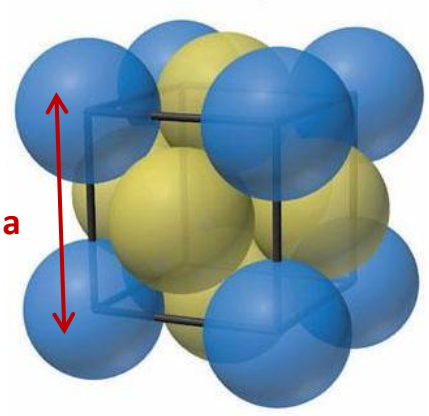
Problem sheet 2

Question 1

The lattice constant (**a**) refers to the constant distance between unit cells in a crystal lattice. Gold has a cubic face-centre-cubic (FCC) crystal structure with 4 atoms per unit cell (1/8 atom at 8 corners and ½ atom at 6 faces).



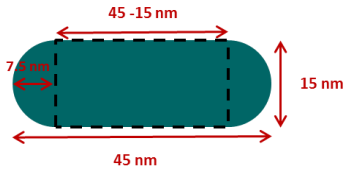
Calculate the lattice constant of gold. (The atomic radius of gold is 0.1442 nm).

Question 2

Taking the approach that there is an outer shell of atoms surrounding the core of the gold nanoparticle and that this shell has a finite thickness assumed to be half the lattice constant (calculated in Question 1), calculate the total number of atoms and the surface atoms of a gold nanoparticle of radius R.
Calculate the surface atom fraction for a 10 nm gold nanoparticle. How about the case of a 2 nm gold nanoparticle? What do you assume the surface atom fraction will be in comparison with the 10 nm?

Question 3

The surface modification of nanoparticles provides diversity in size, shape, solubility, long-term stability, and the possibility of attachment of selective functional groups. The fuctionalization strategies for gold nanoparticles have revolved around the use of thiol (SH) terminated polyethylene glycol (PEG) because of the very high specific binding affinity of gold to SH groups.
PEG-SH ligand has a "footprint" of 0.35 nm^2.[1,2] How many PEG-SH molecules are necessary to create a monolayer in a 15 nm gold nanoparticle? And in a 45×15 nm gold nanorod?



References

(1) Qian, X.; Peng, X. H.; Ansari, D. O.; Yin-Goen, Q.; Chen, G. Z.; Shin, D. M.; Yang, L.; Young, A. N.; Wang, M. D.; Nie, S. *Nature biotechnology* **2008**, *26*, 83.

(2) Wuelfing, W. P.; Gross, S. M.; Miles, D. T.; Murray, R. W. *J Am Chem Soc* **1998**, *120*, 12696.