Uva Wellassa University, Sri Lanka

End Semester Examination – Dec/Jan 2010

CHE 431-1 Multi Scale Modeling Methods in Material Science

Time: one hour

Answer **two (02)** questions **only. All questions carry equal marks**
Total number of questions: Four (04)
All symbols carry standard meanings

Question 1:

In most molecular mechanics software packages, the bond lengths and other geometrical parameters of a molecule are determined by knowledge of the cartesian coordinates of each atom. For example, the bond distance r_{AB} between two atoms A and B can be calculated from the equation

$$(x_A - x_B)^2 + [(y_A - y_B]^2 + (z_A - z_B)^2)^{\frac{1}{2}})$$

where (x_A, y_A, z_A) are the cartesian coordinates of atom A and (x_B, y_B, z_B) are the cartesian coordinates of atom B. Consider a water molecule with atoms having the following cartesian coordinates (in Å):

Atom	x	y	z
O	0	0	0
H1	0.00	-0.65	0.60
H2	0.00	0.65	0.60

(a) For this molecule, calculate the bond distances between pairs of atoms O-H1 and O-H2.

(b) The water molecule is assumed to obey a simple harmonic stretching and bending force field with the following parameters:

k_{OH}	= 700 kcal mol^{-1} Å^{-1}
$r_{OH,equi}$	= 0.93 Å
k_{HOH}	= 100 kcal mol^{-1} radian^{-2}
$\theta_{HOH,equil}$	= 104.5°

What is the stretching energy of water at this geometry? (Include both bonds in the calculation).

(c) What is the bending energy for water at this geometry?
(d) What is the total energy for water at this geometry?

Question 2

In most force fields, the interaction between two non-bonded atoms is described using a function called the Lennard-Jones 6-12 potential. It has the form

$$E_{nb} = -\frac{A}{r^6} - \frac{B}{r^{12}}$$

where A and B are constants which depend on the two interacting atoms and r is the distance between them. For example, for two carbon atoms interacting, $A = 745$ and $B = 2524840$ (these parameters yield energy in kcal/mol if the distance is expressed in angstroms).

a. Sketch the non-bonded energy as a function of distance for the case of two carbon atoms.

b. At approximately what distance does the minimum energy occur for this particular non-bonded interaction?

c. Which of the two terms in the expression for the non-bonded energy is responsible for the attractive part of the interaction? Which term is responsible for the repulsive part of the interaction?

Question 3

(a) State without a derivation Hartree-Fock (HF) equation for a given many body system.

(b) State exchange and coulombic operators.

(c) Introducing a basis set transform the HF equation into Roothann equation (Show all work).

(d) Explain briefly following terms:

(i) CIS (ii) CISD (iii) Full CI (iv) CASCF

Question 4

(a) State briefly the basic idea behind the density functional theory (DFT). How it differs from a wave function?

(b) State two advantages of DFT method over HF.

(c) State the Hohenberg – Kohn theorems (no derivations needed)

(d) Write short notes on following

(i) Kohn Sham electrons (ii) ZDO
(ii) NDDO (iv) MINDO