BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(MID SEMESTER EXAMINATION)

CLASS: B.TECH. **SEMESTER: VII**

BRANCH: CHEMICAL ENGINEERING AND CHEMICAL ENGINEERING (PLASTICS & POLYMER) **SESSION: MO/2022**

SUBJECT : CL413 FUNDAMENTAL OF MOLECULAR SIMULATION

TIME: 2 HOURS **FULL MARKS: 25**

INSTRUCTIONS:
1. The total marks of the questions are 25.
2. Candidates attempt for all 25 marks.
3. Before attempting the question paper, be sure that you have got the correct question paper.
4. The missing data, if any, may be assumed suitably.
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

				CO	BL
Q1	(a)	Write applications of quantum chemistry in process industries.	[2]	1	2
Q1	(b)	The wave function for a free particle in a one-dimensional box is given by $$\psi_n = \mathbf{B}\sin\left(\frac{n\pi x}{a}\right)$$ Where *a* is box length. Find the constant B.	[3]	1	3
Q2	(a)	Write the name of important types of modern electronic structure calculations. How they are different from each other?	[2]	1	2
Q2	(b)	Draw the energy levels, wave functions and probability densities for the free particle in a box for n = 1, 2, and 3.	[3]	1	3
Q3	(a)	Describe the notation 6-31G**.	[2]	1	2
Q3	(b)	Write Hamiltonian operator for helium atom and simplify it in atomic units.	[3]	1	3
Q4	(a)	Briefly describe Molecular modeling and Simulation.	[2]	2	2
Q4	(b)	Differentiate between Monte Carlo simulation and Molecular Dynamics Simulation.	[3]	2	2
Q5		Write a Pseudocode to calculate the value of pi (π) using random number.	[5]	2	3

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