MACHAKOS UNIVERSITY

University Examinations 2023/2024

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

FOURTH YEAR FIRST SEMESTER EXAMINATION FOR BACHELOR OF SCIENCE IN ANALYTICAL CHEMISTRY

SAN 412: ADVANCES IN COMPUTATIONAL CHEMISTRY

DATE: **TIME:**

INSTRUCTIONS:

- The paper consists of **two** sections.
- Section **A** is **compulsory** (30 marks).
- Answer any **two** questions from section **B** (each 20 marks).

SECTION A

QUESTION ONE (30 MARKS)

a) Discuss the following techniques as applied in material computing

i. Semi-empirical techniques **(2 marks)**

iii. Molecular mechanics **(2 marks)**

iv. Molecular dynamics **(2 marks)**

v. Docking **(2 marks)**

b) List two basis functions used most often with Hartree-Fock theory **(2 marks)**

c) Discuss if computational chemistry can replace wet chemistry. **(3 marks)**

d) List two areas of study where molecular dynamics is used **(2 marks)**

e) Define Ab Initio method and write the equation that govern it. **(4 marks)**

f) What makes Density Functional Theory (DFT) very popular **(2 marks)**

g) How has DFT theory been improved over time to overcome its shortcomings **(3 marks)**

h) Define what a force field is and what is meant by parameterizing the force field. **(4 marks)**

i) Which is the scientific problem in adapting the configuration interaction method into a practical one. **(2 marks)**

SECTION B

QUESTION TWO (20 MARKS)

a) State and explain Born-Oppenheimer approximation. **(3 marks)**

b) Explain the consequences of Born-Oppenheimer approximation **(3 marks)**

c) Provide the basis set that you would you use to compute an organic molecule with triple bonds. Explain you answer. **(4 marks)**

d) Compare semi-empirical, Ab initio, DFT and methods by referring to their basic principles. **(5 marks)**

e) Discuss the advantages of DFT over Quantum Monte Carlo methods. **(5 marks)**

QUESTION THREE (20 MARKS)

a) Explain how Quantum Monte Carlo (QMC) addresses making the Hartree-Fock shortcomings. **(3 marks)**

b) Explain what a STO-6G minimal basis set is. **(3 marks)**

c) Explain two approaches used to mitigate limitations of the Hartree-Fock method by going beyond the ansatz of a single-determinant wavefunction. **(2 marks)**

d) State what Thomas and Fermi first explored in improving Density Functional Theory and explain their study focus **(4 marks)**

e) Determine the number of basis functions created when CH_4 is computed using 3-21G basis set. Show your working and explain your answer. **(3 marks)**

f) Explain electron correlation term as applied in Hartree-Fock theory. Write the general equation and correlation energy by adding more slater determinants to the expansion of ψ. **(5 marks)**

QUESTION FOUR (20 MARKS)

a) The energy of a molecule can be determined from the electron density instead of a wave function. Describe the premise behind this level of theory **(2 marks)**

b) "An exact many-body wavefunction, may be written as a linear combination of Slater determinants". Determine the use of Slater determinants in solving the many-body Hamiltonian **(2 marks)**

c) Explain two areas of study where molecular dynamics is applied **(5 marks)**

d) Distinguish between HOMO and LUMO as applied in organic molecules **(4 marks)**

e) Discuss three outputs one can compute using spartan software **(3 marks)**

f) Discuss the following approaches applied in computational chemistry study.

(4 marks)

i. Simulation approach

ii. Complementary approach

QUESTION FIVE (20 MARKS)

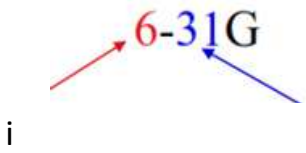
a) Molecular mechanics method has the capabilities of computing large molecules in a short time. Determine how the materials geometry is optimised and treated. **(5 marks)**

b) Atomic simulation reveals at the level of electrons and atoms. Explain six material properties one can work on given an atom. **(6 marks)**

c) Discuss the properties that Semi–empirical method calculations can compute **(3 marks)**

d) Prof. John Pople won the Nobel Prize in Chemistry for his work in quantum chemistry (1998). From his Notation below:

i. Define the terms i and ii **(2 marks)**



e) Write the addational function of angumetative angular momentum type greater than 1 occupied in:

i. Bonding atoms (For N) **(2 marks)**

ii. 2nd and 3rd row of atoms in the periodic table **(2 marks)**