量子化学作业　第十二章　（2016）

12-4. Show that the Hartree-Fock energy is not equal to the sum of the Hartree-Fock orbital energies.

12-22. What is the difference between a double-zeta (DZ) basis set and a double split-valence basis set?

12-23. What is meant by a triple-zeta basis set?

12–24. How many basis functions are used in a 6–31G basis set calculation of an ethane molecule? How many for a propane molecule?

12-26. How many primitive Gaussian functions and how many contracted Gaussian functions are used in a 6-31G basis set calculation of an ethane molecule? How many for a propane molecule?

12–42. Show that the number of singly excited determinants that occur in a configuration interaction calculation is given by $2N(2K - 2N)$ for a molecule with $2N$ electrons and $2K$ spin orbitals. Show that the number of n–tuple excitations is given by

$$\binom{2N}{n}\binom{2K-2N}{n}$$