


Name:			
Enrolment No:			
UPES End Semester Examination, May 2024			
Course: Fundamentals of Computational Material Science Semester: VI Program: B.Sc. (H) Physics Course Code: PHYS 3027P			
			Time : 03 hrs. Max. Marks: 100
Instructions: All questions are compulsory			
SECTION A (5Qx4M=20Marks)			
S. No.		Marks	CO
Q 1	Explain the distinction between engineering stress, stain, and true stress, strain.	4	CO3
Q 2	Explain the concept of dislocations in crystals.	4	CO3
Q 3	Differentiate between modeling and simulations. Give example.	4	CO1
Q 4	Discuss the Kohn-Sham equations in Density Functional Theory.	4	CO4
Q 5	Explain the concept of yield strength and its importance in material design.	4	CO3
SECTION B (4Qx10M= 40 Marks)			
Q 6	Classify the models based on their predictive character.	10	CO1
Q 7	Define grain boundaries in polycrystalline materials and explain their significance in influencing the mechanical strength of a material.	10	CO3
Q 8	Explain the concept of interatomic potential and its significance in molecular dynamics simulations.	10	CO4
Q 9	Describe the interstitial and substitutional diffusion mechanisms.	10	CO3
SECTION-C (2Qx20M=40 Marks)			
Q 10	a) Describe Maxwell-Boltzmann (M-B), Bose-Einstein (B-E), and Fermi-Dirac (F-D) statistics, including their fundamental assumptions, applications, the number of microstates they involve, and the distribution functions associated with each statistical model.	15	CO2
		5	CO2

	b) What will be the average energy U of a one-dimensional quantum oscillator of frequency ω and in contact with a heat bath at temperature T ?		
Q 11	<p>a) State laws of thermodynamics and give physical significance with mathematical expression.</p> <p>b) A monatomic ideal gas at 1700°C is adiabatically compressed to $1/8$ of its original volume. What will be the temperature after compression?</p> <p style="text-align: center;">OR</p> <p>a) What do you mean by configurational entropy of a multi-component system? For a binary system, A-B, find an expression for the configurational entropy. Discuss its importance.</p> <p>b) Define the chemical potential of different components in a binary system A-B. Establish a relation between the chemical potential of a component and its activity.</p>	<p style="text-align: center;">10</p> <p style="text-align: center;">10</p> <p style="text-align: center;">10</p> <p style="text-align: center;">10</p>	<p style="text-align: center;">CO2</p> <p style="text-align: center;">CO2</p> <p style="text-align: center;">CO2</p> <p style="text-align: center;">CO2</p>