Topics in Nanosciences
End Semester Examination: Monsoon 2022
IIIT-Hyderabad

***Full Marks*: 100** **Time: 3 hrs**

Note: Use of a non-programmable scientific calculator is allowed.

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Q.1. (a) Based on the concept of coordination numbers, answer the following and *justify* your answers:
(i) Give the increasing order of the (re)activities of kink, corner, edge, and surface atoms.
(ii) Which of the following is expected to be energetically less favorable: adding an atom to the step vacancy vs. surface vacancy? [3+2]
(b) Why are the 'Hydrodesulfurization (HDS)' catalysts so important? Name an HDS catalyst and briefly describe its mechanism of action. How can an addition of Co improve catalytic performance? [1,2.5,1.5]

Q.2. In the following, the chiral vectors of some CNTs are given:
(i) $c = 9a_1$ (ii) $c = 9a_2$ (iii) $c = 9a_1 + 9a_2$ (iv) $c = 9a_1 + 7a_2$.
(a) What is the type of nanotube formed in each case? Justify. [3.5]
(b) Arrange these tubes in the order of increasing diameter. [3]
(c) Which of these tubes is metallic, and which is semiconducting? Why? [3.5]

Q.3. (a) Mention *two* microscopy (nanoscopy) techniques that can measure/image the surface topography of nanomaterials. [1]
resolution + penetration
(b) Why are high-energy electrons used in electron microscopy techniques? [1.5]
(c) Name a nanoscopy technique whose work environment can be air or liquid, not necessarily vacuum. dls, dynammic light [1]
(d) Mention *three* 'intensive properties' that do not remain 'intensive' in nanomaterials. [1.5]
(e) When do the size effects begin to appear in materials? [1.5]
(f) Why do the surface-interface effects play a great role in determining the material properties in the nanomaterials, unlike bulk materials? [3.5]

Q.4. (a) Define and explain the phenomenon of Ostwald Ripening by using an appropriate thermodynamic expression. [1,3]
(b) What is the effect of Ostwald Ripening on the size distribution (dispersity) of the nanoparticle dispersions? [1]
(c) How does the Cassie-Baxter model differ from the Wenzel model in explaining the superhydrophobicity of a surface? [5]

Q.5. (a) Compare the mechanisms responsible for the appearance of colors in the suspensions of metal and semiconductor nanoparticles. [2]
(b) Discuss the nanoparticle size effects on the nature of (bandwidth, peak height, peak wavelength, etc., of) the LSPR (localized surface plasmon resonance). [3.5]
(c) Two colorless, odorless, and transparent solutions are given to you: one containing an aq. protein solution and the other an aq. solution of the poison, potassium cyanide. How could you distinguish/identify them using the optical property of gold nanoparticles dispersed in water? Use appropriate theoretical relationships to justify your answers. [3.5]

(d) The absorption coefficients of human (aorta) tissue and of water as a function of the excitation wavelength shows that the minimum of the tissue absorption can be found at approximately 800 nm. Some studies have suggested that multiple-photon absorption of gold nanospheres at this wavelength might be advantageous for plasmonic heating (photoinduced hyperthermia). However, monophotonic excitation is advantageous, because its absorption cross-section is several orders of magnitude higher than multiphotonic excitation. What morphologies/shapes of the gold nanostructures do you suggest instead of spheres for this purpose? [1]

afm,stm

Q.6. (a) Name two methods that can be applied for nanoscale distance measurements. [1]
(b) Describe how the assembly-disassembly property of functionalized gold nanospheres can be used for the highly sensitive optical detection of trace amounts of sequence-specific DNA strands. Describe the principles of this sensing method. ed to blue, complimenaty dna [3.5]
(c) Discuss the conditions for the maximum enhancement of the local field on a small spherical plasmonic nanoparticle. [2]
(d) What is "Surface-Enhanced Raman Scattering (SERS)"? Describe its mechanisms. [3.5]

Q.7. (a) Show the full-loop hysteresis curves for ferromagnetic, paramagnetic, and superparamagnetic materials on the same plot. Show all the cardinal points M_s, M_r, and H_c on the hysteresis curves. Compare the salient features of the plots. [3]
(b) Draw a schematic plot showing the variation of the coercivity of a ferromagnetic particle with its size. Justify the nature of the variation. [3]
(c) Show that a particle acts superparamagnetically on the 100 s experimental timescale if it has a volume smaller than the critical volume, $V_{sp} = 25kT_B/K$ (the terms have their usual meanings). [4]

Q.8. (a) Why is Giant Magnetoresistance (GMR) a quantum mechanical and a nanoscale effect? [1.5]
(b) How does the construction of a spin valve differ from the magnetic tunneling junction (MTJ) devices? [2.5]
(c) Discuss the mechanism (with the help of a schematic diagram) of a GMR device composed of the nanoscale ferromagnetic layers of cobalt separated by the nanoscale nonmagnetic layer of copper. [4]
(d) "Currently, the best technology of 'Read' sensors employ the GMR effect." Briefly explain how the GMR effect is used in the 'Reading' head for information retrieval. [2]

Q.9. (a) Derive an expression that shows how the density of states (DOS) function depends on the energy of a *1D* material. [5]
(b) Show that the quantum of electrical conductance is given by $\frac{2e^2}{h}$. [3]
(c) If there exists a finite nonzero resistance in a nano-conductor, why does a superconductor have zero resistance? [2]

Q.10. (a) Mention two advantages of a 'single-electron transistor (SET)'. [1]
(b) Discuss the construction and working principles of a typical SET. [1+3.5]
(c) Calculate the size (radius in nm) of a sphere-shaped Si quantum dot that would produce an observable single electron effect at room temperature (300 K). Given: Dielectric constant of Si = 11.5; Permittivity of vacuum = 8.85×10^{-12} F.m^{-1}; $k = 1.38 \times 10^{-23}$ JK^{-1}; 1 eV = 1.602×10^{-19} J. [4.5]