DEPARTMENT OF MATERIAL SCIENCE & MATTELURGICAL ENGINEERING

UNIVERSITY INSTITUTE OF ENGINEERINGAND TECHNOLOGY, CSJM UNIVERSITY, KANPUR

Subject: Computing Methods in Materials Science, Code-MSE-S4062022-23 (Even Semester) B.Tech. MSME VIII sem Year: 4 Year

End Semester Examination

Time: 3 hours **Maximum marks: 50**

Note: All the questions from Section A is compulsory Attempt all the required questions from section B & C

Section A 10 marks (10 questions of 1 mark each)

1. Define Phase Space.
2. Define Microscopic variable.
3. Make a list of Macroscopic variables.
4. Write down all the types of atomics motions in molecule.
5. Write down Newton Raphson method.
6. Which one is the first MD simulation of realistic system in History?
7. Write down name of all the types of Ensembles.
8. Explain Ergodic Hypothesis.
9. Explain bond stretch.
10. Explain Angle bending

Section B (20 marks (Attempt any 5 questions of 4 marks each)

11. Explain the role of setting up periodic boundary condition in dynamic simulation.
12. Define all the types of Ensembles used in MD Simulation.
13. Draw an algorithm to solve the problem of a non-functioning of light bulb
14. Explain the role of Statistical Mechanics in MD Simulation.
15. Write down time averages: Average Potential Energy & Average Kinetic Energy
16. Explain Thermodynamic State & Phase Space.
17. Explain Ensemble Average & time average.
18. Explain Probability Density Function.
19. Explain Conjugate Gradient energy minimisation method.
20. Write down application of Fourier transform method to transform electron density map into readable form.
21. Write down Braggs law, Definition & general scattering equation.

Section C (20 marks (Attempt any 2 questions of 10 marks each)

22. Define energy minimisation problem & discuss about all the methods of energy minimisation.
23. What is Classical Mechanics. Explain the method of calculating Charm potential energy function.
24. How do we write algorithm after analysing problem (steps of problem solving). Write down an algorithm to attain minimum value on energy surface.
25. Explain the energy term representing the contribution of non-bonded interactions in the CHARMM potential function which have two components.
26. What is solvation shell? explain process of active site solvation. Discuss about Mesoscale simulation.
27. Wrote down the steps of setting up and running a Molecular Dynamics Simulations & explain them in detail. Discuss about its application in Material Science
28. What is free energy? Discuss about the End point & pathway methods of calculating Gibbs Free Energy
29. Write down all the functions of MATLAB programming to calculate potential energy function & minimum energy of any material form.