

Topics in Nanosciences
Mid Sem Exam: Monsoon 2023
IIIT-Hyderabad

Full Marks: 60

Time: 1:30 hrs

Important notes:

1. *Use of non-programmable scientific calculators is allowed.*
2. Some Formulas/Equations are given at the end of the questions paper. You may pick one or more appropriate ones for your answers. Write the significance of the terms used in these expressions while using them.

Q1. (a) Why does the surface play a crucial role in determining the material properties in the nanomaterials unlike bulk materials? (3)

(b) For a spherical particle of radius R , derive the expression for the ratio of surface atoms (N_s) to total atoms (N_v). Using the expression, calculate the approximate number of atoms that will be at the surface of a spherical particle of radius, 5 nm, having around 8,000 atoms. (3+2)

(c) Name the zero-dimensional (0D) and two-dimensional (2D) nanocarbon systems. (2)

Q2. (a) What is Young's contact angle? (2)

(b) Under which conditions does a hydrophilic surface become more hydrophilic whereas a hydrophobic surface become more hydrophobic? Use an appropriate model and illustrate with examples to justify your answer. (5,3)

Q3. (a) Show that the molar Gibbs energy of the whole particle, μ_P , is given by the sum of the chemical potential of the particle bulk, μ_s , and a term that accounts for the molar surface energy contribution. Also, show that the surface energy contribution becomes significant for nanoparticles. (8)

(b) How do the melting temperature and the solubility of a nanoparticle depend on its size? (2)

Q4. (a) What should be the equilibrium shape of an fcc nanocrystal seed? Why? Starting with this fcc seed crystal and an appropriate capping agent, how can one prepare an octahedron-shaped nanoparticle? Explain. (1,2,4) (3)

(b) Discuss how one can obtain branched nanoparticles. (3)

Q5. (a) Draw a schematic LaMer plot and explain what happens in various stages both along the x- and y-axes. (6)

(b) Discuss how one can prepare smaller nanoparticles out of a given quantity of (monomer) precursor. (2.5)

(c) Why is it necessary to control the size and shape of a nanoparticle? (1.5)

Q.6. (a) In case of formation of an epitaxial phase, what kind of nucleation happens? (1)

(b) In the case of formation of an epitaxial phase, describe the commonly observed mechanisms of nucleation and overgrowth. (9)

Equations/Formulas:

The number of atoms per shell is $= \frac{4}{3} (10n^2 + 2)$.

$$r_c = -\frac{2\gamma}{\Delta G_v} = \frac{2\gamma V_m}{RT \ln S}$$

$$dG = VdP - SdT + \sum_i \mu_i dn_i + \gamma dA$$
