BIRLA INSITITUTE OF TECHNOLOGY AND SCIENCE, PILANI
SEMESTER-I, 2023-24
CHE F497: Atomic and Molecular Simulations
(Closed Book)

DURATION: 90 mins **DATE:** 09/10/2023 **F.M.:** 90

Instructions: For suitable data wherever necessary, take the necessary assumptions.
Do *not* write anythings in the question paper.

Part--A : Objective answer questions (1 mark each)
Write only in the answer book

[10 Marks]

1) Matrix formulation of quantum mechanics was developed by _____.

2) When light is interpreted as particle, it is called _____.

3) To simulate bulk properties, _____ is applied during MD simulations.

4) The wave function evolves according to _____ equation.

5) The first step of Kohn-Sham equation is _____ .

6) the soft sphere potentials contain no repulsive part. (True/False)

7) In planewaves DFT calculation, the calculation time will increase with

a) number of atoms b) occupied volume

c) unoccupied volume d) all of these

8) During MD simulations, we solve _____ equation.

9) In molecular dynamics simulations, the ions interact each other via _____ interaction.

10) After MD equilibration, the calculated thermodynamics parameters should not have fluctuations. (True/False)

Part--B : Short answer questions (2 marks each)

[10 Marks]

1) Describe square-well potential with schematic.

2) What is the ergodic hypothesis of MD simulations in thermodynamic averaging.

3) Describe Verlet neighbour list.

4) What is the basic difference between Schrödinger equation and Kohn-Sham equation.

5) Name any two methods to perform geometry optimization in DFT.

Part--C : Long answer questions (50 Marks)

[5+5]

1) a) Write down the equation of Lennard-Jones potential and draw the function indicating all the important parameters. b) Find out the value of r at which the repulsive and attractive parts get separated.

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[5+5+5]

2) a) Write down the important advantage and drawback back of truncation of pair-wise potential. b) How to overcome that drawback of truncation in MD simulations. c) Draw the schematic.

[5]

3) Name and draw all the potentials for a molecular system.

[5]

4) Discuss velocity Verlet algorithm.

[5]

5) Write down all the steps of AIMD simulation.

[5+5]

6) a) Define the second Hohenberg–Kohn theorem. b) Discuss how it is useful in quantum mechanics.

Part--D : Problem Solving Questions (20 marks)

[5 Marks]

1) Calculate the interaction parameters for carbon-oxygen based on the given parameters.

Interacting molecules	ε (kJ/mol)	σ (nm)
Oxygen – Oxygen	0.51799	0.32407
Carbon – Carbon	0.4257	0.335

[15 Marks]

2) The following is the output of a MD simulations, where in 1st column the MD steps and in 2nd column the pairwise energies are printed. Assume timestep is 2 fs. a) Plot them to divide the total run in two categories. b) Calculate the average energy.

Step	E_{pair}
0	-275933.85
1000	-270866.08
2000	-264764.23
3000	-260814.71
4000	-258023.55
5000	-256774.91
6000	-255834.09
7000	-255856.71
8000	-255800.98
9000	-255870.3
10000	-255880.99