Uva Wellassa University of Sri Lanka
Faculty of Applied Sciences
Department of Science and Technology
400 level 1st Semester Examination – July/Aug 2019
SCT 454-2 Multiscale Modelling Techniques

Uva Wellassa University

Instructions to candidates
Duration: 02 hours
Number of questions: Part I: 10 Structured questions , Part II: 4 Essay questions
Mark allocation: 100 marks
Use standard notations without a definition.
Part I: Answer all questions in the spaces given.
Part II: Answer in the sheets provided.

Index No:

PART – I

1. Write an expression in Dirac notation to calculate expectation (average) value of observable, $\hat{O}$.

(02 marks)

2. State the Hamiltonian of a H_2 molecule using classical and quantum mechanics.

(02 marks)

3. Write a generalized expression to denote electronic Hamiltonian of a generic molecule.

(02 marks)

4. State two differences between Hatree and Hartree Fock methods.

(02 marks)

5. What is meant by self-consistent field optimization?

(02 marks)

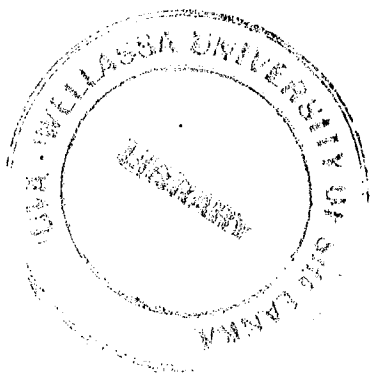
6. State an expression for variation principle according to Hartee -Fock and density functional theory methods.

(02 marks)

7. Prove that the Verlet algorithms of MD calculations are fourth order accurate.

(02 marks)

8. Write a Slater Determinant for He.



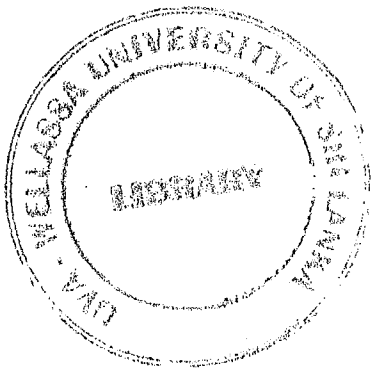
(02 marks)

9. Name scientists who won the Nobel Prize for the density functional theory.

(02 marks)

10. How binding energy of a molecular system is calculated in ab intio molecular dynamics codes.

(02 marks)



PART - II

1. Nobel Prize in Chemistry in 2013 is awarded for computational development of multi-scale modeling methods. Answer following questions.
   i. Name the Nobel Laurates.
   ii. How they perform computational experiment to resolve complex calculations.
   iii. How the potential energy surface is defined?
   iv. Discuss the methods that Laurates used to resolve complexity of the computational problem.

   (20 marks)

2.
   i. Define the term electron density in standard notation. Why density functional calculations are faster than other ab inito methods.
   ii. State Hohenberg-Kohn theorems of electron density.
   iii. State the functional of total energy of a system. Describe how each term is used (no mathematical formulations are required).
   iv. Comment on the LDA and GGA approximations used in DFT computation.

   (20 marks)

3.
   i. According to classical mechanics atoms do not exist. Prove it using H atom classical Hamiltonian.
   ii. Quantum mechanics suggests the atomic model. Explain it using H atom. State the application of Heisenberg Principle of Uncertainty.
   iii. State the wave function of a crystal using Einstein convention.
   iv. Discuss scaling of the computation theory in the calculations of nano composites, pharmaceuticals, and molecules

   (20 marks)

4.

i. Define following terms as needed for multi scale modeling of solids
    a. Reciprocal lattice
    b. Band structure
    c. Brillouin zone
ii. State the principle of ab intio molecular dynamics method with the help of a flow diagram.
iii. Draw energy level diagrams for Si solid demarcating energy gap zones. Identify the positions correspond to C, Sn and Pb in the diagram.
iv. The band structure and density of state computations of Si crystal are shown below. Answer following questions.
    a. Label the diagrams that correspond to density of state and band structures
    b. Show first Brillouin zone.
    c. Mark Fermi level only in the diagram.
    d. Deduce the band gap energy of Si
    e. Comment on the properties of Si solid.

(20 marks)