Name: **Enrolment No:**	

UPES

End Semester Examination, May 2025

Course: Fundamentals of Computational Material Science — **Semester : VI**

Program: BSc (Hons.) Physics — **Time : 03 hrs**

Course Code: PHYS3027P — **Max. Marks : 100**

Instructions: *Read the questions clearly and provide needed details only.*

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	Differentiate between dislocations and grain boundaries.	**4**	**CO1**
Q 2	List all the assumptions utilized in molecular dynamics simulations.	**4**	**CO1**
Q 3	Discuss how molecular dynamics simulations are better than the density function theory (DFT) calculations.	**4**	**CO2**
Q 4	Explain the distinction between engineering stress-strain and true stress-strain.	**4**	**CO2**
Q 5	Explain any 4 types of ensembles with proper schematics.	**4**	**CO1**
	SECTION B **(4Qx10M= 40 Marks)**		
Q 6	Explain the concept of forcefields and their significance in molecular dynamics simulations.	**10**	**CO3**
Q 7	List governing equations of 4 different types of forcefields with their meaning.	**10**	**CO3**
Q 8	State Maxwell's thermodynamics relations, and give physical significance with mathematical expressions.	**10**	**CO4**
Q 9	Discuss Velocity-Verlet and Verlet algorithms for integrating equations of motion in molecular dynamics simulations.	**10**	**CO4**
	SECTION-C **(2Qx20M=40 Marks)**		
Q 10	Discuss in detail all the 3 steps of the molecular dynamics method.	**20**	**CO5**
Q 11	Differentiate between (a) Steepest-descent method vs Conjugate Gradients method, and (b) Abstract Model vs Concrete Model.	**2 x 10**	**CO5**