UNIVERSITY OF GHANA

BSc. MATERIALS SCIENCE & ENGINEERING

SECOND SEMESTER EXAMINATIONS: 2016/2017

SCHOOL OF ENGINEERING SCIENCES

DEPARTMENT OF MATERIALS SCIENCE & ENGINEERING

MTEN 304: COMPUTATIONAL MATERIALS SCIENCE (2 CREDITS)

INSTRUCTIONS:

ANSWER QUESTION 1 (SECTION A) IN THE ANSWER BOOKLETS PROVIDED AND (SECTION B) USING THE DESKTOP COMPUTER PROVIDED. SAVE YOUR WORK USING YOUR INDEX NUMBERS ON TO YOUR DESKTOP COMPUTERS

TIME ALLOWED: TWO (2) HOURS

SECTION A

ANSWER ALL QUESTIONS FROM SECTION A

1.

a. Briefly describe what you understand by the term *basis sets*. **[2 Marks]**

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

[2 Marks]

c. 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

[6 Marks]

d. Explain what you understand by the following;

   i. Geometry optimization

   ii. Iteration process

iii. Convergence.

[6 Marks]

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

[4 Marks]

SECTION B

ANSWER ALL QUESTIONS FROM SECTION B ON YOUR DESKTOP COMPUTER PROVIDED

1.

a. Compute the Lennard-Jones energy curve for a system of two Argon (Ar) atoms using the CP2K code with an input file labelled on your desktop computer as *energy.inp*. Use a distance intervals of 1 Å to 8 Å for your coordinates files. From your Lennard-Jones curve, determine the;

i. minimum equilibrium energy for the two argon (Ar) atoms,

ii. equilibrium bond length.

iii. What type of calculation are you performing? **[40 Marks]**

b. If you were to do geometry optimization, what will you be doing as compared to computation of the Lennard-Jones curve above? **[5 Marks]**

c. Give the advantages of using empirical potential methods as compared to ab-initio methods using your own understanding of Lennard-Jones potential in your calculation. **[5 Marks]**