Name: **Enrolment No:**	

UPES

End Semester Examination, May 2025

Course: Computational Tools: Atomistic Simulation Techniques

Semester: VI **Time : 03 hrs.**

Course Code: PHYS 3028P **Max. Marks: 100**

Instructions: All questions are compulsory.

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q1	Write Hohenberg-Kohn Theorems.	**4**	**CO1**
Q2	Distinguish between Verlet and Velocity Verlet algorithms in MD. What are their uses?	**4**	**CO2**
Q3	Explain Molecular Mechanics and its uses.	**4**	**CO2**
Q4	What is a variable? What are the rules for naming a variable?	**4**	**CO3**
Q5	Write python code to read and write in a file. Also close the file.	**4**	**CO3**

SECTION B
(4Qx10M= 40 Marks)

Q6	Explain how to create a dictionary in python? Write a few methods that are used in Python Lists. How are lists updated in Python?	**10**	**CO3**
Q7	Explain the Hartree and Hartree-Fock methods, highlighting their key assumptions, differences, and significance in quantum chemistry.	**10**	**CO1**
Q8	Write and prove Variational principle. OR For a particle in a box in its ground state, calculate the expectation value of the a. *position,* b. the *linear momentum,* c. the *kinetic energy,* and d. the *total energy*	**10** **10**	**CO1**
Q9	Explain different types of interatomic forces, their variation with distances. Give examples.	**10**	**CO2**

SECTION-C
(2Qx20M=40 Marks)

Q10	Create a class BankAccount with attributes: account number, holder name, and balance. Include methods for deposit and withdrawal. Demonstrate its use with example data.	**20**	**CO3**
Q11	(a) What do you understand by Molecular dynamics. Assuming initial positions and velocities, explain a MD Cycle. (b) Define ensemble. With the help of diagrams and examples explain different types of ensembles. OR (a) What do you understand by potential in MD and MM? Explain the stiffness of a bond and bond angle and then mention in detail different bonded and non-bonded interactions. (b) Differentiate in detail between MD and DFT. Give three example cases to explain when to use MD, MM or DFT.	**10** **10** **10** **10**	**CO2**