BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION MO 2022)

CLASS: B.TECH. **SEMESTER : VII**
BRANCH: CHEMICAL ENGG./CHEMICAL ENGG. (P&P) **SESSION : MO-2022**

SUBJECT: CL413 FUNDAMENTALS OF MOLECULAR SIMULATION

TIME: 03 HOURS **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Tables/Data handbook/Graph paper etc., if applicable, will be supplied to the candidates**

			CO	BL
Q.1(a)	Explain the physical significance of the wave function.	[2]	1	2
Q.1(b)	Describe the Self-Consistent Field (SCF) algorithm to solve the Hartree-Fock equations for many-body electronic systems.	[3]	1	2
Q.1(c)	Suppose that a particle in a box is in the state represented by the normalized state function. $$\Psi(x) = [(30)/(a^5)]^{0.5}\, x(a-x);\ 0 \le x \le a$$ $$0 \qquad ;\ \text{otherwise}$$ Calculate the average energy of this system.	[5]	1	3
Q.2(a)	Define Markov Processes.	[2]	2	2
Q.2(b)	Explain the technique used in molecular simulation to simulate the bulk system using only a small number of molecules.	[3]	2	2
Q.2(c)	Briefly describe the Metropolis Monte Carlo simulation.	[5]	2	3
Q.3(a)	What are the commonly used ensembles in Monte Carlo Simulation? Write a pseudo code for simulating Monte Carlo simulation in a Canonical (NVT) ensemble.	[3]	3	3
Q.3(b)	Write a Monte Carlo simulation pseudo code for simulating phase equilibria in the Gibbs ensemble.	[7]	3	3
Q.4(a)	Describe the force field. Write the names of the different force fields used in molecular simulation.	[2]	2	2
Q.4(b)	Explain the working of molecular dynamics with the help of a pseudo code.	[3]	4	3
Q.4(c)	What are the different integrating algorithms in Molecular Dynamics Simulation? Briefly describe the Verlet algorithm and Velocity Verlet algorithm.	[5]	2	3
Q.5(a)	Explain the .pdb file and .data file used for simulating molecular systems in LAMMPS.	[2]	5	2
Q.5(b)	Explain the following code:	[3]	5	3

```
----------------------------------
filetype pdb
output packing.pdb
tolerance 2.5

structure waternew.pdb
  number 500
    inside box 0 0 0 40 40 40
end structure
----------------------------------
```

PTO

Q.5(c) Explain the following keywords used in the LAMMPS input file: [5] 5 3

```
boundary        p  p  p
pair_style      lj/cut/coul/long 12
bond_style      harmonic
read_data       water.data
velocity        all create 298 4567712 mom yes rot yes dist gaussian
fix             1 all npt temp 298 298 ${tempdamp} iso ${presset} ${presset}
dump            1 all atom 1000 dump.lammpstrj
restart         500000 restart.*.equil
run             1000000
```

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