MACHAKOS UNIVERSITY

University Examinations for 2021/2022 Academic Year

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

THIRD YEAR FIRST SEMESTER EXAMINATION FOR

BACHELOR OF SCIENCE IN ANALYTICAL CHEMISTRY

SAN 304: COMPUTATIONAL CHEMISTRY AND MOLECULAR MODELLING

DATE: 31/8/2022 **TIME: 8.30-10.30 AM**

INSTRUCTIONS:

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

QUESTION ONE (COMPULSORY) (30 MARKS)

a) Distinguish between Quantum mechanics and Molecular mechanics (4 marks)

b) Density functional theory (DFT) has become very popular in recent years. Explain

i. What makes Density Functional Theory (DFT) very popular (2 marks)

ii. The DFT shortcoming (2 marks)

iii. How has DFT theory been improved over time to overcome the above shortcomings (2 marks)

c) Discuss the properties theoretical a chemist can attempt to calculate ggiven a set of nuclei and electrons. (5 marks)

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

e) Distinguish between conduction band and valence band (2 marks)

f) Explain how Quantum Monte Carlo (QMC) avoid making the Hartree-Fock mistakes. (3 marks)

g) Define a functional as used in Density Functional Theory (2 marks)

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

i) Determine the method of solving the many-body Hamiltonian that is based on this observation "an exact many-body wavefunction, may be written as a linear combination of Slater determinants".. (2 marks)

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

   i. Simulation approach

   ii. Complementary approach (2 marks)

QUESTION TWO (20 MARKS)

a) The Schrödinger equation, which is given by $H\Psi = E\Psi$, is the foundation of mechanical approach. Define all the units in the equation. (2 marks)

b) Discuss the theory that uses best approximation to the true wave function, where each electron occupies an orbital. (2 marks)

c) Determine the approach that is perceived as a series of atoms joined by bonds like a spring when materials are being geometry optimised. (2 marks)

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

e) Discuss the design constrains of molecular dynamics (4 marks)

f) The perturbation theory and the theory based on the variational principle by assuming a single-determinant form the wavefunction are applied in which main theory and what do they neglect (2 marks)

g) List from the Born-Oppenheimer approximations the three terms in Hamiltonian operator (3 marks)

h) The most common force fields (FFs) are OPLS, MM3, MM2, AMBER, CHARMM and GROMOS MOMEC, SHAPES and VALBOND. Classify the above common force field applied in each of the following: liquids, Proteins and inorganic elements. (3 marks)

QUESTION THREE (20 MARKS)

a) Discuss the deficiencies/limitations of DFT and how they can be corrected. (4 marks)

b) i. Explain what reflex powder diffraction module in Materials studio calculates. (2 marks)

ii. Define a Fermi Level and discuss its significance in materials study. (6 marks)

c) There are two key theorems in defining a model:

1. External potential v(r) and electron density n(r) one-to-one correspondence - result, a "reductio ad absurdum," i.e., reduction to absurdity

2. F_{HK} $[n]$ the functional that delivers the ground state energy of the system deliver the lowest energy if and only if the input density is the true ground state density no. The determination of density and ground-state energy would be easy if the electron density and universal functional (F_{HK} $[n]$) of n(r) in external potential were known. However, the determination of $F_{HK}[n]$ are associated with the complexities of the many-electron problem.

Based on the two theorems:

i. Discuss what the 1st theorem proofs (2 marks)

ii. Determine where the two key theorems belong. (2 marks)

d) Discuss the theoretical (Fig.1) verses experimental results (Fig.2) below. (4 marks)

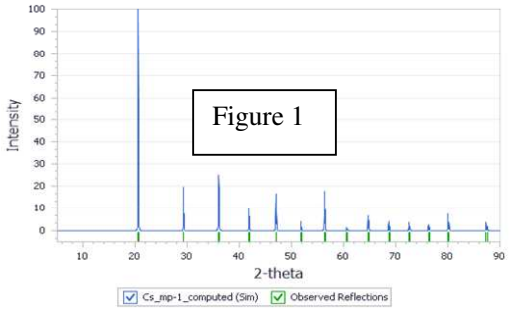


Figure 1

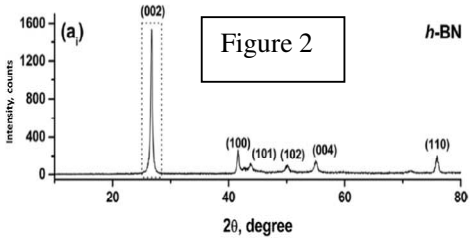


Figure 2

QUESTION FOUR (20 MARKS)

a) Determine the software that predicts optimized docked conformer using total energy of the system property**.** (2 marks)

b) Explain the significance of a band gap in a given material. (2 marks)

c) Explain how the band gap is calculated. (3 marks)

d) Define DOS, PDOS and Band structure electronic structure calculations and state their significance in materials analysis (6 marks)

e) Explain what Thomas and Fermi first explored in improving Density Functional Theory and discuss their study focus (3 marks)

f) The coupled-cluster method is one of the most important practical advances over the Configuration interaction method. Discuss where it is applied and the problems it solves (4 marks)

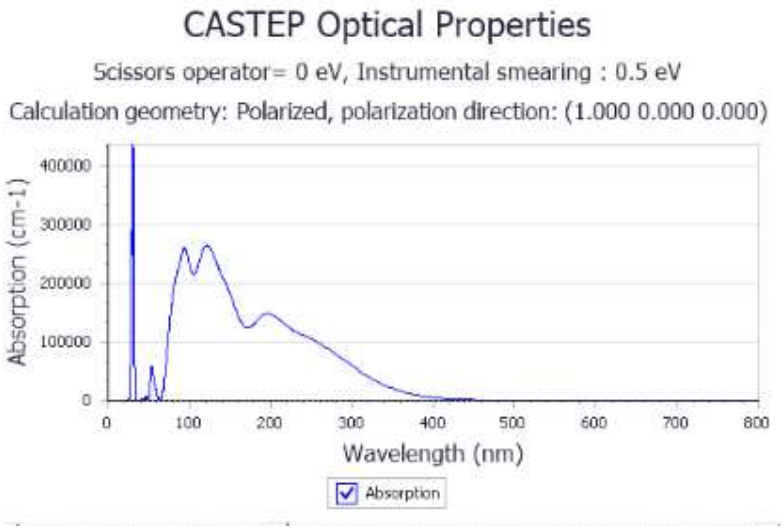
QUESTION FIVE (20 MARKS)

a) Discuss the approximations used in Quantum Monte Carlo to obtain accurate data during analysis. (2 marks)

b) Explain the Hartree-Fock Theory. (2 marks)

c) Explain the scientific problem in adapting the configuration interaction (CI) method. (2 marks)

d) Discuss the optical analysis results below for TiO_2 (2 marks)



e) Discuss Kohn and Sham derived set of differential equations that enables the ground state density to be computed. (6 marks)

f) Name the four comprehensively utilized docking tools employed in search algorithms. (4 marks)

g) Explain how Born-Oppenheimer approximates solution to the Schrödinger equation (2 marks)