BIRLA INSITITUTE OF TECHNOLOGY AND SCIENCE, PILANI
SEMESTER-I, 2023-24
BITS F497: Atomic & Molecular Simulations
Part–-A (Closed Book)

DURATION: 120 mins **DATE:** 06/12/2023 **F.M.:** 85

Instructions: For suitable data wherever necessary, take the necessary assumptions.

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1. *Objective answer questions (1 mark each)*

(*Write only in the answer book*) **[10 Marks]**

1.1) Monte Carlo simulation is used for solving:

(a) Stochastic problems where passage of time plays no substantive role.

(b) Deterministic problems where passage of time plays substantive role.

(c) Stochastic problems where passage of time plays substantive role.

(d) All of the above

1.2) In the Heisenberg uncertainty principle, which two measurable properties of a particle cannot be observed precisely at the same time? _____ and _____

1.3) Number of particles are not constant in _____ thermodynamic ensemble.

1.4) To calculate the pair correlation function, we divide the pairwise density distributions by _____.

1.5) During MD simulations, diffusion coefficient of a molecule is calculated from _____.

1.6) Implementation of _____ is essential to control the temperature during MD simulations.

1.7) _____ is the widely used optimized barostat in MD simulation.

1.8) Monte Caro simulates phase space. (True/False)

1.9) Equilibrium uptake of a gas molecule in a porous bed can be well predicted using _____ simulation technique.

1.10) The term *Importance Sampling* is important in _____ simulation technique.

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2. *Short answer & Critical Thinking questions (25 Marks)*

[5 Marks]

2.1) Name two different random moves of particle during MC simulations. Explain the significance of considering rigid and nonrigid molecules during MC trial moves.

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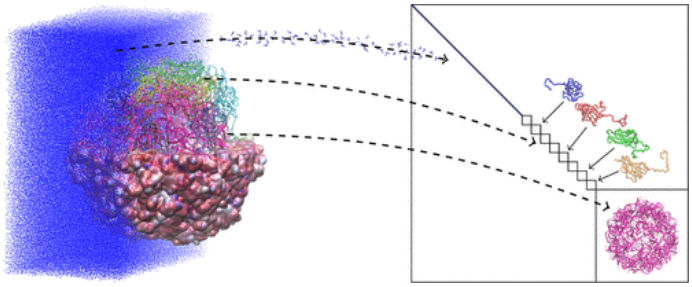
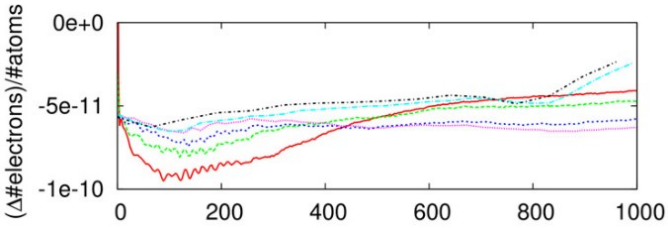
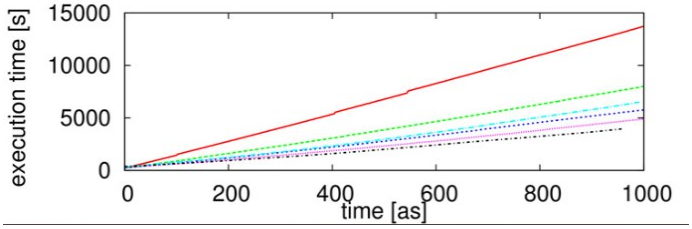
[10 Marks]

2.2) The transient electronic transport effects in nanoscale devices have been studied for TiO_2 nanoparticles in acetonitrile solution as shown in the side picture. →



Which simulation method you think will be best suited for the calculation and why? The outcomes of the





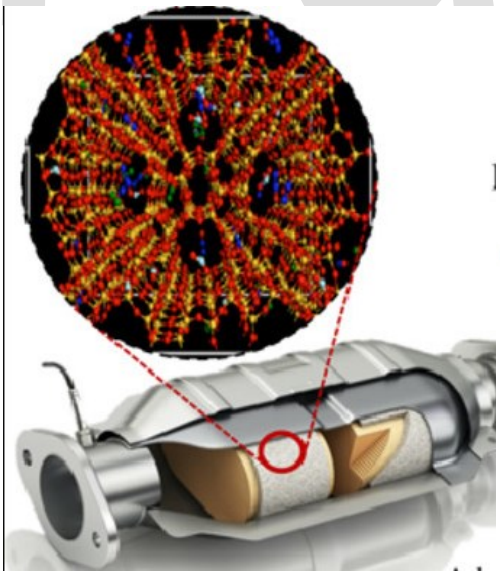
simulations are plotted.

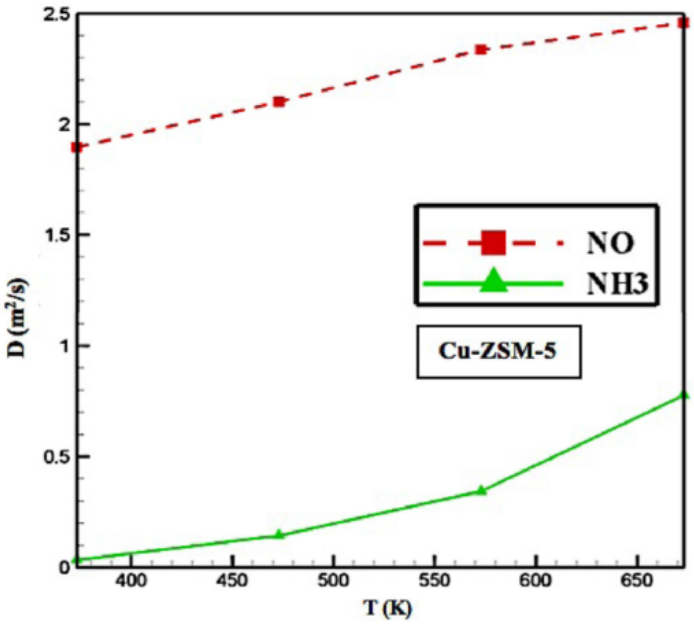
[5 Marks]

2.3) Describe Metropolis algorithm.

[5 Marks]

2.4) Gas diffusivity (D) has been calculated in a porous solid adsorbent as shown in the below picture. Which simulations technique is depicted. Justify.





Gas adsorbed in a solid adsorbent

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3. *Problem Solving Questions (50 marks)*

[5+5+8+5+ 5+2=30 Marks]

3.1) The production rate of an automobile company is approx. 100 cars per day which vary day to day basis. The probability distribution of the car production per day is given below.

Production/day	95	96	97	98	99	100	101	102	103	104	105	106
probability	0.03	0.05	0.07	0.10	0.15	0.20	0.15	0.10	0.07	0.05	0.03	0.06

a) Based on the given probability, calculate the respective cumulative probabilities.
b) Plot the cumulative probabilities in % on a single graph paper.
c) You need to do MC simulation to predict the outcomes for next 15 days. To do that you need to fire 15 random numbers to simulate each day outcome. Please consider the range of the random number 0 – 99. Based on the random number find out the production/day for all the 15 samplings.
d) At the end of the day, the cars produced each day are transported by a ferry. The ferry has a capacity of 101 cars. For each day of the 15 samplings, find out the number of cars shipped by the ferry and number of empty car spaces on the ferry.
e) Finally, find out the average number of cars shipped and the average number of empty car spaces on the ferry.
f) Comment, what will be the effect on the predicted outcomes if you simulate for 20 days instead of 15 days.

[10 Marks]

3.2) For Argon atom the following information are provided.

$$\epsilon/k_B = 119.8\ \text{K}, \sigma = 3.405 \times 10^{-10}\text{m}, M = 0.03994\ \text{kg/mol}$$

In reduced unit, the temperature, pressure and density are reduced to unity.
Find out the value of temperature, density and pressure in real units with help of statistical thermodynamics.

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[5+5=10 Marks]

3.3) Four different potentials are provided for a short chain molecule as described below.

(i) the bond-stretching potential,

$$V_{\text{stretch}}(d) = \tfrac{1}{2} k_{\text{d}} (d - d_0)^2, \tag{1}$$

where d_0 is the equilibrium bond length and d is the actual bond length, (ii) the bond-bending potential,

$$V_{\text{bend}}(\theta) = \tfrac{1}{2} k_{\theta} (\theta - \theta_0)^2, \tag{2}$$

where θ_0 is the equilibrium bond angle and θ is the bond angle between three adjacent atoms, (iii) the torsional potential,

$$V_{\text{torsion}}(\phi) = \tfrac{1}{2} k_{\phi} [1 - \cos(3\phi)], \tag{3}$$

where ϕ is the dihedral angle formed by four consecutive atoms, and (iv) the 12-6 Lennard-Jones potential between atoms separated by more than two bonds along the same chain and between atoms in different chains,

$$V_{\text{LJ}}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right], \tag{4}$$

where r is the distance between atoms. The values of all the parameters are listed in the table.

Parameter	Value	Unit
d_0	0.153	nm
θ_0	1.2310	rad
k_{d}	70 000	kcal/nm^2·mol
k_{θ}	100	kcal/rad^2·mol
k_{ϕ}	2.0	kcal/mol
ϵ	0.1984	kcal/mol
σ	0.362 39	nm

a) Plot the torsional potential in a graph paper. (b) calculate the minimum interaction diameter for pair-wise potential.

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Part–B (Open Book/Laptop)

DURATION: 60 mins **DATE:** 06/12/2023 **F.M.:** 35

Instructions: For suitable data wherever necessary, take the necessary assumptions.

[35 Marks]

Q1. You need to study O_2/N_2 separation using a carbon nanotube (CNT) with the help of atomic and molecular simulation at 298 K and 100 atm. Set the bulk gas mixture to O_2/N_2 : 21/79 to mimic air composition. Place the gas mixture on top of the CNT and observe how the diffusion, adsorption and separation is happening.

(a) Draw a schematic of the problem statement in the answer book.

(b) Draw a (4,4) carbon nanotube consisting of 1- or 2- repeating units, one O_2 and one N_2 using Avogadro/VMD. Save the coordinates.

(c) Run MD simulations for the first 5×10^3 cycles for equilibration and the last 500 cycles for taking ensemble averages. You may consider timestep of 1 fs. Consider the CNT as a single rigid molecule. Non-bonded interaction parameters are given in the below table.

Atom	σ (Å)	ϵ(kcal/mol)	$q(e)$
C	2.80	0.054	0.70
O	3.05	0.157	-0.35
N	3.31	0.072	0

The Lorentz–Berthelot mixing rules were employed for pairwise interactions. Coulomb potentials may be ignored. A Nose–Hoover thermostat can be used to keep temperature constant. Try to keep total number of gas molecules restricted to 1000. N–N chemical bond can be modeled as a harmonic spring with constant k_b = 22.95 N/cm and length r_0 equal to 1.10 Å.

O–O chemical bond can be modeled as a harmonic spring with constant k_b = 11.77 N/cm and length r_0 equal to 1.208 Å.

(d) Calculate *g(r)* of O_2 and N_2 from CNT. Plot the potential energy with time. (You need to upload the two *g(r)* plots and potential energy plot with time)

(e) Comment on your results.

(f) Compress and upload the *working folder* in the Google classroom.