Name: **Enrolment No:**	

UPES

End Semester Examination, December 2023

Course: Computational Tools: Atomistic Simulations Techniques **Semester: V**

Program: B.Sc (H) Physics **Time : 03 hrs.**

Course Code: PHYS3028 **Max. Marks: 100**

Instructions: All questions are compulsory

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	(i) Write differences between list and tuples. (ii) Explain the difference between 'append ()' and 'extend ()' methods.	**2+2**	**CO3**
Q 2	Write a python program to check Armstrong number.	**4**	**CO3**
Q 3	State Hohenberg Kohn theorems.	**2+2**	**CO2**
Q 4	State variational principle.	**4**	**CO1**
Q 5	Discuss variation of DOS for a non-relativistic particle in two-dimensional motion.	**4**	**CO2**

SECTION B
(4Qx10M= 40 Marks)

Q 1	(i) Write a python program to check whether a number is prime or not. (ii) Write a python program to find area of a circle.	**5+5**	**CO3**
Q 2	(i) Give the mathematical description of DFT. (ii) Explain Kohn Sham equations.	**5+5**	**CO2**
Q 3	(i) State and prove crystallographic restriction theorem. (ii) Determine Miller indices of plane that makes an intercept 3 A^o, 4A^o & 5A^o on coordinate axis of orthorhombic crystal with a:b:c = 1:2:5.	**5+5**	**CO2**
Q 4	(i) What are the differences between crystalline and amorphous solids? (ii) List seven Bravais lattices in 3D with their characteristics.	**3+7**	**CO2**

SECTION-C
(2Qx20M=40 Marks)

Q 1	(i) State and prove Hellman Feynman principle.	**10+10**	**CO1**

	(ii) With the help of Hellman Feynman principle prove that the average kinetic energy of a harmonic oscillator is equal to its average potential energy.		
Q 2	(i) Write a python program to calculate factorial of a number. (ii) Write a python program for temperature converter (^{o}C to ^{o}F) **OR** (i) What are the common built-in data types in Python? Explain with examples. (ii) What is the purpose of "for" and "while" loop in python and how it is used? Explain with examples.	**10** **10** **10** **10**	**CO3**