MACHAKOS UNIVERSITY

University Examinations 2021/2022

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

FOURTH YEAR SECOND SEMESTER EXAMINATION FOR BACHELOR OF SCIENCE (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 (COMPULSORY)(30 MARKS)

a) Determine the method that calculates the probability density for the electrons and interpret as the square of the wave function Ψ. (2 marks)

b) Discuss why in molecular mechanics methods electrons are not treated explicitly. (4 marks)

c) Write an equation representing the Hamiltonian operator H and define the Laplacian operator. (4 marks)

d) Does Hartree–Fock theory use the simple approximation to the true many–body wave Function? How does it solve the many–body Hamiltonian. (5 marks)

e) Define the two types of Quantum Monte Carlo approaches. (2 marks)

f) List five commonly used semi–empirical methods. (5 marks)

g) What do the following applications do in play molecule docking software:

i. Deepsite

ii. Kdeep (4 marks)

h) Distinguish what the non–local functionals and the local density functionals (LDA) rely on to improve DFT (4 Marks)

SECTION B

QUESTION TWO (20 MARKS)

a) Explain the following Exchange–Correlation Functionals

i. Local Density Approximation (LDA) (2 marks)

ii. Generalised Gradient Approximation (GGA) (2 marks)

iii. The Meta–GGAs (2 marks)

iv. The Hybrid Functionals (2 marks)

b) The goal of atomic simulation is to understand the level of electrons and atoms.

i. What materials properties can one work on. (3 marks)

ii. List three classifications of materials one can find from materials studio structures. (3 marks)

c) Explain what the following tests reveals, when using spartan software

i. HOMO (2 marks)

ii. LUMO (2 marks)

iii. Electrostatic potential (2 marks)

QUESTION THREE (20 MARKS)

a) Define the approximations to the Schrödinger equation. (2 marks)

b) Modelling and analysis involve builders and analysis. What does each of the following reveal in analysis:

i. Geometry and dynamics trajectories. (2 marks)

ii. Band structures and DOS (2 marks)

iii. Electron and spin density (2 marks)

iv. Potential and Fermi surface (2 marks)

v. Phonons and transition states (2 marks)

c) Provide the major challenge faced by analysts when using density functional theory approach. (4 marks)

QUESTION FOUR (20 MARKS)

a) Task servers compute properties of a material. State what each of the listed servers compute:

i. VASP (2 marks)

ii. MOPAC (2 marks)

iii. GiBBS (2 marks)

iv. LAMMPS (2 marks)

b) Using Perdew proposed variation of functionals ("Jacob's ladder") explain the following categories:

i. Dependence on Virtual Orbitals Functional (2 marks)

ii. Meta-GGAs (2 marks)

iii. Local Density Approximation Functional (2 marks)

iv. From Jacobs ladder above, which is most expensive and why? (2 marks)

c) To predict the binding affinity of a set of ligands docked in a protein using a state-of-the-art neural network-based predictor we use which application in play molecule (4 marks)

QUESTION FIVE (20 MARKS)

a) Discuss the properties semi–empirical calculations can compute. (2 marks)

b) Explain what semi–empirical calculations neglect. (2 marks)

c) The electrons kinetic energy is computed from the equation

$$T[n] = C_F \int n^{5/3}(r)dr,$$

i. define C_F in the above equation (2 marks)

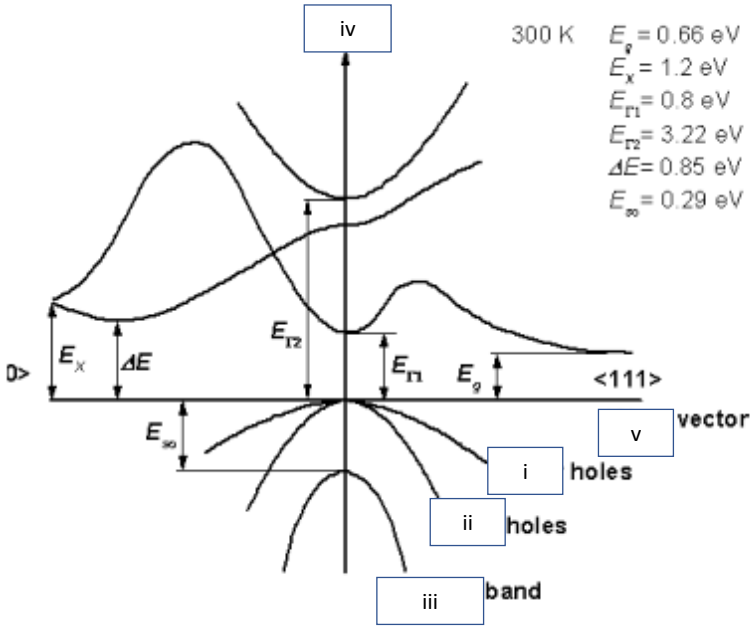
ii. In which model does it belong? (2 marks)

d) Kohn and Sham further developed the DFT theory in the mid–1960s to improve on a theory that had failed in its explanation of the kinetic energy

i. Provide the theory that had failed. (2 marks)

ii. Discuss how the problem was solved (3 marks)

e) The figure below represents the band structure for TiO_2. Identify what the roman numbers i-iii represent and the x and y axis (iv and v). (5 marks)


iv
300 K
E_g = 0.66 eV
E_χ = 1.2 eV
$E_{\Gamma 1}$ = 0.8 eV
$E_{\Gamma 2}$ = 3.22 eV
ΔE = 0.85 eV
E_∞ = 0.29 eV
$E_{\Gamma 2}$
E_χ
ΔE
$E_{\Gamma 1}$
E_g
<111>
vector
E_∞
v
i
holes
ii
holes
iii
band

END