Name : Dipesh Digwal

Roll No. : 170121015

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Quantum Dots

Objectives

- Calculate the band gap energy of CdSe quantum dot
- Study the variation of band gap energy of CdSe quantum dot with the size of the strucure
- Calculate the fundamental absorption wavelength with the size of CdSe quantum dot.
- Study some applications of quantum dots in industry.

Theory

- ## Methodology used for making Quantum Dot

The organic synthesis method uses pyrolysis to engineer quantum dots by infusing organometallic reagents into hot coordination fluid (300°C) such as triocytlphosphine (TOP) and triocytlphosphine oxide (TOPO), these are also called capping reagents and the reaction medium. These hydrophobic organic molecules helps in the prevention of formation of bulk semiconductor by coordinating with the unsaturated metal atoms on the surface of quantum dots. For maintaining the optical properties of the quantum dot triocytlphosphine oxide (TOPO) and triocytlphosphine (TOP) organic ligands are used. These ligands also protect core from the medium

- ## Characterisation used for determining band-gap

For describing properties of semiconductors , I am using model of free electrons and free holes. The lowest unoccupied and highest occupied band have energy difference defined by Eg(bulk). Expecting energy diversion relations to be still parabolic in quantum dot. The energy levels of a quantum dot are approximated by particle in a box model.

$$E_{\text{well, 3d(cube)}} = 3\ E_{\text{well, 1d}} = 3/8\ h^2/md^2$$

For a spherical box of diameter d , equations can be written as

$$E_{\text{well, 3d(sphere)}} = 1/2\ h^2/md^2$$

$$E_{\text{well}} = h^2/2m^*d^2$$

$$1/m^* = 1/m_e + 1/m_h$$

For calculating energy amount required in creating an electron-hole pair, columbic energy is considered

$$E_{\text{Coul}} = -1.8\ e^2/2\pi\varepsilon\varepsilon_0 d$$

Thus energy gap in quantum dot will be

$$E_g(\text{dot}) = E_g(\text{bulk}) + E_{\text{well}} + E_{\text{Coul}}$$

$$E_g(d) = E_g(\text{bulk}) + h^2/2m^*d^2 - 1.8\ e^2/2\pi\varepsilon\varepsilon_0 d$$

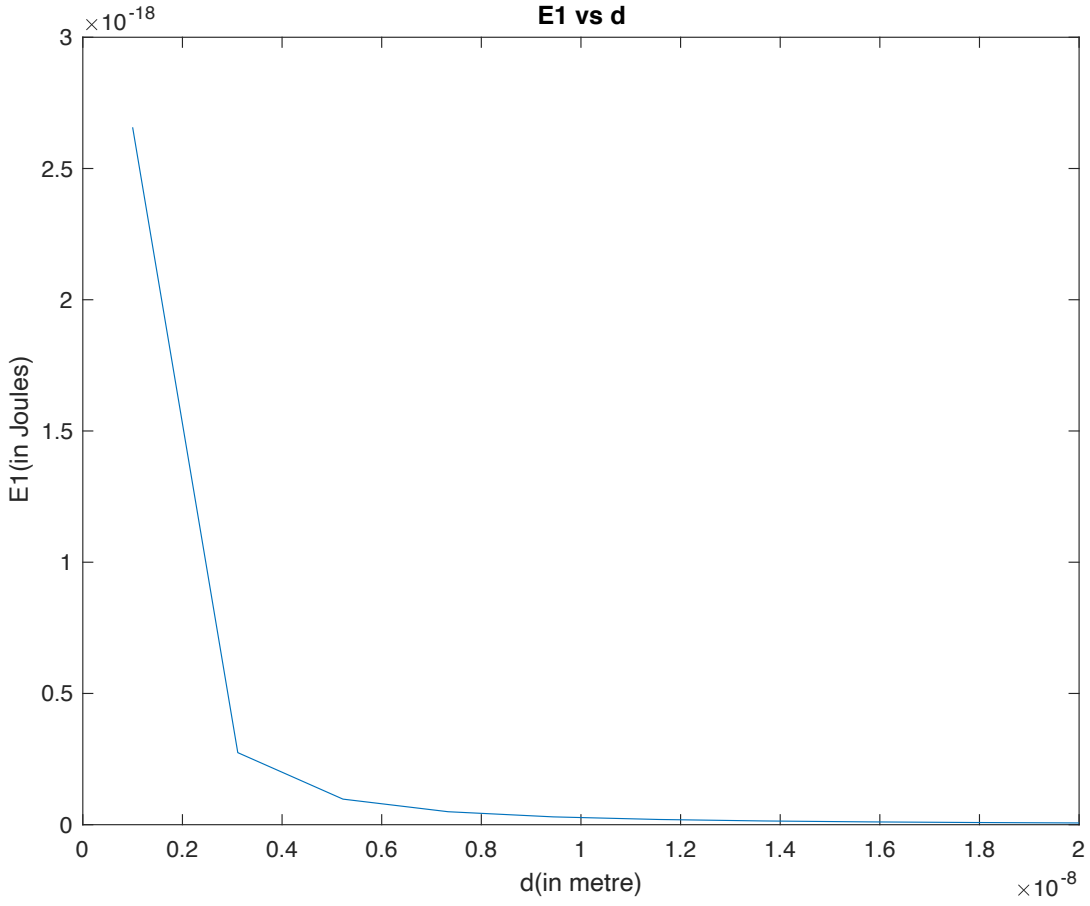
Calculation

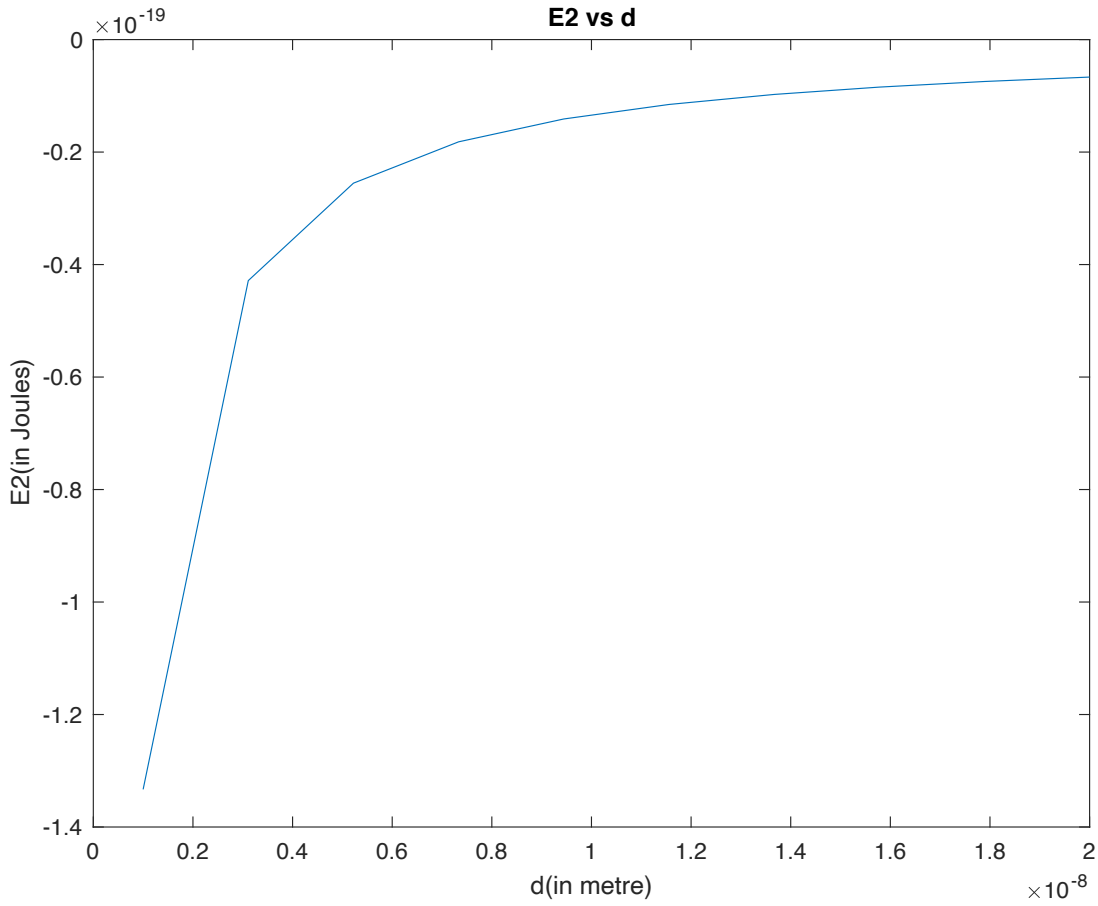
MATLAB Code:

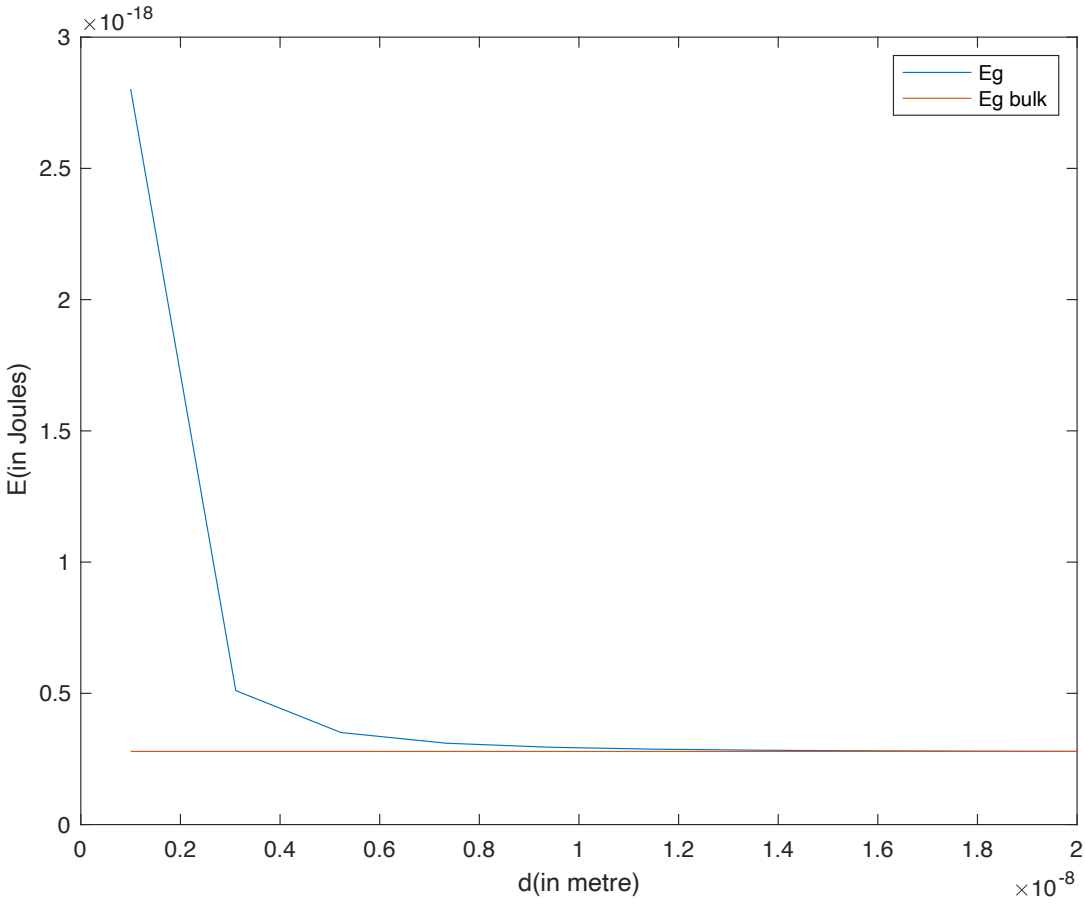
```
1)  sympref('FloatingPointOutput',true);
2)  syms d E1(d) E2(d) E(d) lambda(d);
3)  Eg_bulk=1.74*1.60218e-19;
4)  h=6.62607015e-34; %plank's constant
5)  e=1.602176634e-19; %electronic charge
6)  epsilon_0=8.854187817e-12; %epsilon not
7)  pi=3.141592653589793238;
8)  c=299792458; %speed of light(metre/sec)
9)
10) %CdSe constants
11) Me=0.13*9.10938356e-31; %effective mass of electron
12) Mh=0.3*9.10938356e-31; %effective mass of hole
13) epsilon=6.23; %epsilon for CdSe
14)
15) %band gap energy dependence on crystal size
16) E1(d)=((h^2/(2*d^2))*(Me^-1+Mh^-1));
17) E2(d)=-((0.9*e^2)/(pi*epsilon*epsilon_0*d));
18) E(d)=Eg_bulk+E1(d)+E2(d);
19) lambda(d)=(h*c)/E(d); %absorption wavelength
20)
21) %get values of E,E1,E2,lambda with variation of d in range[1-20](nanometres)
22) d1=linspace(1e-9,20e-9,10)';
23) E11=double(E1(d1));
24) E22=double(E2(d1));
25) EE=double(E(d1));
26) lambda2=double(lambda(d1));
27) t=table(d1,E11,E22,EE,lambda
```

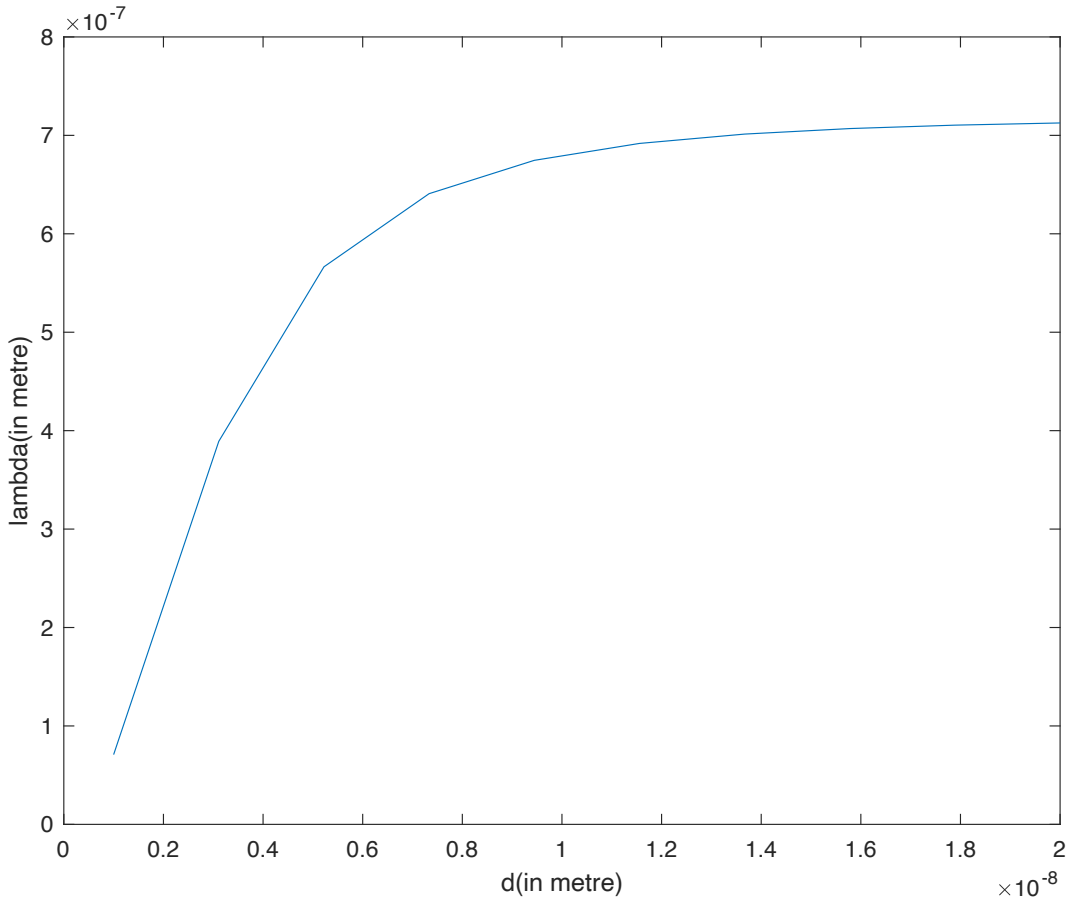
Table and Figures

	1 d	2 E1	3 E2	4 E	5 lambda	6
1	1.0000e-09	2.6570e-18	-1.3331e-19	2.8025e-18	7.0881e-08	
2	3.1111e-09	2.7451e-19	-4.2851e-20	5.1044e-19	3.8916e-07	
3	5.2222e-09	9.7429e-20	-2.5528e-20	3.5068e-19	5.6646e-07	
4	7.3333e-09	4.9408e-20	-1.8179e-20	3.1001e-19	6.4077e-07	
5	9.4444e-09	2.9788e-20	-1.4116e-20	2.9445e-19	6.7462e-07	
6	1.1556e-08	1.9898e-20	-1.1537e-20	2.8714e-19	6.9180e-07	
7	1.3667e-08	1.4226e-20	-9.7547e-21	2.8325e-19	7.0130e-07	
8	1.5778e-08	1.0673e-20	-8.4495e-21	2.8100e-19	7.0691e-07	
9	1.7889e-08	8.3029e-21	-7.4524e-21	2.7963e-19	7.1038e-07	
10	2.0000e-08	6.6426e-21	-6.6657e-21	2.7876e-19	7.1261e-07	
11						
12						
13						
14						
15						




E2 vs d
×10^-19
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
E2(in Joules)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
d(in metre)
×10^-8


×10^-18
3
2.5
2
1.5
1
0.5
0
E(in Joules)
Eg
Eg bulk
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
d(in metre)
×10^-8


×10^-7
8
7
6
5
4
3
2
1
0
lambda(in metre)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
d(in metre)
×10^-8

Applications

- Making light sensing devices like we have photovoltaics made from semiconductor diodes.
- In Biology, quantum dots can be used as organic dyes because of their flexibility over traditional methods.
- In chemistry, quantum dots can be used as photocatalysis to finely control the reaction of light driven reactions.

Conclusion

- From the plot of E1 vs d and E2 vs d we can conclude that band gap energy variation is only prevalent at size of around 10nm and below.
- Similarly plot of E vs d(with Eg(bulk) denoted) shows that for only sizes below 10nm the variation in bandage energy of quantum dot are seen.
- From the wavelength spectra variation with size it can be seen that light can be emitted in the visible region of electromagnetic spectrum very easily by just controlling size.
- Applications of quantum dots in industry are truly explored.

References

1. https://www.sigmaaldrich.com/technical-documents/articles/materials-science/nanomaterials/quantum-dots.html ————————(types of QDs)
2. Baskoutas, Sotirios & Terzis, Andreas. (2006). Size-dependent band gap of colloidal quantum dots. Journal of Applied Physics. 99. 013708 - 013708. 10.1063/1.2158502.
3. http://bme240.eng.uci.edu/students/07s/yokabe/synthesis.htm