Assignment 12

The due date for submitting this assignment has passed.
As per our records you have not submitted this assignment.

1) Which of the following tricks removes the surface effect in computer simulations?
   - minimum image convention  
   - periodic boundary condition  
   - cut-off condition  
   - surface boundary
   Score: 2 points
   Accepted Answers:
   - periodic boundary condition

2) The two most basic inputs for molecular dynamics (MD) simulations are:
   - Initial coordinates and potential energy parameters  
   - Potential and kinetic energy parameters  
   - Kinetic energy parameters and solvent description  
   - Initial coordinates and cut-off values
   Score: 2 points
   Accepted Answers:
   - Initial coordinates and potential energy parameters

3) Metropolis algorithm is used in:
   - Brownian dynamics  
   - Molecular dynamics simulations  
   - Monte-Carlo simulation  
   - Quantum calculation
   Score: 2 points
   Accepted Answers:
   - Monte-Carlo simulation

4) Which of the following statement is true for verlet algorithm?
   - It is used to calculate explicit velocity  
   - It is used to calculate new coordinates  
   - It is used in Monte-Carlo simulations  
   - It is used in Brownian Dynamics simulations
   Score: 2 points
   Accepted Answers:
   - It is used to calculate new coordinates

5) Force fields used in MD simulations contains the terms for
   - Lennard-Jones potential  
   - Coulombic interaction  
   - Bonded interactions  
   - All of the above
   Score: 2 points
   Accepted Answers:
   - All of the above

6) A system starts with a W of 2000. Two kJ of heat are transferred into the system reversibly at 298 K. What is the W (thermodynamic probability) now?
   - Assume $k_B = 1 \text{ JK}^{-1}$
   Score: 2 points
   Accepted Answers:
   - $1.64 \times 10^5$
   - $1.64 \times 10^7$
   - $1.64 \times 10^7$
   - $1.64 \times 10^9$

7) A system has a partition function of 1.3 at 293 K. At that temperature, an energy level is populated by 10% of the molecules. What is the energy of that level? Assume $k_B = 1 \text{ JK}^{-1}$
   - 410 J  
   - 628 J  
   - 257 J  
   - 650 J
   Score: 3 points
   Accepted Answers:
   - 410 J