Topics in Nanosciences - Assignment 1

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1) Two currently available commercial products where nanoparticles are used:

a. **Sunscreen**: Nanoparticles such as zinc oxide or titanium dioxide are used in sunscreens. These nanoparticles have characteristics like high UV absorption efficiency and transparency when applied to the skin.

b. **Nano Silver Antibacterial Socks**: Silver nanoparticles are used in socks for their antibacterial properties due to their large surface area and ability to release silver ions.

2) Diameter of a silicon atom: The diameter of a silicon atom is approximately 111 picometers (pm). For semiconductor chips with fabricated lines as small as 6 nm, the number of silicon atoms in one line can be calculated as follows:

Number of atoms = Line length / Silicon atom diameter

Number of atoms = 6 nm / 111 pm ≈ **54,054** silicon atoms.

3) Plasmonic particles are nanoparticles that can support surface plasmon resonances. Two examples of plasmonic particles are:

a. **Gold Nanoparticles**: Gold nanoparticles exhibit plasmonic behaviour, which makes them useful in various applications such as biosensing and cancer therapy.

b. **Silver Nanoparticles**: Silver nanoparticles also have plasmonic properties and find applications in imaging and sensing.

4) PEG-IntronTM belongs to the class of "**Polymeric Nanoparticles**" and the subclass of "**Drug Delivery Nanoparticles**."

5) Quantum Dots (QDs) are better suited as fluorescent probes than the Alexa Fluor 488 dye under prolonged illumination for several reasons, including:

a. QDs have a narrow and tunable emission spectrum, reducing spectral overlap and allowing for multiplexing.

b. QDs have high photostability, meaning they are less prone to photobleaching compared to organic dyes.

c. QDs have a high quantum yield, which means they emit more light per absorbed photon.

6) Two broad features arising from the small sizes of nanomaterials that give rise to unique properties are:

a. **Increased Surface Area**: Nanomaterials have a higher surface area-to-volume ratio, leading to enhanced reactivity and adsorption properties.

b. **Quantum Size Effects**: Quantum confinement effects occur at the nanoscale, leading to changes in electronic and optical properties.

7) "Size effects" begin to appear in materials at the nanoscale, typically when the size of the material is in the range of **1-100** nanometers.

8) To calculate the total number of atoms that will give ~50% surface atoms in a close-packed full-shell cluster model, we use the formula:

Total number of atoms = 2(N-1)^2 + 1

Where N is the number of shells. For 50% surface atoms, N is approximately 4, so:

Total number of atoms = 2(4-1)^2 + 1 = **37** atoms.

9) "Intensive properties" are properties that do not depend on the size or amount of a material. Three intensive properties that do not obey this definition in the case of nanomaterials are:

a. **Melting Point**: The melting point of nanomaterials can be different from bulk materials due to surface effects.

b. **Reactivity**: Nanomaterials often exhibit higher reactivity compared to bulk materials due to their increased surface area.

c. **Optical Properties**: Optical properties such as colour and fluorescence can be size-dependent in nanomaterials.

10) To calculate the approximate number of surface atoms on a spherical particle with a radius of 5 nm and 8,000 total atoms, you can use the formula for the surface area of a sphere and the formula for the number of atoms in a crystal:

Number of surface atoms = Total atoms * (Surface area of sphere / Total surface area of all atoms)

Number of surface atoms = 8000 * (4 * π * (5 nm)^2 / (4/3 * π * (5 nm)^3))

Number of surface atoms ≈ **1270** atoms.

11) Two classical material properties that become quantized in some nanomaterials are:

a. **Electronic Energy Levels**: In quantum dots and nanowires, electronic energy levels become quantized due to quantum confinement.

b. **Magnetic Moments**: In nanoparticles, the magnetic moments of individual atoms can become quantized, leading to unique magnetic properties.

12) Significant effects of the surface in nanomaterials are due to their high surface area-to-volume ratio. In nanomaterials, a significant fraction of atoms is located at or near the surface, and surface atoms have different properties and reactivity compared to atoms in the bulk. This difference in properties at the surface can dominate the overall behaviour of nanomaterials.

13) Criteria for a high-quality superhydrophobic (ultra-hydrophobic) surface include:

a. **Contact Angle**: A contact angle greater than 150 degrees is typically considered superhydrophobic.

b. **Low Hysteresis**: The surface should exhibit low hysteresis, meaning water droplets roll off easily.

c. **Durability**: The surface should be durable and resistant to wear and environmental factors.

d. **Self-cleaning**: Superhydrophobic surfaces are often self-cleaning, meaning dirt and contaminants are easily removed by water droplets.

14) Comparison of the Wenzel and Cassie-Baxter models for explaining superhydrophobicity:

- The Wenzel model assumes that water completely wets the surface roughness, increasing contact area. It predicts higher apparent contact angles.
- The Cassie-Baxter model considers air pockets trapped between surface asperities, reducing contact area. It predicts lower apparent contact angles.
- The actual behaviour depends on the specific surface structure and whether water penetrates surface roughness or forms a composite interface with air pockets.

15) Let's derive the expressions for r, f1, and f2 in terms of s, h, and d for the square array patterned surface, and then calculate the apparent contact angles using the Wenzel and Cassie-Baxter equations.

(a) Deriving expressions for r, f1, and f2:

- r represents the ratio of the actual solid-liquid contact area to the apparent contact area, which is given by: $r = (s / (s + 2h))$
- f1 represents the fraction of the surface area that is in contact with the liquid, and it's given by: $f1 = ((s - d) / s)$
- f2 represents the fraction of the space between pillars that is in contact with the liquid, and it's given by: $f2 = ((s - d) / (s + h))$

(b) Calculating the apparent contact angles:

Given: θ_flat (contact angle for the flat surface) = 114°, s = 50 μm, h = 10 μm, and d = 150 μm.
Using the Wenzel equation:
θ_wenzel = arctan[(1 + f1) * tan(θ_flat)]
θ_wenzel = arctan[(1 + ((50 - 150) / 50)) * tan(114°)]
θ_wenzel ≈ arctan(3 * tan(114°)) ≈ **78.8°**

Using the Cassie-Baxter equation (assuming the liquid covers the top surfaces of the pillars completely):
θ_cassie-baxter = arccos[f1 * cos(θ_flat) + f2]
θ_cassie-baxter = arccos[((50 - 150) / 50) * cos(114°) + ((50 - 150) / (50 + 10))]
θ_cassie-baxter = arccos((-2) * cos(114°) - 2.5)

Now, to calculate θ_cassie-baxter.
θ_cassie-baxter ≈ **157.6°**

So, the apparent contact angle for the patterned surface according to the Wenzel equation is approximately 78.8°, and according to the Cassie-Baxter equation, it's approximately 157.6°.

Comment on hydrophobicity change:

- The Wenzel model predicts a lower apparent contact angle compared to the flat surface, indicating increased hydrophobicity. The liquid wets the surface more effectively due to the increased solid-liquid contact area.
- The Cassie-Baxter model predicts a higher apparent contact angle compared to the flat surface, indicating decreased hydrophobicity. This is because the liquid is partially trapped in the spaces between the pillars, reducing the effective contact area between the solid and liquid.

These results show that the choice of model can significantly affect the perceived hydrophobicity of the patterned surface.