List of concepts to be familiar with for the Spring Semester 2023 CHE 525/PHY 567 final exam

Potential energy surface

Geometry optimization

Global vs local minima

Transition state

Harmonic vibrational frequencies

Primitive and contracted Gaussians

Single-zeta, double-zeta, triple-zeta, valence double-zeta, etc

Polarization functions (What are they? What are they good for?)

Diffuse functions (What are they? What are they good for?)

Pople and Dunning basis sets and abbreviations (What do they mean?)

Representation of molecular orbitals as linear combinations of atomic orbitals

The variational theorem (What is it? When does it apply?)

Antisymmetry

Hartree product (What is it? Why is it no good?)

Slater determinant (What is it? Why is it better than a Hartree product?)

Hartree-Fock theory (What is it? When does it work? When does it fail?)

Exchange interaction

The dissociation catastrophe

Restricted vs. unrestricted Hartree-Fock theory

Electron correlation

Static vs. dynamic correlation

Coulomb hole correlation (What kind of correlation is it? Which methods describe it and which can't?)

London dispersion forces (What kind of correlation is it? Which methods describe it and which can't?)

Configuration interaction

Full configuration interaction

Truncated configuration interaction (What is it? What are its strengths and weaknesses?)

Size extensivity/consistency (What is it? What methods are or aren't size extensive/consistent?)

Coupled cluster theory (What is it? What are its strengths and weaknesses?)

Moller-Plesset perturbation theory (What is it? What are its strengths and weaknesses?)

Multireference methods (What are they? What are their strengths and weaknesses?)

Complete active space self-consistent field method

Density functional theory (What is it? What about DFT is exact and what isn't? What are its strengths and weaknesses in practice?)

First and second Hohenberg-Kohn Theorems (What are they?)

Kohn Sham approach to DFT (What is the basic idea?)

Jacobs Ladder of DFT (What differentiates the different functional "rungs?")

Know the following abbreviations:

CISD

CCSD

MP2

DFT

CASSCF