, Spring 2024
Quantum Chemistry: Theory and Practice

Tentative Lecture Schedule

Week	Date	Lecture Topic (Detailed)	Readings	Problem Sets
1	23-Jan	Intro to many-electron quantum mechanics ❖ Brief history of quantum chemistry ❖ Non-relativistic molecular Hamiltonian ❖ Born-Oppenheimer approximation and electronic Hamiltonian ❖ Difficulties in obtaining exact solution	Szabo and Ostlund Chapter 2.	
	25-Jan	Hartree-Fock (Self-consistent Field) Theory I ❖ Linear combination of atomic orbitals (LCAO) and atomic basis sets ❖ Electronic Hamiltonian in Atomic Orbitals Basis ❖ Spatial and Spin orbitals, Slater-Condon rule	Szabo and Ostlund Chapter 3.	PS1 out
2	30-Jan	Hartree-Fock (Self-consistent Field) Theory II ❖ Variational Principle and Hartree-Fock (HF) Theory ❖ Restricted, Unrestricted, and Generalized HF. Fukutome's classification.		
	1-Feb	Density Functional Theory (DFT) I ❖ Hohenberg-Kohn Theorem ❖ Thomas-Fermi theory and kinetic energy functionals ❖ Kohn-Sham DFT and orbital-free DFT	Parr and Yang Chapter 3, 7, 8.	PS1 due / PS2 out
3	6-Feb	Density Functional Theory (DFT) II ❖ DFT Ladder: LDA, GGA, mGGA ❖ Self-interaction error, hybrid functionals, and range-separation ❖ Dispersion interactions and non-local correlation functionals		
	8-Feb	Density Functional Theory (DFT) III ❖ Practical Implementation for DFT (atom-centered quadrature, etc.) ❖ Computational cost, performance, and limitations		PS2 due / PS3 out
4	13-Feb	Perturbation Theory for electron Correlation I ❖ Second Quantization for fermions	Fetter and Walecka	

		❖ Wick's Theorem ❖ Rayleigh-Schrodinger, Brillouin-Wigner	Chapter 1,2. Szabo and Ostlund Chapter 6.	
	15-Feb	Perturbation Theory for electron Correlation II ❖ Size-consistency and size-extensivity ❖ MP2 and Hylleraas variational principle ❖ Computational costs and Density Fitting ❖ Improvements on MP2 (SCS, SOS, OO, etc.) ❖ Computational cost, performance, and limitations		PS3 due / PS4 out
5	20-Feb	Non-perturbative Electron Correlation Theory I ❖ Excitation hierarchy ❖ Strong and Weak Correlation ❖ Configuration Interaction (FCI, truncated CI, and selected CI)	Piela Vol. 2 Chapter 2.	
	22-Feb	Non-perturbative Electron Correlation Theory II ❖ Active-space method, multi-reference method, and MCSCF method ❖ Coupled-Cluster (CC) theory (various types of CC expansion) ❖ Relationship between CI and CC ❖ Computational cost and performance		PS4 due / PS5 out
6	27-Feb	Electronic excited states I ❖ Time-dependent variational principle ❖ Linear-response theory, time-dependent HF, and CI singles ❖ Runge-Gross theorem	Chem. Rev. 2005, 105, 4009.	
	29-Feb	Electronic excited states II ❖ Time-dependent DFT ❖ Electron correlation effects in excited states (CIS(D), EOM-CC, etc.) ❖ Computational cost and performance		PS5 due / PS6 out
7	5-Mar	Exploration of Potential Energy Surface I ❖ Potential Energy Surface ❖ Force Calculations for variational and non-variational method ❖ Coupled-perturbed SCF equations and z-vector equation	Piela Vol. 2 Chapter 6.	
	7-Mar	In-class Exam 1		
8	12-Mar	Spring Break		
	14-Mar	Spring Break		
9	19-Mar	Exploration of Potential Energy Surface II	Piela Vol. 2	PS6 due /

		❖ Optimization methods for minima and transition structures ❖ Reaction paths and intrinsic reaction coordinate ❖ String methods for reaction path finding ❖ Variational transition state theory and reaction path Hamiltonian	Chapter 6.	PS7 out
	21-Mar	Electronic Structure of Extended System I ❖ Lattice, Brillouin zone, and band structure ❖ Bloch's theorem ❖ Crystalline orbitals (an extension of LCAO)	Piela Vol. 2 Chapter 1. Angew. Chem., Int. Ed. Engl.,26,1987, 805.	Project Discussion
10	26-Mar	Electronic Structure of Extended System I ❖ Periodic HF theory and periodic MP2 ❖ Intuitive understanding of band structure from MO theory ❖ Computational costs and performance		PS7 due / PS8 out
	28-Mar	Analysis of Electronic Structure Calculation I ❖ Population analysis based on basis functions, ESP, and electron density ❖ Natural atomic orbital and natural bond orbital analyses ❖ Orbital localization	Jensen Ch. 10.	
11	2-Apr	Analysis of Electronic Structure Calculation II ❖ Energy Decomposition Analysis ❖ Correlation Effects (natural orbital occupation analysis) ❖ Excited states (natural transition orbitals)		PS8 due / PS9 out
	4-Apr	Emerging Electronic Structure Methods I ❖ Stochastic electronic structure methods (Quantum Monte Carlo and stochastic Resolution of Identity)		
12	9-Apr	Emerging Electronic Structure Methods II ❖ Tensor network methods (DMRG, PEPS, etc.)		
	11-Apr	Emerging Electronic Structure Methods III ❖ Quantum algorithms for quantum chemistry (Variational Quantum Eigensolver and Quantum Phase Estimation)		
13	16-Apr	In-class Exam 2		PS9 due
	18-Apr	Student Project Presentation I		
14	23-Apr	Student Project Presentation II		
	25-Apr	No Class (Reading Period)		