Homework #3

Spring 2016

Due date: April 11^{th} in class (hard copy print out).

ECE 6307 – Nanomaterials and Solar Energy, CHEE6320 -Introduction Nanomaterials Engineering, MTLS6320 - Nanomaterials Engineering, CHEE5320 – Introduction to Nanomaterials Engineering
ECE5320 - Introduction to Nanomaterials Engineering, MECE5320- Introduction to Nanomaterials Engineering,

Student Name ____

Student ID ____

Instructions: The first page of this HW assignment has to be incorporated into your material HW. Make sure this page is signed and has your information. Students, your work (hard copy) has to be handed to the instructor at the indicated due date. Make sure your HW is typed in MS work or similar software. Handwritten submission will not be accepted. Exceptions applies to sketches that should be explanatory to your derivations or problem posting. Only independent work will be granted points. Work in the group, consulting among the students, or other type of collaboration is strictly forbidden. Student who violate this rule will be subject to the college academic honesty hearing. Problems with * marking indicate also the question that could occur on your midterm/final exam. Bonus problems are not mandatory, but could bring you extra points.

Student Signature ____

Points________________/_______________

Designation	Symbol	Value	Units*
Atomic mass unit	u	1.660 566 (−27)	kg
Avogadro's constant (number)	N	6.022 045 (+26)	$kmol^{-1}$
Boltzmann constant	k	1.380 662 (−23)	$J \cdot K^{-1}$
Electric field constant	ϵ_0	8.854 223 (−12)	$C^2 \cdot N^{-1} \cdot m^{-2}$
Electronvolt	eV	1.602 190 (−19)	J
Electron charge	e^-	1.602 190 (−19)	C
Faraday constant	$\mathscr{F}$	9.648 456 (+07)	$C \cdot kmol^{-1}$
Gravitational acceleration	g	9.806 650 (+00)	$m \cdot s^{-2}$
Gravitational constant	G	6.672 000 (−11)	$N \cdot m^2 \cdot kg^{-2}$
Magnetic field constant	μ_0	1.256 640 (−06)	$N \cdot A^{-2}$
Mass of electron (rest)	m_e	9.109 534 (−31)	kg
Mass of neutron (rest)	m_n	1.674 954 (−27)	kg
Mass of proton (rest)	m_p	1.672 649 (−27)	kg
Planck constant	h	6.626 176 (−34)	$J \cdot s$
Speed of light in vacuum	c	2.997 925 (+08)	$m \cdot s^{-1}$
Speed of sound in air, 0°C	c_s	3.313 621 (+02)	$m \cdot s^{-1}$
Standard atmosphere	atm	1.013 250 (+05)	Pa
Standard kilomole volume	V_0	2.241 383 (+01)	$m^3 \cdot kmol^{-1}$
Thermochemical calorie	cal	4.184 000 (+00)	J
Universal gas constant	R	8.314 410 (+03)	$J \cdot K^{-1} \cdot kmol^{-1}$

Problem 1. (2)

The measurements of the index of refraction of polymer-TiO2 NP composite as a function of TiO2 NP concentration is shown in the table below. Using this data, after reading material from the book, determine the index of refraction of TiO2-NP, and polymer matrix. Explain your approach in detail.

n_R	1.5	1.52	1.54	1.55	1.56	1.57	1.58	1.59	1.60
C / vol%	0	3	5	7	8	9	10	11	12

Problem 2. (1)

Assuming that you solved problem 1, and that you know the refractive index of your TiO2-NP and your polymer matrix, find out what is $P_{scatter}/(\kappa \cdot P_0)$ ratio for this composite for light with wave length 600 nm (vacuum) if the size of TiO2-NP is 100 nm. Calculate your result for each concentration of TiO2-NP shown in the table above. If the nanoparticle size is decreased 2 times, and light wavelength is decreased 6 times, how many times the $P_{scatter}/(\kappa \cdot P_0)$ ratio for this composite will change?

*Problem 3. (1)

Using particle in the box approach to calculate the energy of an electron as a function of the quantum level n, and size of the system L, calculate the wavelength of the light that would be required to excite the electron from the ground state with quantum number n, to an excited state with quantum number n+3. If the size of the NP changes 4 times, how many times will change the wavelength of the light required for this excitation.

*Problem 4. (1) BONUS

Explain the meaning of the common term stating that the wavelength of the absorbed light by NP is "blue shifted" as compared to the wavelength of the light absorbed by bulk material.

*Problem 5. (2)

In the table below the results from the measurements of the light absorption for two different average size of CdS nanoparticle population are presented. Find out what is the difference between band gap energies of these two population of CdS NP.

Photon Energy/eV	4.5	4.7	5	7.1	8	8.6	9
5 nm CdS NP/$(\alpha h\nu)^n$	0.15	0.25	0.4	1.45	1.9	2.2	2.4
10 nm CdS NP / $(\alpha h\nu)^n$	0.45	0.55	0.7	1.75	2.2	2.5	2.7

*Problem 6. (1)

For PbS NP, the luminescence intensity is a function of NP size. Explain how the intensity of luminescence changes if the PbS NP size decreases and why?

*Problem 7. (2) BONUS

Consider ZrO2-NP/PMMA combination. Luminesce peak of ZrO2 NP/PMMA is measured as a function of ZrO2 NP size. Data are shown in the table below. Using this data and reading a book, find out what should be luminescence of 2 nm and 70 nm ZrO2-NP/PMMA.

NP size/ nm	10	20	30	40	50
Peak, λ / nm	312	386	396	398	399

*Problem 8. (1)

In one or two sentences explain what is the plasmon?

Problem 9. (1)

Explain how the electroluminescence light intensity depends on current density of the device for CdSe/PPV multilayer system.

*Problem 10. (1)

What are the typical photochromic and electrochromic materials? Explain why? (no more than 100 words)

Problem 11 (2) BONUS

In the table below the characterization measurements for two stacks of Fe2O3 NP are shown. In the first set, the Fe2O3 NP have mean size of 10 nm, and the angle of polarized light rotation passing through the stack of NP (Faradays effect) is measured as a function of magnetic field. In the second set the of data, the stack of Fe2O3 NP with unknown size is investigated using the same measurements. What is the size of NP in the second experiment?

Exp 1.

B / T	0.1	0.3	0.5	1	1.5	2
β/ rad	0.1	0.3	0.5	1	1.5	2

Exp.2

B / T	0.2	0.3	0.4	0.5	0.7	0.85
β/ rad	0.7	1.05	1.4	1.74	2.45	NA

*Problem 12 (1).BONUS

What is the role of TiO2 NP in the Gratzel Cell. (2-3 sentences).

Problem 13 (1).

Draw the structure of typical dye molecule used in the Gratzel Cell

Problem 14 (1)

What is the purpose of I_3^-/I^- redox couple in Gratzel Cell (2-sentences).

Problem 15(1)

Draw the relative to each other the energy level of the TiO2 conduction band, energy level of LUMO of the dye, and energy of the HOMO of I^- complex.