Chemistry for Engineers
CHEM 141
Lab 8: CdS Nanoparticles

Dr. Hahn

Use wavelength of light to get size (r = radius) of CdS nanoparticles

Cd S bulk

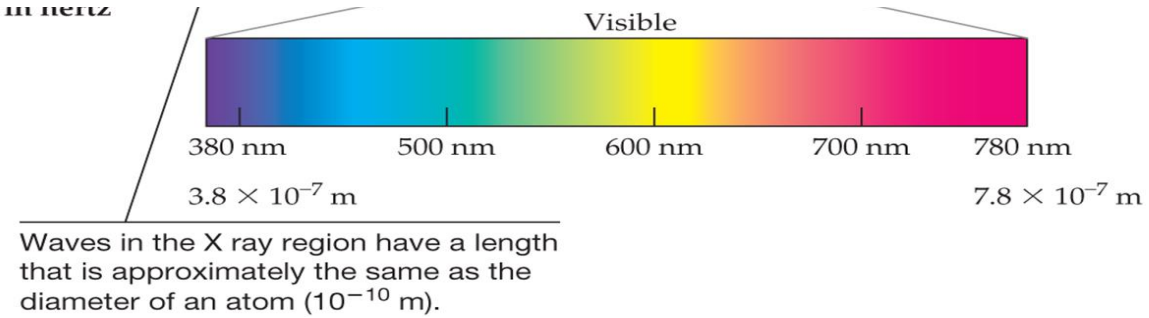
$CdCl_2 + Na_2S$

CdS nano in micelles

orange (I do)

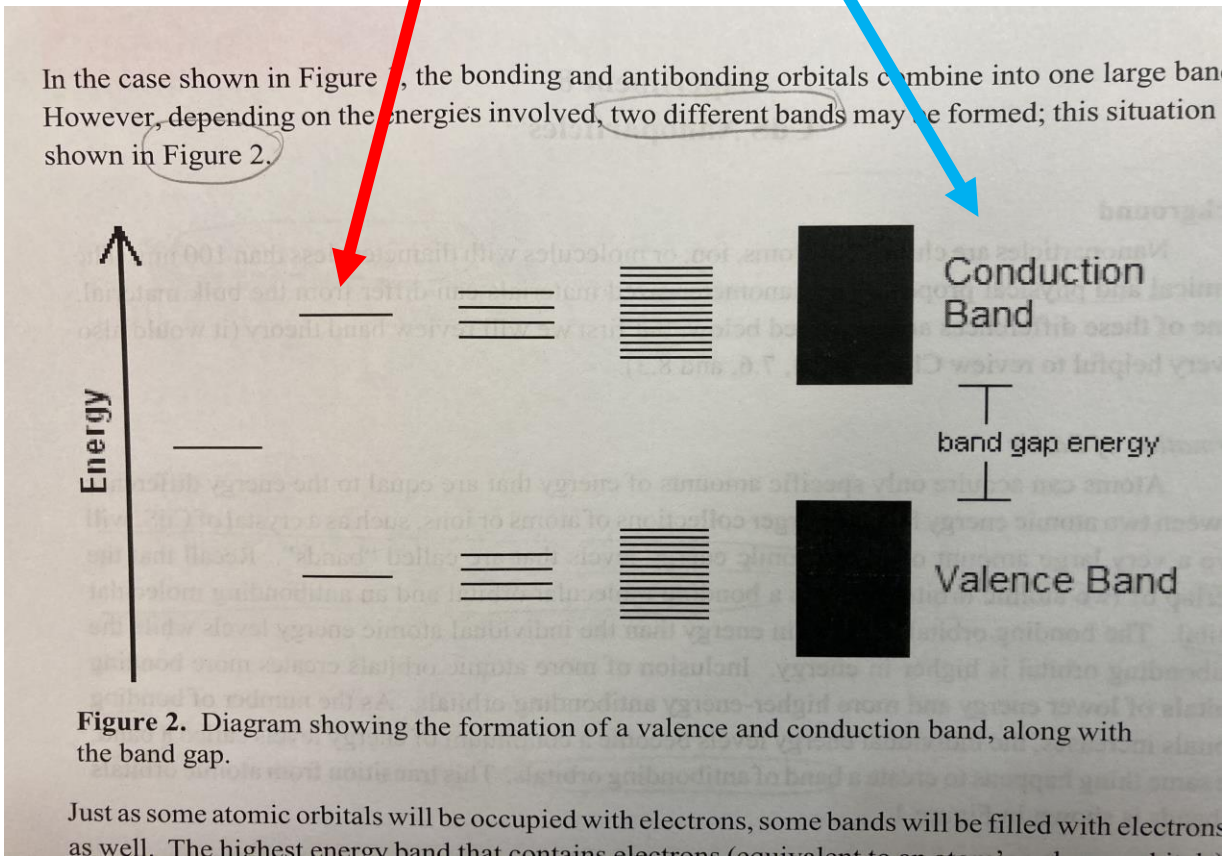
blue shift (higher Energy) (nano higher E band gap)

yellow (you do)



Waves in the X ray region have a length that is approximately the same as the diameter of an atom (10^{-10} m).

Energy difference between bonding & antibonding molecular orbitals but with a large number of molecules goes to valence band & conduction band



Energy difference between valence band & conduction band - larger for smaller broken down nano size (in micelle) CdS than for normal sized (bulk) CdS

In the case shown in Figure 1, the bonding and antibonding orbitals combine into one large ban
However, depending on the energies involved, two different bands may be formed; this situation
shown in Figure 2.

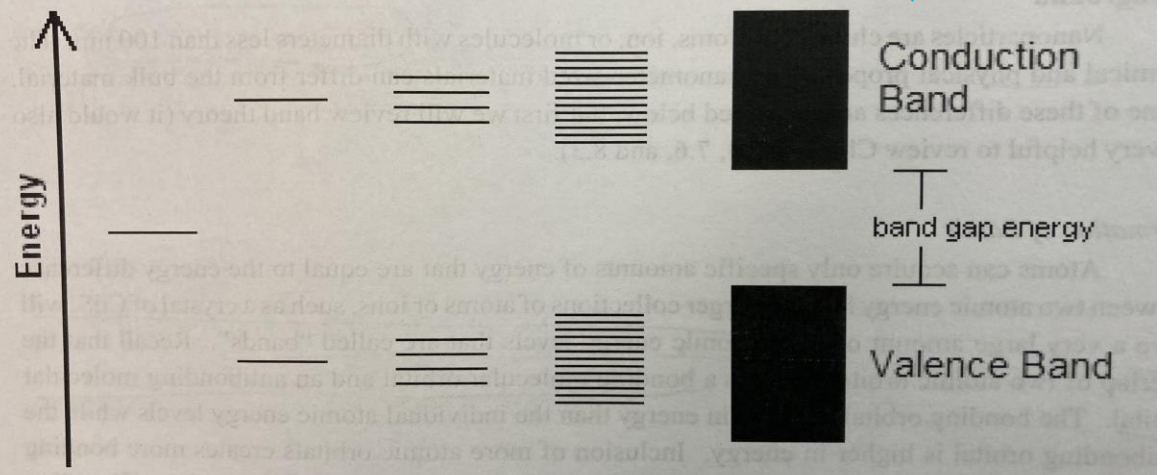
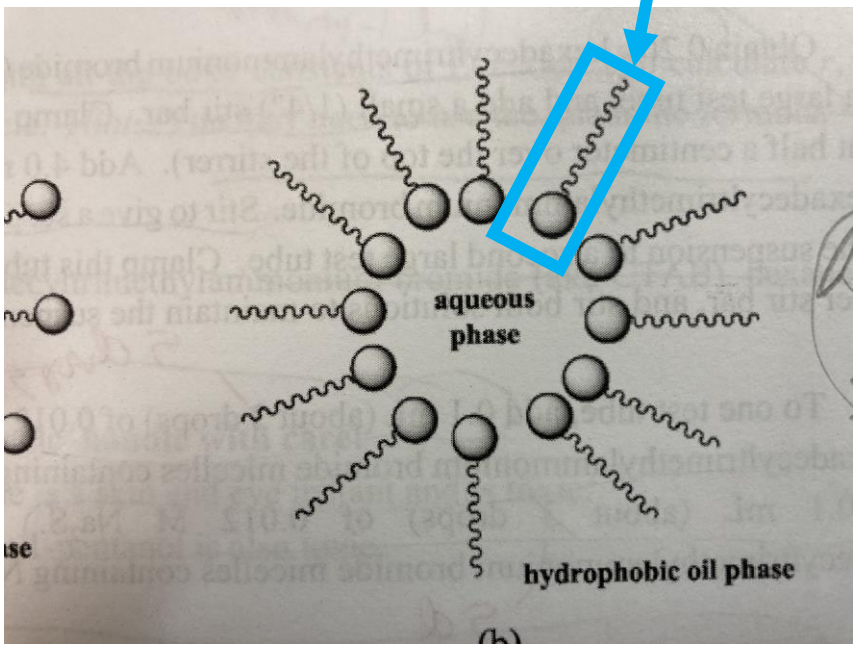


Figure 2. Diagram showing the formation of a valence and conduction band, along with the band gap.

Just as some atomic orbitals will be occupied with electrons, some bands will be filled with electrons
as well. The highest energy band that contains electrons (equivalent to an atom's

How do you get nano size CdS , use micelles (using hexadecyl trimethyl ammonium bromide)



Bulk CdS (I make) orange

- 1 mL of 0.012 M CdCl2 + 1 mL of 0.012 M Na_2S

  small energy difference in band gap

Nano CdS (you make) yellow

No water in your test tubes (TT) – MUST BE DRY – clamp to stand, use magnetic stirrer inside TT (modifications verbally from lab coordinator – Jim Wilkerson)

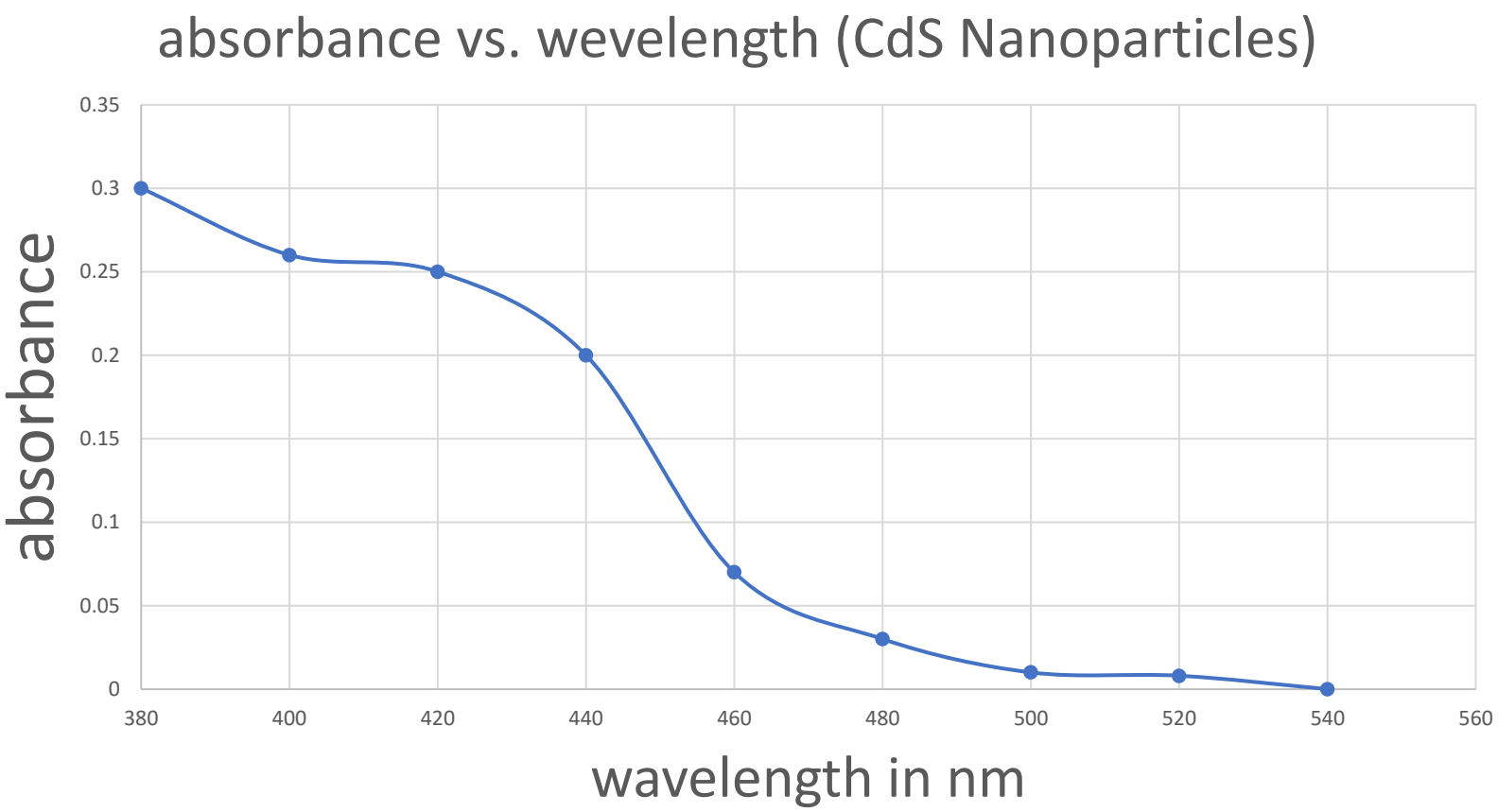
(a) TT1: Get about 0.20 g CTAB (between 0.20 to 0.15 grams)+ 4.0 mL hexane + 1.0 mL 1-pentanol (use 10 mL graduated cylinder)
(b) TT2 = ½ of TT1
(c) TT1: add 3 drops of 0.012 M $CdCl_2$
(d) TT2: add 5 drops of 0.012 M Na_2S
(e) Combine TT1 & TT2 into TT1
(f) Get 2 cuvettes
(g) cuvette 1 = hexane cuvette 2 = your nano CdS
(h) Manually set wavelength to 530 nm: hexane zero spectrometer (every time) & then do nano CdS & write down wavelength & Absorbance #

530 nm, 510 nm, 490 nm, 470 nm, 450 nm, 430 nm, 410 nm, 390 nm, 380 nm

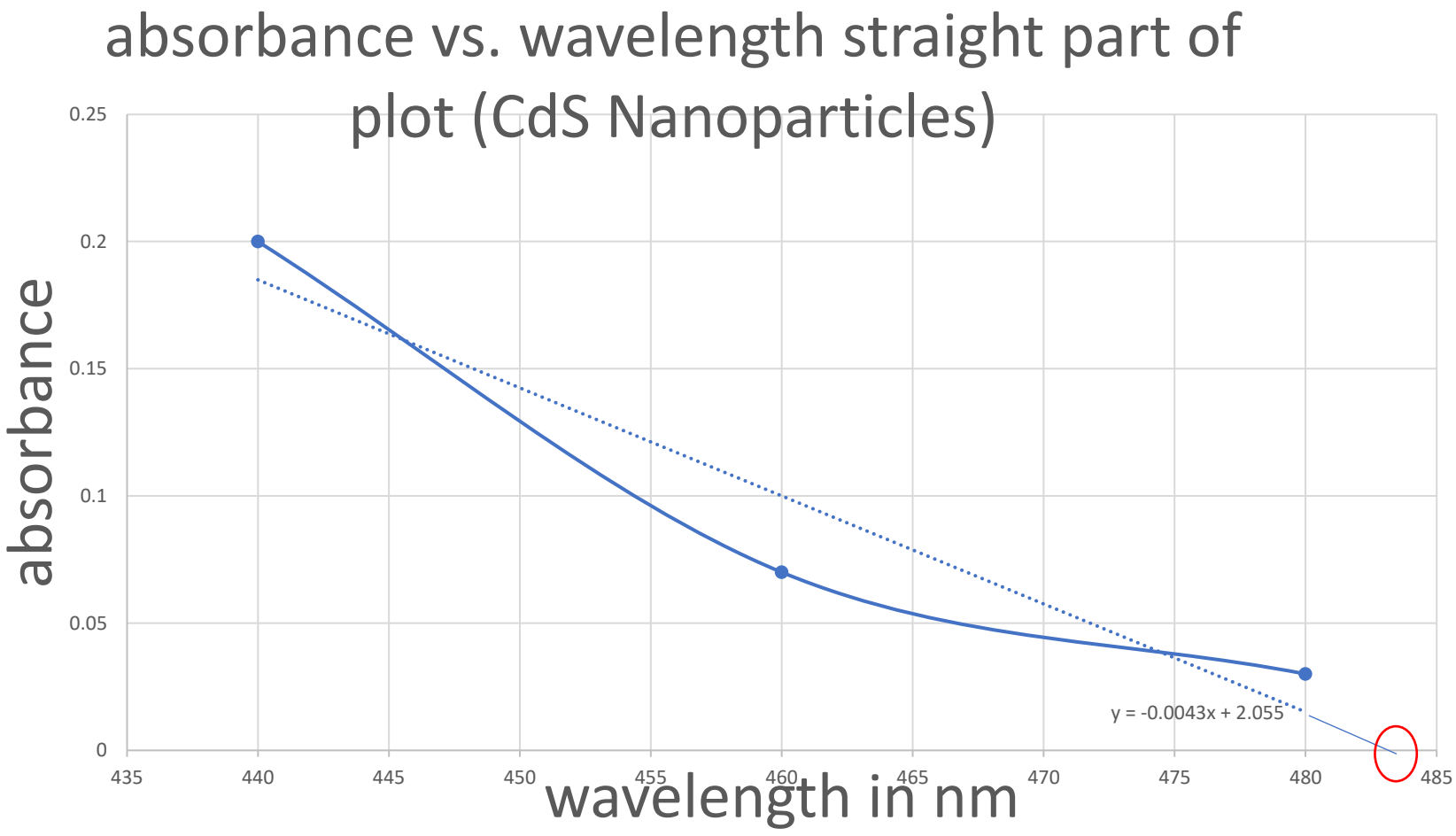
Expected Good Data collected during lab.

wavelength	Absorbanc
380	0.3
400	0.26
420	0.25
440	0.2
460	0.07
480	0.03
500	0.01
520	0.008
540	0

Final Plot of Spectra



Plot straight line over linear part of plot – showing cutoff wavelength of 483 nm cross zero Absorbance (correct is around 474.8 nm)



Solve for r (radius of the nano particle)

$$E_g^{nano} = E_g^{bulk} + \frac{h^2}{8r^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] - \frac{1.8\,e^2}{4\pi\,\mathcal{E}\,\mathcal{E}_o\,r}$$

$E = \frac{hc}{\lambda}$ $h = 6.626 \times 10^{-34}$ Js $c = 3.00 \times 10^{8}$ m/s

$\lambda = 474.8$ nm (from published JCE 2007)

(use your data λ here from your plot) = 4.19×10^{-19} J

$E_g^{bulk} = 3.88 \times 10^{-19}$ J $m_e^* = 1.73 \times 10^{-31}$ kg

$m_h^* = 7.29 \times 10^{-31}$ kg $e = 1.602 \times 10^{-19}$ c

$\pi = 3.14159$ $\mathcal{E} = 5.7$

$\mathcal{E}_o = 8.854 \times 10^{-12}$ $c^2\,s^2/(kg\,m^3)$

After algebra:

$0 = 3.93 \times 10^{-37} - (r)7.29 \times 10^{-29} - (r^2)(4.19 \times 10^{-19} - 3.88 \times 10^{-19})$

$0 = c \quad - r * b \quad - \quad r^2$ (a)

Use quadratic → $r = 2.56 \times 10^{-9}$ m

(CdS nano particle radius)

$$r = \frac{-b +/- \sqrt{b^2 - 4ac}}{2a}$$

$E = \frac{hc}{\lambda}$ $h = 6.626 \times 10^{-34}$ Js $c = 3.00 \times 10^{8}$ m/s

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(use your data λ here from your plot) = 4.19×10^{-19} J