Reg. No. \_\_\_\_\_\_\_\_\_\_\_\_



**End Semester Examination – Nov / Dec – 2019**

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| **Code :** | **14NT3019** | **Duration :** | **3hrs** |
| **Sub. Name :** | **INTRODUCTION TO MOLECULAR SIMULATION** | **Max. Marks :** | **100** |

**ANSWER ALL QUESTIONS (5 x 20 = 100 Marks)**

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| **Q. No.** | **Sub Div.** | **Questions** | **Course**  **Outcome** | **Marks** |
| 1. |  | Give an overview of molecular simulation and thereby mention the salient features of molecular dynamics simulation method with necessary examples. | CO1 | 20 |
| **(OR)** | | | | |
| 2. | a. | Monte Carlo is one of the well known method among other molecular simulation techniques. With a simple program explain the important features of Monte Carlo simulation. | CO1 | 10 |
| b. | Discuss the factors that should be considered in order to obtain a better algorithm which is necessary to integrate the Newton’s equations of motion. | CO1 | 10 |
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| 3. |  | Explain in detail the interaction potentials involved in a system of atoms. Calculate the potential energy using the concept of Lennard-Jones for a pair of atoms in liquid argon. | CO2 | 20 |
| **(OR)** | | | | |
| 4. | a. | Define a constraint. Explain how they are treated using algorithms in simulation. | CO2 | 10 |
| b. | Describe how the distribution of velocities from all the atoms are determined at equilibrium using Maxwell’s velocity distribution in molecular dynamics. | CO2 | 10 |
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| 5. |  | Mention the need for algorithms in simulation. Give a detailed account on the algorithms that are involved in MD simulation. | CO3 | 20 |
| **(OR)** | | | | |
| 6. | a. | Verlet algorithm is the most commonly used method of integrating the equations of motion and it gives the direct solution to the second order equations. Validate the sentence. | CO3 | 10 |
| b. | State the advantage of using metropolis algorithm in molecular dynamics simulation by explaining it in detail. | CO3 | 10 |
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| 7. |  | Discuss briefly the ensemble especially based on the thermodynamic condition and statistical mechanics concept. | CO3 | 20 |
| **(OR)** | | | | |
| 8. | a. | To simulate a system at constant pressure in molecular dynamics the volume is considered as a dynamic variable that changes during simulation. Explain the concept in detail. | CO3 | 10 |
| b. | Discuss the Nose-Hoover thermostat as an illustration of an extended-Lagrangian formulation in molecular dynamics. | CO3 | 10 |
|  | | **Compulsory**: |  |  |
| 9. |  | Give an overview of Monte Carlo simulation and explain its formulation and Structural characterization. | CO3 | 20 |