

GERMANIUM NANOCCLUSERS AS A PROMISING NANO OPTOELECTRONIC MATERIAL: INSIGHTS FROM DFT

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Abstract

Germanium - based nanostructures have attracted significant attention due to their tunable electronic and optical properties arising from strong quantum confinement effects. This paper presents the structural, electronic, and optical properties of germanium nanocluster (GeNCs) investigated using density functional theory (DFT) within the Quantum Espresso simulation package. The optimized GeNC structure has a cohesive energy of -3.596 eV and an average Ge-Ge bond length of 2.32 Å, indicating high structural stability. Analysis of the electronic band structure and density of states (DOS) shows discrete energy levels and a finite DOS at the Fermi level, revealing weak semimetallic behavior due to Ge-H hybridization effects. The charge density distribution indicates that Ge-Ge bonds have a covalent character. The HOMO (Highest Occupied Molecular Orbital) states are mainly localized in the central region, while the LUMO (Lowest Unoccupied Molecular Orbital) states are extended toward the surface. The optical spectra exhibit absorption peaks at 1.6 eV, 2.2 eV, and 4.5 eV, with a maximum absorption coefficient of approximately $2.5 \times 10^5 \text{ cm}^{-1}$. The JDOS spectrum shows several peaks between 0.9 and 9.4 eV, confirming energy discretization and the presence of internal plasmon resonance. These results demonstrate that GeNCs possess strong optical activity and show potential for applications in nano-optoelectronic devices and optical sensors.

Keywords: density functional theory, electronic structure, germanium nanoclusters, optical properties, quantum confinement, quantum espresso.

1. Introduction

In recent years, the study of quantum dots (QDs) or nanoclusters (NCs) has attracted considerable attention from researchers. QDs or NCs are nanometer-scale structures that exhibit quantum confinement effects, leading to electronic and optical properties distinct from those of bulk 2D or 3D materials. Various types of QDs have been investigated, focusing on their electronic and optical characteristics, as well as on how these properties depend on size or doping, with potential applications in optoelectronics and sensing. Cadmium selenide (CdSe) quantum dots, one of the earliest studied II-VI semiconductor systems, show size-dependent optical shifts under hydrostatic pressure, where quantum

confinement becomes significant below approximately 3 nm, while the crystal structure remains stable and optical changes are reversible (Chen et al., 2023). Studies on perovskite QDs (such as CsPbX_3 , where $X = \text{Cl, Br, I}$) have demonstrated remarkable properties, including very high photoluminescence quantum yield, narrow emission spectra, and superior color purity compared to other QDs, indicating strong potential for applications in LEDs, solar cells, and nanolasers (Stephen et al, 2024). Carbon quantum dots (CQDs) exhibit excellent biocompatibility, low toxicity, and high solubility in aqueous media. CQDs can be synthesized using various methods, and their photoluminescence can be tuned by controlling size and surface functionalization. These features make CQDs suitable for bioimaging, sensing, and photocatalytic applications (Kong et al., 2024; Elugoke et al., 2024; Pechnikova et al., 2025). Graphene quantum dots (GQDs) have been shown to possess strong photoluminescence, high photostability, and tunable optical properties through elemental doping such as sulfur or nitrogen (Mondal et al., 2024; Das et al., 2022). Cadmium-free QDs, including InP/ZnS , $\text{CuInS}_2/\text{ZnS}$, and ZnSe/ZnS , have also gained significant interest due to their environmental friendliness and strong optical performance (Xu et al., 2014; He et al, 2025; Mei et al., 2019).

Although numerous experimental and theoretical studies have been conducted on different types of quantum dots (QDs), research on germanium nanoclusters (GeNCs) remains limited. Detailed investigations into their structural, electronic, and optical characteristics are still scarce. The effects of quantum confinement and surface reconstruction on the band gap and optical absorption spectra of GeNCs have not been clearly understood. In this study, the structural, electronic, and optical properties of GeNCs are examined using the density functional theory (DFT) method implemented in the Quantum Espresso simulation package. The atomic structure is fully optimized, followed by calculations of the electronic band structure, density of states (DOS), and optical dielectric functions, to clarify the relationship between geometric configuration and optoelectronic behavior. The obtained results provide theoretical insights into the quantum confinement effects in GeNCs and offer useful guidance for potential applications in optoelectronic materials, solar cells, and advanced semiconductor devices, as well as for future experimental studies.

Despite extensive studies on semiconductor quantum dots and nanocrystals, the electronic and optical properties of very small hydrogen - passivated germanium nanoclusters remain insufficiently understood. In particular, the relationship between atomic structure, frontier orbital distribution, and optical absorption features in ultrasmall Ge clusters has not been fully clarified from first-principles calculations. Therefore, this study aims to systematically investigate the structural stability, electronic structure, charge density distribution, and optical response of a hydrogen-passivated Ge nanocluster using density functional theory. The results provide insights into the quantum confinement behavior and optoelectronic characteristics of Ge - based nanosystems at the cluster scale.

2. Model and computational method

The GeNC structure was constructed based on the hexagonal crystal lattice of germanium, consisting of 13 Ge atoms and 9 H atoms, within a cubic supercell of $20 \times 20 \times 20 \text{ \AA}^3$ to eliminate periodic interactions between neighboring dots. Hydrogen atoms were added to passivate surface dangling bonds, thereby removing unsaturated electronic states and ensuring structural stability. The initial configuration was optimized, and self-consistent field (SCF) calculations were performed until convergence in both energy and forces was

achieved. All calculations were carried out using the Quantum Espresso (QE) simulation package, an opensource software suite for material modeling based on Density Functional Theory (DFT) with the plane-wave pseudopotential method (Giannozzi et al., 2020). The exchange-correlation functional was treated within the Perdew-Zunger Local Density Approximation (LDA) (Perdew et al., 1981). Norm conserving pseudopotentials were used for both Ge and H atoms to describe the ion valence electron interactions. The plane-wave energy cutoff was set to 40 Ry, and the charge density cutoff to 480 Ry to ensure convergence. A $1 \times 3 \times 3$ Monkhorst-Pack k-point grid was used for Brillouin zone sampling. The Marzari Vanderbilt (mv) smearing method with a degauss value of 0.02 Ry was applied to improve energy convergence. The total energy and charge density convergence thresholds were set to 2.2×10^{-4} Ry and 4.4×10^{-9} Ry, respectively. After achieving SCF convergence, non-self-consistent field (NSCF) calculations were performed to obtain detailed electronic distributions across the Brillouin zone. Subsequently, the electronic band structure and density of states (DOS) were computed. The charge density was extracted to visualize the electronic distribution and analyze the bonding characteristics within the GeNC system. Linear optical properties were also evaluated. The complex dielectric function, $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, was calculated within the Random Phase Approximation (RPA), neglecting excitonic effects. The real part, $\epsilon_1(\omega)$, was obtained using the Kramers-Kronig relation, while the imaginary part, $\epsilon_2(\omega)$, was derived directly from the transition matrix elements between electronic states. From these, the joint density of states (JDOS) and the optical absorption spectrum $\alpha(\omega)$ were determined. This approach allows the simulation of absorption and reflectivity spectra consistent with previous DFT-RPA studies (Gajdoš et al., 2006). The optimized atomic configuration of the GeNC model is illustrated in figure 1.

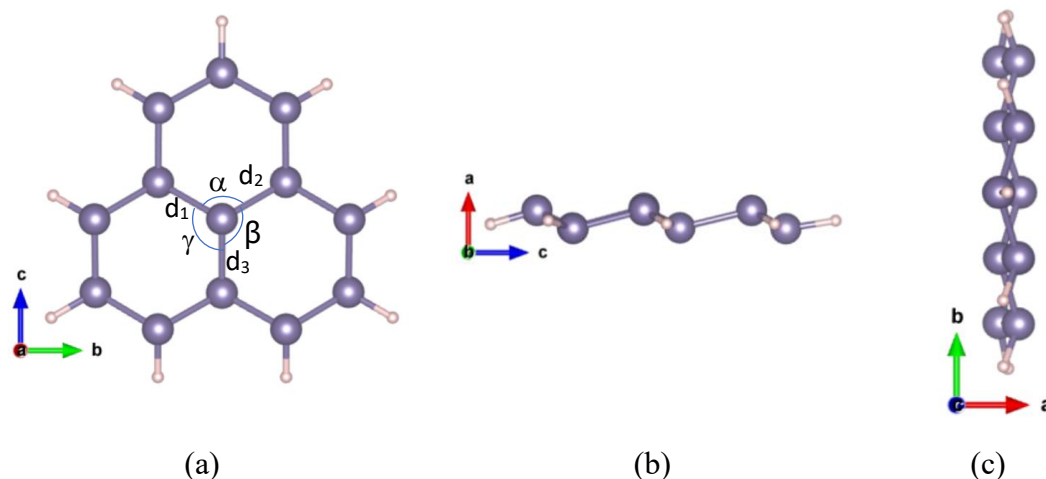


Figure 1. Optimized geometric structure of GeNC in different directions

3. Results and Discussion

3.1. Structural properties

Figure 1 shows the optimized GeNC structure from different orientations. Table 1 lists the fundamental geometric parameters of the GeNC after optimization. The bond lengths of $d_1 = 2.32104$ Å, $d_2 = 2.32098$ Å, and $d_3 = 2.32097$ Å are nearly identical, indicating that the structure achieves high symmetry and geometric equilibrium. These bond lengths are slightly shorter than the Ge-Ge bond length in bulk germanium (approximately 2.45 Å), reflecting the typical bond contraction that occurs when the size decreases to the

nanoscale, a common feature of quantum dot systems due to the higher electron density around surface bonds. This result is consistent with previous DFT studies on Ge nanoclusters, which reported a 4-5% reduction in bond length compared to bulk germanium (Titantah et al., 2004).

Table 1. Fundamental structural parameters of optimized GeNC

Parameters	$d_1(\text{\AA})$	$d_2(\text{\AA})$	$d_3(\text{\AA})$	$\alpha(^{\circ})$	$\beta(^{\circ})$	$\gamma(^{\circ})$	$\delta(\text{\AA})$	$E_{\text{coh}}(\text{eV})$
GeNC	2.321	2.320	2.320	113.334	113.402	115.309	0.636	-3.596

The bond angles $\alpha = 113.330^{\circ}$, $\beta = 113.400^{\circ}$, and $\gamma = 115.310^{\circ}$ deviate slightly from the ideal tetrahedral angle of 109.470° , indicating local lattice distortion caused by the small-size effect and hydrogen passivation. This suggests that although the GeNC framework maintains its fundamental tetrahedral geometry, it tends to adopt a partially planar configuration, similar to what has been observed in Ge nanoflakes and monolayer Ge (Cahangirov et al., 2009). The structural buckling amplitude of $\delta = 0.636 \text{ \AA}$ helps reduce the total energy of the system by minimizing surface stress and enhancing electrostatic stability. The cohesive energy of $E_{\text{coh}} = -3.596 \text{ eV}$ indicates that GeNC is thermodynamically stable. The large negative value of the cohesive energy reflects the formation of strong Ge-Ge and Ge-H bonds within the system. Compared to bulk germanium (-3.85 eV/atom), the slight reduction in cohesive energy is reasonable, arising from surface effects and the reduced coordination number of surface atoms. However, this small difference confirms that the GeNC remains highly stable and robust. Overall, the structural results demonstrate that the GeNC possesses a stable and highly symmetric geometry, with bond lengths and angles within the expected range for Ge-Ge tetrahedral networks. The slight bond contraction, the presence of buckling distortion, and the cohesive energy collectively indicate the influence of quantum confinement and surface effects at the nanoscale.

3.2. Electronic properties

Figure 2(a) shows the electronic band structure, and figure 2(b) presents the electronic density of states (DOS) of the GeNC. The results reveal clear quantum characteristics of the nanosystem, where the energy levels appear as discrete bands rather than continuous ones as in bulk or 2D germanium. The appearance of these discrete levels arises from the quantum confinement effect when the particle size becomes smaller than the exciton Bohr radius of Ge (approximately 24 nm), causing electronic states to become spatially confined and energy levels to separate into discrete states. The valence and conduction bands are nearly in contact at the Fermi level, resulting in a nonzero DOS near the Fermi energy in the DOS plot (figure 2b). The existence of a finite DOS around the Fermi level indicates that GeNC does not exhibit a true band gap or possesses a very narrow gap. The relatively flat energy bands reflect strong localization of the electronic states, a typical feature of spatially confined quantum dot systems. At the Γ point, a slight overlap between the valence and conduction bands is observed, suggesting that GeNC exhibits a hybrid behavior between semiconductor and semimetal. This phenomenon has also been reported in small Ge nanoclusters ($n < 30$ atoms), where strong surface effects and hydrogen passivation lead to mixing of Ge-H energy states within the band gap region.

The DOS analysis further supports this observation. In the energy range from -0.5 eV to 0.5 eV around the Fermi level, the DOS does not vanish completely but shows several small peaks, indicating the presence of electronic states near this level. These states are

typically formed due to asymmetry in surface reconstruction or incomplete hybridization between Ge 4p and H 1s orbitals. The DOS region below -2 eV exhibits higher intensity, corresponding to Ge 4s states, while the energy range from -2 eV to 0 eV is mainly dominated by Ge 4p states, with distinct DOS peaks arising from energy splitting between sp^3 -hybridized orbitals. The conduction band region above 0 eV shows lower DOS values, reflecting the discrete nature of excited electronic levels in the confined system. The presence of finite DOS at the Fermi level indicates that GeNC exhibits weak electrical conductivity or semimetallic behavior, in contrast to bulk germanium, which is an indirect semiconductor. This property suggests that the electronic characteristics of GeNCs can be further tuned through doping, strain engineering, or surface functionalization.

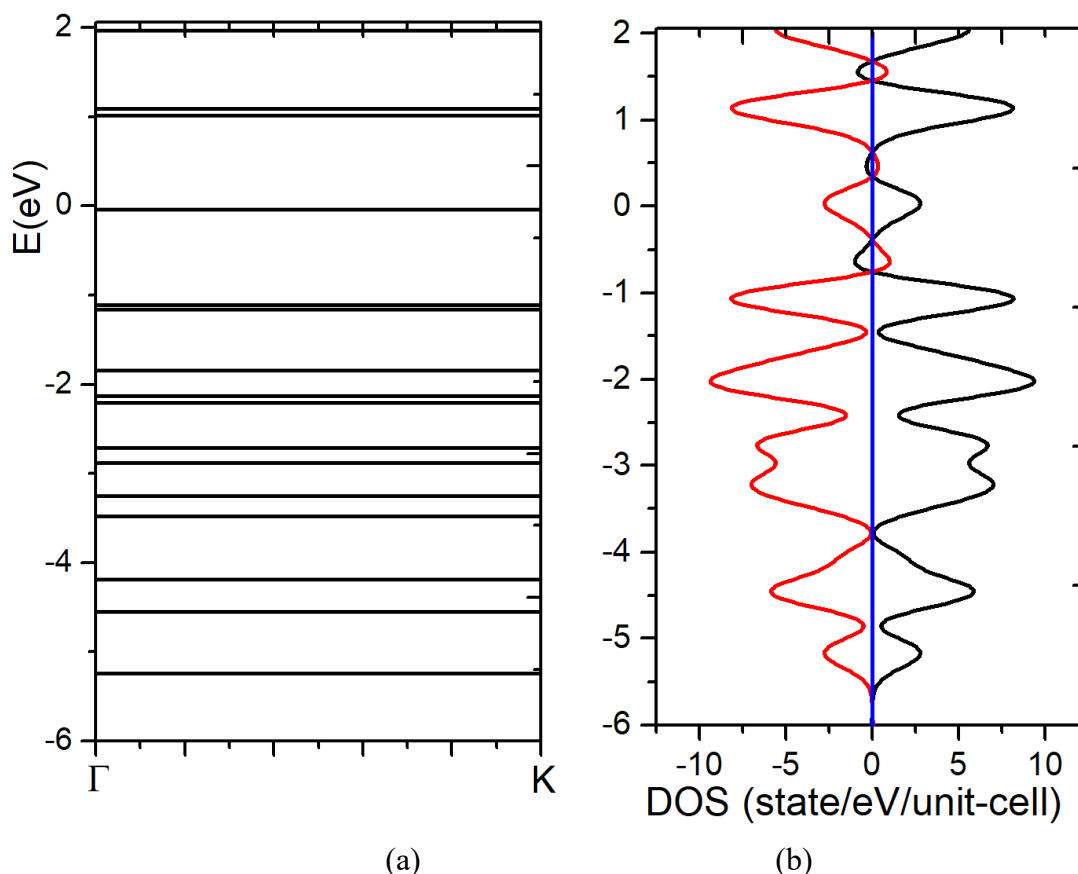


Figure 2. (a) Molecular orbital energy levels of the Ge nanocluster and (b) density of states (DOS) of GeNC

3.3. Charge density distribution

Figure 3 illustrates the charge density distribution of the GeNC system. Figures 3(a) and 3(b) show the three-dimensional charge density in the xy-plane and xz-plane, respectively, while figures 3(c) and 3(d) present two dimensional contour maps, where charge density intensity is represented by a color scale ranging from red (high density) to blue (low density). The results reveal that the charge density is primarily concentrated along the Ge-Ge bonds, indicating that covalent bonding is the dominant interaction within the system. The dense iso-surfaces connecting neighboring Ge atoms reflect strong overlap between the 4s and 4p orbitals, forming stable σ bonds characteristic of sp^3 hybridization in germanium. This behavior is fundamentally different from that in materials dominated by ionic or weak van der Waals interactions. The dark red regions

between Ge atoms correspond to the highest charge density zones, where bonding electrons are strongly localized between Ge nuclei, a signature of covalent σ bonding. In contrast, the light blue regions located at the hexagonal voids represent spatially empty regions where electron density is nearly zero. The sixfold symmetric distribution of charge density reflects the structural stability of the system and indicates the absence of abnormal electronic localization at the surface, confirming that GeNC maintains high electronic stability. At the outer region, where Ge atoms are passivated by hydrogen, the charge density is lower than that in the inner region. The electron clouds surrounding H atoms are oriented toward Ge atoms, showing weak electron sharing between Ge and H. The Ge-H bonds are weakly covalent and slightly polarized, with electrons slightly attracted toward H due to its higher electronegativity, effectively saturating the dangling orbitals of surface Ge atoms.

Figure 4 shows the charge density distribution corresponding to the frontier orbitals: HOMO (Highest Occupied Molecular Orbital) in figures 4(a-c) and LUMO (Lowest Unoccupied Molecular Orbital) in figures 4(d-f) for the GeNC. The charge density associated with the HOMO is mainly concentrated around the central Ge atoms and distributed along the Ge-Ge bonds, indicating strong bonding characteristics. The electron clouds are symmetrically shaped around the Ge-Ge bonds, with high density localized between adjacent atoms, a typical feature of σ bonds formed through strong overlap of 4p orbitals. This also indicates that the highest occupied electronic states (HOMO) have an intrinsic covalent bonding nature, primarily arising from sp^3 hybridized orbitals within the Ge network. The HOMO region does not extend toward the hydrogen atoms at the edges, suggesting that H atoms do not significantly contribute to the main valence orbitals but rather serve to passivate surface dangling bonds. This confirms that hydrogen functionalization effectively removes unstable surface states while maintaining the bulk-like covalent nature of the HOMO levels. The localization of the HOMO charge density near the core region also provides evidence of strong quantum confinement, where valence electrons are spatially confined within a small region, resulting in an upward shift of the HOMO energy compared to that in 2D or bulk germanium.

In contrast, figures 4(d-f) show that the charge density distribution of the LUMO exhibits clearly different characteristics. The LUMO electron clouds are more widely distributed and strongly extend toward the surface region, particularly along the Ge-H bonds. This indicates that the LUMO states possess antibonding character and a delocalized nature, meaning that excited electrons can spread over a larger portion of the structure. These LUMO orbitals are mainly formed by weak overlap between the Ge 4p and H 1s orbitals, resulting in Ge-H antibonding states. The electron density tends to concentrate at the surface and along the vertical direction, rather than in the core region as observed for the HOMO. The distinct spatial separation between HOMO and LUMO distributions demonstrates that the HOMO-LUMO electronic transition in GeNC is spatially directional, where excited electrons move from the core toward the surface upon optical excitation. This suggests that the photoexcitation process in GeNCs involves charge transfer from the interior to the surface region, an important factor influencing their photoelectronic and photocatalytic activity.

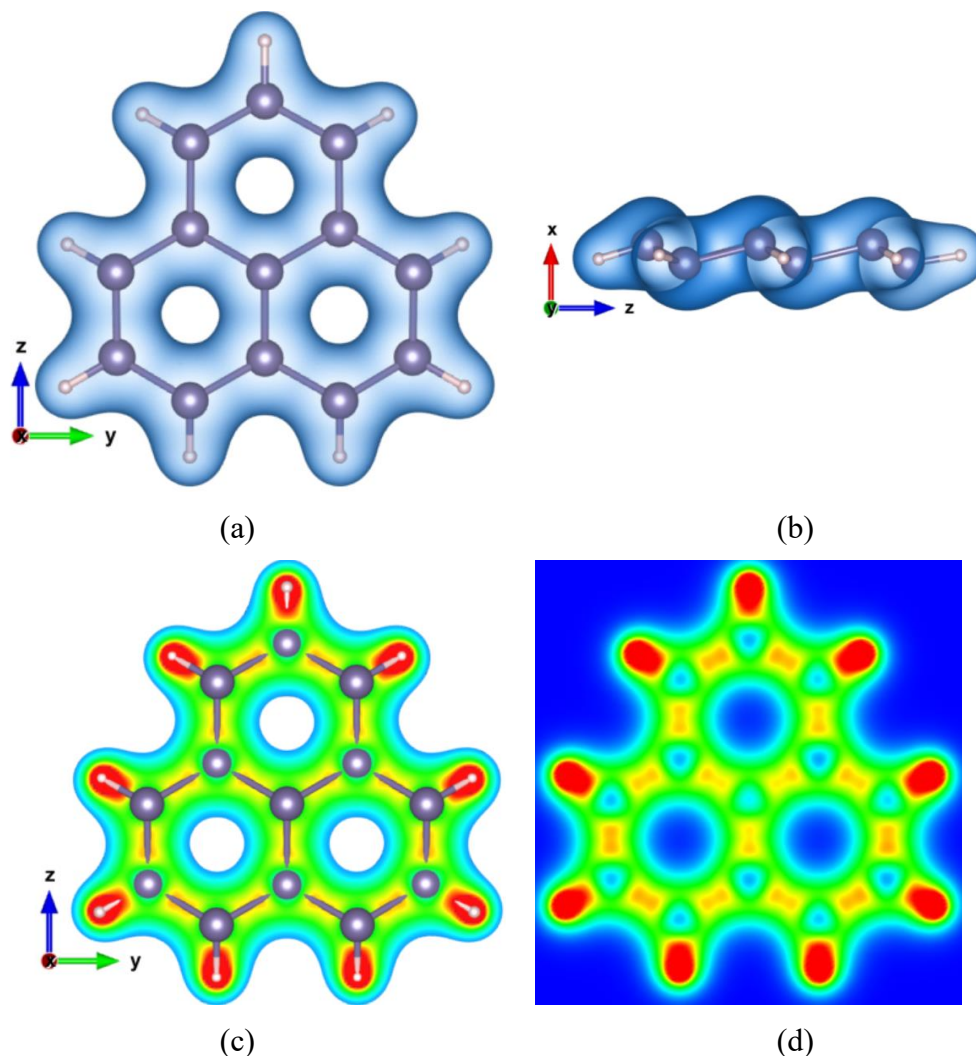


Figure 3. Charge density distribution of GeNC

The energy separation between the HOMO and LUMO defines the effective band gap (HOMO-LUMO gap) of the system, which is approximately 1.7 eV. The clear spatial distinction between the HOMO (localized in the core) and the LUMO (distributed at the surface) indicates that GeNC may exhibit asymmetric exciton behavior, where electrons and holes are confined in different spatial regions. This phenomenon often leads to reduced non-radiative recombination and enhanced photoluminescence efficiency, which is a key advantage of well-passivated quantum dots. The extended distribution of the LUMO beyond the surface also suggests a strong potential for interaction with the surrounding environment, such as adsorption or solvent effects. GeNCs with such HOMO-LUMO characteristics show promising potential for applications in optical sensing, photocatalysis, and light-emitting materials.

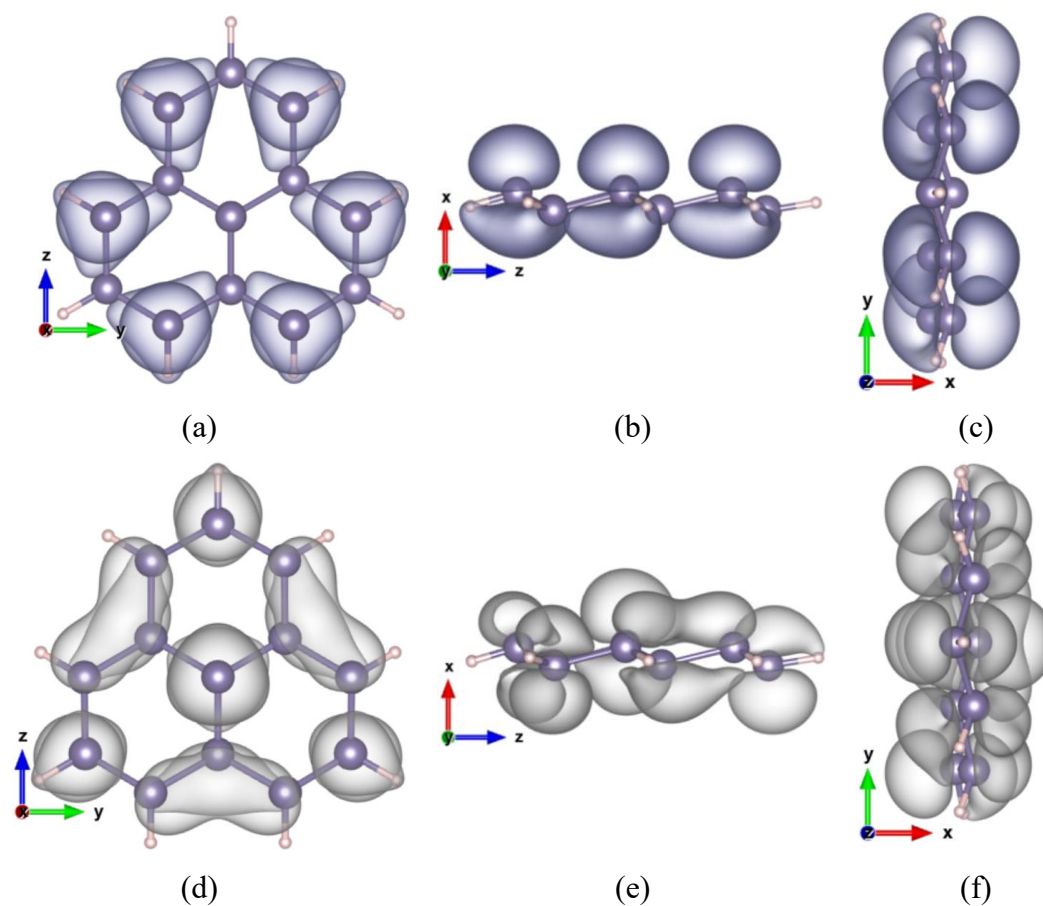


Figure 4. Charge density distribution of HOMO (a-c) and LUMO (d-f) states in GeNC

3.4. Optical properties

Figure 5 presents the fundamental optical characteristics of the GeNC. Figures 5(a) and 5(b) show the real part, $\epsilon_1(\omega)$, and the imaginary part, $\epsilon_2(\omega)$, of the complex dielectric function, respectively, while figures 5(c) and 5(d) display the absorption coefficient, $\alpha(\omega)$, and the reflectivity, $R(\omega)$, as functions of photon energy in the 0-10 eV range. The results were analyzed along the three incident light directions (x, y, and z). The real part, $\epsilon_1(\omega)$, reaches its first maximum at around 1.2 eV, then decreases and oscillates near a value of 1.0 in the range of 2-6 eV. This first peak corresponds to electronic transitions from the HOMO to LUMO states, matching the previously determined energy gap, and marks the onset of optical absorption in GeNC. A secondary peak is observed at 2.2 eV, representing transitions between deeper valence states and higher conduction states, primarily involving Ge(4s) to Ge(4p) electronic excitations. For photon energies above 6 eV, $\epsilon_1(\omega)$ becomes more stable. The static dielectric constant, $\epsilon_1(0)$, is approximately 2.8, which is lower than that of bulk germanium, indicating that GeNC possesses a significantly reduced polarizability. This reduction is consistent with the quantum confinement effect, which decreases the free electron density and weakens charge screening.

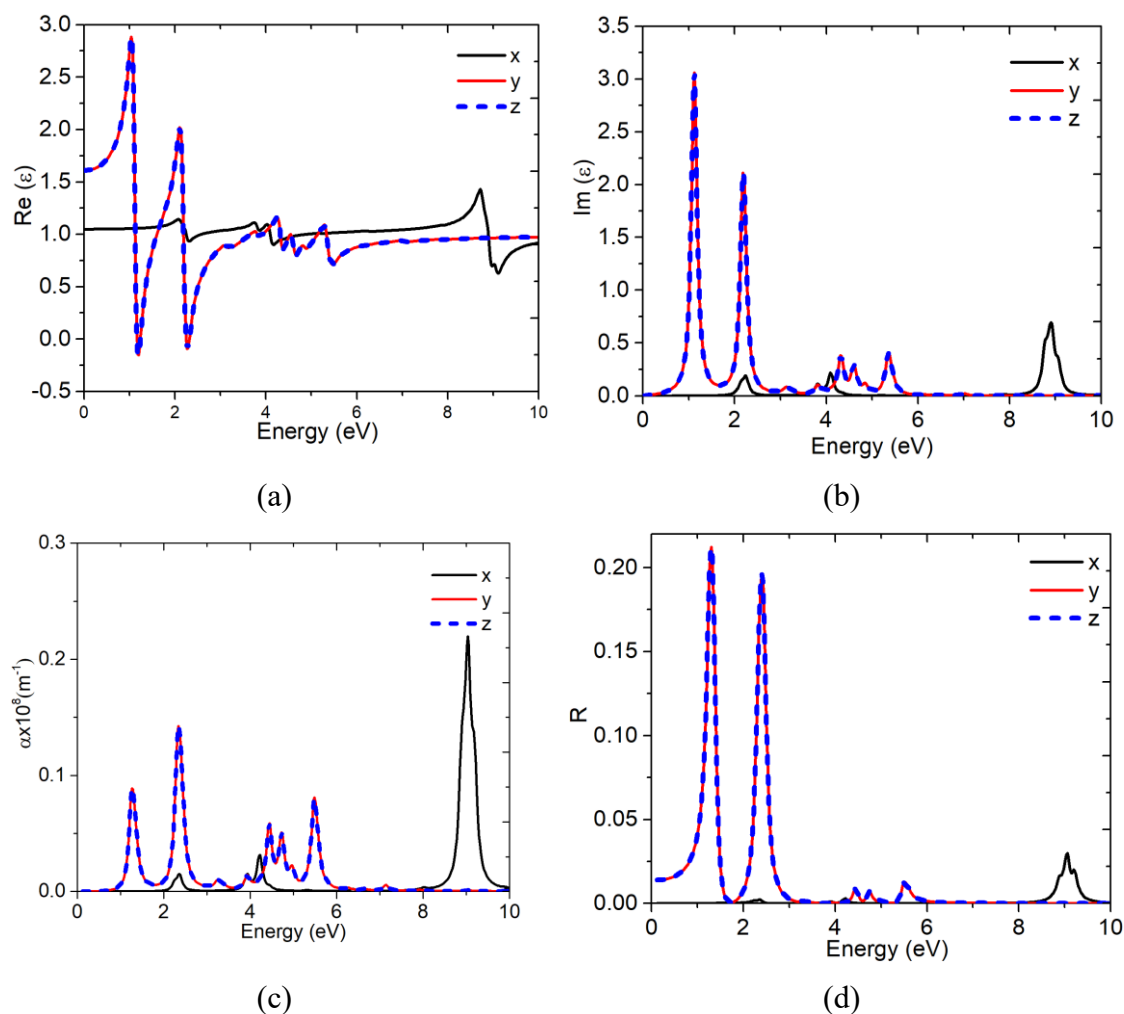


Figure 5. (a) Real and (b) imaginary parts of dielectric function, (c) absorption coefficient, (d) reflectivity of GeNC

The imaginary part, $\epsilon_2(\omega)$, reflects the photon energy absorption capability arising from electronic transitions. The $\epsilon_2(\omega)$ curve exhibits three prominent absorption peaks at 1.6 eV, 2.2 eV, and 4.5 eV. The first peak corresponds to the direct transition from the HOMO to the LUMO, representing the optical absorption edge of the GeNC. The second peak is associated with transitions from deeper valence states (HOMO-1, HOMO-2) to higher conduction states (LUMO+1, LUMO+2), which are hybridized Ge 4p-4s orbitals. The third peak arises from Ge 4s to 4p high-energy transitions, corresponding to strong absorption in the visible and near-ultraviolet regions. The presence of multiple distinct peaks in $\epsilon_2(\omega)$ indicates the involvement of several electronic states in the optical absorption process, which is a typical feature of quantum dots in the nanoscale regime.

The absorption spectrum $\alpha(\omega)$ shows a similar trend to $\epsilon_2(\omega)$. The first peak marks the absorption threshold, corresponding to the GeNC band gap edge. The second peak represents strong absorption in the visible range, mainly related to transitions involving Ge-H hybridized surface states. The third peak appears in the ultraviolet region and corresponds to deep Ge 4s to 4p transitions associated with intraband plasmon oscillations in the nanostructure. The maximum absorption coefficient reaches approximately $2.5 \times 10^5 \text{ cm}^{-1}$, demonstrating that GeNCs have strong absorption in the visible region, suggesting potential for use in optical absorber materials and photovoltaic devices.

The reflectivity spectrum $R(\omega)$ exhibits three peaks at 1.2 eV, 2.4 eV, and 8.6 eV, corresponding to the main absorption peaks in $\epsilon_2(\omega)$ and $\alpha(\omega)$. The maximum reflectivity is about $R \approx 0.22$, which is lower than that of bulk germanium ($R \approx 0.40$ at the same photon energy), indicating that GeNCs reflect less light but absorb more strongly, consistent with the quantum confinement effect that enhances light-matter interaction. The reflectivity peak at 8.6 eV corresponds to intraband plasmon resonance, also observed in $\epsilon_1(\omega)$, representing the collective oscillation energy of electrons in the system. The exciton binding energy can be estimated as the difference between the electronic gap (HOMO, LUMO gap about 1.7 eV) and the first optical absorption peak (1.6 eV). This yields an approximate exciton binding energy of about 0.1 eV. Such a value indicates that the electron hole pair is moderately bound within the confined nanocluster, which is consistent with previous studies on semiconductor nanoclusters where spatial confinement enhances excitonic interactions.

Figure 6 shows the Joint Density of States (JDOS) of the GeNC in the photon energy range of 0-10 eV. The JDOS describes the number of possible pairs of occupied and unoccupied states that can participate in photon absorption processes, providing essential information for understanding the origin of the absorption peaks in the dielectric function and the optical absorption coefficient.

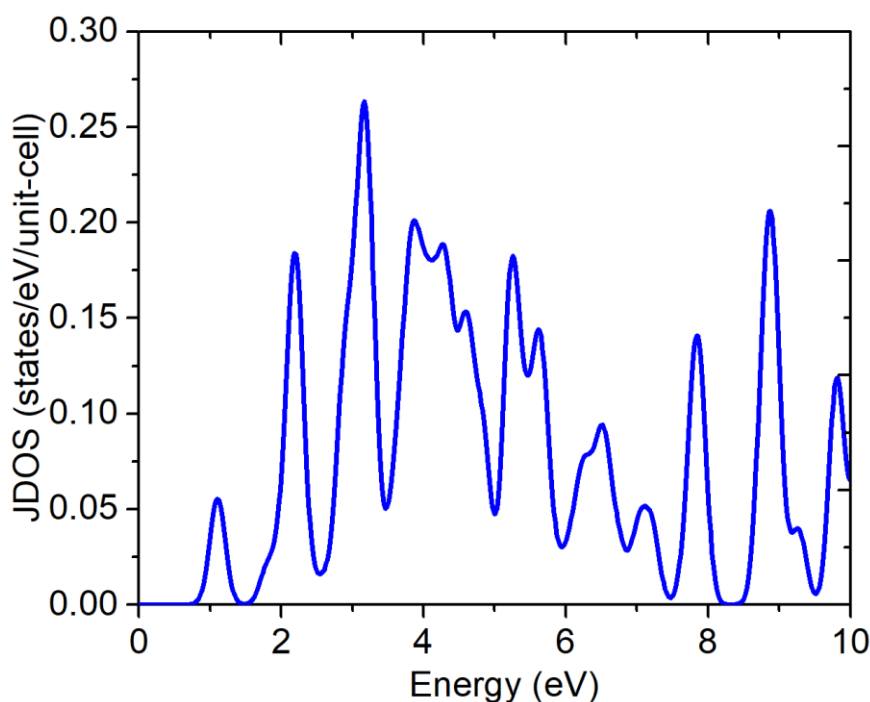


Figure 6. Joint Density of States – JDOS

The results show several prominent peaks at approximately 0.9 eV, 2.1 eV, 3.4 eV, 4.8 eV, 6.2 eV, 8.3 eV, and 9.4 eV, indicating the presence of multiple discrete electronic transitions between the valence and conduction bands. The first peak at 0.9 eV corresponds to the first optical absorption threshold (HOMO to LUMO transition), confirming the narrow band gap nature of GeNC. The next two peaks, at 2.1 eV and 3.4 eV, have the strongest intensities and represent transitions between hybridized Ge 4p-4s and Ge 4s-4p orbitals. These transitions mainly contribute to absorption in the visible and

near-ultraviolet regions. In particular, the 3.4 eV peak (JDOS ≈ 0.26 states/eV/unit-cell) indicates a high density of excited states, consistent with the main absorption maximum in the optical spectrum.

The peaks at 4.8 eV and 6.2 eV correspond to deeper electronic transitions and orbital overlap between Ge 4s-4p and Ge 4d states, while the two high-energy peaks at 8.3 eV and 9.4 eV are associated with intraband plasmon oscillations, representing the collective electronic response to high-energy photon excitation. Overall, the JDOS spectrum of GeNC exhibits clear energy discretization, with a dense distribution of transition states in the 1-4 eV range and plasmonic resonances in the 8-9 eV region. These findings confirm the quantum confinement effect and the strong optical absorption capability of GeNCs.

All figures and tables in this article are the results of the authors' own research.

4. Conclusion

This paper presents a study of the structural, electronic, and optical properties of germanium quantum dots (GeNCs) using the density functional theory (DFT) method implemented in the Quantum ESPRESSO simulation package. The structural, electronic, and optical characteristics of GeNCs were calculated and analyzed in detail. The results show that GeNC has a stable structure with a large negative cohesive energy and strong covalent Ge-Ge bonding. The quantum confinement effect is clearly evident from the discretization of the energy spectrum and the noticeable reduction in bond length compared to bulk germanium. Analysis of the electronic band structure and density of states (DOS) reveals a finite electronic density near the Fermi level, indicating weak semimetallic behavior originating from surface effects and Ge-H hybridization. The charge density and HOMO-LUMO distributions show a clear spatial separation between valence and conduction regions, suggesting directional electron transfer and stable exciton recombination. The optical spectra demonstrate that GeNCs exhibit strong absorption in the visible and near-UV regions, with characteristic absorption peaks in the range of 1.6-4.5 eV. The JDOS spectrum shows multiple discrete peaks between 0.9 eV and 9.4 eV, indicating pronounced quantum effects and intraband plasmon resonances typical of nanomaterials. Overall, these findings confirm that GeNCs are promising materials for optoelectronic applications, with strong potential for use in next-generation devices such as solar cells, optical sensors, light-emitting diodes (LEDs), and energy storage systems.

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