Department of Materials Science and Engineering
Norwegian University of Science and Technology

TMT4320 Nanomaterials, fall 2015

EXERCISE 3

Guidance: Wednesday 9th September, 18:15-20:00, H3
Due date: Friday 11th September, 14:00, boxes outside R7 or on it's learning

PROBLEM 1

a) When nanoparticles are reduced in size below a certain level, their properties can no longer be described in terms of bulk properties. Explain why this happens. And why can a metal nanoparticle become a semiconductor below a certain size?

b) In the first approximation, the quantum-size effect can be described by a simple "quantum box" model, in which the electron motion is restricted in all three dimensions by impenetrable walls. For a spherical QD with radius R, this model predicts that a size-dependent contribution to the energy gap is simply proportional to $1/R^2$, implying that the gap increases as the QD size decreases. The following equation can be used to calculate the energy gap (E_g) for a semiconductor quantum dot, assuming the dot is a perfect sphere

$$E_g(\mathrm{QD}) = E_{g0} + \frac{\hbar^2\pi^2}{2m_{eh}R^2}$$

$$m_{eh} = \frac{m_e m_h}{m_e + m_h}$$

m_e = effective electron mass

m_h = effective hole mass

Given the values: $m_e = 0.19m$, $m_h = 1.21m$ and $E_{g0} = 3.2$ eV, calculate and graph E_g(QD) vs R for a ZnO quantum dot with a maximum size of 5 nm and a minimum size of 5Å. Here m = electron mass = 9.11×10^{-31} kg and $\hbar = 6.5821 \times 10^{-16}$ eV·s = 1.0546×10^{-34} J·s.

c) From the graph in the previous problem, find the critical radius where quantum size effects start to appear. Explain your answer.

PROBLEM 2

What is a zeolite? Describe the general structure and composition and give a few examples of technological applications of these materials.

PROBLEM 3

a) What is the difference between homogeneous and heterogeneous catalysis.

b) How does the catalyst affect the reaction path from reactants to products? Draw energy vs reaction path diagrams to explain how the catalyst accelerates the reaction.

c) Energetically, what is the main requirement for a reaction to take place, regardless of a catalyst being present or not?