International Institute of Information Technology - Hyderabad

Question Paper

***Subject:* SC2.401 Topics in Nanosciences**

Mid-Semester Examination: Monsoon 2025

Max. Time: 1.5 Hr **Max. Marks: 60**

Note:

1. Answer all questions.
2. Make appropriate assumptions where required.
3. Use of nonprogrammable scientific calculators is allowed.
4. Some information is given at the end of the question paper that may be used if needed.

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Q1. (a) When does the 'size effect' begin to appear in materials properties? [2]

(b) Why do the roles of the surface become more significant in determining the properties of the nanomaterials than their bulk counterparts? [2]

(c) For a spherical particle of radius R, show that the ratio of surface atoms (N_s) to total atoms (N_v) is given by $\approx 1/R$. [2]

(d) Consider a spherical gold nanoparticle that contains 500 atoms. If the diameter of an atom is approximately 3 Å, what fraction of the gold atoms in the particle are on the surface? [2]

(e) Define "intensive properties". Mention two intensive properties that behave like 'extensive properties' in nanomaterials. [1,1]

Q2. (a) Starting from Gibbs free energy function, show that the molar Gibbs free energy of the whole particle, μ_P, is given by the sum of the chemical potential of the bulk, μ_S, and a term that accounts for the molar surface energy contribution. Use the expression to show that the surface energy contribution becomes significant at the nanoparticles. [6,2]

(b) Predict the size effects on the oxidation potentials of nanoparticles. Justify your answer. [2]

Q3. (a) What is meant by a "superhydrophobic self-cleaning surface"? Write down the conditions in terms of the dynamic contact angles and the roll-off angles. [1,2]

(b) Discuss the role of 'air trapping' in causing superhydrophobicity of a surface using an appropriate model. [7]

Q4. (a) Mention three classical material properties that show quantum behavior in some nanomaterials. [1.5]

(b) What is the largest size (edge length) of a cubic metal particle where quantization effects would be observed at room temperature. [4.5]

(c) Define density of states (DOS). What is the density of states at zero energy for 3-D, 2-D, and 1-D systems? [1,3]

Q5. (a) What is meant by a 'single-electron transistor (SET)'? Mention two advantages of SETs. [1,1]

(b) Discuss the construction and working principles of a typical SET. [4]

(c) Why does one need quantum dots for the SETs? [2]

(d) Calculate the energy change when the quantum dot is charged from n to $(n + 1)$ electrons. [2]

Q6. (a) Define a quantum dot. [1]

(b) Why are the quantum dots called artificial atoms? [2]

(c) Compare surface plasmon resonance (SPR) and localized surface plasmon resonance (SPR) (LSPR). [3]

(d) Bi reacts with the cysteine in hair to make Bi_2S_3 (bismuth sulfide). Bi_2S_3 is a nontoxic metal chalcogenide semiconductor with band gap of ~ 1.5 eV. Can one use Bi compound as hair coloring (black) agent? Justify your answer. [4]

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Given: k_B (Boltzmann constatnt) = 1.38×10^{-23} JK^{-1} = 8.63×10^{-5} eVK^{-1} = 1.38×10^{-16} erg K^{-1}.

1 eV = 1.6×10^{-19} J. 1 J = 1 kg m^2/s^2. 1 eV = 1240/λ (wavelength in nm)

$h = 6.6 \times 10^{-34}$ J s. $m_e = 9.1 \times 10^{-31}$ kg. $e^2/4\pi\varepsilon_0 = 1.44\times10^{-9}$ eV m.

Electronic charge = 1.6×10^{-19} Coulomb. ε_0 (vacuum) = 8.8542×10^{-12} F/m.

$D(E) \approx E^{[(d/2)-1]}$. $C = (4\pi\varepsilon_0\varepsilon_r)\cdot r = 4\pi \times 8.85\times 10^{-12}\ \text{F.m}^{-1} \times 11.5 \times r$

$$E = \frac{\pi^2\hbar^2}{2m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2 + \left(\frac{n_z}{L_z}\right)^2\right]$$

$$E = E_g + \frac{\pi^2\hbar^2}{2\mu r^2}$$