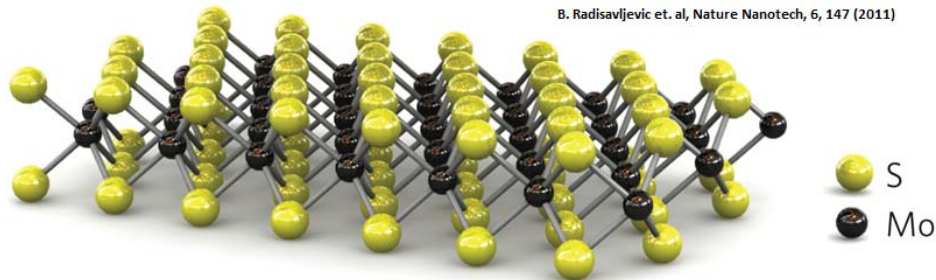


1. (40 points) After getting into a fight with your PhD adviser over the future of graphene ( $E_g=0$  eV) in electronic device applications, you now only have one weekend to prove that  $\text{MoS}_2$  ( $E_g=1.8$  eV, shown in figure) is a superior 2D optoelectronic materials platform. To do so you first need to assess  $\text{MoS}_2$  properties:



**Molybdenum disulfide is periodic.**

Image courtesy of Nature. From: Radisavljevic, B., A. Radenovic, et al. *Nature Nanotechnology* 6 (2011): 147–50 . Used with permission.

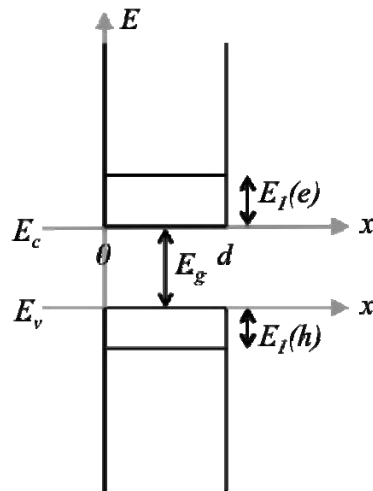
- a. (5 points) What is the general form for the wavefunctions of electrons in this material (given its symmetries)? Is momentum conserved in this material?
- b. (10 points) Assuming free electron behavior, derive the (2D) density of states for this material.

c. (10 points) Using your derived D.O.S. and the occupation probability function sketch the density of electrons in the conduction band at 0 K, room temperature, and high temperature.

d. (5 points) Considering the equation for conductivity in semiconductors, what properties are important for application of MoS<sub>2</sub> in electronics?

e. (10 points) What parameter(s) determine the emission spectra of MoS<sub>2</sub> for applications in optoelectronic devices such as LEDs? What color light would MoS<sub>2</sub> LED operate at? Why are you convinced that MoS<sub>2</sub> is a better choice for optoelectronics than graphene?

2. (40 points) Needless to say you have proven your adviser wrong, since you have successfully completed your PhD and joined your grad school buddy Kapsid at Samsung's ultra-thin display research group. Kapsid can't help but wonder how come his virus-based BioBulb display barely glows, while your quantum dot (QD) light emitting devices (LEDs) shine in brilliant colors at device thicknesses  $< 10$  nm. To save your friendship you need to explain the materials science behind your success to Kapsid. As you approach the board, you hope that your 3.024 memories haven't gotten too rusty....



- a. (10 points) Electrons and holes in QDs can be approximated as particles in infinite potential wells shown above. Then the bandgap in a QD can be calculated as  $E_g' = E_g + E_n(e) + E_n(h)$ , where  $E_n(e/h)$  are the energy levels of the particle in a 1D infinite well. Find the general expressions for  $E_n(e)$  and  $E_n(h)$ .

- b. (10 points) Assume  $n = 1$  for both  $E_n(e)$  and  $E_n(h)$ . Calculate the QD diameters that would allow you to achieve band gaps corresponding to  $\lambda = 460$  nm (blue), 530 nm (green), 630 nm (red) using only CdSe as your material.

Useful CdSe properties:

Bulk band gap  $E_g = 1.73$  eV

Electron effective mass  $m_e^* = 0.13m_e$

Hole effective mass  $m_h^* = 0.45m_e$

- c. (5 points) Could we have used GaN ( $E_g=3.4$  eV,  $m_e^*=0.19m_e$ ,  $m_h^*=0.6m_e$ ) instead of CdSe for these LEDs?
- d. (15 points) In your QD-LED display, the QDs are embedded in a polymer binder with a refractive index  $n_{poly}=1.6$ . The refractive index of the display glass is  $n_{glass}=1.5$ . Choose the best refractive index for the anti-reflection coatings at the polymer-glass (5 points) and glass-air interfaces (5 points) ( $n_{air}=1$ ). What would be the optimal thickness of each for  $\lambda=530$  nm light (5 points)?

3. (40 points) *Despite your best intentions your friendship with Kapsid was shattered by a scientific dispute. To your surprise you (now a professor at MIT) meet Kapsid (now a professor at Stanford) at the research grant completion for the next best infrared photodetector at the Army Research Office (ARO). While Kapsid's proposal focuses on trendy photosynthesis-based Virabsorbers, your results indicate that thin-film Ge ( $E_g=0.67$  eV,  $\rho=4.4\times 10^{22}$  cm<sup>-3</sup>,  $n_i=2.0\times 10^{13}$  cm<sup>-3</sup>) outperforms the biological counterpart. Now all you need is for the ARO to agree with you, so go to work:*
- a. (5 points) You decided to fabricate a Ge *pn*-junction for the IR photodetectors. Pick appropriate dopants for *p* and *n* regions of your detector. (Please use only non-volatile compounds as dopants).
- b. (10 points) Draw the band diagram for Ge doped with 1 ppm of donors on the *n*-side and 5 ppm of acceptors on the *p*-side. What is the built-in potential?

- c. (15 points) Draw the charge density profile in the depletion region. Is the width of the depletion region symmetric with respect to the position of the  $p$  and  $n$  materials' junction (7 points)? How do you expect it to change when we apply voltage in the direction of built-in potential (4 points)? In the direction opposing the built-in potential (4 points)?
- d. (10 points) Draw the characteristic current-voltage plot for this device. How does it change under  $\lambda=2500$  nm illumination (5 points)? What about  $\lambda=1500$  nm (5 points)? Label the important features of the  $I$ - $V$  curve under illumination.

4. (30 points) Crushed by his scientific losses Kapsid tries to boost his powers with genetic modification. Unfortunately, in addition to giving him the regenerative powers his experimental protocol also turns him into the vicious monster, Genomod. Now, it's up to you and Major Riker (an attractive Navy officer) to stop him from destroying the planet. Where the bullets and bombs have failed to stop Genomod's regenerative powers, only the uniformly dispersed heating from hysteretic power losses in single-domain ferromagnetic nanoparticles might succeed. As you signal to Riker to throw the switch on the World's largest magnetic field generator, you inject the monster with iron oxide ( $\text{Fe}_3\text{O}_4$ ) nanoparticles and frantically run through the calculations once more in your head:

Lattice constant  $a = 8.4 \text{ \AA}$

Exchange integral  $J = 100 \text{ meV}$

Anisotropy energy density  $K_u = 1.4 \times 10^4 \text{ J/m}^3$

- a. (10 points) Draw the  $M$  vs.  $H$  curves for the single-domain ferromagnetic nanoparticles for the cases when  $H$  is parallel to the easy magnetic axis or the hard magnetic axis (7 points). For which direction of the applied field will the energy dissipation be maximized (3 points)?
- b. (10 points) For iron oxide, find the upper limit of power dissipation in the nanoparticles by using the area of the maximum hysteresis loop from part (a) in a 1 MHz alternating magnetic field (don't forget to use/include appropriate limits) (7 points). Does this area depend on the magnitude of the applied field? (3 points)



- c. (10 points) How small do these nanoparticles actually need to be so we can approximate them as single domain ferromagnets, which you used for calculations in (a) and (b) (Single-domain = cannot contain a domain wall).

The energy of the domain wall is given by:  $\sigma_{BW} = \sigma_{BW}^{ex} + \sigma_{BW}^a = JS^2 \frac{\pi^2}{a^2 N} + \frac{NK_u a}{2}$ ,

where  $N$  is the number of the lattice cells constituting the domain wall,  $a$  is a lattice constant, you can use  $S = \frac{1}{2}$ , the exchange integral  $J$  and the magnetic anisotropy energy density  $K_u$  are given above. The domain wall size is defined by the minimum wall energy.

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3.024 Electronic, Optical and Magnetic Properties of Materials  
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