Name: **Enrolment No:**	

UPES

End Semester Examination, May 2025

Course: Advanced applications of Nanotechnology — **Semester : VIII**

Program: B.Tech.-AM-NT. — **Time : 03 hrs**

Course Code: MECH4050 — **Max. Marks : 100**

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

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	Define Embedded Atom Method (EAM) in detail.	**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 Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM).	**4**	**CO2**
Q 5	Explain and mention various types of ensembles with proper schematics.	**4**	**CO1**
SECTION B **(4Qx10M= 40 Marks)**			
Q 6	Explain the concept of forcefields and its significance in molecular dynamics simulations.	**10**	**CO3**
Q 7	List governing equations of 4 different types of forcefields with their meaning.	**4 x 2.5**	**CO3**
Q 8	Derive the diameter and chiral angle formulas for a single walled carbon nano-tube (CNT). Evaluate the same for (9,5) CNT.	**2 x 5**	**CO4**
Q 9	Discuss Velocity-Verlet and Verlet algorithms for integrating equations of motion in molecular dynamics simulations.	**2 x 5**	**CO4**
SECTION-C **(2Qx20M=40 Marks)**			
Q 10	Discuss in detail all the 3 steps of the molecular dynamics method.	**20**	**CO5**
Q 11	Describe in detail the term “nano-composites”. Mention any one self-healing mechanism operating in their domain.	**20**	**CO5**