UNIVERSITY OF GHANA

FACULTY OF ENGINEERING SCIENCES

BSc. (ENG) MATERIALS SCIENCE AND ENGINEERING

END OF SECOND SEMESTER EXAMINATIONS: 2013/2014

MTEN 304: COMPUTATIONAL MATERIALS (2 CREDITS)

TIME ALLOWED: 2 HOURS

Answer ALL Questions

Question 1

a) In the use of a DFT method for materials simulation, it is important to understand the approximations you are using in order to meaningfully interpret the results. From your laboratory experience on the use of DFT, list the approximations and briefly explain them.

b) State clearly the difference between Hartree-Fock (HF) and Density Functional Theory (DFT).

c) What is the difference between a plane wave basis and a gaussian basis?

d) Explain what you understand by the following:

 (i) Geometry optimisation (ii) Iteration process and (iii) Convergence.

18 Marks

Question 2

a) Give at least 2 real examples for each of these types of errors common to computer simulation;
   (i) systematic and
   (ii) statistical errors.

b) How is diffusion Monte Carlo different from Hartree-Fock, variational Monte Carlo, and post-Hartree Fock methods?

c) What does adding correlation do? What is the leading order effect in the wavefunction?

d) State the major difference between an 'ab initio' method and semi-empirical approach.

e) Differentiate between molecular mechanics and molecular dynamics.

10 Marks

Question 3

a) Write the time independent Schrödinger equation and clearly define all the terms in the equation. What is the use of this equation in computer simulation?

b) To solve the Schrödinger equation for many-body electrons, approximations are necessary. List all the approximations and explain them briefly.

c) List three (3) simulation codes you know and explain any one.

d) Explain what a Lennard-Jones potential is used for. Sketch this type of potential using two atomic species.

12 Marks

Question 4

a) Briefly describe what you understand by the term basis sets.

b) Give the major difference between Slater type orbital and Gaussian orbital. Use graphical representation to explain your answer(s).

c) You have been tasked with a materials problem that requires computer simulation in which you are provided with two different basis sets; STO-3G and 6-31++G.

    (i)   Give an explanation to the basis sets designation.

    (ii)   Which one of the two will you use in a simulation experiment if one requires accurate results with respect to the simulation?

    (iii)   Will your choice of basis set also affect the computational time? Explain your answer.

    d.   Give at least 2 examples of simulations where you should employ periodic boundary layer (PBC) and 2 examples where you should not (or at least need not).

20 Marks