CLASS: IMSC   SEMESTER : V
BRANCH: CHEMISTRY   SESSION : MO/2022

SUBJECT: CH306 MOLECULAR MODELLING & DRUG DESIGN
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)	What are the compoutational methods for theoritcal calculation or for the molecular modeling.	[2]	1	1
Q.1(b)	Briefly discuss the term "structural coordinates" and "stationary point"	[3]	2	2
Q.1(c)	Explain the term Potential Energy Surface (PES). Draw the PES diagram of H2O to discuss the stationary point.	[5]	4	3
Q.2(a)	What is L-J Potential, and how it is useful to control the convergence of modeling calculations.	[2]	1	3
Q.2(b)	Explain the role of Triad Tools in Molecular Modeling Calcuation.	[3]	2	3
Q.2(c)	What is geometrical optimization or molecular minimization. Explain with energy diagram.	[5]	3	2
Q.3(a)	What is meant by Periodic boundary condition?	[2]	2	1
Q.3(b)	How can the initial velocity and position be assigned to a given system in a molecular dynamics simulation ?	[3]	3	2
Q.3(c)	What is meant by Force Fields? Explain in detail how intramolecular and intermolecular interactions are represented by force fields in a given molecular simulation.	[1+4]	4	3
Q.4(a)	What is a permutation operator ?	[2]	2	1
Q.4(b)	Explain briefly the Hohenberg-Kohn Theorem. What is meant by a functional ?	[2+1]	3	2
Q.4(c)	Explain why local density approximation (LDA) may not predict correct chemical behavior of a given system. Why GGA is needed in density functional theory?	[2+3]	4	5
Q.5(a)	Explain how velocity could be evaluated from Velocity-Verlet algorithm in a given molecular simulation.	[2]	2	2
Q.5(b)	Explain physically the meaning of Markov process. What is meant by detailed balance ?	[2+1]	4	2
Q.5(c)	Explain physically the reason of employing sampling methods in a Monte-Carlo simulation. Explain in detail what is meant by i) 6-31G(d,p) ii) aug-cc-pvtz iii) 6-311++G(d,p) basis sets ?	[2+3]	5	5