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Size-dependent Energy Gap in Some Semiconductor Nanomaterials

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Abstract

This study deals with the change of energy gaps as a result of the difference in the size of nanoparticles for CdS, GaAs, InN, and InP using a theoretical model, which has been measured theoretically from a model based on energy differences between nanoparticles and their corresponding bulks. This study clearly reveals that band gap energy is not a particular value, but rather it varies strongly with the size of particles. That is to say, what has become increasingly clear from this theoretical study is an increase in the band gap energy for smaller particles of the studied materials in this research. This phenomenon is related to the synthesis of semiconductor nanomaterials. Predictions from this model have worked fairly well in earlier experiments, offering significant encouragement regarding its validity.

1. Introduction:

Many years ago, some semiconductor nanomaterials were synthesized. While some of them have been synthesized many years ago, the contemporary scientific literature abounds with the wonders of semiconductor nanomaterials that find applications in electronics [1], optics, and even mechanics. An extremely vital property of the materials is what is known as a band gap, which determines, in essence, how they would behave both electrically and optically. So that we can get the full benefit of the little buggers, we had better take a firm grip on how to go about screwing around with or adjusting this band gap. And so that we can get the full benefit we probably can out of the little buggers, we had better take a good grip on the way to go about screwing around with or adjusting this band gap [2], [3], [4].

Probably the most interesting aspect concerning the nanomaterials is that their band gap energy does not always stay constant as the size becomes smaller, but on the contrary, it rises as we reduce the size of the particle. An explanation of the phenomenon in terms of quantum confinement effects, where a dimension reduction alters the electronic structure, can be given. When using bulk material, the Eg is always constant, but in nanomaterials, optical and electronic properties can be finely tuned through variation of particle size. This makes them stand out in terms of advanced applications potentials that extend to high-performance solar cells to personalized devices of light-emitting [5], [6], [7].

Once the materials become so small, as in the nanoscale, their characteristics become fundamentally altered, providing a new realm of unheard-of technologies whose features can be fine-tuned [8], [9], [10]. Such inventions are particularly promising for optoelectronic devices. As an example, semi-

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conductor nanomaterials are in use today in solar cells and in the ultra-small electronic component parts of the modern logic and memory [11], [12].

Scientists have theoretically modeled why the bandgap of a semiconductor decreases with its diminution up to the nanoscale and most of them adopt the relation of ΔEg(D) = Eg(D) – Eg(∞) [8]. In which bandgap is given as: ΔEg, nanoparticle bandgap Eg(D), and bulk material bandgap Eg(∞). The exciting aspect of nanomaterials is that their behavior is strongly size and shape-dependent in a particular way and not dependent in some other way as would be predicted by traditional theories [9].

Some of these special capabilities are because nanomaterials have a very large surface-to-volume ratio compared to their bulk counterparts, and it is this high ratio that determines their behavior. The band gap is one of the most significant characteristics of a semiconductor since it determines its electrical and optical properties. This is why it is important to comprehend how the band gap increases in semiconductor compound nanomaterials (SCNs), which would be instrumental in realizing their full potential. These semiconductors are very diverse and find application in very diverse technologies because their band gaps can be tailored [13].

The bond theory model explains the importance of dangling bonds on the surfaces of materials at the nanoscale in determining their behavior in the nanoscale. The size of particles of a semiconductor has always been shown to have a direct correlation with its energy bandgap. In particular, the nanoscale structure of materials normally has a broader bandgap than the bulk structure of the same material [14], [15], [16], [17].

Numerous studies have investigated this correlation between the size of a nanomaterial and its band gap. Scientists have measured photoluminescence spectra to investigate the changing band gap with the diameter of nanowires, comparing their results with experimental evidence from semiconductors such as CdS, InN, InP, and GaAs, using different theoretical predictions [11]. At the nanoscale, two relevant processes occur: enhancing the surface effects and enabling quantum confinement, which is a purely quantum mechanical process that begins to become significant when objects are very small, and the actual scale depends on the chemical composition and intrinsic properties of the material. This leads to a binding of a pair of electrons and holes to give rise to excitons (or bound pairs), and this makes the band gap increase when the nanoparticle becomes smaller [18].

A variety of theoretical models have been considered by scientists because they want to determine how to tune the band gap in nanomaterials [19], [20], [21], [22], [23]. Nevertheless, lots of methods that have thermodynamics as their foundation are not capable of duplicating the entire picture. They can easily miss out on such small details as the effects occurring at the surface, particularly, the so-called dangling bonds, and the way atoms are organized in the crystal structure, and how nanoparticles are not necessarily perfectly spherical. Because energy is central to the characteristics of a material [24], a more detailed thermodynamic study of the nanoscale would provide us with a far better insight into the manner in which the band gap varies with the size and shape of the particles. Nanocrystals have a wide range of applications in the real world, and the size of nanocrystals plays a significant role in determining their optical properties. These optical properties are directly associated with the dynamics of electrons on the edges of the band of semiconductors. Considering this close relationship, one of the main goals in semiconductor nanocrystal studies has been to have a complete understanding of the behavior of the band gap as well as the exciton energy shift with changes in particle size.

In the current investigation, we introduce a theoretical framework that can be used in predicting the band gap energy of semiconductor nanomaterials based on cohesive energy, especially without any adjustable parameters. Our model examines the variation of band gap with particle size, and we have experimented on a range of materials such as CdS, GaAs, InN, and InP, in various forms such as nanoparticles, nanowires, and nanofilms. These findings validate the fact that the band gap is actually controllable easily by merely changing the size of the particles. We have compared the theoretical predictions of the model with available experimental data of different sizes and found that they have a strong correlation. This great agreement justifies the validity of our suggested model. Due to its precision, this method may turn out to be an efficient sprouting map of determining band gap energies, especially in cases where experimental data is limited.

2. Theory of Analysis:

The total cohesive energy of a nanomaterial is the sum of contributions from both its interior and surface atoms. This can be mathematically represented as [25]:

$$E_{tot} = E_o(n-N) + \frac{1}{2}E_oN \tag{1}$$

In this case, n is the number of atoms in a nanosolid, and N is the number of atoms on its surface. Thus, (n - N) provides the number of atoms on the inside. E_o is the abbreviation of the cohesive energy per atom of the bulk material. To state this energy in per mole basis, equation 1 may be rewritten as below:

$$AE_{tot}/n = AE_o(1-N/n) + \frac{1}{2n}AE_oN \tag{2}$$

In which A is the number of Avogadro, AE_{tot}/n is the cohesive energy per mole of the nanomaterial (E_n), and AE_o

is the cohesive energy per mole of the bulk material (E_b). Replacing them with equation 2 will give:

$$E_n = E_b(1 - N/2n) \tag{3}$$

It is believed that the linearly dependent variable on melting temperature is cohesive energy [26], [27]. Therefore, the melting temperature of a nanomaterial (T_{nm}) can be written in terms of the bulk melting point (T_{bm}) as follows:

$$T_{nm} = T_{bm}(1 - N/2n) \tag{4}$$

Additionally, the electrical conductivity (σ(D,T)), which depends on particle size (D) and temperature (T), follows the Arrhenius equation [28]:

$$\sigma(D,T) = \sigma_o exp(-E_a(D)/k_B T) \tag{5}$$

The symbols σ_o and E_a(D) used in this equation mean the pre-exponential constant and size-dependent electrical migration activation energy in nanocrystals, respectively, and k_B is the Boltzmann constant. Activation energy is determined to be E_a(D) = E_c - E_F, with E_c the conduction band energy, and E_F the Fermi energy. By assuming that melting temperature and particle size do not affect the electrical conductivity [29], the conductivity of the nanomaterials and that of bulk materials can be regarded as equal at their respective melting temperatures. T_{nm} here is the melting temperature of the nanomaterial, and T_{bm} is the melting temperature of the bulk material of the same material with an infinite size. Replacement of this assumption in Equation 5 brings out the following relationship.

$$\sigma_o \sigma_o(D) exp(-E_a(D)/k_B T_{nm}) = \sigma_o(\infty) exp(-E_a(\infty)/k_B T_{bm})$$

If we disregard the influence of size effects on σ_o, we obtain the relationship $E_a(D)/E_a(\infty) = T_{nm}/T_{bm}$. Since the Fermi level typically resides near the middle of the band gap in most semiconductors, the activation energy can be approximated as $E_a = E_g/2$. This means that any variation in activation energy is directly related to changes in the band gap [30]. As a result, we can express this relationship in a more appropriate form:

$$E_g(D)/E_g(\infty) = |\Delta E_a(D)/E_a(\infty)| \tag{6}$$

where ΔE_g is the difference in energy band gap. Then, Equation 6 may be written as

$$\Delta E_g(D)/E_g(\infty) = |(E_a(D)E_a(\infty))/E_a(\infty)|$$

Or

$$\Delta E_g(D)/E_g(\infty) = 1(T_{mn}/T_{mb}) \tag{7}$$

Using Equation 4, and 7 may be written as

$$E_g(D) = E_g(\infty)(1 - \frac{N}{2n}) \tag{8}$$

The ratio N/2n varies depending on the size and shape of the nanomaterials [25]. In the case of spherical nanosolids, N/2n can be expressed as 2d/D, where d represents the atomic diameter and D is the diameter of the nanosphere. For nanowires and nanofilms, N/2n takes the forms 4d/3l and 2d/3h, respectively, with l being the nanowire's diameter and h the thickness of the nanofilm. By substituting these N/2n values into Equation 8, we derive the following expressions:

$$E_g(D) = E_g(\infty)(1 + \frac{2d}{D}) \tag{9}$$

$$E_g(l) = E_g(\infty)(1 + \frac{4d}{3l}) \tag{10}$$

$$E_g(h) = E_g(\infty)(1 + \frac{2d}{3h}) \tag{11}$$

The energy band gap for spherical nanosolids, nanowires, and nanofilms is described by Equation 9, 10, 11, which Equations 9, 10, 11 clearly indicate that the band gap increases inversely with different nanoscale dimensions (D, l , h). This observation aligns with the concept of quantum confinement, where reducing the size increases the ground state energy of electrons and holes, and consequently widens the band gap. In this study, we use these equations to analyze how the band gap energy of semiconductor compound nanomaterials varies depending on their shape and size.

3. Results and Discussions:

Depending on the Equations 9, 10, 11, respectively, based on the input parameters provided in Table 1 and Figures 1, 2, 3, 4, illustrate how the energy band gap varies with size for CdS, InN, InP, and GaAs in both spherical nanoparticles (NPs) and nanowires (NWs). Our computational results were compared with existing experimental data and simulations from previous studies [7], [8], [9], [10], [11], [12], [13], [14], showing good agreement. The band gap of nanomaterials increases as particle size decreases due to the quantum confinement effect, where electrons and holes are restricted to a very small region. This confinement raises their energy levels

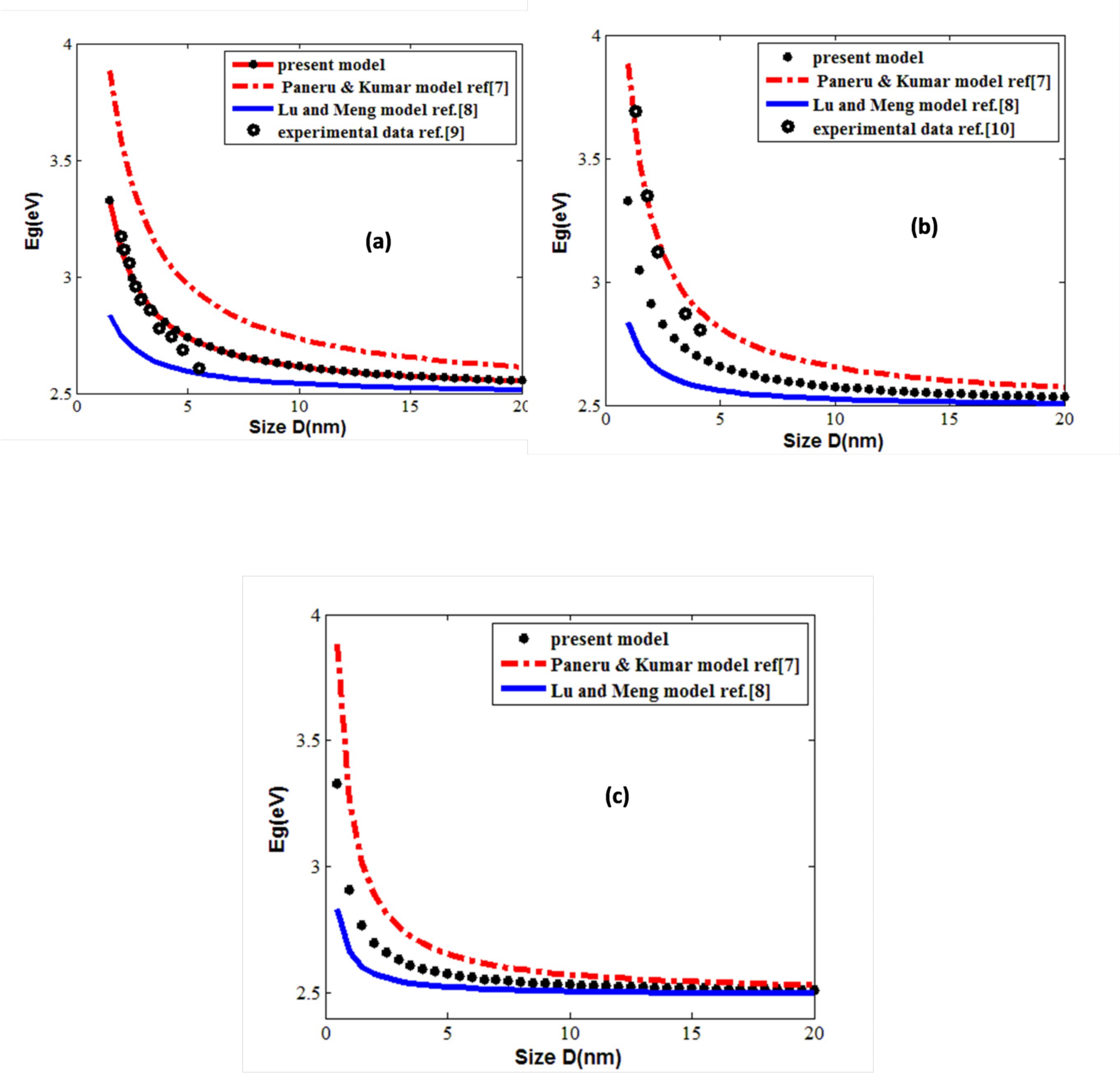

Figure 1. Size dependent of Bandgap of, (a) Spherical, (b) Nanowire, and (c) Nanofilm CdS.

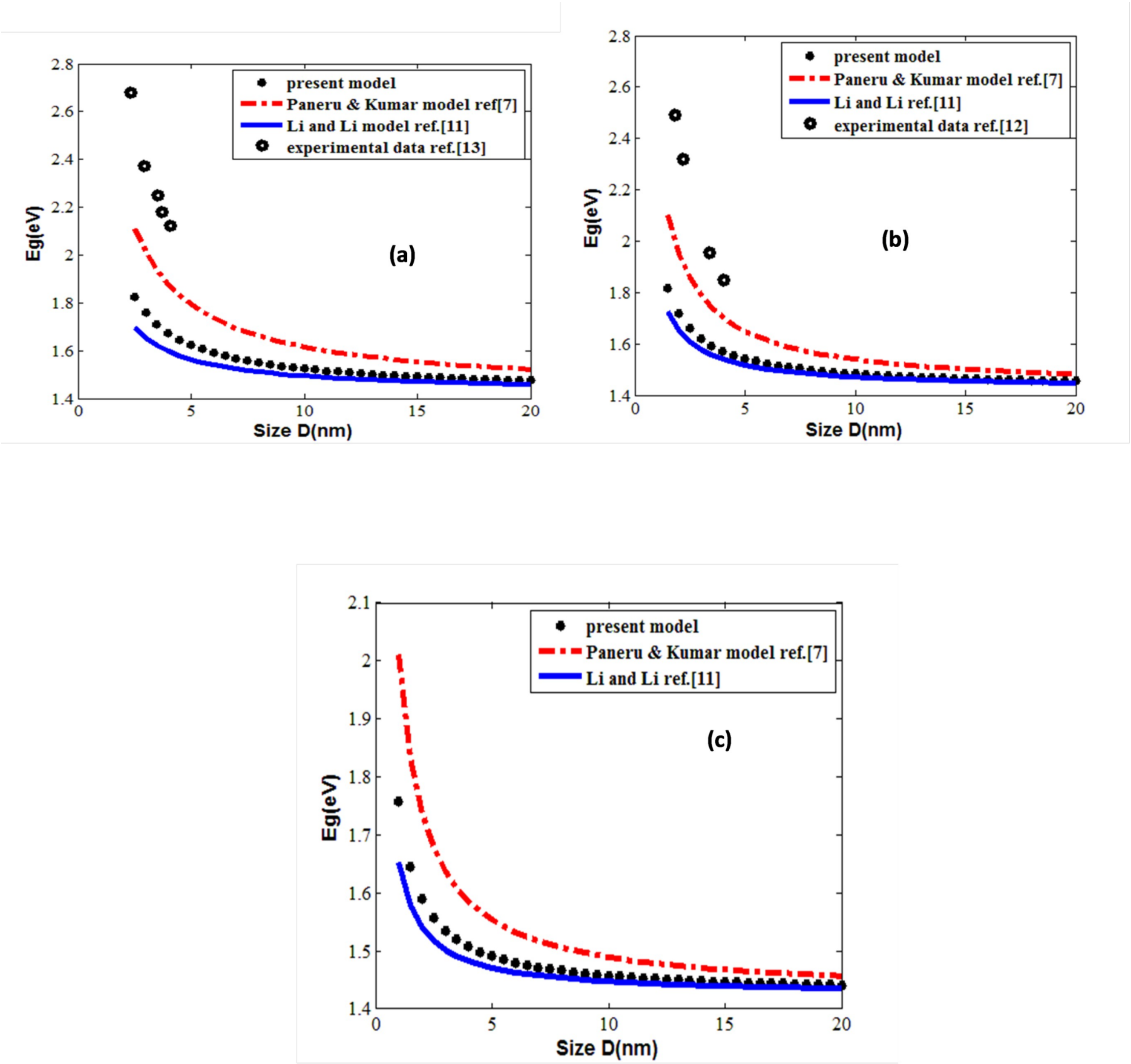

Figure 2. Size dependent of Bandgap of, (a) Spherical, (b) Nanowire, and (c) Nanofilm GaAs.

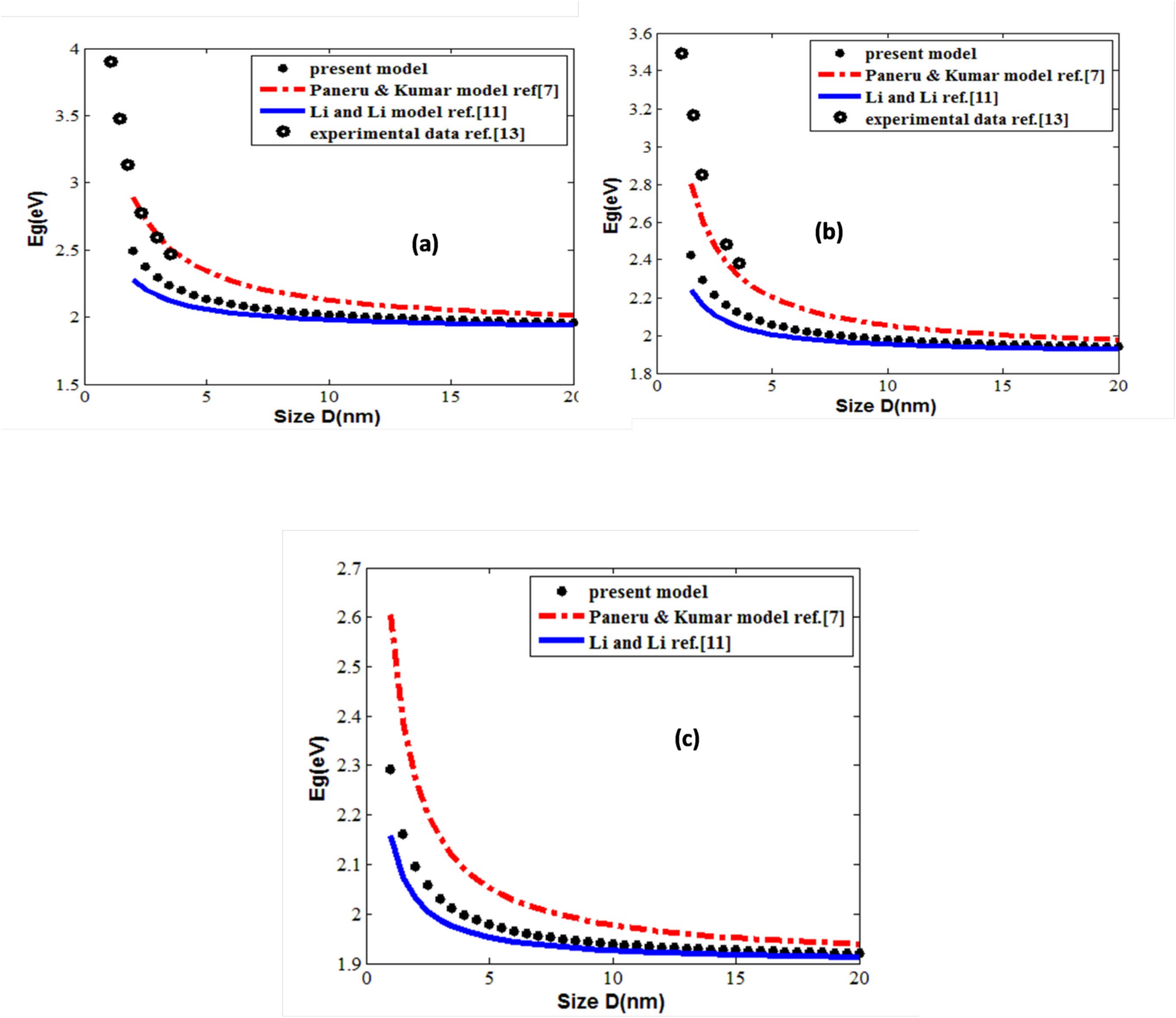

Figure 3. Size dependent of Bandgap of, (a) Spherical, (b) Nanowire, and (c) Nanofilm InN.

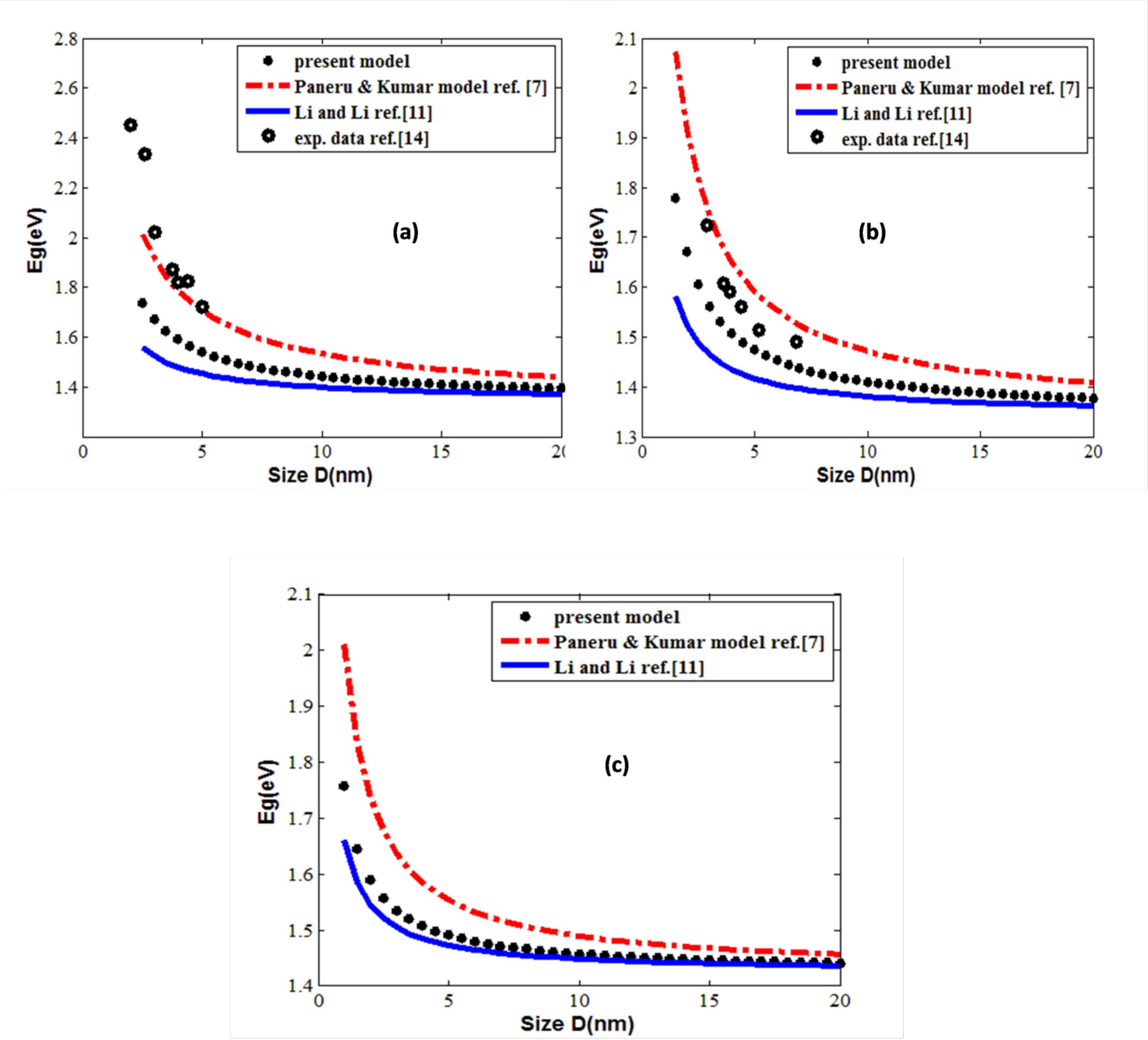

Figure 4. Size dependent of Bandgap of, (a) Spherical, (b) Nanowire, and (c) Nanofilm InP.

Table 1. Input parameters used in the present work [7], [8], [9], [10], [11].

Material	Energy gap of bulk size Eg(∞) (eV)	Atomic diameter d (nm)
CdS	2.49	0.252
GaAs	1.424	0.35
InN	1.9	0.31
InP	1.344	0.364

and increases the energy required for an electron to transition from the valence band to the conduction band. It further leads to the proximity of the electron-hole pairs, strengthens the Coulombic interaction, and adds to their kinetic energy. Even though exciton effects play a role in optical behavior, the scaling effect of any optical effect, quantified by the widening band gap in smaller nanostructures, be it nanoparticles or nanowires, is the scaling effect of kinetic energy due to spatial confinement. This applies to a variety of nanostructures, such as be nanoparticles in the form of spheres or nanowires in the form of thin ones [30].

In order to test the performance of our model, we tested it on a series of semiconductor nanomaterials. We ensured we used materials where experimental evidence had been done before, so that we could compare our results with the previous studies [7], [8], [9], [10], [11], [12], [13], [14]. This enabled us to determine the appropriateness of our theoretical approach. We have demonstrated in Figures 1, 2, 3 and 4 our calculated values of the bandgap values, $E_g(D)$, together with the experimental and simulation data. We predict that we agree with previous theoretical studies and experimental data on the whole size scale, particularly with CdS, InN, InP, and GaAs, where a large amount of experimental data is present.

The distance between the neighboring ions is important in defining the extent to which their electron wave functions overlap, which in turn affects the energy band structure. The electron-phonon interaction is another parameter that is important and depends on the size of the particle as a result of variation in the lattice vibrations- a process called size-dependent lattice vibration (SDLV). Basically, SDLV could be measured by measuring as the measure of the mean displacement of the atoms with respect to their equilibrium positions known as size-dependent mean-squared displacement (SDMSD). This lattice vibration effect is sometimes referred to as Debye-Waller (DW) screening, which contains the effect of a lattice vibration upon the effective potential that electrons feel [31].

Lastly, in bulk materials, energy bands are created as a result of the aggregation of many atoms and molecules, via which adjacent energy levels become combined. But, in the process of reducing the particles to the nanoscale, they consist of a very small number of atoms or molecules. Consequently, the overlap between orbitals and energy levels is reduced, which results in narrower bands. Such narrowing of the band width raises the energy difference between the conduction and the valence band, and that is why the band gap of nanoparticles (NPs) is usually larger than the band gap of their bulk counterparts. The band gap, being a forbidden region of energy to the electrons, a larger band gap would create more constraints on the movement of electrons. As a result, nanoparticles have a lower electrical conductivity than the bulk material their creation is out of. Moreover, this widened band gap results in a change of the absorption spectrum to shorter wavelengths-popularly referred to as blue shift.

From Figures 1, 2, 3 and 4, it's clear that the band gap is wider in the given size range, is strongest for nanoparticles, and moderate for nanowires and nanofilms display weaker increasing in bandgap for all materials used in this work, because size-dependent band gap modulation varies significantly with dimensionality due to differences in electronic confinement. Spherical nanoparticles exhibit the strongest quantum confinement because electrons and holes are restricted in all three spatial directions, producing an approximately ($1/R^2$) dependence. Nanowires show a more moderate dependence since carriers are confined only in the radial directions while remaining free along the axial direction. In contrast, nanofilms display the weakest size-induced band gap shift, as quantization occurs solely along the film thickness. These trends reflect the dimensionality-dependent curvature imposed on electronic wavefunctions at the boundaries: as the number of confined directions increases, this leads to an increase in carrier kinetic energy and, consequently, the wider the band gap, the greater the number of confined directions, the larger the increase in carrier kinetic energy, and, consequently, the wider the band gap.

4. Conclusion:

The behavior of the band gap in nanoscale semiconductors of different sizes and geometries is accurately described by the proposed model. The findings are consistent with experimental data and other theoretical models and suggest the relevance of the mathematical approach used in the given study. This is because the quantum confinement of a band gap increases strongly with the size of a particle. It was found that the particles of different sizes such as the spherical, nanowires and nanofilms have different behavior in the bandgap as a result of their different electronic degrees of freedom. Therefore, the present model provides a powerful predictive method of designing and optimizing the electronic characteristics of new materials in a high-order optical and microelectronic technology, which is a great advance in the field.

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Data Availability Statement: All of the data supporting the findings of the presented study are available from the corresponding author on request.

Declarations:

Conflict of interest: The authors declare that they have no conflict of interest.

Ethical approval: This research did not include any human subjects or animals.

Author Contributions: All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

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الفجوة الطاقية المعتمدة على الحجم في بعض المواد النانوية شبه الموصلة

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الخلاصة

يتناول هذا البحث دراسة التغير في فجوة الطاقة نتيجة لاختلاف حجم الجسيمات على المستوى النانوي لكل من (CdS ، $GaAs$ ، InN و InP)، والذي تم قياسه نظرياً بالاعتماد على نموذج نظري يستند الى فروق الطاقة بين الجسيمات النانوية ونظيراتها في الحالة السائبة. هذه الدراسة توضح أن طاقة فجوة النطاق ليست قيمة ثابتة، وإنما تتغير بصورة جوهرية تبعاً لحجم الجسيمات. وقد بينت هذه الدراسة النظرية بوضوح أن طاقة فجوة النطاق تزداد مع تناقص حجم الجسيمات في المواد المدروسة في هذا البحث. ويرتبط هذا السلوك ارتباطاً وثيقاً بآليات تحضير اشباه الموصلات النانوية. كما أظهرت التنبؤات المستخلصة من هذا النموذج توافقاً ملحوظاً مع نتائج التجارب السابقة، مما يعزز من مصداقيته ويؤكد جدواه العلمية.

الكلمات الدالة : فجوة الطاقة، المواد النانوية، الاعتماد الحجمي

التمويل: لايوجد.

بيان توفر البيانات: جميع البيانات الداعمة لنتائج الدراسة المقدمة يمكن طلبها من المؤلف المسؤول.

اقرارات:

تضارب المصالح : يقر المؤلفون أنه ليس لديهم تضارب في المصالح.

الموافقة الأخلاقية: لم يتضمن هذا البحث أي تجارب على البشر أو الحيوانات، بالتالي لم يكن من الضروري الحصول على موافقة اخلاقية.

مساهمات المؤلفين: قام جميع المؤلفين بمراجعة النسخة النهائية المراد نشرها ووافقوا على تحمل المسؤولية عن جميع جوانب االعمل.