

Introduction to Computational Quantum Chemistry: Theory

Tutorial Problems 2

Wednesday 31st May 2006

- (1) Why are Gaussian functions used in quantum chemistry software packages? How do GTOs differ from STOs?
- (2) Place the following basis sets in order of increasing size: 6-31G(*d,p*), 6-311+G(3*df*,2*p*), STO-3G, 6-31+G(2*d,p*), 3-21G
- (3) What are polarized basis sets, and what advantages do they have over minimal basis sets? Use a sketch to show the effects of *d* polarization functions on a *p* orbital. What sort of bonding would benefit from this sort of polarization?
- (4) Describe as fully as possible the basis set 6-311++G(*d*). What advantage does this basis set have over 6-311G*?
- (5) Consider the 6-31G basis set. How many primitives are used to describe the core and valence orbitals respectively? Why are so many primitives required to model the core?
- (6) What are the advantages of using an effective core potential (ECP)?
- (7) What is the difference between local and gradient corrected density functionals? Give examples of each and explain why the local approximation works better than you might expect,
- (8) What are the differences and similarities between Hartree-Fock theory and DFT?
- (9) What are the key advantages and disadvantages of DFT over a wavefunction based correlated method such as CCSD?
- (10) The Hohenberg-Kohn theorems tell us that we should be able to obtain the energy from the density only. Why then does the hybrid functional B3LYP perform better than the GGA functional BLYP.
- (11) Explain why LDA overbinds.

