



## Research Paper

# Modeling Size and Dimension Dependence of Electrical and Optical Properties of Semiconductor Materials at Nanoscale

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Received: 22/Apr/2023; Accepted: 24/May/2023; Published: 30/Jun/2023

**Abstract-** Semiconductor nanomaterials show changing behavior when the size of materials decreases from bulk to nanoscale. Inspired by this, we developed a model free from adjustable parameters to calculate the optoelectrical properties of CdSe, CdS, ZnSe, Si, and ZnO semiconductor nanosolids. Cohesive energy varies by reducing the particle size, based on this we established a model to calculate the dielectric constant, phonon frequency, and energy band gap of semiconductor nanomaterials. In our calculations, we incorporated the shape factor, which changes from a spherical shape to an octahedral shape. It is reported that the energy band gap increases on decreasing the size of the particle and the effect is more when the shape changes from spherical to tetrahedral to octahedral on the same size. Also, it is observed that there is an appreciable change in the properties of the semiconductor materials when the size is near 10 nm. Our results are compared with the existing experimental and simulation data. It is reported that the model prediction agrees well with the experimental data, which validates the theory developed.

**Keywords-** Dangling bonds, Cohesive energy, Bandgap, Phonon frequency, Nanomaterials, Shape factor.

## 1. Introduction

The surface area exhibits a vital role to predict the physical, thermal, electrical, magnetic, and electronic properties of solids as dimension diminishes to the nano level. In fact, on the reduction of particle dimension, the surface-to-volume ratio changes appreciably. Consequently, the cohesive energy changes of the materials as we lower the size of the solids. Semiconductor nanomaterials show changing behavior when the size of materials decreases from bulk to nanoscale. Stimulated by this, we developed a model free from adjustable parameters to calculate the optoelectrical properties of CdSe, CdS, ZnSe, Si, and ZnO semiconductor nanosolids. Cohesive energy changes by reducing the particle size, based on this we established a model to calculate the dielectric constant, phonon frequency, and energy band gap of semiconductor nanomaterials. In our calculations, we incorporated the shape factor, which changes from a spherical shape to an octahedral shape. It is reported that the energy band gap increases on decreasing the size of the particle and the effect is more when the shape changes from spherical to tetrahedral to octahedral on the same dimension. In the present paper, we reported a model, which not only depends upon the dimension but also shows the substantial changeable behavior on the shape factor. In our model, we opted for a spherical shape, wire shape, film shape, regular tetrahedral,

regular hexahedral, and regular octahedral shapes. It is predicted that optoelectrical properties exhibit variable behavior to the nano level, especially up to the size of 2 nm. Our predicted model also applies to semiconductor materials with missing experimental data.

## 2. Related Work

It has been discussed by earlier researchers that the electrical and thermal properties of solid material at nano level show wonderful behavior [1-9]. Using thermodynamical properties, Guisbiers *et al.* have studied the variable behavior bandgap energy and the melting point of TiO<sub>2</sub> nano solid on downing the size to the nanoscale [10]. Depending upon the cohesive energy the dimension-dependent valence band energy and conduction band energy of nano solids have been analyzed. By quantum confinement properties, the electronic behavior of the diamond crystal at the nano level is projected by earlier researchers, which opens the door to discussing the energy band gap by the quantum confinement behavior [11-12]. In the above theories on changing the dimension of the particles the dangling bonds increase which is related to the cohesive energy of the materials. The melting temperature of the solid materials at the nano level is predicted to reduce as the surface area to volume ratio increases and of quantum

confinement effect on downing the size of nano solids [13-15]. For semiconductor devices, the bandgap, dielectric constant, and phonon frequency are very important because they affect optical and electrical behavior. The dielectric constant of semiconductors does not remain fixed but reduces as the material size is decreased. The suppression of the dielectric constant increases the Coulomb energy between the charge carrier, the electrons, the holes, and the impurities which are ionized. Because of the quantum confinement treatment, it has been debated by earlier scientists that the conduction bands and the valance bands of the semiconductors are confined by their respective electrons and hole, which restrict the movement of the charge carriers, consequently changing the properties of the nano solids [ 16-20]. In the past, it has been argued that the electrical and mechanical actions of the nanostructured materials show differently with the effect of dimension and structure of the semiconductors [21-22]. To describe the suppression of dielectric constant, various efforts have been done along with many proposed theoretical models. Using the sound-recognized connection of the electrical susceptibility with the energy band gap which depends on the cohesive energy of the crystal, a dependence of dielectric constant and refractive index on the cohesive energy was observed [6, 2, 23-25].

### 3. Mathematical Model

The electrical conductivity  $\sigma(D,T)$  which depends upon dimension and temperature is specified by Arrhenius manifestation, which is recited as [26]:

$$\sigma_e(D,T) = \sigma_{e0} \exp(-E_{ac}(D)/k_B T) \tag{1}$$

Here,  $E_{ac}(D)$  is the dimension-dependent activation energy, which is and  $\sigma_{e0}$  is a pre-exponential constant for electrical migration for solids at a nano size. , which is recited as  $E_{ac}(D) = E_{ce} - E_{Fe}$ , where  $E_{Fe}$  and  $E_{ce}$  are designated as the Fermi energy and the energy of the conduction band. Agreeing on the independency of size and melting of electrical conductivity. We get  $\sigma_e(D, T_{mn}) = \sigma_e(\text{bulk}, T_{mb})$ , where  $T_{mn}$  and  $T_{mb}$  are the melting temperatures of nanomaterials and corresponding bulk materials, respectively [27]. Thus, from Eq. (1) one can get

$$\sigma_{e0}(D) \exp\left[-\frac{E_{ac}(D)}{k_B T_{mn}}\right] = \sigma_{e0}(\text{bulk}) \exp\left[-\frac{E_{ac}(\text{bulk})}{k_B T_{mb}}\right]$$

Studying the dimension effect  $\sigma_{e0}$ , we get  $\frac{E_{ac}(D)}{E_{ac}(\text{bulk})} = \frac{T_{mn}}{T_{mb}}$ . For most semiconductors, it is predicted that the fermi level exists in the mid-way of the valence and the conduction bands [28].

we analyze that the Fermi level lies in the middle of the band gap [28]. Consequently, the energy of activation is read as  $E_{ac} = E_g / 2$ , by which we can say that there is a linear relation between band gap energy and the activation energy. Thus, we have the proper equation given as

$$\Delta E_g(D) / E_g(\text{bulk}) = |\Delta E_{ac}(D) / E_{ac}(\infty)| \tag{2}$$

Here,  $\Delta E_g$  is defined as the band gap energy of semiconductor materials.

Or, Eq. (2) is read as:

$$\Delta E_g(D) / E_g(\text{bulk}) = |(E_{ac}(D) - E_{ac}(\infty)) / E_{ac}(\infty)| \tag{3}$$

Lu *et al.* [29] have proposed the relation of cohesive energy which depends upon dimension and the structure of nanomaterials, which is given as:

$$\frac{E_{cn}}{E_{cb}} \approx \frac{T_{mn}}{T_{mb}} \approx \left\{ 1 - \frac{1}{(12D/D_0) - 1} \right\} \exp \left\{ -\left(\frac{2}{3}\right) \lambda \left(\frac{S_m}{R}\right) \frac{1}{\left(\frac{12D}{D_0}\right) - 1} \right\} \tag{4}$$

Here,  $E_{cb}$ ,  $S_m$  and  $R$  are defined as the bulk cohesive energy, entropy of evaporation of bulk, and the gas constant of the solid materials respectively. Symbol  $D_0$ , which is read as

$$D_0 = 2h(3-d),$$

known as the critical size of the nanosolids.

Also, the value of  $d$ , which is the degree of freedom, depends upon the shape of the nanostructured materials, which is 0, 1, and 2 for the spherical shape, wire shape, and film shape respectively. Here,  $h$  is the atomic diameter of the nanostructured materials. Rose *et al.* reported that there is a linear relation between the melting temperature and the cohesive energy of bulk which is read as [30]:

$$E_c \propto T_m$$

Or,  $\frac{E_{cn}}{E_{cb}} = \frac{T_{mn}}{T_{mb}}$  (5)

Therefore, we have

$$\frac{T_{mn}}{T_{mb}} = \left\{ 1 - \frac{1}{\left(\frac{12D}{D_0}\right) - 1} \right\} \exp \left\{ -\left(\frac{2}{3}\right) \lambda \left(\frac{S_m}{R}\right) \frac{1}{\left(\frac{12D}{D_0}\right) - 1} \right\} \tag{6}$$

Hence, by Eqs. (3) to (6), we get

$$\Delta E_g(D) / E_g(\text{bulk}) = 1 - \left\{ 1 - \frac{1}{\left(\frac{12D}{D_0}\right) - 1} \right\} \exp \left\{ -\left(\frac{2}{3}\right) \lambda \left(\frac{S_m}{R}\right) \frac{1}{\left(\frac{12D}{D_0}\right) - 1} \right\} \tag{7}$$

The movement of electrons from the valence band to the conduction band is triggered by the dielectric constant [31]. The optical response of semiconductors materials is caused by the energy and momentum conservations which reflects how strongly the conduction electrons in the excited state are coupled by the valence electrons. It is debated by earlier

researchers that energy band gap and the dielectric constant are directly related to each other [31].

Extending the approximation of  $\chi(\infty) \propto \{1/E_g(\infty)\}^2$  relationship and the  $\varepsilon(\infty) = \chi(\infty) + 1$  at nanoscale, where  $\chi$  is the electrical susceptibility, we obtained the relation of dielectric constant between bulk and nanostructured materials.

$$\varepsilon(D) = (\varepsilon(\text{bulk}) - 1) \left\{ 1 - \frac{1}{\left(\frac{12D}{D_0}\right)^{-1}} \right\} \exp \left\{ -\left(\frac{2}{3}\right) \lambda \left(\frac{S_m}{R}\right) \frac{1}{\left(\frac{12D}{D_0}\right)^{-1}} \right\} + 1 \tag{8}$$

As size decreases, Raman frequency undergoes a redshift [32]. In solid, the Cohesive energy of bulk and the phonon frequency of the electrons of the atoms are proportional to each other [33]. Henceforth, one can say that there is a proportionality between the phonon frequency of nanostructured semiconductor materials and the phonon frequency of the electrons in the bulk materials, which is read as:

$$\omega(D) = \omega(\text{bulk}) \left\{ \left[ 1 - \frac{1}{\left(\frac{12D}{D_0}\right)^{-1}} \right] \exp \left\{ -\left(\frac{2}{3}\right) \lambda \left(\frac{S_m}{R}\right) \frac{1}{\left(\frac{12D}{D_0}\right)^{-1}} \right\} \right\}^{1/2} \tag{9}$$

### 4. Results and Discussion

Based on cohesive energy and Lu *et al.* model [29], we derived equations to explain the change in bandgap energy, frequency of phonon, and dielectric constant with dimension and shape of CdSe, CdS, ZnSe, Si, and ZnO semiconductors solids at the nanoscale. The needed input parameters utilized in computations are introduced in Table 1 [32-40]. Values of  $S_m$  vary as the temperature reaches the melting point of the materials, particularly those of the semiconductor materials. Therefore, in our calculation, we have assumed the value of  $S_m$  is 13R, which is the mean value [36].

**Table1.** Input parameters used in the calculation [32-40]

Semiconductors	$\omega(\text{bulk})(\text{cm}^{-1})$	$h(\text{nm})$	$E_g(\infty)(\text{eV})$	$\varepsilon(\text{bulk})$
CdSe	212	0.262	1.74	6.2
CdS	303	0.252	2.42	8.7
ZnSe	255	0.245	2.58	6.6
Si	350	0.234	3.16	9.6
ZnO	570	0.264	3.37	7.6

$\Delta E_g(D)$ ,  $\omega(D)$  and  $\varepsilon(D)$  are estimated by Eqs. (7), (8), and (9) on decreasing dimensions of the semiconductors in different shapes like spherical, nanowire, film, regular tetrahedral, regular hexahedral, and regular octahedral. The graphical representation of the energy band gap  $\Delta E_g(D)$  of

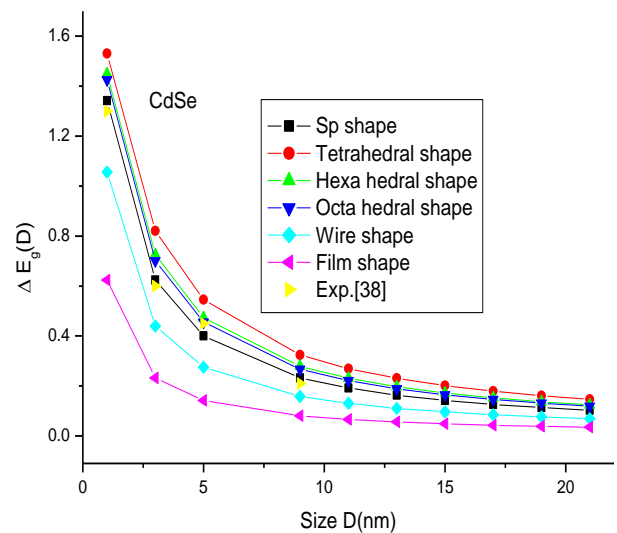
CdSe, CdS, ZnSe, Si, and ZnO of nano solid semiconductors with decreasing sizes and in different shapes are projected in Figs. 1-5 respectively with the existing experimental and simulation data to prove our proposed model. In Fig.1, the band gap energy of CdSe nanosolids is calculated by Eq. (7) and the results are projected along with the existing simulation and experimental data for the comparison purpose at the nanoscale [38]. Increasing behavior of the  $\Delta E_g(D)$  is projected with the reduction of particle size at nano level. Also, it is observed that the effectiveness of the energy band gap is near 8nm size. Additionally, the effect is catalyzed when the shape is changed from spherical to film to regular octahedral shape, which reveals that the variation of the energy band gap is a function of shape also. For the support of our results, it was debated that the transition of the charge carriers from the top of the valance band to the lower of the conduction band increases because of the quantum confinement of the electrons and holes charge carriers. However, it was reported in the case of bulk materials energy levels are closely spaced [37]. The model prediction using Eq. (7) for the particle size-dependent energy band gap  $\Delta E_g(D)$  of CdS nanostructured semiconductor material along with the simulation and existing experimental data are projected in Fig. 2 [24]. In our calculations the shape factors  $\lambda$  are incorporated whose values are in spherical ( $\lambda = 1$ ), wire ( $\lambda = 1$ ), film ( $\lambda = 1$ ), octahedral ( $\lambda = 1.18$ ), hexahedral ( $\lambda = 1.24$ ), and tetrahedral ( $\lambda = 1.49$ ) shapes. It is reported that the band gap energy not only depends upon the dimension of the particle but also varies with the shapes of the nanostructured materials [36-37]. Moreover, from Fig. 2, it is monitored that the band gap energy effect is more appreciable below 8nm, while above 8nm variation is feeble. It is uncovered that the drift is similar to that of the nanoparticles with a slight deviation to the experimental value. By the theory of earlier researchers, it is realized that because of the quantum confinement treatment, consequently loss of dimensions, energy variation is weakened from the spherical -to-film shape of the semiconductors [41]. The trend of increasing  $\Delta E_g(\infty)$  is the same as that of nano solids in a spherical shape. Results show that on moving from a regular tetrahedral to a spherical shape the effect of size is not substantial. Although such type of behavior is expected because of the reduction of particle size there is an increase in surface-to the -volume ratio of the CdS semiconductor. It is revealed in Fig.2 that our calculated projections are more closely related to the existing experimental and simulation findings for the considered semiconductor [25].  $\Delta E_g(D)$  computed by Eq. (7) for ZnSe nano solid is reported in Fig. 3. Theory reveals that the increasing behavior of  $\Delta E_g(D)$  with the decreasing dimension of the appreciable on shifting film to tetrahedral shape of the considered nanostructure materials. Moreover, prediction explains that at the particular particle size, the increase of energy band gap is more in tetrahedral shape as compared to the film shape of ZnSe nanostructured materials. Infact there is a discrete in energy levels and separation increases between the valance band and the conduction band because of quantum

confinement on going to the nanoscale, henceforth energy levels show the increase in gap. The  $\Delta E_g(D)$  of Si semiconductor nano solid on changing the shape factor and down to the nanoscale, the computed results by Eq. 7 are reported in Fig. 4 with the existing data for the support of our theoretical results. Moreover, results reveal that there is a close agreement between the theory and existing findings [2]. Band gap energy variations of ZnO nanocrystals by Eq. 7 are reported in Fig. 5, it is seen that when the particle size is less than 10 nm, our model predictions are very close to the results available for the spherical shape [42]. Additionally, for the other shape such as tetrahedral, hexahedral, and octahedral shapes are also plotted on the shape graphs for comparison purposes, it is seen that the trend is similar. The prediction shows that around size 4nm there is a more increase of energy band gap because the particle size becomes comparable to the exciton radii. The fact is that when the size of the particle tends to be below 4nm, the energy level become discrete and the band widens.

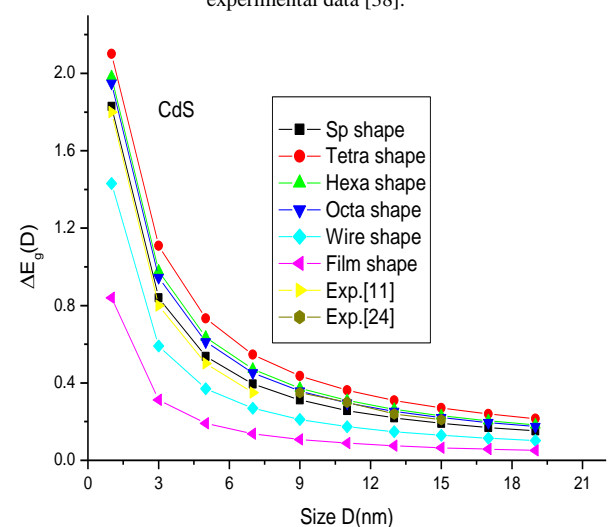
The predictions of the dielectric constants are reported in Figs. 6-9 by Eq. (8) for the CdSe, CdS, Si, and ZnO nanostructured materials at Nano lane. The dielectric constant shows the behavior of the electron polarization on applying the external field. Likewise, variation of the dielectric constant depends upon the electron-phonon coupling and the bindings which characterize the optical response [43]. Fig. 6 explains the trend of the variation of the CdSe nano solids in different shapes and particles size. It is seen that on reduction of particle size and changing the shape of nanosolids, the dielectric constant decreases and the trend is the same as that of the existing data [44]. Characteristics of the dielectric constants of CdS, Si, and ZnO are reported using Eq. (8) in Figs. 7-9. Model predictions are compared with the existing computational and experimental data [42, 45]. It is observed that the theoretical findings ate very close to the existing experimental results, which validated the findings. Besides, the shape factor added the nature of the decreasing trend of dielectric constant on reducing the particle size. The reason is that on reducing the particle size, the surface area increases and the cohesive energy decreases which is the measure of bond strength, consequently dielectric constant decreases. The crystal size effect is studied by the phonon confinement theory for the nanostructured materials on phonon Raman spectra [32]. Evaluation of the phonon frequency of CdSe, CdS, and Si, nanosolids with particle dimensions and the effect of shape are demonstrated in Figs. 10-12, by Eq. (9). Validity of our model predictions is compared with the computational and experimental reports by the earlier researchers [14, 19]. For the clarity of our model, spherical shape, film shape, tetrahedral shape, and octahedral shapes are plotted on the same graphs. Graphs reveal that on going down to the nanoscale, the trend of phonon frequency drops. Furthermore, the shape factor enhanced the decrement of phonon frequency by decreasing the particle dimension. Physical properties of the nanostructured material are enhanced by the reduction of particle size consequently the quantum confinement effect and the increase in surface area to volume ratio, further increase the surface energy of the

solid materials at the nano level [ 23, 46]. The graphical prediction of variation in phonon frequency is shown in Fig. 11 along with the computational results using Eq. (9). The variation trend is similar to that of the simulated data [14]. Our theory reports that at the particular particle size, the effect is minimum on tetrahedral shapes and maximum on film shapes. Such type of behavior can be explained by the bond theory model, which changes the cohesive energy on the effect of the shape and size of the Nano solids.

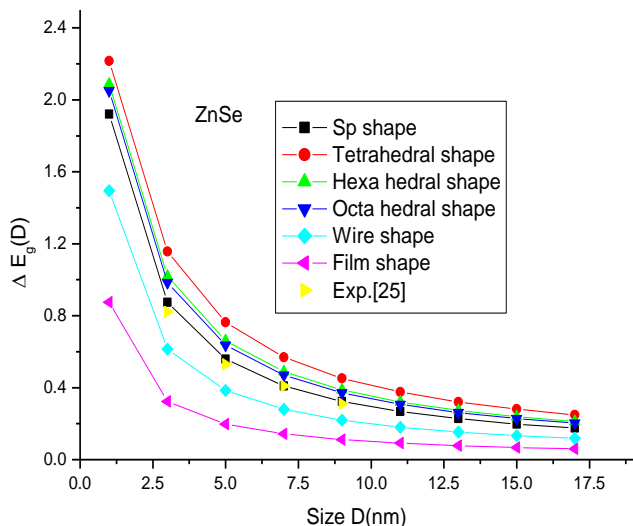
In light of Eq. (9), the theory reports for the Si semiconductor nanostructured solids are projected in Fig. 12 in variable particle size and the shapes such as spherical to film to regular octahedral. Our findings are compared to judge the predictions in reducing the order of the grain size. Furthermore, the effect is studied on increasing the shape factor. Predictions show that our theory validates throughout the range of the particle size at the nanoscale.



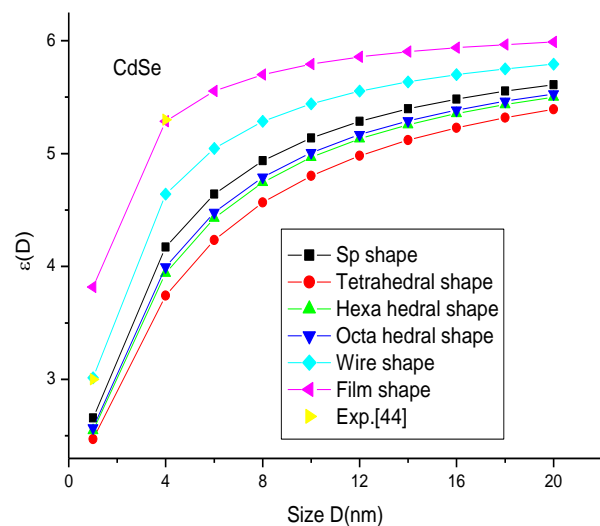
**Figure 1.** Band gap energy variations of of CdSe semiconductor nanosolid. The lines with symbols represent  $\Delta E_g(D)$  . Symbols (yellow arrow) show experimental data [38].



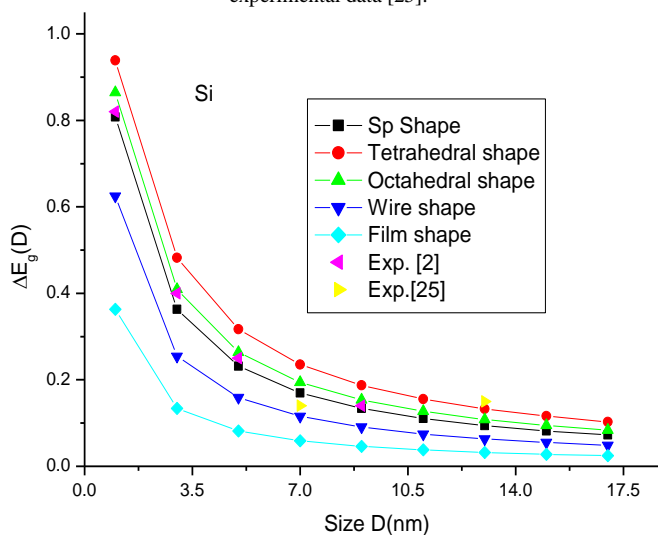
**Figure 2.** band gap energy variations of CdS semiconductor nanosolid. The lines with symbols represent  $\Delta E_g(D)$  . Symbols (yellow arrow and solid circle) show experimental / simulated data [11,24].



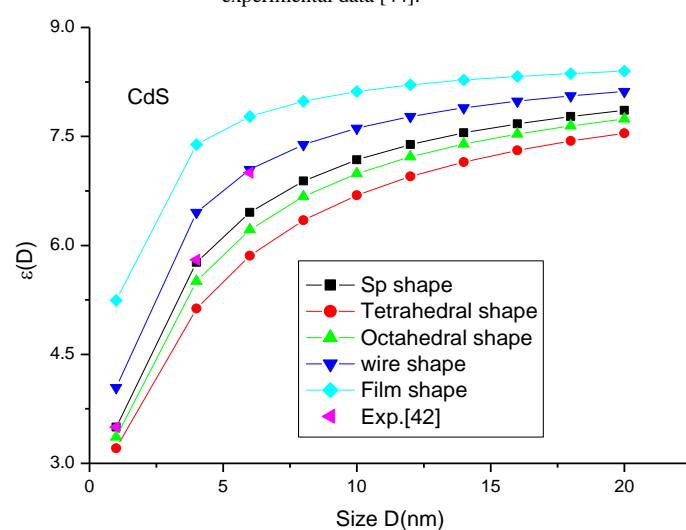
**Figure 3.** Band gap energy variations of ZnSe semiconductor nanosolid. The lines with symbols represent  $\Delta E_g(D)$ . Symbols (yellow arrow) show experimental data [25].



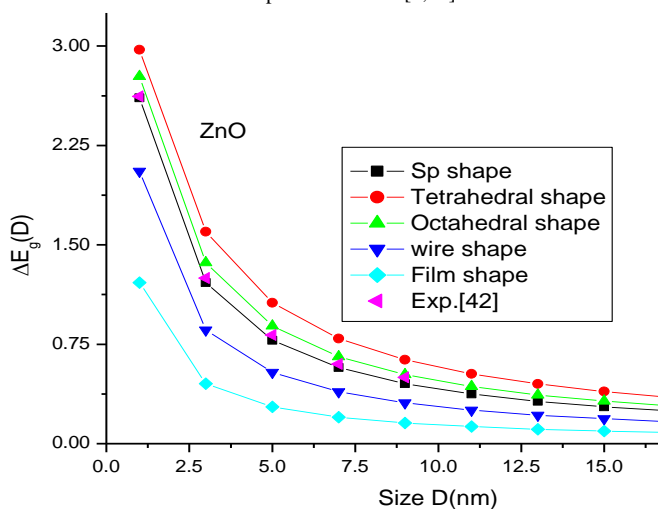
**Figure 6.** Dielectric constant variations of CdSe semiconductor nanosolid. The lines with symbols represent  $\epsilon(D)$ . Symbols (yellow arrow) show experimental data [44].



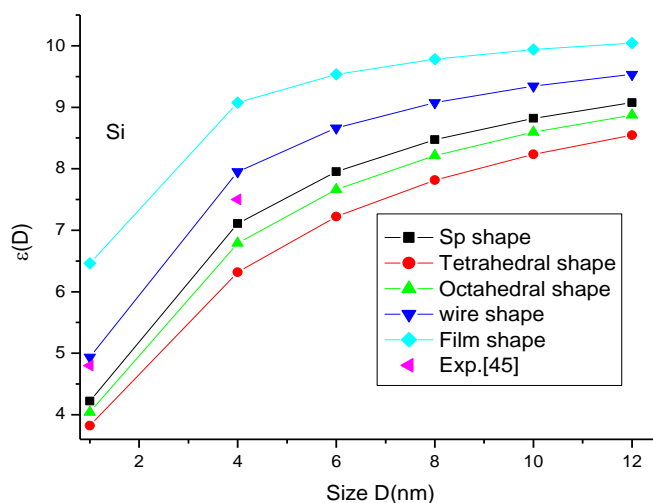
**Figure 4.** Band gap energy variations of Si semiconductor nanosolid. The lines with symbols represent  $\Delta E_g(D)$ . Symbols (yellow and pink arrow) show experimental data [2,25].



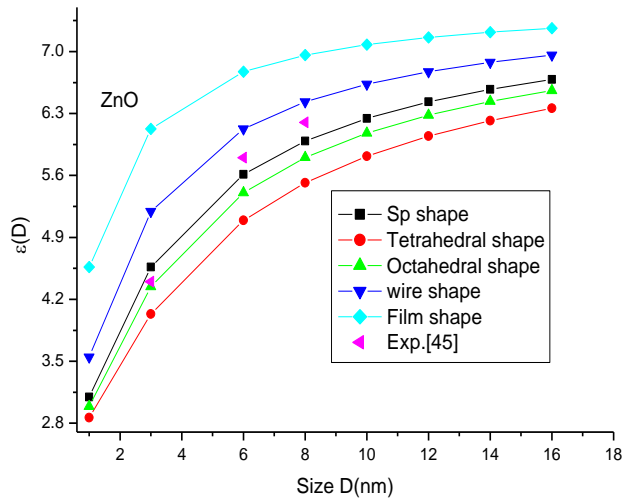
**Figure 7.** Dielectric constant variations of CdS semiconductor nanosolid. The lines with symbols represent  $\epsilon(D)$ . Symbols (pink arrow) show experimental data [42].



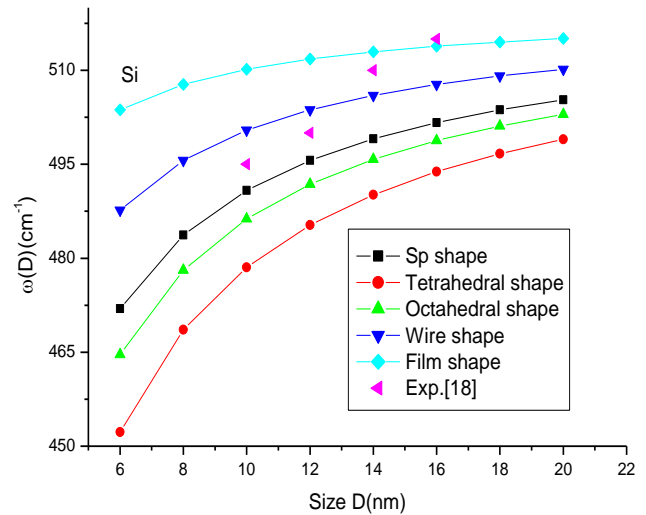
**Figure 5.** Band gap energy variations of ZnO semiconductor nanosolid. The lines with symbols represent  $\Delta E_g(D)$ . Symbols (pink arrow) show experimental data [42].



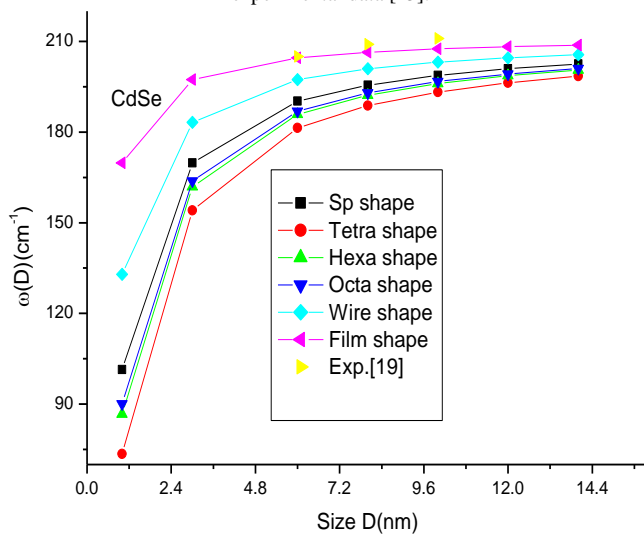
**Figure 8.** Dielectric constant variations of Si semiconductor nanosolid. The lines with symbols represent  $\epsilon(D)$ . Symbols (pink arrow) show experimental data [45].



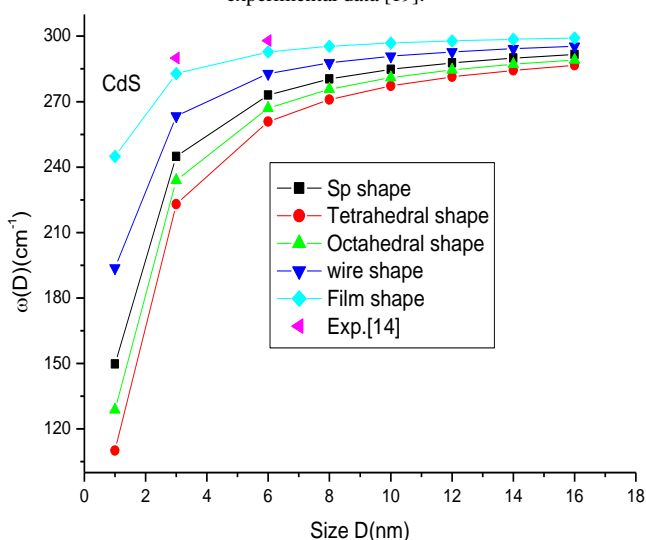
**Figure 9.** Dielectric constant variations of ZnO semiconductor nanosolid. The lines with symbols represent  $\epsilon(D)$ . Symbols (pink arrow) show experimental data [45].



**Figure 12.** Phonon frequency variations of Si semiconductor nanosolid. The lines with symbols represent  $\omega(D)$ . Symbols (pink arrow) show experimental data [18].



**Figure 10.** Phonon frequency variations of CdSe semiconductor nanosolid. The lines with symbols represent  $\omega(D)$ . Symbols (yellow arrow) show experimental data [19].



**Figure 11.** Phonon frequency variations of CdS semiconductor nanosolid. The lines with symbols represent  $\omega(D)$ . Symbols (pink arrow) show experimental data [14].

### 5. Conclusions

In the present paper, considering the cohesive energy and the Lu *et al.* model, we derived a relation to calculate the optoelectrical properties of the semiconductor nanostructured materials. It is found that  $\Delta E_g(D)$  increases as  $D$  decreases in the nanosolids. However,  $\epsilon(D)$  and  $\omega(D)$  decrease in the reduction of the particle size. Moreover, the effect of the dimension of dielectric constant and phonon frequency of film shape of semiconductors is feeblor in comparison to the spherical shape of the materials. Furthermore,  $\epsilon(D)$  and  $\omega(D)$  are stronger in hexahedral and octahedral shape because of the surface-to-volume ratio or surface effect. Here it is reported that the effect of dimension and shape is most significant up to the particle size of 10 nm. Consistency between the model prediction and accessible experimental and simulated data confirms the rationality of the concept.

### Conflict of Interest

The authors declare that there is no conflict of interest.

### Authors' Contributions

Dr Madan Singh developed the mathematical model and discussed the results. Mr. Sekhants'o Lara was involved in data analysis and referencing. Dr. Naleli Jubert Matjelo worked on plotting the graphs and writing the introduction. Mr. Moruti Kao and Ms. Limakatso Lepekola were involved in data collection. Ms. Mampesi Thato Matobako researched review literature. The current manuscript is reviewed and edited by all authors and agreed on the final version of it.

### Acknowledgment

Our work is supported by the National University of Lesotho, Southern Africa.

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