Chalcogenide Letters Vol. 21, No. 5, May 2024, p. 407- 411

Cohesive energy model for the optical properties in nanostructured materials of zinc sulfide and cadmium selenide

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Applying the cohesive energy model, this research theoretically studies how the size of nanoparticles affects their optical characteristics. The findings demonstrate that optical characteristics are size-dependent for nanoparticles, with an exponentially growing energy gap for nanoparticles on a scale of less than 4 nm. As the size of nanoparticles is reduced, the absorption wavelength also decreases. Compounds undergo a transition to a higher energy spectral area (blue shift) when their wavelength decreases; this change can make these compounds effective in certain optical nanodevices.

(February 23, 2024; Accepted May 10, 2024)

Keywords: Energy band gap, quantum dot (QD), Model of cohesive energy and optical characteristics

1. Introduction

The utilization and examination of low-dimensional nanostructures have been made feasible by the fast advancement of nanotechnology in the past few years. Some notable structures that fall under this category include quantum dots (QDS), quantum wells (QWS), and quantum nanowires (QWR) [1-2]. Quantum dots show promise for sensing applications because of their unique optical, chemical, and structural features [3]. Semiconductor crystals smaller than 10 nm are known as quantum dots; these tiny particles exhibit unique electrical and optical characteristics not seen in bulk materials [4]. Nanostructured semiconductors have extensive application in LEDs, sensors, and solar cells. The ability to tune the size of the particles enables management of the energy gap, which is the most notable property of these materials [5-6]. In semiconductors, quantum confinement effects manifest when charge carriers (holes and electrons) are contained in tiny spaces with confinement dimensions smaller than the charge carriers' de Broglie wavelength or an equal value [7-8].

2. Theoretical framework

A molecule's cohesive energy is the amount of power needed to disassemble it due to the strength of its atomic connections. The collective cohesive energy of nanoparticles is affected differently by atoms on the inside and the outside.
This equation describes the overall cohesive energy of a nanoparticle:

$$E_{Total} = E_{\circ}(n - N) + \left(\frac{1}{2}\right) E_{\circ} N \quad (1)$$

N: is the number of atoms on the surface, n: is the total number of atoms in the nanosolid, and E_°: is the cohesive energy of the bulk semiconductor per atom. Where n - N is the number of atoms contained inside the nanomaterial. It follows that Eq. 1 may be written as:

$$E_n = E_b\left(1 - (N/2n)\right) \quad (2)$$

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https://doi.org/10.15251/CL.2024.215.407

For nanomaterials, the equivalent cohesive energy per mole is En, whereas for materials of a more conventional size, it is E_b.

Here is the expression for the solution of the previous equation for semiconductors having a nanostructure:

$$E_{g(D)} = E_{g(bulk)}(1 + N/2n) \tag{3}$$

The energy gap of semiconductors of varying sizes may be determined using the aforementioned equation. (9) and (10) here.As a function of nanomaterial size and form, the value of N/2n for spherical nanomaterials changes, the value of n $= \frac{4/3\pi(D/2)^3}{4/3\pi(d/3)^3} \approx {D^3}/{d^3}$ and $N = \frac{4\pi(D/2)^2}{4/3\pi(d/2)^3} = 6\frac{D^2}{d^2} \approx {4D^2}/{d^2}$. So the ratio N/2n becomes:

$$\frac{2d}{D}, \tag{4}$$

$$E_{g(D)} = E_{g(bulk)}\left(1 + \frac{2d}{D}\right) \tag{5}$$

where Nanoenergy gap: E_g(D); the nanosolid's diameter is D, while an atom's diameter is d. In addition to the quantum dots' size, the absorption wavelength is affected by the quantum dots' substance. The wavelength of the absorbed or emitted light (blue offset) decreases as the quantum dots' size decreases [11]. This relation gives the absorption wavelength [12].

$$\lambda = \frac{hc}{E_{g(D)}} \tag{6}$$

3. Results

To investigate how nanomaterial size impacts optical characteristics (energy gap, absorption wavelength), a model was developed based on the cohesive energy model. We chose fifteen different nanoparticle sizes to use as quantum dots.

Table 1. Illustrates the characteristics of the materials made use of [13-14].

Material	$E_{g(bulk)}$ (eV)	d(nm)
ZnS	3.68	0.234
CdSe	1.74	0.268

4. Discuss the results

4.1. Energy gap

Figures (1, 2) illustrate the correlation between particle size and the energy gap; the latter varies somewhat for nanoparticles larger than 20 nm and exhibits a dramatic rise for those less than 10 nm. The cohesive energy model explains the variation in the energy gap at various sizes by using the second term of Equation 5, which stands for the ratio of the atomic diameter to the particle size, or the surface-to-total atomic number, as an analogy. The cohesive energy decreases and the energy gap increases when the particle size is smaller than 10 nm because the number ratio is present on a greater surface. When it comes to zinc sulfide, this energy band gap analysis prediction model is in good agreement with experimental data [15].

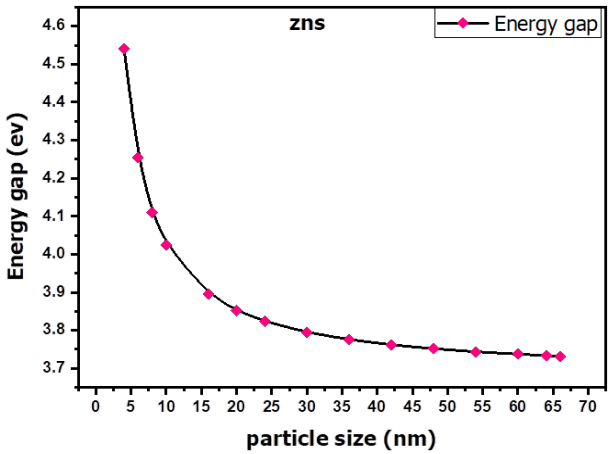

Fig. 1. Shows the fluctuation in the energy gap of zinc sulfide (ZnS) as a function of nanoparticle size.

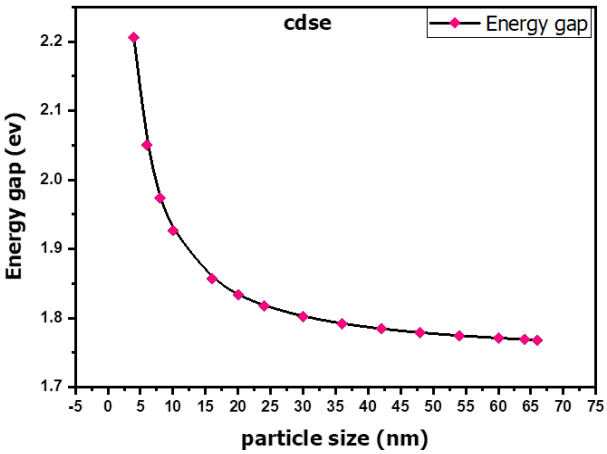

Fig. 2. Shows the fluctuation in the energy gap of cadmium selenide (CdSe) as a function of nanoparticle size.

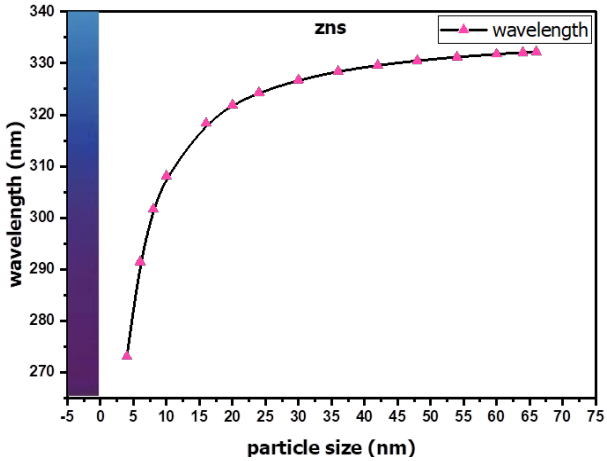

Fig. 3. The variation in the wavelength of zinc sulfide (ZnS) as a function of Nono particle size.

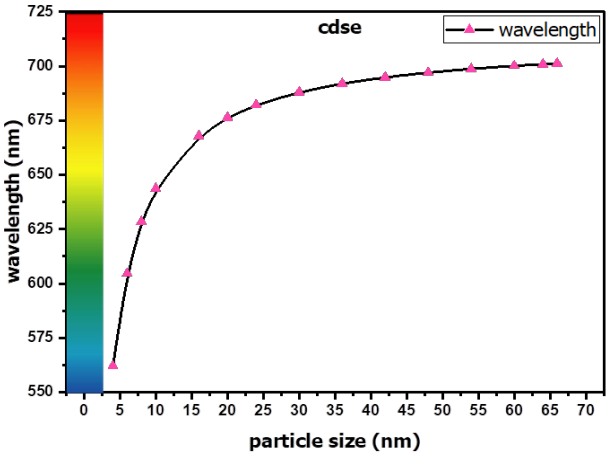

Fig. 4. The variation in the wavelength of cadmium selenide (CdSe) as a function of nano particle size.

4.2. Wavelength

The relationship between the absorption wavelength and the volume of quantum dots (QDs) of cadmium selenide and zinc sulfide, two semiconductor materials, is illustrated in Figures (3, 4). Additionally, the figures demonstrate the potential for wavelength adjustment by quantum dot size tuning. As the quantum dots shrink in size, their displacement towards an area of greater energy decreases and their absorption wavelength shrinks. The experimental findings are in agreement with the theoretical prediction that the absorption wavelength of zinc sulfide at 4 nm nanoparticles is 265 nm [16].

5. Conclusion

As the particle size lowers, the data reveal that the energy gap widens. Additionally, the data show that the wavelength decreases as the particle size increases. The absorption spectra of cadmium selenide are seen to change towards shorter wavelengths, the absorption spectra of zinc sulfide are seen to shift towards a higher energy area, and the visible region is shifted from the ultraviolet region to the visible region near the visible region. These findings have important implications for photovoltaic applications, as they suggest that the size of quantum dots may affect both the energy gap and the absorption wavelength. The cohesion energy model makes it easy to see how these characteristics vary as one moves along the nanoscale.

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