UNIVERSITY OF GHANA

FACULTY OF ENGINEERING SCIENCES

BSc. (ENG) MATERIALS SCIENCE AND ENGINEERING

END OF SECOND SEMESTER EXAMINATIONS: 2012/2013

MTEN 304: COMPUTATIONAL MATERIALS (2 CREDITS)

TIME ALLOWED: 2 HOURS

Answer ALL Questions

Question 1

a) How would you simulate the following systems/properties? List which code(s), approach(es), and any details you can think of;
   (i) Mechanical energy transfer rate between two carbon nanotubes
   (ii) Band gap as a function of diameter, crystal growth direction, and surface termination of Si nanowires.
   (iii) Phase transition in liquid Argon.
   (iv) Strength of nanoscale materials with defects.

b) Mention three (3) challenges of computer simulation.

c) Explain what you understand by the following:
   (i) Geometry optimisation (ii) Iteration process and (iii) Convergence.

12 Marks

Question 2

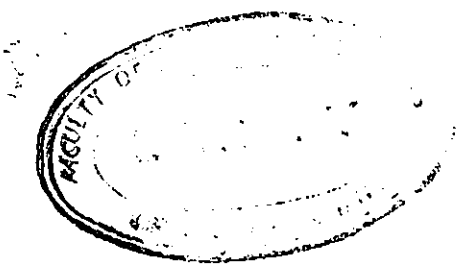
a) Give five (5) physical properties that can be calculated from doing a computer simulation.
b) How is diffusion Monte Carlo different from Hartree-Fock, variational Monte Carlo, and post-Hartree Fock methods?
c) What does adding correlation do? What is the leading order effect in the wavefunction?
d) State the major difference between an 'ab initio' method and semi-empirical approach.
e) Differentiate between molecular mechanics and molecular dynamics.

18 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) Describe briefly two (2) 'ab initio' methods you know of.
d) Explain what a Lennard-Jones potential is used for. Sketch this type of potential using two atomic species.

20 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) Compare the computational expense with respect to the number of basis function for the following methods;

(i) Hartree-Fock (ii) DFT (iii) MP2 (iv) MP3.

20 Marks