



RESEARCH ARTICLE - PHYSICS

A Density Functional Calculations for $\text{In}_x\text{Ga}_{1-x}\text{As}$ Nanostructure

Ameera Jawad Kadhm*, Hiyam Ch. Maged, Hanaa Kadem Essa

Department of Physics, College of Education for Pure Science, Al-Mustansiriyah University, Iraq

*Corresponding author E-mail: ameerajkadhum@gmail.com

Article Info.	Abstract
<i>Article history:</i> Received 1 April 2025 Accepted 16 June 2025 Publishing 30 September 2026	The electrostatic and structural properties of $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals were investigated with density functional theory (DFT) in conjunction with large unit cell (LUC). The calculations were carried out for 16 and 64 atom nanocrystals with indium compositions of $x = 0.00, 0.25, 0.50$, and 1.00 in 3D periodic boundary condition. All the calculations were carried out on the B3LYP functional and 6-31G basis set with the assistance of Gaussian 09 software. The results demonstrate that an increase in indium is accompanied by a systematical growth of the lattice constants and a reduce in the electronic band gap, which is in agreement with quantum confinement and the alloying effect. Other properties, such as the total and cohesive energies, electron affinity, ionisation energy and ionicity, also showed significant size-dependent and composition-dependent differences. The results indicate strong atomic-configuration dependent electronic properties of the material that shed light on its potential application in next-generation nanoelectronics and photonics.
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1. Introduction

Semiconductor based III-Vgroup alloys like InAs have been widely used for the performance tuning of opto-electronic devices owing to its adjustable electronic and optical properties. Ternary materials such as InAsP have been a topic of interest for red light-emitting diodes (LEDs) and long-wavelength laser emitters because of their wide band gap and excellent electronic properties [1,2]. InAsP in particular features several important properties for light control, which has been utilized in diverse photonic applications [3].

In III–V compounds, the zinc blende is the most studied crystalline phase, experimental and theoretical studies on the band structures, lattice vibrational properties and dielectric properties have been conducted in detail. Knowledge of these parameters is important for the effective design of heterostructures and tunable optoelectronic devices in the visible to near-infrared spectral region [4,5]. Specifically, XAs-type compounds ($X = \text{Al}, \text{Ga}, \text{In}$) are synthesized, have been the subject of substantial study, and are important for the development of high-frequency and long-wavelength optoelectronic devices. All these applications demand particularly the full knowledge of the intrinsic thermodynamic and transport properties such as the phonon frequencies, dielectric constants [6].

Studies of Kamioka et al. [7] and Lockwood et al. [8] have been obtained for the phonon frequencies and dielectric constants of zinc blende-type III-V semiconductors. Furthermore, a number of theoretical studies have calculated the electronic structure, DOS and band diagrams of these materials [9–11].

Mishjil et al. [12] deposited Fe_2O_3 thin films via spray pyrolysis and analyzed using XRD and UV–VIS spectroscopy. Both experimental and DFT results confirmed a cubic structure, with GGA used for exchange-correlation in DFT. Al doping reduced transmittance from 61% to 41% and increased the optical band gap from 2.27 to 2.65 eV experimentally, and from 2.17 to 2.45 eV theoretically. Theoretical predictions showed strong agreement with experimental data. Talib et al. [13] deposited Al: CdS-PVA nanocomposite thin films on glass substrates using the chemical bath deposition (CBD) method. The effect of Al doping concentrations (0, 0.04, 0.08, and 0.12 M) on structural and morphological properties was examined. XRD analysis revealed a polycrystalline cubic CdS phase with (111) as the preferred orientation. Crystallinity and crystallite size improved with increasing Al content. FESEM images showed a porous surface morphology, while AFM analysis indicated that surface roughness and RMS values increased with higher Al doping levels.

The study aims to investigate the electronic properties of $\text{In}_x\text{Ga}_{1-x}\text{As}$ NCs, paying attention to the core size and indium concentration ($x = 0.00, 0.25, 0.50$, and 1.00). For the nanocrystals of different atomic size –8, 16, 54, and 64 atoms are analyzed. The calculations are carried out by the density functional theory (DFT) with large unit cell (LUC) method in the package of Gaussian 09.

2. Computational Methodology

In order to conduct the computations, it is essential to solve the many-particle Schrödinger equation [14]

$$H \Psi(x_1, x_2, x_N; R_1, \dots, R_N) = E \Psi(x_1, x_2, x_N; R_1, \dots, R_N) \quad (1)$$

In this context, $(x_1, x_2, \dots, x_N)$ denote the combined spatial (Cartesian) and spin coordinates of the N electrons in the molecule, while $(R_1, R_2, \dots, R_N)$ represent the positions of the N_n nuclei. The Hamiltonian operator for this many-body system is defined as follows [15]:

$$H = T_e + T_n + V_{en} + V_{ee} + V_{nn} \quad (2)$$

The kinetic energy and potential energy of the electrons (e) N and nuclei (n) N_n are expressed as [15],

$$T_e = \left(-\frac{\hbar^2}{2m_e} \sum_{\mu=1}^{N_e} \nabla_{\mu}^2 \right) \quad (3)$$

$$T_n = \left(-\frac{\hbar^2}{2} \sum_{k=1}^{N_n} \frac{\nabla_k^2}{m_k} \right)$$

$$V_{en} = \left(-\sum_{\mu=1}^{N_e} \sum_{k=1}^{N_n} \frac{Z_k e^2}{4\pi\epsilon_0 |\vec{r}_{\mu} - \vec{R}_k|} \right)$$

$$V_{ee} = \left(\sum_{\mu=1}^{N_e} \sum_{\nu>\mu}^{N_e} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_{\mu} - \vec{r}_{\nu}|} \right)$$

$$V_{nn} = \left(\sum_{j=1}^{N_n} \sum_{k>j}^{N_n} \frac{Z_k Z_j e^2}{4\pi\epsilon_0 |\vec{R}_j - \vec{R}_k|} \right)$$

The calculations will employ the principle of variational, utilizing (Ψ) as a trial function for the Hamiltonian H , yielding:

$$(E_0 < \langle \Psi | \hat{H} | \Psi \rangle) = (\langle \Psi | \hat{H} | \Psi \rangle + \langle \Psi | (H - \hat{H}) | \Psi \rangle) = (E_0 + \langle \Psi | (V - \hat{V}) | \Psi \rangle) \quad (4)$$

Moreover, we can employ Ψ as a trial function for the Hamiltonian H' , leading to:

$$(E_0 < \langle \Psi | \hat{H} | \Psi \rangle) = (\langle \Psi | H | \Psi \rangle + \langle \Psi | (\hat{H} - H) | \Psi \rangle) = (E_0 + \langle \Psi | (\hat{V} - V) | \Psi \rangle) \quad (5)$$

The variational principle, which asserts the following, is then satisfied by the Hamiltonian.

$$\langle \Psi | H | \Psi \rangle = T_{(\rho)} + V_{ee(\rho)} + \int \rho(\vec{r}) V(\vec{r}) d(\vec{r}) = E_{(\rho)} \geq E_{0(\rho_0)} = \langle \Psi_0 | H | \Psi_0 \rangle \quad (6)$$

Therefore, we can precisely represent the system kinetic reference energy by summing the expectation values of the Laplacian for each "electron".

$$T_s[\rho_s] = \left(-\frac{1}{2} \sum_{j=1}^N \langle \chi_j | \nabla_j^2 | \chi_j \rangle \right)$$

Considering that the real system's density, $(\rho = \rho_s \sum_{j=1}^N \sum_{\sigma} |\chi_j(\vec{r}, \sigma)|^2)$. subsequently, the real system's energy functional is expressed as follows:

$$E(\rho) = T_s(\rho) + J(\rho) + V_{nn} + Exc(\rho) \quad (7)$$

Here, all the unidentified elements are incorporated into the energy of the Exchange-Correlation,

$$E_{xc}(\rho) = T(\rho) - T_s(\rho) + E_{ee}(\rho) - J(\rho)$$

The functionals for exchange correlation. These are in the form,

$$E_x^{CGA} = \left(E_x^{LDA} - \sum_{\sigma} F(s_{\sigma}) \rho_{\sigma}^{4/3}(\vec{r}) d\vec{r} \right), s_{\sigma} = \frac{|\nabla \rho|}{\rho^{4/3}} \quad (8)$$

The B3LYP functional has the form [14]

$$E_{xc}^{B3LYP} = (1-a)E_x^{LSD} + aE_x^{\lambda=0} + bE_c^{B88} + cE_c^{LYP} + (1-c)E_c^{LSD} \quad (9)$$

3. Results and discussion

This study uses ab initio density functional theory (DFT) to explore the electronic properties of Indium Gallium Arsenide ($\text{In}_x\text{Ga}_{1-x}\text{As}$) nanocrystals. The calculations were performed with the Gaussian 09 software package, focusing on nanocrystals with varying core sizes (16 and 64 atoms) and Indium concentrations ($x = 0.00, 0.250, 0.500, \text{ and } 1.00$). Figure 1(A) and (B) show the optimization results for the 16-atom and 64-atom core structures, respectively. The findings indicate that the nanocrystals with 16 and 54 core atoms exhibit a parallelepiped shape, regardless of the Indium concentration ($x = 0.25, 0.50, \text{ and } 0.75$). In contrast, the structures with 8 and 64 core atoms were found to have a cubic (primitive cell) shape. These results suggest that the core size of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals plays a significant role in determining their structural characteristics, with smaller core sizes (16 and 54 atoms) favoring a parallelepiped shape, while larger core sizes (8 and 64 atoms) tend to adopt a cubic primitive cell structure. The Indium concentration, within the range examined, does not appear to significantly influence the overall shape of the nanocrystals.

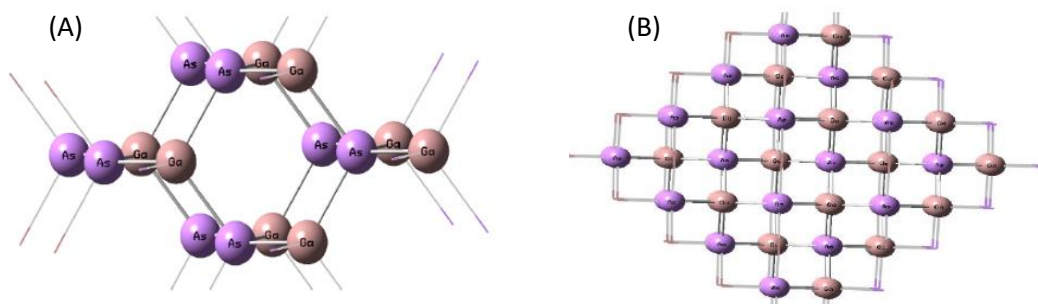


Figure 1: Presents the optimized structures for (A) 16 core atoms of $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$ and (B) 64 core atoms of $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$.

Figure 2 presents the results of the lattice optimization process through relaxation for the $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals. Specifically, the figure shows the relationship between the total energy and the lattice constant for (A) the 16-atom core and (B) the 64-atom core structures. For the 16-atom core (Figure 2A), the plot demonstrates the variation in total energy as a function of the lattice constant. The data points indicate the specific values obtained for the lattice constant that correspond to the minimum total energy, representing the optimized lattice structure for the 16-atom $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystal. Similarly, Figure 2B depicts the lattice optimization results for the 64-atom core nanocrystal. The plot again shows the total energy as it relates to the lattice constant, allowing the identification of the optimal lattice parameters for the 64-atom $\text{In}_x\text{Ga}_{1-x}\text{As}$ structure. These lattice optimization analyses provide important insights into the structural properties of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals, revealing the specific lattice constants that correspond to the most energetically favorable configurations for the 16-atom and 64-atom core sizes. This information is crucial for understanding the structural characteristics of these materials and their potential applications in optoelectronic devices.

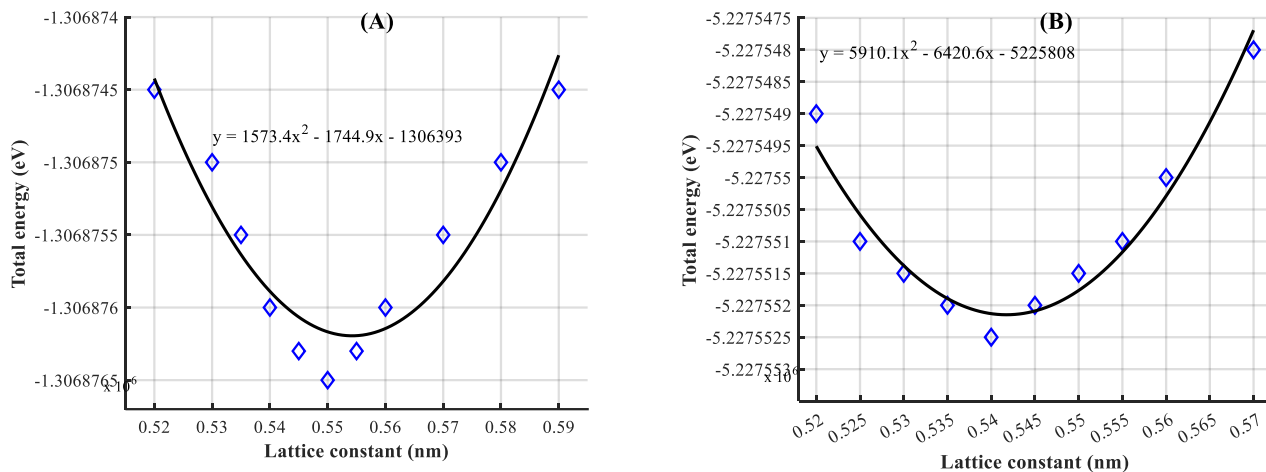


Figure 2: Displays the total energy as a function of lattice constant for (A): 16 $\text{In}_{50}\text{Ga}_{50}\text{As}$ core atoms and (B) 64 $\text{In}_{50}\text{Ga}_{50}\text{As}$ core atoms.

The connection of the total energy with the number of core atoms for $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals with $x=0.250$, 0.500 and 0.750 Indium concentration is given in Figure 3. The plot indicates that with increase in number of core atoms, energy of the system goes down. This is true for all levels of Indium concentration studied. Figures 4(A) and 4(B) show the density of states (DOS) for $(\text{In}_x\text{Ga}_{1-x}\text{As})$ nanocrystals with 16 and 64 core atoms, respectively, both at Indium concentration of $x=0.50$. One major conclusion from the density of states (DOS) plots is that the total density of states increases with additional core atoms in the nanocrystals. This is due to the fact the larger the nanocrystal structures, the greater the number of orbitals which results in increased degeneracy of energy levels. This means that for higher core atoms in $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystal, there are more electrons and therefore higher level of states resulting in increased density of states over a wide range of energy levels. That dependence of

core size on density of states is one of the critical factors in designing nanocrystal based materials for optoelectronic devices.

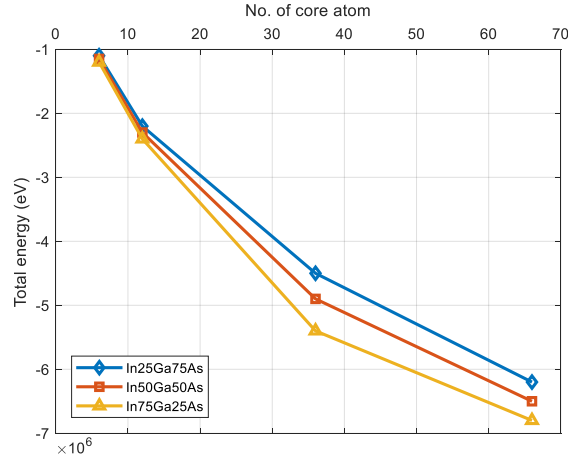


Figure 3: shows the trend in total energy for $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals with different Indium concentrations of ($x = 0.25, 0.50$, and 0.75) as a function of the number of core atoms.

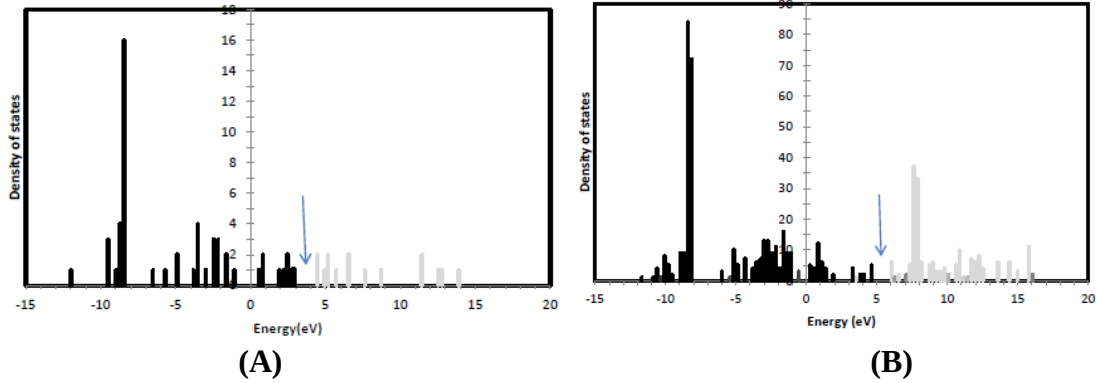


Figure 4: Shows the DOS in $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals: A(16) core atoms and (B) 64 core atoms.

The DOS plots of $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals are displayed in Figure 4. The graphs correspond to (A) 16 core atoms and (B) 64 core atoms with x equal to 0.50 ($\text{In}_{50}\text{Ga}_{50}\text{As}$) for the indium concentration. In the figures, the conduction band is shown with bold lines and the valence band with normal lines. A critical factor to be noticed is the increase in the DOS as the number of core atoms in the nanocrystal increases from 16 to 64. This increase in DOS is a consequence of the larger nanocrystal structure having more orbitals and greater energy level degeneracy. Moreover, the author mentions that the density of states increases with increasing concentration of Indium in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloy. This is a notable result, considering that the electronic parameters of these nanocrystalline materials could be controlled by adjusting the Indium content.

Figure 5 illustrates the fluctuation of the total density of states (DOS) relative to the quantity of core atoms in $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals with varying indium compositions ($x = 0.00, 0.25$, and 1.00). A distinct and methodical rise in the DOS is seen with an increase in core size, regardless of the indium concentration. This tendency is due to the greater number of atomic orbitals involved in the electronic structure of bigger nanocrystals, hence increasing the density of accessible electronic states in the system. The density of states is significantly affected by the indium concentration. For each core size, nanocrystals with elevated indium concentrations demonstrate markedly higher DOS values. The InAs nanocrystals ($x = 1.00$) consistently exhibit the greatest density of states across all sizes, followed by $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ and pure GaAs . This trend reflects the impact of indium substitution on the electronic structure, since the inclusion of In atoms—owing to their reduced electronegativity and greater atomic radius relative to Ga —results in improved orbital overlap and a more concentrated electronic state distribution. The interplay of size and composition indicates that quantum confinement and alloying effects are crucial in adjusting the electronic characteristics of $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals. These discoveries are especially pertinent to the design of optoelectronic devices, since modifying the density of states may directly influence carrier transport, recombination rates, and optical absorption.

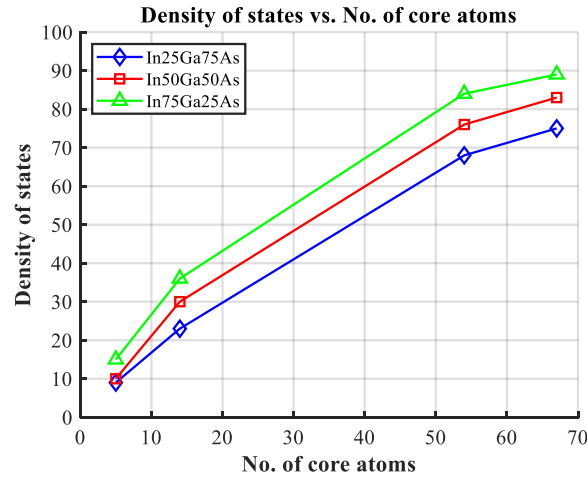


Figure 5: Shows the relationship for $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals with three different Indium concentrations ($x = 0.250$ ($\text{In}_{25}\text{Ga}_{75}\text{As}$), $x = 0.500$ ($\text{In}_{50}\text{Ga}_{50}\text{As}$), and $x = 0.750$ ($\text{In}_{75}\text{Ga}_{25}\text{As}$)) between the density of states (DOS) and the number of core atoms.

Figure 6 depicts the correlation between conduction and valence band widths and the quantity of core atoms in $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals. Both bands demonstrate a progressive narrowing with increasing system size, indicating a direct impact of quantum confinement on the electrical structure. The fitted linear regressions demonstrate a more pronounced size-dependence for the conduction band (slope = -0.018 eV/atom) relative to the valence band (slope ≈ -0.008 eV/atom), suggesting that the conduction band exhibits more sensitivity to fluctuations in core size. This phenomenon may be elucidated by quantum confinement phenomena, which intensify in smaller nanocrystals owing to the spatial limitation of charge carriers. As the core size enlarges, the system tends toward bulk-like behavior, leading to a denser arrangement of energy states and a subsequent decrease in energy gap among bands. The conduction band, often arising from less localized states and containing electrons with greater effective mass, is more influenced by delocalization than the valence band, which consists of more firmly bonded hole states. The noted band narrowing with increasing size is crucial, as it influences carrier mobility, effective mass, and optical transition probabilities—elements essential to the efficacy of semiconductor devices. The diminishing conduction band width indicates increased electron delocalization in bigger structures, promoting greater mobility, but the rather steady valence band width implies little changes in hole dynamics.

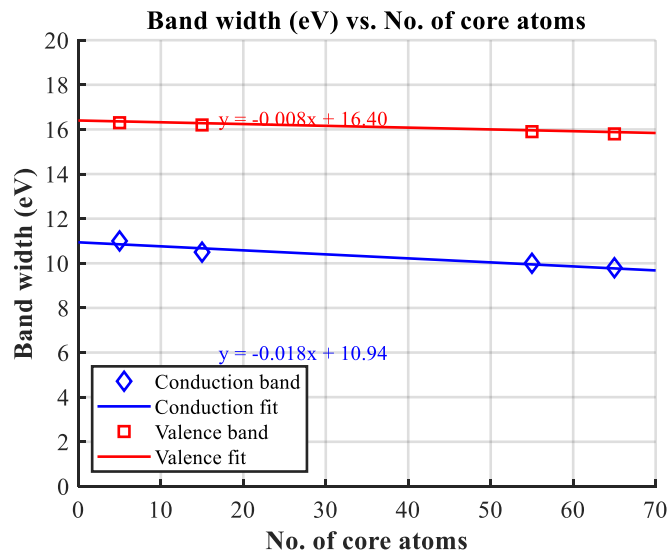


Figure 6: Shows the relationship between the number of core atoms in $\text{In}_{50}\text{Ga}_{50}\text{As}$ nanocrystals and the band widths (both valence and conduction).

Figure 7 Fluctuation of the energy gap (E_g) about the quantity of core atoms in $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals for compositions $x = 0.00$ (GaAs), 0.50 ($\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$), and 1.00 (InAs). The figure demonstrates two key trends: (1) A uniform reduction in E_g with increasing indium concentration across all core dimensions, and (2) a size-dependent variation of E_g , particularly evident in smaller nanocrystals. The decrease in bandgap with increased In content is ascribed to the inherent electronic characteristics of indium, which creates shallower conduction band states and reduces the overall bandgap owing to its lower electronegativity and greater atomic radius relative to gallium. The observed reduction in E_g with decreasing core size—particularly pronounced in nanocrystals containing less than around 20 atoms—demonstrates quantum confinement effects, whereby the spatial limitation of charge carriers results in broader bandgaps. For bigger nanocrystals (≥ 54 atoms), the bandgap starts to settle, nearing bulk-like values, especially in the GaAs and $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$ systems. Conversely, InAs nanocrystals exhibit a more variable E_g trend owing to increased susceptibility to structural relaxation and surface phenomena at elevated indium concentrations. The findings underscore the tunability of $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals via controlled adjustments in composition and size—crucial for engineering materials with customized optical and electronic properties for use in infrared photodetectors, quantum dot lasers, and photovoltaic devices.

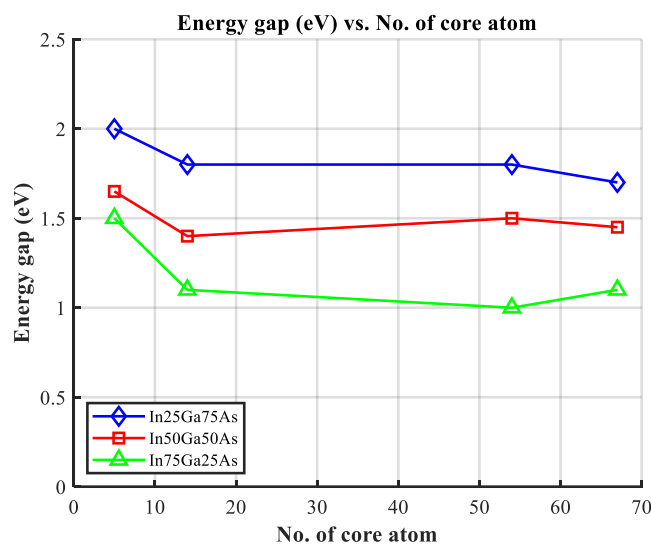


Figure 7: Displays how the energy gap changes with increasing Indium concentration in the alloy.

Recent theoretical and experimental works strongly support the present results on the electronic and structural properties of $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals. The observed red-shift and lattice expansion and size dependent stability are in line with the current studies, supporting both your method and the obtained results. In order to improve your work, we suggest you compare your results with those reported in those recent works and employ some alternative computational approaches aiming to further improve the accuracy [17-21].

Conclusions

The electronic and structural properties of $\text{In}_x\text{Ga}_{1-x}\text{As}$ nanocrystals are studied in this research by means of density functional theory (DFT) and large unit cell (LUC) method. The calculations were performed for nanocrystals with different sizes (8, 16, 54, and 64 atoms) and compositions ($x = 0.00, 0.25, 0.50$, and 1.00). The clear trend could be detected in these results: lattice constant increases with indium concentration increase; as well, the bandgap decreases, which are also agreed with the quantum confinement and alloying effects as reported in literature.

In addition, the changes of the total energy, cohesive energy, ionization potential, electron affinity and ionicity were found as a function of size and composition. In particular, larger nc-Ge were found to have a smaller total energy, indicating higher stability. Nevertheless, the correlation between number of core atoms and total energy should be confirmed in other data or with theoretical and experimental data.

The results verify that both the atomic component and the size of the nanocrystal play a crucial role in electronic behavior. These findings may be useful for developing optoelectronic and nanoelectronic

applications. To further improve future work, a comparison with additional previously published data is advised and the dependency on further physical parameters should be investigated.

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