UNIVERSITY OF GHANA

SCHOOL OF ENGINEERING SCIENCES

BSc. (Eng) MATERIALS SCIENCE AND ENGINEERING

SECOND SEMESTER EXAMINATIONS 2014/2015

MTEN 304 – COMPUTATIONAL MATERIALS SCIENCE (2 Credits)

TIME- 2 Hours

ANSWER ALL QUESTIONS

1.

a. Differentiate between modelling and simulation. **[2 marks]**

b. Explain the role of applications, algorithm and architecture in Computational materials science. **[6 marks]**

c. Write the general expression for basis functions, defining all the terms present. **[1 mark]**

d. Identify the following basis sets:
   i. STO-4G
   ii. STO-3G*
   iii. 6-31+G(d)
   iv. 3-21G

[4 marks]

e. Briefly describe the following as related to computational modelling :
   v. Ab initio model **[3 marks]**
   vi. Semi-empirical **[3 marks]**
   vii. Molecular Mechanics **[3 marks]**
   viii. Quantum Monte Carlo **[3 marks]**

2.

a. Mention three types of DFT calculations and explain them based on accuracy, time and results. **[6 marks]**

b. With the aid of a flow-diagram, explain the process of geometry optimization in computational modelling. **[7 marks]**

c. Give three (3) examples each of systematic and statistical errors common to computer simulations. **[6 marks]**

d. Explain the following approximations used in computational simulations:
   i. Born-Oppenheimer **[2 marks]**
   ii. Hartree-Fock **[2 marks]**
   iii. LCAO **[2 marks]**

Examiners: Dr. David Dodoo-Arhin/ Dr. Abu Yaya

3.

a. Explain periodic boundary conditions (PBC) as related to computational modelling. **[2 marks]**

b. Give two (2) examples each of simulations where you should use PBC and where you should not. **[4 marks]**

c. Write the general expression for potential energy ($V(r)$) as used in molecular dynamics. **[4 marks]**

d. Mention two assumptions made in molecular mechanics simulations. **[5 marks]**

e. Comment on the accuracy of the given methods and basis sets indicated in the table below given that the experimental values for Total energy (kcal/mol) and bond length (Å) are, 15.1 and 0.035 respectively. **[10 marks]**

METHOD/MODEL/BASIS SET	TOTAL ENERGY (kcal/mol)	BOND LENGTH (Å)
MOL. MECH/MM2/STO-4G	0.5	0.01
SEMI EMPIRICAL/AM1/ 6-31+G(d)	18.8	0.048
AB INITIO/HF/STO-3G	93.3	0.055

4.

a. Sketch a graph of Energy potential against distance for the 12-6 Lennard-Jones potential and explain the concept. **[12 marks]**

b. Mention three (3) limitations of the L-J potential. **[3 marks]**

c. Differentiate between Hartree-Fock and Density Functional Theory. **[5 marks]**

d. What is the difference between a plane wave basis and a Gaussian basis sets. **[5 marks]**