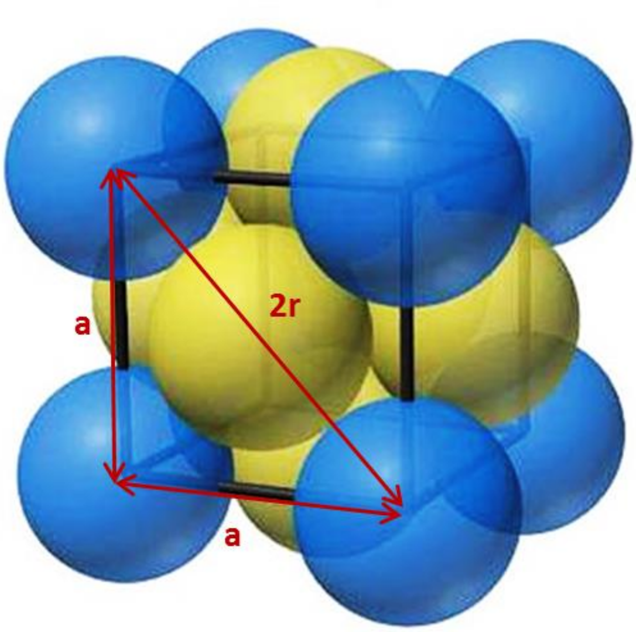
Model Answers

Question 1 - solution

a = lattice constant

r = radius of gold atom = 0.1442 nm



$$(4r)^2 = a^2 + a^2 \Leftrightarrow 16r^2 = 2a^2 \Leftrightarrow 8r^2 = a^2 \Leftrightarrow a = \sqrt{8}r$$

$$r \approx 0.1442 \text{ nm}$$

$$a = \sqrt{8}r = \sqrt{8}r \approx \sqrt{8} \times 0.1442 \approx 0.4079 \text{ nm}$$

Question 2 – solution

The shell thickness is half of the lattice parameter, and 0.2039 nm.

The total volume of the nanoparticle of radius R is:

$$V_{total} = \frac{4}{3}\pi R^3$$

The volume of the core after accounting for the finite shell thickness is:

$$V_{core} = \frac{4}{3}\pi(R - 0.2039)^3$$

The volume of the shell is the difference between the total volume and the volume of the core, *i.e.*:

$$V_{sheel} = V_{total} - V_{core} = \frac{4}{3}\pi R^3 - \frac{4}{3}\pi(R - 0.2039)^3$$

Now since the lattice constant of the Au unit cell is 0.4079 nm the volume of a single unit cell is:

$$V_{unit} = 0.4079R^3$$

The number of unit cells making up the shell can be calculated from:

$$\text{Unit cells}_{sheel} = \frac{V_{sheel}}{V_{unit}}$$

Since the number of atoms per unit cell is 4, the total number of surface atoms is:

$$\text{Atoms}_{surface} = 4 \times \text{Unit cells}_{sheel}$$

To calculate the total number of atoms in the entire particle, first it is necessary to find the total number of unit cells.

$$\text{Unit cells}_{total} = \frac{V_{total}}{V_{unit}}$$

The number of atoms per unit cell is 4 giving the total number of atoms in the particle:

$$\text{Atoms}_{total} = 4 \times \text{Unit cells}_{total}$$

Thus, the fraction of surface atoms is:

$$f = \frac{\text{Atoms}_{surface}}{\text{Atoms}_{total}}$$

For a 10 nm gold nanoparticle:

$$V_{total} = \frac{4}{3}\pi R^3 = \frac{4}{3}\pi(5)^3 \approx 523.6 \ \text{nm}^3$$

$$V_{core} = \frac{4}{3}\pi(5 - 0.2039)^3 \approx 462.1\ \ nm^3$$

$$V_{sheel} = V_{total} - V_{core} = 523.6 - 462.1 = 61.5\ \ nm^3$$

$$V_{unit} = 0.4079^3 \approx 0.068\ nm^3$$

$$\text{Unit cells}_{sheel} = \frac{V_{sheel}}{V_{unit}} = \frac{61.5}{0.068} \approx 904$$

$$\text{Atoms}_{surface} = 4 \times \text{Unit cells}_{sheel} = 4 \times 904 = 3616$$

$$\text{Unit cells}_{total} = \frac{V_{total}}{V_{unit}} = \frac{523.6}{0.068} = 7700$$

$$\text{Atoms}_{total} = 4 \times \text{Unit cells}_{total} = 4 \times 7700 = 30800$$

$$f = \frac{\text{Atoms}_{surface}}{\text{Atoms}_{total}} = \frac{3616}{30800} \approx 0.12$$

For a 2 nm gold nanoparticle:

$$V_{total} = \frac{4}{3}\pi R^3 = \frac{4}{3}\pi(1)^3 \approx 4.2\ \ nm^3$$

$$V_{core} = \frac{4}{3}\pi(1 - 0.2039)^3 \approx 2.1\ \ nm^3$$

$$V_{sheel} = V_{total} - V_{core} = 4.2 - 2.1 = 2.1\ \ nm^3$$

$$V_{unit} = 0.4079^3 \approx 0.068\ nm^3$$

$$\text{Unit cells}_{sheel} = \frac{V_{sheel}}{V_{unit}} = \frac{2.1}{0.068} \approx 31$$

$$\text{Atoms}_{surface} = 4 \times \text{Unit cells}_{sheel} = 4 \times 31 = 124$$

$$\text{Unit cells}_{total} = \frac{V_{total}}{V_{unit}} = \frac{4.2}{0.068} = 62$$

$$\text{Atoms}_{total} = 4 \times \text{Unit cells}_{total} = 4 \times 62 = 248$$

$$f = \frac{\text{Atoms}_{surface}}{\text{Atoms}_{total}} = \frac{124}{248} \approx 0.50$$

Question 3 – solution

The surface area of a 15 nm gold nanoparticle is:

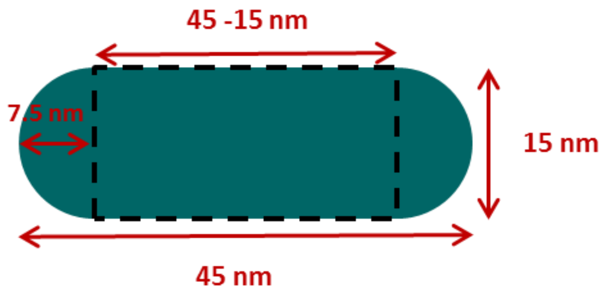
$$S_{sphere} = S_{15\ nm\ nanosphere} = 4\pi R^2 = 4\pi(7.5)^2 \approx 706.9\ nm^2$$

Thus, the number of PEG-SH molecules necessary to create a monolayer in a 15 nm gold nanosphere, $N_{SH\ 15\ nm\ nanosphere}$, is given by:

$$N_{SH\ 15\ nm\ nanosphere} = \frac{S_{15\ nm\ nanosphere}}{\text{Footprint}_{PEG-SH}} = \frac{706.9}{0.35} = 2020$$

The surface area of a 45×15 nm gold nanorod is:

$$S_{45\times15\text{ nm gold nanorod}} = S_{\text{lateral of cilinder}} + S_{\text{sphere}} = 2\pi Rh + 4\pi R^2$$
$$= 2\pi \times 7.5 \times (45 - 15) + 4\pi(7.5)^2 \approx 2120.6\text{ nm}^2$$



Thus, the number of PEG-SH molecules necessary to create a monolayer in a 45×15 nm gold nanorod, $N_{\text{SH }45\times15\text{ nm nanorod}}$, is given by:

$$N_{\text{SH }45\times15\text{ nm gold nanorod}} = \frac{S_{45\times15\text{ nm gold nanorod}}}{\text{Footprint}_{\text{PEG-SH}}} = \frac{2120.6}{0.35} = 6059$$