Name: **Enrolment No:**	

UPES

End Semester Examination, May 2024

Course: Computational Tools: Atomistic Simulation Techniques

Semester: VIII

Program: BSc (H) Physics **Time :** 03 hrs.

Course Code: PHYS4032P **Max. Marks:** 100

Instructions: All questions are compulsory

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	State variational method.	**4**	**CO1**
Q 2	Write a function that accepts two numbers and returns their sum.	**4**	**CO3**
Q 3	Draw a flow chart to plot PDOS (projected density of states)	**4**	**CO2**
Q 4	Show that the operator -ihd/dx is a linear operator.	**4**	**CO1**
Q 5	What are the different types of operators in Python?	**4**	**CO3**
	SECTION B **(4Qx10M= 40 Marks)**		
Q 6	Write a Python program using a loop to print first N numbers divisible by five.	**10**	**CO3**
Q 7	Write Kohn-Sham equations of DFT implementation.	**10**	**CO2**
Q 8	Mention four reserve keywords in Python. Give an example of assigning a variable value to another.	**10**	**CO3**
Q 9	Derive the expression for energy of a particle in a box (one-dimensional infinite square well potential).	**10**	**CO1**
	SECTION-C **(2Qx20M=40 Marks)**		
Q 10	a) State and prove Hellman Feynman principle. b) Using this principle prove that the average potential energy of a one-dimensional linear harmonic oscillator is equal to its average kinetic energy.	**10** **10**	**CO1**
Q 11	a) What do you understand by LDA and GGA approximations? b) Write the Hamiltonian of a many-body problem and define each term involved in it.	**10** **10**	**CO2** **CO2**

	Or a) Given the structure of any material, mention steps in computing, visualization and plotting the electronic bandstructure using DFT methodology as implemented in the Quantum Espresso software package with the help of an example. b) Explain exchange-correlation in DFT.	**15** **5**	**CO2** **CO2**