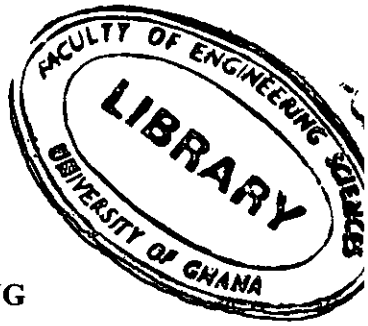

UNIVERSITY OF GHANA

BSC. MATERIALS SCIENCE & ENGINEERING
SECOND SEMESTER EXAMINATIONS: 2015/2016
SCHOOL OF ENGINEERING SCIENCES
DEPARTMENT OF MATERIALS SCIENCE & ENGINEERING
MTEN 304: COMPUTATIONAL MATERIALS SCIENCE (2 CREDITS)

INSTRUCTIONS: ANSWER ALL QUESTIONS

TIME ALLOWED: TWO (2) HOURS

1.

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

b. Give the major difference between a *plane wave basis* and *gaussian basis* sets.

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. Mention two (2) criteria for selecting basis functions.

e. As a computational materials engineer, you have been involved in a project that requires the use of computational modelling. How would you approach this project?

30 Marks

2.

a. As you may have learned, not everything can be optimized for all properties. Mention for the simulations below what potential term(s) are most important to get 'right';

   i. Liquid water
   ii. Protein
   iii. Hard Spheres

b. Three (3) types of Density Functional Theory (DFT) calculations exist. Name them and comment on their appropriateness in using each for computational simulation.

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.

30 Marks

3.

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

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

c. Explain what you understand by the following;

   i. Geometry optimization
   ii. Iteration process
   iii. Convergence.

d. Explain what you understand by 'periodic boundary conditions' (PBC).

e. Briefly describe what a Lennard-Jones potential is used for. Sketch this type of potential using two atomic species.

30 Marks