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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 entails pyrolysis to make quantum dots by injecting organometallic reagents into hot coordination fluid (300˚C) such as triocytlphosphine (TOP) and triocytlphosphine oxide (TOPO), which are used as capping reagents and the reaction medium [2,9]. These hydrophobic organic molecules prevents the formation of bulk semiconductor formation by coordination with the unsaturated metal atoms on the surface of quantum dots [2]. The TOPO and TOP organic ligands in the inner surface of quantum dots are important for maintaining the optical properties of the dot and also protects the core from the medium

- ## Characterisation used for determining band-gap

Some basic properties of semiconductors can be described by model of free electrons and free holes.the lowest unoccupied and highest occupied band are separated by band gap Eg(bulk). Expecting energy diversion relations to be still parabolic in quantum dot. The energy levels a quantum dot are estimated 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

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

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

$$1/m^* = 1/m_{\text{e}} + 1/m_{\text{h}}$$

In order to calculate energy required to create an electron-hole pair, columbic energy has to be considered

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

Thus energy gap in quantum dot will be

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

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

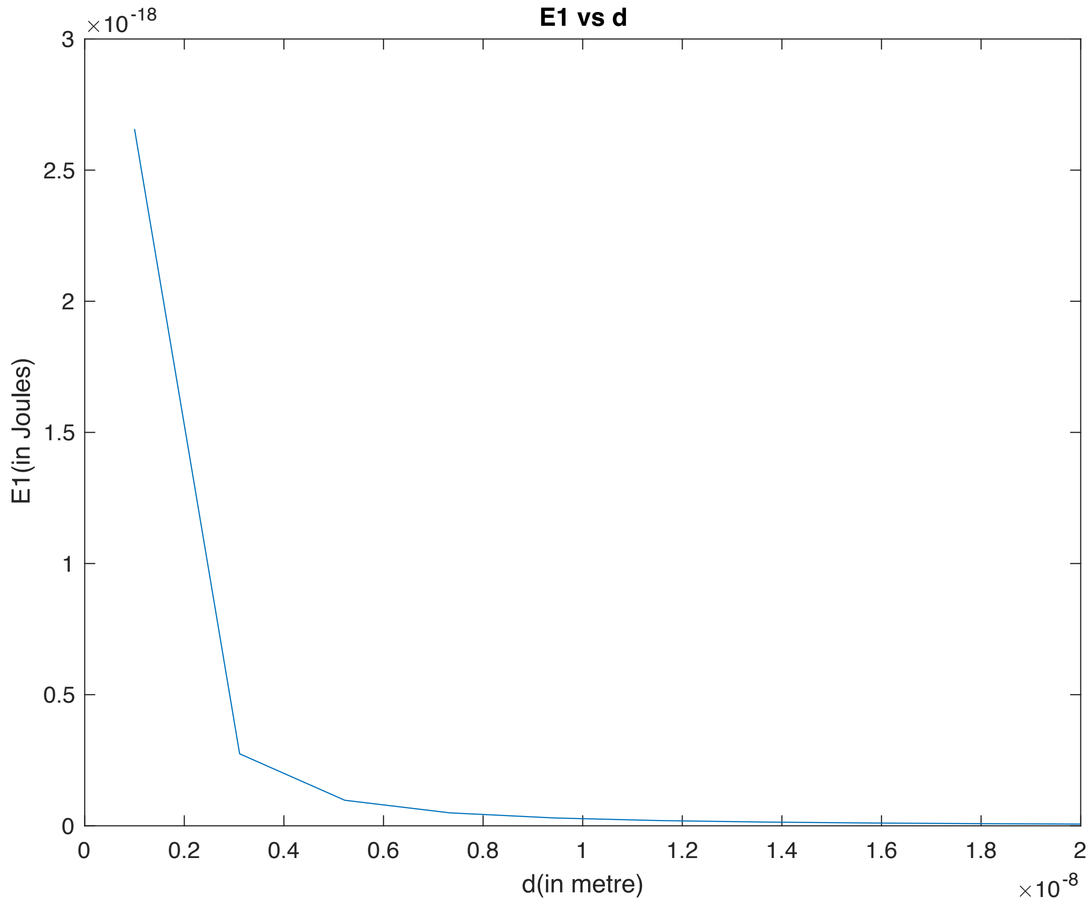
Calculation

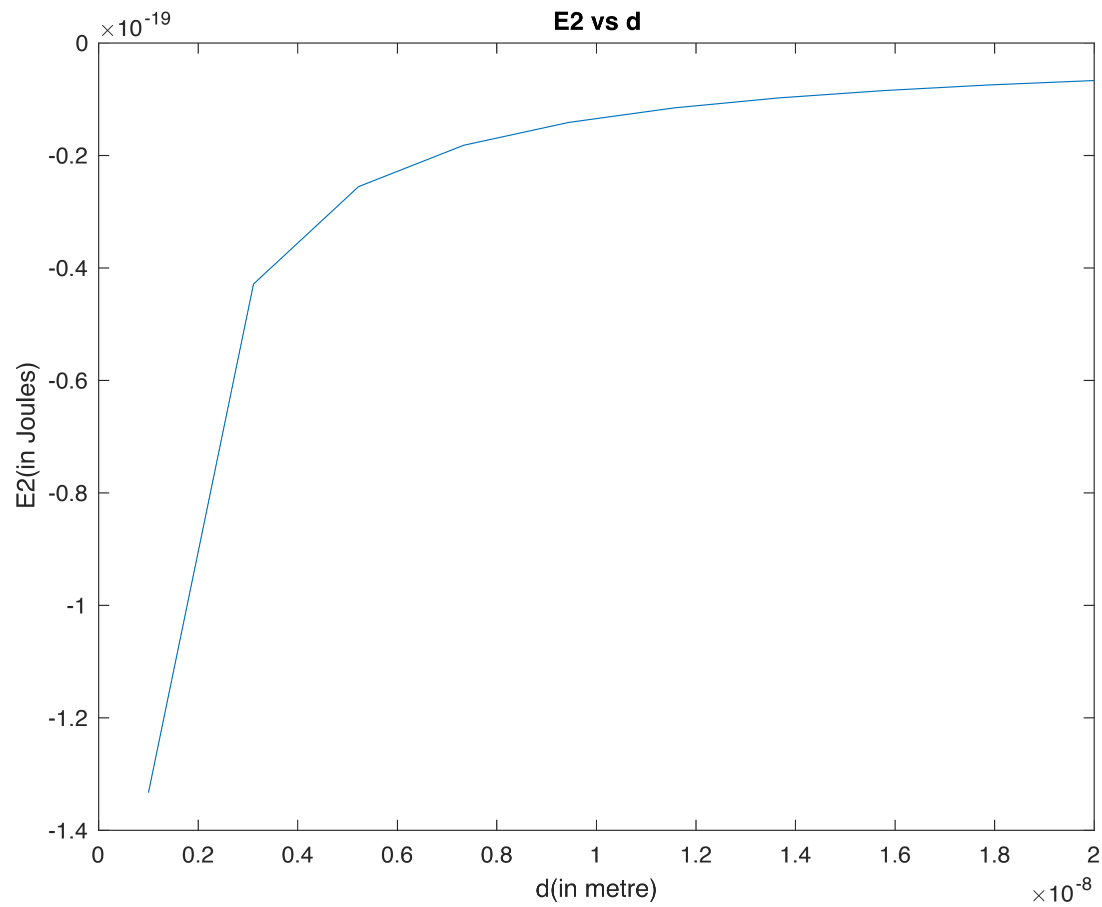
MATLAB Code:

```
sympref('FloatingPointOutput',true);
syms d E1(d) E2(d) E(d) lambda(d);
Eg_bulk=1.74*1.60218e-19;
h=6.62607015e-34; %plank's constant
e=1.602176634e-19; %electronic charge
epsilon_0=8.854187817e-12; %epsilon not
pi=3.1415926535897932 38;
c=299792458; %speed of light(metre/sec)

%CdSe constants
Me=0.13*9.10938356e-31; %effective mass of electron
Mh=0.3*9.10938356e-31; %effective mass of hole
epsilon=6.23; %epsilon for CdSe

%band gap energy dependence on crystal size
E1(d)=((h^2/(2*d^2))*(Me^-1+Mh^-1));
E2(d)=-((0.9*e^2)/(pi*epsilon*epsilon_0*d));
E(d)=Eg_bulk+E1(d)+E2(d);
lambda(d)=(h*c)/E(d); %absorption wavelength

%get values of E,E1,E2,lambda with variation of d in range[1-20](nanometres)
d1=linspace(1e-9,20e-9,10)';
E11=double(E1(d1));
E22=double(E2(d1));
EE=double(E(d1));
lambda2=double(lambda(d1));
t=table(d1,E11,E22,EE,lambda
```

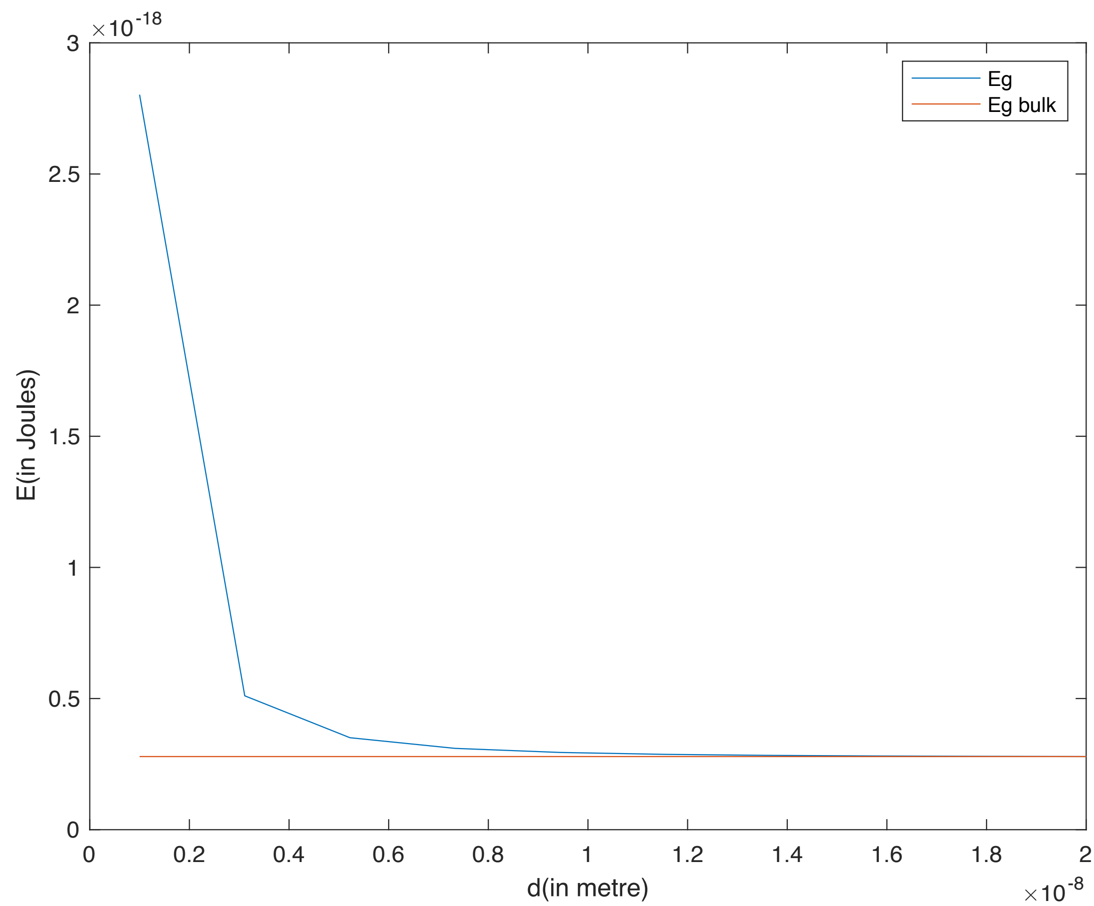
Table and Figures

	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						

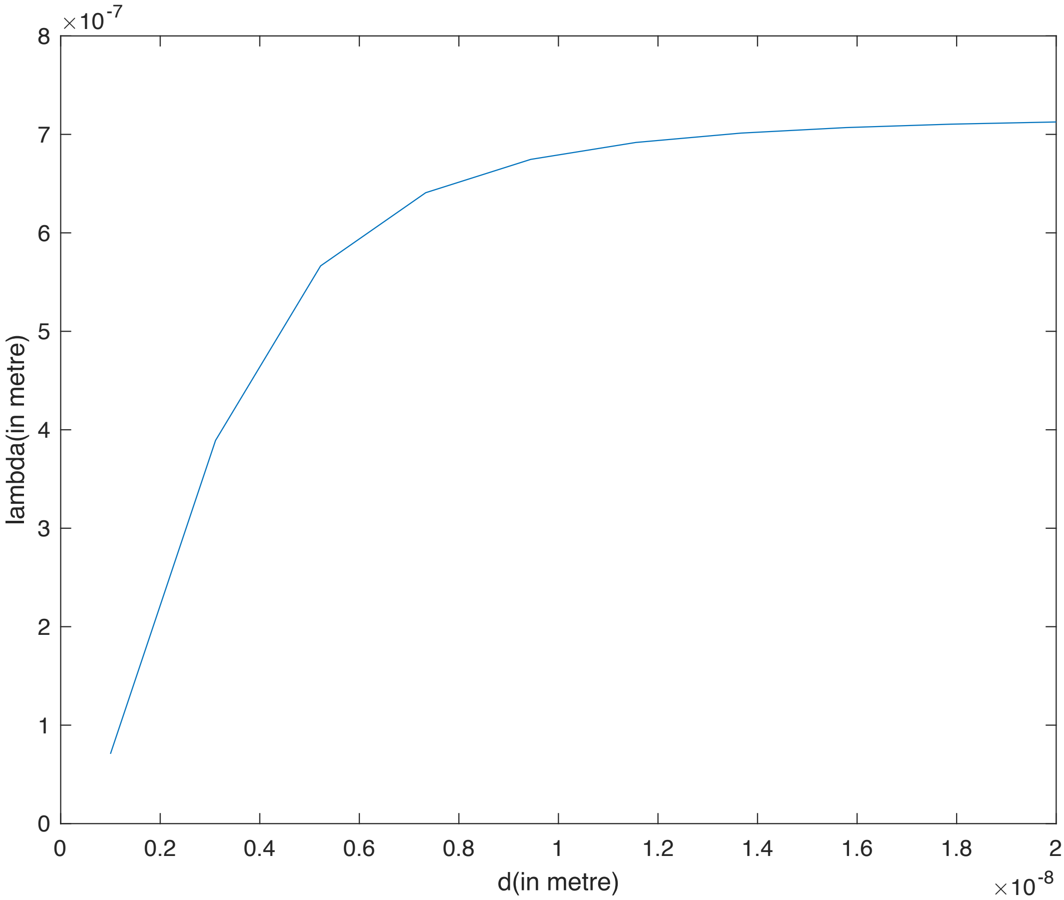




E2 vs d
E2(in Joules)
×10^-19
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
d(in metre)
×10^-8



E(in Joules)
×10^-18
3
2.5
2
1.5
1
0.5
0
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