Dr. Abhishek K Gupta

Roll No:

9/5/2023

E

199

NATIONAL INSTITUTE OF TECHNOLOGY, HAMIRPUR, H.P

Department of Materials Science and Engineering

End -Term Examination

Computational Materials Science (MS-324)

Duration: 3 hrs **Maximum Marks: 50**

Attempt all the following questions.

Q.1 Draw a schematic showing four typical methods used in computational materials modelling in terms of size and time scale? *(4)*

Q.2 Explain the potential function used to simulate the interactions between two Neon atoms. Draw the schematic of this potential function and explain the several features when these two atoms approach each other from a long distance? *(2+2+2)*

Q.3 Derive Verlet algorithm? How are the velocities updated after new positions and accelerations in Velocity-Verlet algorithm? *(2+2)*

Q.4 Explain the concept of molecular dynamics simulation. Draw the flow chart of an MD run and explain the different steps to be considered while setting up a molecular dynamics simulation of a crystal/molecule. *(3+3+4)*

Q.5 (a) A computational materials scientist is investigating the probability of a certain type of defect occurring in a crystal structure. Based on previous simulations, the probability of the defect occurring in a single unit cell is 0.02. If the scientist examines a random sample of 100 unit cells, what is the probability that there are exactly 5 unit cells with the defect? (Hint: Binomial theorem: $n_{C_k} p^k (1-p)^{n-k}$) *(2)*

(b) Evaluate the above problem by Monte Carlo simulation describing the different steps (Not code!) used to achieve the final probability? *(4)*

Q.6 Draw a flowchart of Monte Carlo simulation of the Ising model. Describe the simulation steps detailing the use of Markov chain of states and Metropolis algorithm to obtain the expected value of magnetisation? *(4+6)*

Q.7 Using Runge-Kutta of 2nd order method, find y(1) for the equation

$$\frac{dy}{dx} = y - 2x^2 + 1; y(0) = 0.5 \; with \; step \; size \; h = 0.2$$

Construct a Table showing the Predicted and Corrected values with final solution of 'y(1)' at the end. *(10)*