

Questions Regarding Computational Quantum Chemistry

Read handout: "Computational Quantum Chemistry", Ch 11, pp. 410-433;
in *Physical Chemistry, a Molecular Approach*, by D. McQuarrie and J.D. Simon

1. Know the definitions and usage of the following:
 - a. Molecular orbital approximation
 - b. Hartree product wavefunction
 - c. Slater determinant (Hartree-Fock) wavefunction
 - d. Hartree-Fock equations
 - e. Self-consistent m.o. theory
 - f. L.C.A.O. theory; Roothaan-Hartree-Fock equations
 - g. *Ab initio* vs semiempirical calculations
 - h. Correlation energy
2. What are Slater-type orbitals (STO's) and Gaussian-type orbitals (GTO's)? What are the advantages and disadvantages of each as an LCAO basis set?
3. What compromise is used in the STO-NG basis sets?
4. Which basis set, STO-3G, STO-5G, or STO-6-31G** would provide a better description of a molecular wavefunction? Why? (note Table 11.6)
5. What techniques are used to go beyond the Hartree-Fock limit in order to calculate correlation energies?
6. Describe (note) the success of the GAUSSIAN method in the *ab initio* calculation of molecular geometries (Table 11.10, 11.11, and 11.12)