

Unit 14 - Week 12

Course outline
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Assignment 12

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

Due on 2020-12-09, 23:59 IST.

- 1) For a random walk model of polymer, the mean square end to end distance $\langle R^2 \rangle$ of a chain of N segments with segment length ℓ is given by (where C_∞ is Flory's characteristics ratio) 1 point
- (a) $\langle R^2 \rangle = C_\infty N$
 (b) $\langle R^2 \rangle = C_\infty N \ell$
 (c) $\langle R^2 \rangle = C_\infty \ell^2$
 (d) $\langle R^2 \rangle = C_\infty N \ell^2$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (d)
- 2) The radius of gyration (R_g) for a sphere of radius R will be 1 point
- (a) $\frac{R}{2}$
 (b) $\frac{R}{\sqrt{2}}$
 (c) $\frac{3R}{5}$
 (d) $\sqrt{\frac{3}{5}}R$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (d)
- 3) For a two-dimensional excluded volume chain, the value of the Flory exponent will be 1 point
- 3/7
 0
 1/2
 3/4
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 3/4
- 4) According to Liouville's theorem any phase space function A evolves as (here, H corresponds to the Hamiltonian of the system) 1 point
- (a) $\frac{dA}{dt} = \{A, H\}$
 (b) $\frac{dA}{dt} = [A, H]$
 (c) $\frac{dA}{dt} = \{H, A\}$
 (d) $\frac{dA}{dt} = [H, A]$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (a)
- 5) Liouville operator L is 1 point
- Anti-Hermitian operator
 Unitary operator
 Hermitian operator
 Non-Unitary operator
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 Hermitian operator
- 6) We are unable to calculate total energy at each timestep of molecular simulation when we use 1 point
- Velocity Verlet algorithms
 Leap frog algorithms
 Position Verlet algorithms
 Predictor-corrector algorithms
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 Leap frog algorithms
- 7) The interaction potential energy between charge and induced dipole varies with the separation between them (r) as 1 point
- (a) $\frac{1}{r}$
 (b) $\frac{1}{r^2}$
 (c) $\frac{1}{r^3}$
 (d) $\frac{1}{r^4}$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (d)
- 8) While performing MD simulation in Canonical ensemble which of the following relation holds between momentum fluctuation (σ_p^2) and momentum (p) 1 point
- (a) $\frac{\sigma_p^2}{\langle p^2 \rangle} = \frac{2}{3}$
 (b) $\frac{\sigma_p^2}{\langle p^2 \rangle} = \frac{1}{3}$
 (c) $\frac{\sigma_p^2}{\langle p^2 \rangle} = \frac{2}{3}$
 (d) $\frac{\sigma_p^2}{\langle p^2 \rangle} = \frac{5}{3}$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (a)
- 9) Suppose, we have a system having temperature $T(t)$ at time t and the temperature at which the system needs to bring is T_{ref} . To achieve the required temperature we can rescale the velocities of the particles by multiplying λ , where λ is 1 point
- (a) $\sqrt{T_{ref}}$
 (b) $\sqrt{T_{ref} T(t)}$
 (c) $\sqrt{T(t) / T_{ref}}$
 (d) $\sqrt{T_{ref} / T(t)}$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (d)
- 10) If p be the momentum of the particle of mass 'm' at temperature T, then the value of $\langle p^2 \rangle$ is 1 point
- (a) $2mk_B T$
 (b) $3mk_B T$
 (c) $4mk_B T$
 (d) $mk_B T$
- (a)
 (b)
 (c)
 (d)
- No, the answer is incorrect.**
 Score: 0
 Accepted Answers:
 (b)