

MAGNETIC AND OPTICAL BEHAVIOR OF CE- AND TE- DOPED GaSb (110) SLABS FOR ADVANCED OPTOELECTRONIC APPLICATIONS

N.A. ISMAILOVA ^{1,2*}, S. ASADULLAYEVA ^{1,3,4}, SH. AMIROV ⁵, A.S. ALEKPEROV ⁶,
A.N. JAFAROVA ³, Q.Y. EYYUBOV ¹

¹ Institute of Physics, Ministry of Science and Education Republic of Azerbaijan, 131 H.Javid avenue, Baku, AZ-1143, Azerbaijan

² Azerbaijan University of Architecture and Construction, 26 Mammad Rahim Str., AZ-1073, Baku, Azerbaijan

³ Azerbaijan State Oil and Industry University, 20 Azadliq Avenue, AZ-1010, Baku, Azerbaijan

⁴ Khazar University, Department of Physics and Electronics, 41 Mehseti Str., Baku, Azerbaijan

⁵ Department of Medical and Biological Physics, Azerbaijan Medical University, 165 Samad Vurgun Str., AZ-1022, Baku, Azerbaijan

⁶ Baku Engineering University, Khirdalan, 120 Hasan Aliyev Str., AZ-0101, Baku, Azerbaijan

*Corresponding author: isnarmin106@gmail.com

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Abstract. We investigate the electronic, optical, and magnetic properties of finite-thickness GaSb(110) slabs doped with Ce, Te, and Ce+Te using first-principles calculations. The pristine 7-layer GaSb(110) slab has a calculated band gap of 0.76 eV. Ce doping narrows the gap to 0.64 eV and introduces occupied, localized Ce 4f states below the Fermi level, along with empty acceptor-like states near the gap, indicating acceptor-like electronic character. Te doping gives a band gap of 0.72 eV and shifts the Fermi level toward the conduction-band side, consistent with donor-like behavior. Ce+Te co-doping modifies the electronic structure through donor-acceptor compensation, while the magnetic behavior is mainly associated with Ce-derived states. The optical response shows doping-induced changes in the low-energy spectral region, which may relate to dopant-derived electronic states. Photoluminescence measurements of GaSb and Ce-doped GaSb nanocrystals under 785 nm excitation reveal a pronounced temperature dependence of the emission, with higher PL intensity at 70 K than at 300 K. Gaussian fitting of the photoluminescence (PL) spectra provides good agreement for GaSb ($R^2=0.954$) at 70 K and ($R^2=0.964$) at 300 K while the lower fitting quality for Ce-doped GaSb at 300 K ($R^2=0.939$) reflects its more complex and asymmetric spectral profile. The main emission feature remains in the near-infrared region around 1530–1550 nm, whereas Ce incorporation primarily broadens and asymmetrizes the PL band. These changes may reflect modifications in carrier localization and recombination processes arising from dopant-related states, surface defects, and structural inhomogeneity. Because PL measurements were available only at 70 and 300 K, we did not attempt a quantitative activation-energy analysis. These results clarify how rare-earth and donor co-doping can tune the electronic, magnetic, and optical response of GaSb(110) slab models for optoelectronic and spintronic applications.

Keywords: Magnetism, first-principles calculations, optoelectronic properties, bandgap engineering, co-doping

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1. Introduction

Gallium antimonide (GaSb) is a promising III-V semiconductor with a narrow bandgap, making it well-suited for optoelectronic applications, including infrared detectors, thermophotovoltaic devices, and high-speed transistors [1-3]. With a room-temperature bandgap of around 0.72 eV [4,5], GaSb is particularly suitable for near-infrared optoelectronic applications [6].

However, to unlock GaSb's full potential for these applications, its electronic properties must be optimized, and one of the most effective approaches is doping with rare-earth elements like cerium (Ce) [7]. Cerium is a rare-earth element with unique properties that

significantly impact the electronic characteristics of semiconductors. In GaSb, Ce doping has been shown to enhance the material's p-type conductivity by introducing Ce-related acceptor states [8]. This is particularly valuable because it reduces the concentration of native acceptors, such as gallium vacancies, which can otherwise limit the material's performance. As an acceptor, Ce modifies the electronic structure of GaSb, potentially improving its performance in optoelectronic applications [7]. While Ce doping has been widely studied in bulk GaSb crystals, research on its effects in reduced-dimensional systems, such as GaSb slabs, remains limited. Experimental studies have confirmed the feasibility of forming nanoscale GaSb thin films. Chusovitin et al. reported forming a thin, continuous GaSb film on Si(001) using solid-phase epitaxy, showing that a 20 nm GaSb film can remain continuous with crystalline grains of 9–16 nm [9]. These findings motivate studies of reduced-dimensional GaSb slab-type models and their dopant-induced structural, electronic, magnetic, and optical properties. Nanosheets offer distinct advantages over bulk materials, particularly because quantum confinement effects alter their electronic properties [10–13]. These effects can significantly change the material's electronic band structure, density of states (DOS), and optical behavior [14]. Additionally, the larger surface-to-volume ratio in slabs introduces new opportunities to control defects and surface states, which can further influence the material's properties and performance. Studies on Ce-doped GaSb crystals have shown that cerium forms weak bonds with both gallium and antimony atoms in the GaSb lattice, leading to the formation of a Ce–Ga intermetallic phase on the surface. This interaction not only influences the material's intrinsic properties but also promotes oxidation of the GaSb surface, which can further affect defect formation [7]. By offering new insights into the role of Ce as an acceptor dopant in GaSb slabs, this study contributes to the design of materials for next-generation quantum devices and energy-efficient technologies [7,14]. In parallel, tellurium (Te) is a well-established donor dopant in GaSb, commonly used to induce n-type conductivity. Te substitution at Sb sites has been shown to reduce resistivity and modify optical transitions by interacting with native acceptor defects [15]. Experimental studies indicate that Te incorporation can neutralize gallium-related defect complexes at low concentrations, while higher Te concentrations may form complex defect states that significantly alter GaSb's optical and structural properties. These findings highlight the delicate balance between defect compensation and Te-induced defect generation. While Ce and Te doping have been studied extensively independently, the combined effect of rare-earth and donor dopants in GaSb has received limited attention, particularly at the nanoscale. Co-doping with Ce and Te offers a promising pathway to simultaneously control carrier type, defect chemistry, and electronic structure through complementary substitution mechanisms – Ce replacing Ga atoms and Te replacing Sb atoms [16]. This co-doping strategy is expected to introduce competing and cooperative interactions between acceptor- and donor-like states, potentially leading to tunable electronic behavior that single-element doping cannot achieve. Furthermore, GaSb slabs provide an ideal platform to study these effects because of their reduced dimensionality and enhanced sensitivity to defects and dopants. Quantum confinement and surface effects in slabs can significantly amplify dopant-induced modifications, offering new opportunities for engineering electronic, optical, and magnetic properties. However, experimental exploration of such systems is challenging, making first-principles calculations an essential tool for understanding dopant behavior at the atomic level.

2. Method of calculation

We investigated the electronic, optical, and magnetic properties of Ce-, Te-, and Ce+Te co-doped GaSb(110) slabs using density functional theory (DFT) implemented in the QuantumATK package [17]. We described the exchange-correlation interactions using the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional [18]. We performed the calculations using the Linear Combination of Atomic Orbitals (LCAO) approach with a high-accuracy basis set. We used a real-space density mesh cutoff of 150 Hartree. We used PseudoDojo pseudopotentials for Ga, Sb, Ce, and Te atoms. To account for the localized nature of Ce 4f electrons, we applied a Hubbard correction (DFT+U) only to the Ce 4f orbitals. We set the Hubbard parameter to $U = 4.5$ eV, based on previously reported theoretical studies of localized Ce 4f states [19, 20]. Because the calculated electronic structure may depend on the selected U value, we performed additional calculations with $U = 3.5$ and 5.5 eV. We constructed the pristine GaSb slab from bulk zinc-blende GaSb using the Surface (Cleave) builder in QuantumATK with Miller indices (110). The resulting structure corresponds to the GaSb(110) surface. We introduced the non-periodic direction along the [110] surface-normal direction by adding a vacuum region, while the in-plane directions of the (110) surface correspond to $[1\bar{1}0]$ and $[001]$. We first investigated slabs with 3, 5, 7, and 9 atomic layers to assess the thickness dependence of the electronic properties (Fig. 1). Based on these convergence calculations, we selected the seven-layer slab as the host structure for all subsequent doping calculations.

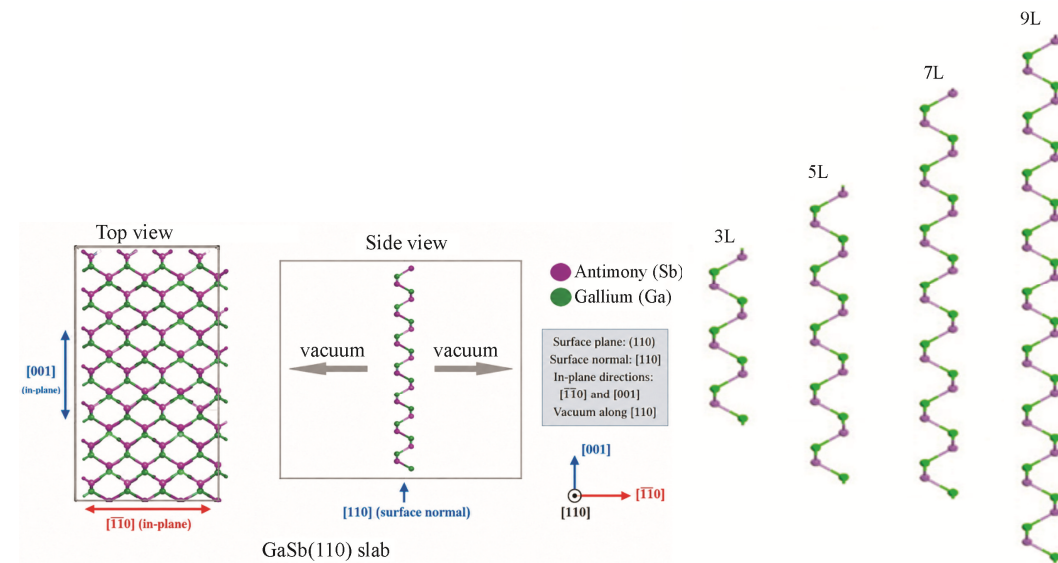


Fig. 1. Top and side views of the pristine GaSb(110) slab model constructed using the QuantumATK Surface (Cleave) builder with Miller indices (110). The crystallographic orientation and vacuum direction are indicated for clarity. The [110] direction represents the surface normal, while $[1\bar{1}0]$ and $[001]$ define the two in-plane directions of the (110) surface.

We repeated the primitive slab using a $4 \times 4 \times 1$ surface supercell, yielding a 104-atom model with 52 Ga and 52 Sb atoms. We applied periodic boundary conditions along the two in-plane crystallographic directions. We treated the [110] surface-normal direction as non-periodic using the corresponding slab boundary conditions in QuantumATK. We included a $15 \text{ \AA}$ vacuum region along the surface-normal direction to provide adequate separation between the slab and the non-

periodic boundaries. We applied no dipole correction because we built the slab model without an external electric field, and the vacuum separation was sufficient to minimize interactions between periodic images. We fully optimized the atomic structures until the residual force on each atom was below $0.02 \text{ eV}/\text{\AA}$, and we set the total-energy convergence threshold to 10^{-6} eV . We examined the influence of k-point sampling using $2 \times 2 \times 1$, $4 \times 4 \times 1$, and $6 \times 6 \times 1$ Monkhorst–Pack grids at a fixed density mesh cutoff of 150 Hartree. We selected the $6 \times 6 \times 1$ grid for subsequent calculations. In the doped configurations, Ce atoms substituted Ga sites, whereas Te atoms substituted Sb sites (Fig. 2). Substituting two Ga atoms with Ce corresponds to a Ce concentration of 3.85% of the Ga sublattice (1.92% of the total atoms). Similarly, substituting one, two, or three Sb atoms with Te corresponds to Te concentrations of 1.92%, 3.85%, and 5.77% of the Sb sublattice, respectively. For the co-doped configurations, the Ce concentration remains 3.85% of the Ga sublattice, while the Te concentration varies depending on the number of substituted Sb atoms (Table 1). We examined several possible dopant arrangements and selected the energetically most favorable configurations based on calculated formation energies.

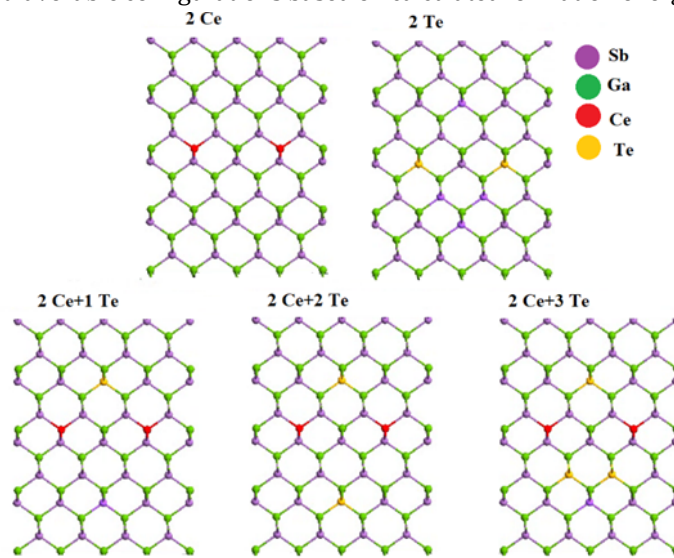


Fig. 2. Atomic structure of GaSb (110) slabs with different Ce and Te substitutional doping configurations.

Table 1. Composition and dopant concentration of pristine, Ce-, Te-, and Ce+Te-doped GaSb(110) slab models.

Model	Composition	Ce concentration	Te concentration
Pristine	$\text{Ga}_{52}\text{Sb}_{52}$	–	–
2Ce	$\text{Ga}_{50}\text{Ce}_2\text{Sb}_{52}$	3.85% Ga sites	–
1Te	$\text{Ga}_{52}\text{Sb}_{51}\text{Te}$	–	1.92% Sb sites
2Te	$\text{Ga}_{52}\text{Sb}_{50}\text{Te}_2$	–	3.85% Sb sites
3Te	$\text{Ga}_{52}\text{Sb}_{49}\text{Te}_3$	–	5.77% Sb sites
2Ce+1Te	$\text{Ga}_{50}\text{Ce}_2\text{Sb}_{51}\text{Te}$	3.85% Ga sites	1.92% Sb sites
2Ce+2Te	$\text{Ga}_{50}\text{Ce}_2\text{Sb}_{50}\text{Te}_2$	3.85% Ga sites	3.85% Sb sites
2Ce+3Te	$\text{Ga}_{50}\text{Ce}_2\text{Sb}_{49}\text{Te}_3$	3.85% Ga sites	5.77% Sb sites

We performed spin-polarized calculations for all structures to analyze magnetic behavior. For each Ce-containing slab, we examined two initial magnetic configurations by assigning parallel and antiparallel spin orientations to the two Ce atoms. Band structures and DOS were calculated to separate host valence/conduction bands from dopant-induced defect states. Mulliken population analysis was performed to estimate charge transfer and atomic contributions to the magnetic moments. Optical properties were evaluated from the energy-dependent dielectric function within the independent-particle approximation. The imaginary part was obtained from interband transitions, while the real part was derived through the Kramers–Kronig relation. The optical response was analyzed for the two in-plane polarization directions of the GaSb(110) surface, corresponding to the $[1\bar{1}0]$ and $[001]$ crystallographic directions. The dielectric tensor components were interpreted according to the crystallographic coordinate system of the GaSb(110) slab, where the out-of-plane component corresponds to the $[110]$ surface-normal direction.

3. Results and discussion

The band structure and DOS provide detailed insight into the electronic properties of pristine and doped GaSb(110) slabs. To evaluate the effect of slab thickness, we first calculated pristine slabs with 3, 5, 7, and 9 atomic layers (Fig. 3). The band gap gradually decreases with increasing thickness, reflecting reduced quantum-confinement effects. The 3-layer slab exhibits a direct band gap of about 1.77 eV, whereas the 7-layer and 9-layer slabs show gaps much closer to the narrow-gap behavior of bulk GaSb [21–24]. This thickness dependence indicates that sufficiently thick slabs recover a bulk-like interior while retaining surface-related relaxation effects. To confirm the dynamical stability of the selected slab models, we calculated phonon dispersion along the Γ –X–S–Y– Γ path (Fig. 3). We observed no imaginary phonon frequencies, and the acoustic modes smoothly approach zero at Γ . These results confirm that the pristine slabs are dynamically stable and provide a valid host structure for subsequent doping studies. Based on this convergence analysis, we selected the 7-layer slab as the host structure for all further dopant calculations. This thickness balances computational efficiency and accuracy, ensuring the slab sufficiently represents bulk electronic properties while still allowing exploration of surface- and layer-dependent effects from Ce, Te, and Ce+Te doping. In more detail, the corresponding DOS shows a clear separation between the valence and conduction bands, with the Fermi level within

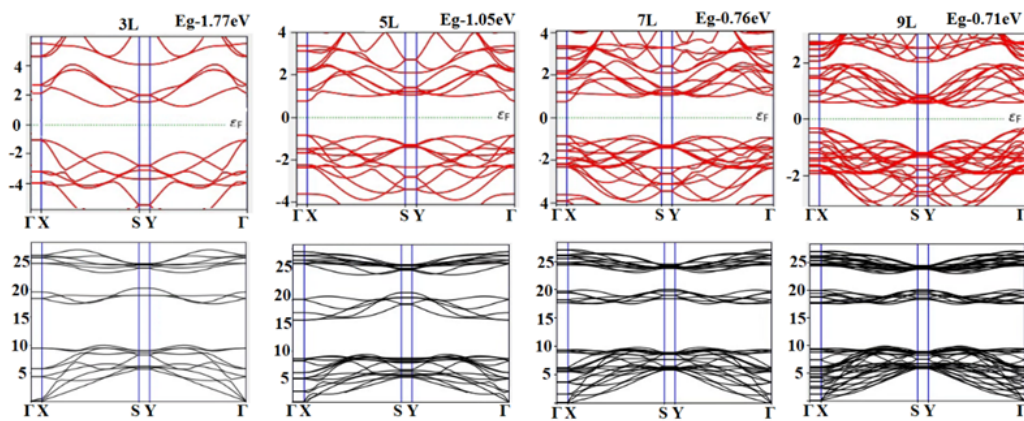


Fig. 3. Electronic band structures (upper panels, red curves) and phonon dispersions (lower panels, black curves) of pristine GaSb(110) slabs containing 3, 5, 7, and 9 atomic layers.

the gap, confirming the pristine system's semiconducting character. To further examine the role of electron correlation, we compared band structures obtained with standard GGA-PBE and GGA-PBE+U. We applied the Hubbard correction only to the localized Ce 4f states, since standard GGA-PBE does not adequately describe these strongly correlated orbitals. Including the Hubbard term moderately widens the band gaps in the Ce-containing systems. To account for localized Ce 4f states, we applied a single on-site Hubbard parameter of 4.5 eV to the Ce 4f shell using the DFT+U implementation in QuantumATK. This value was selected as a literature-supported modeling parameter rather than as a uniquely determined value for Ce-substituted GaSb [19, 20]. To evaluate the sensitivity of the results, additional calculations were performed using $U=3.5$ and 5.5 eV (Fig. 4). The qualitative ordering and character of the Ce-derived states remained unchanged over this interval, although moderate quantitative changes in the spin-resolved band gaps were observed.

For example, in the 2Ce configuration, the spin-resolved band gaps increase from 0.76/0.58 eV in GGA-PBE to 0.85/0.64 eV in GGA-PBE+U (Fig. 5). Similarly, for the co-doped systems, the corresponding changes are from 0.69/0.66 eV to 0.76/0.75 eV for 2Ce+1Te, from 0.64/0.52 eV to 0.68/0.62 eV for 2Ce+2Te, and from 0.74/0.66 eV to 0.76/0.71 eV for 2Ce+3Te. These results indicate that the Hubbard correction improves the description of the Ce-derived localized states and leads to a more reliable electronic structure for the Ce-containing systems. In contrast, for the Te-only configuration, we applied no Hubbard U correction because we introduced the U term in this study specifically for the Ce 4f orbitals. Therefore, we treated the 2Te system within standard GGA-PBE, for which the calculated spin-up and spin-down band gaps are 0.72 eV. The doped configurations show direct or quasi-direct band-gap characteristics because the valence-band maximum and conduction-band minimum are located at the same or nearly the same k -point along the Γ -X-S-Y- Γ path. The relatively flat band edges indicate weak band dispersion, which is consistent with the reduced dimensionality of the slab and the localized nature of dopant-induced states. For Ce-doped GaSb(110), the Fermi level shifts toward the valence-band side, reflecting the introduction of Ce-related states (Fig. 5). Importantly, these states should be separated into occupied localized Ce 4f states below the Fermi level and empty acceptor-like states above or near the Fermi level. The empty acceptor-like states drive the p-type tendency, whereas the occupied localized 4f states mainly affect the DOS and magnetic behavior and do not directly

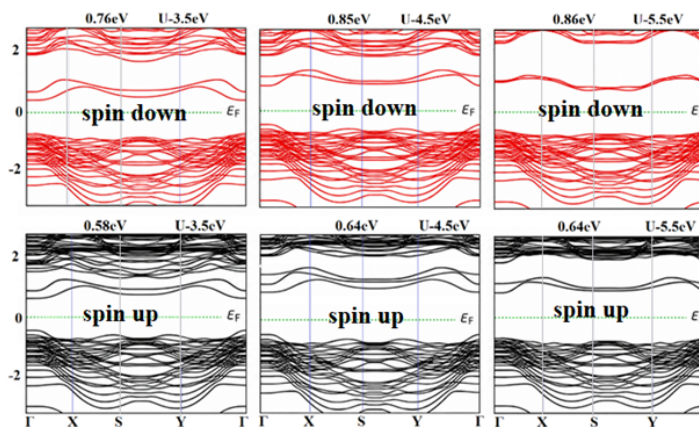


Fig. 4. Spin-resolved electronic band structures of Ce -doped GaSb(110) slabs calculated using different Hubbard U parameters.

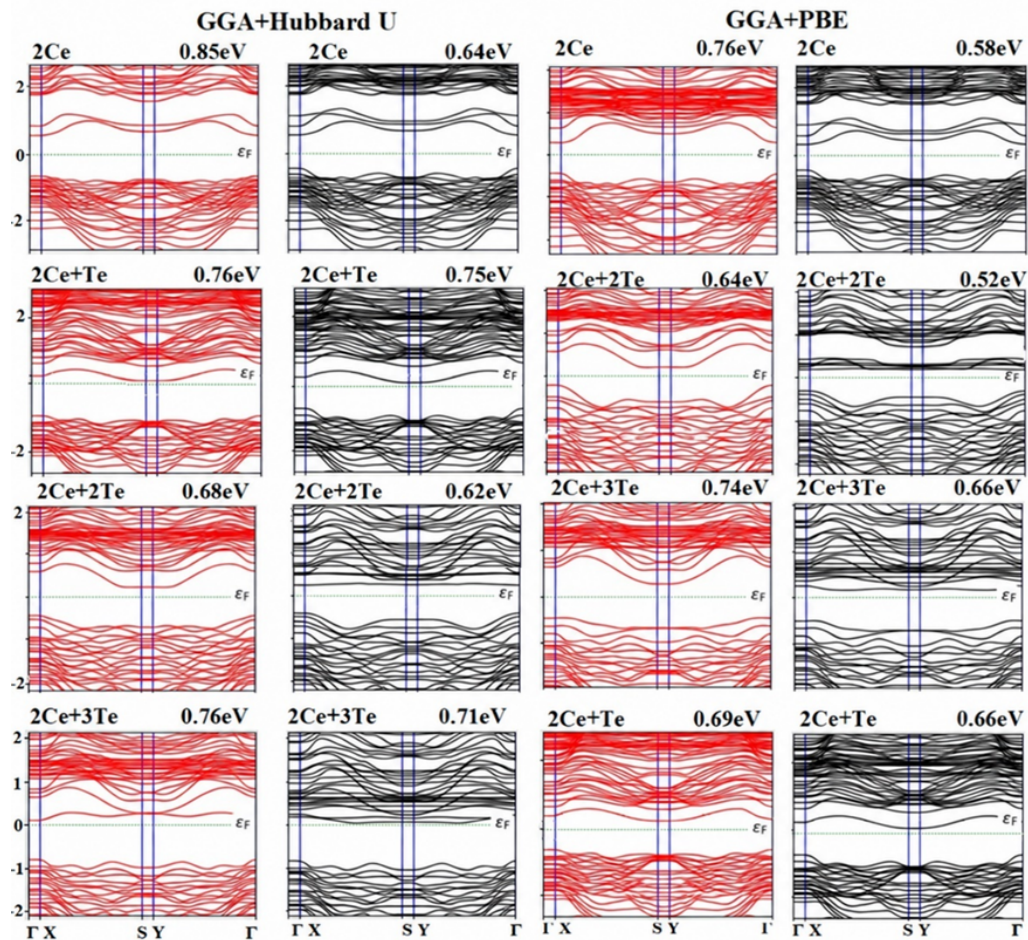


Fig. 5. Comparison of the spin-resolved electronic band structures of Ce-containing GaSb(110) slabs calculated using GGA-PBE+U and GGA-PBE. The Hubbard correction ($U = 4.5$ eV) was applied only to the Ce 4f orbitals. Red and black curves represent the spin-down and spin-up channels, respectively.

provide free carriers. The calculated band gap narrows from 0.76 eV in the pristine 7-layer slab to approximately 0.64 eV in the Ce-doped slab, consistent with previous reports on Ce-modified GaSb [7,8].

In Te-doped GaSb(110), the Fermi level shifts toward the conduction band, consistent with donor-like behavior and an n-type tendency. This result agrees with earlier studies of Te-doped GaSb [15, 25]. Te introduces donor-related states near the conduction-band edge and reduces the effective band gap to about 0.72 eV. These donor states increase the electron density near the conduction band but should still be distinguished from the host conduction band itself. For Ce+Te co-doped 7-layer GaSb(110), the Fermi level lies near the middle of the gap because Ce-induced acceptor-like states and Te-induced donor-like states compensate one another. The DOS includes contributions from both types of dopant-related states near the Fermi energy; however, these states are largely localized and do not imply simultaneous strong electron and hole conduction (Fig. 6).

The calculated electronic structures are consistent with donor-acceptor compensation in the Ce+Te co-doped slabs. However, the present calculations do not determine free-carrier concentrations, defect ionization energies, or transport properties. The Ce- and Te-related

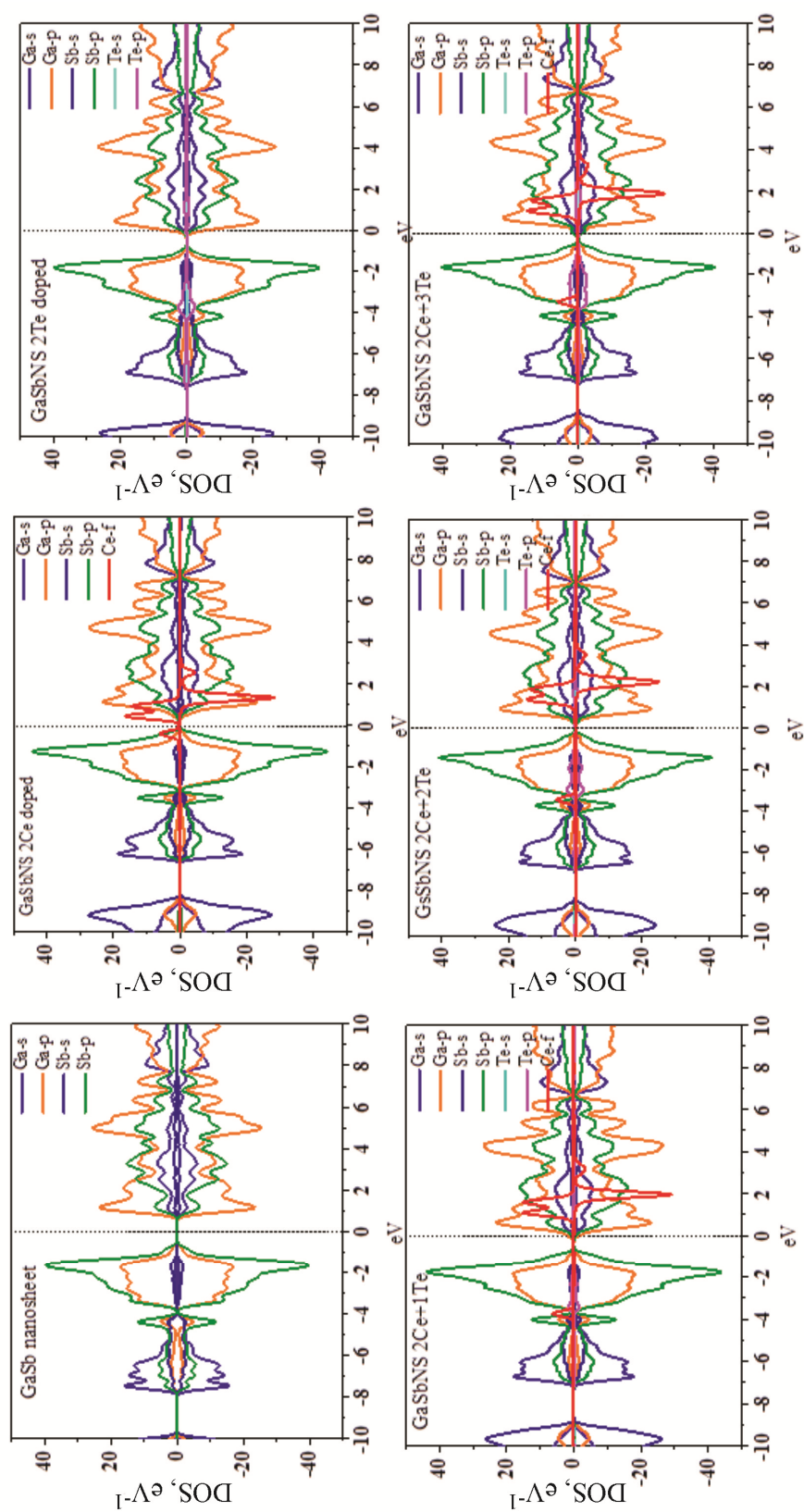


Fig. 6. DOS of Ce-, Te-, and Ce+Te co-doped GaSb (110) slabs.

states are therefore described as acceptor-like and donor-like, respectively, rather than as evidence of effective p-type or n-type conductivity [26]. In particular, the present results do not establish whether the Ce-related acceptor-like states are shallow acceptors or deep traps. The band gap of the co-doped slab is reduced to approximately 0.62 eV for the 2Ce+2Te, with slightly higher values for other dopant ratios. The formation energy of a doped GaSb(110) slab is defined relative to the pristine slab and the selected elemental reservoirs as follows: $E_{\text{form}} = E_{\text{doped}} - E_{\text{pristine}} + n_{\text{Ce}}\mu_{\text{Ga}} + n_{\text{Te}}\mu_{\text{Sb}} - n_{\text{Ce}}\mu_{\text{Ce}} - n_{\text{Te}}\mu_{\text{Te}}$. Here, E_{doped} and E_{pristine} are the total energies of the doped and pristine GaSb(110) slabs, respectively. The quantities μ_{Ga} , μ_{Sb} , μ_{Ce} , and μ_{Te} denote the elemental chemical potentials, while n_{Ce} and n_{Te} are the numbers of substituted Ce and Te atoms. The elemental chemical potentials were taken as the calculated total energies per atom of bulk α -Ga, rhombohedral Sb, face-centered-cubic Ce, and trigonal Te. To evaluate the energetic tendency for successive Te incorporation into the 2Ce-doped slab, we calculated the sequential incorporation energy as $\Delta E_{\text{inc}}(m) = E(2\text{Ce} + m\text{Te}) - E[2\text{Ce} + (m-1)\text{Te}] + \mu_{\text{Sb}} - \mu_{\text{Te}}$, $m=1,2,3$, where $m=1,2,3$ denotes the number of Te atoms successively incorporated into the 2Ce-doped GaSb slab. In this expression, one additional Te atom substitutes for one Sb atom at each incorporation step. A negative value of ΔE_{inc} indicates that the corresponding substitution is exothermic relative to the selected elemental reservoirs. The calculated sequential incorporation energies are -4.199, -3.810, and -2.544 eV for the first, second, and third Te atoms, respectively. These values indicate that successive Te substitution is energetically favorable relative to the selected elemental reservoirs, with a decreasing energy gain for each additional Te atom. However, they should not be interpreted as direct predictions of equilibrium dopant solubility. Experimental realization will additionally depend on Ga-rich or Sb-rich growth conditions, competing Ce- and Te-containing phases, defect charge states, diffusion barriers, surface kinetics, and growth temperature.

To assess the influence of spin-orbit coupling (SOC), additional calculations were performed for the pristine and 2Ce-doped GaSb(110) slabs. Fig. 7 compares the electronic band structures calculated without and with SOC. Panels (a) and (b) show the pristine GaSb(110) slab without and with SOC, respectively, whereas panels (c) and (d) show the corresponding results for the 2Ce-doped slab. Including SOC produces visible splittings of selected valence- and conduction-band states, with characteristic splittings of approximately 0.06–0.10 eV. For the pristine slab, the calculated band gap decreases from 0.76 eV without SOC to 0.71 eV with SOC. For the 2Ce-doped slab, the calculated band gap decreases from 0.64 eV without SOC to 0.59 eV with SOC. Thus, SOC changes the calculated gap values by approximately 0.05 eV, while the overall band topology and the main features associated with the Ce-derived states remain qualitatively preserved. These results indicate that SOC introduces a modest but non-negligible quantitative correction to the electronic structure. Therefore, to reduce the computational cost, the remaining calculations were performed without SOC and are used primarily to discuss qualitative doping-induced trends.

Mulliken population analysis was performed to quantify charge redistribution [27, 28] and magnetic contributions in the doped GaSb(110) slab. For Ce-doped systems, most of the magnetic moment originates from Ce 4f states, while neighboring Sb atoms show only weak induced spin polarization. Te contributes little to the magnetization, consistent with the calculated DOS and Mulliken spin populations. In the 2Te-doped slab, the total magnetic moment is zero. In the 2Ce+1Te system, the total magnetic moment is approximately 2.21 μ_B . This fractional value should not be interpreted as an ideal isolated-ion spin state. It arises from the integrated spin

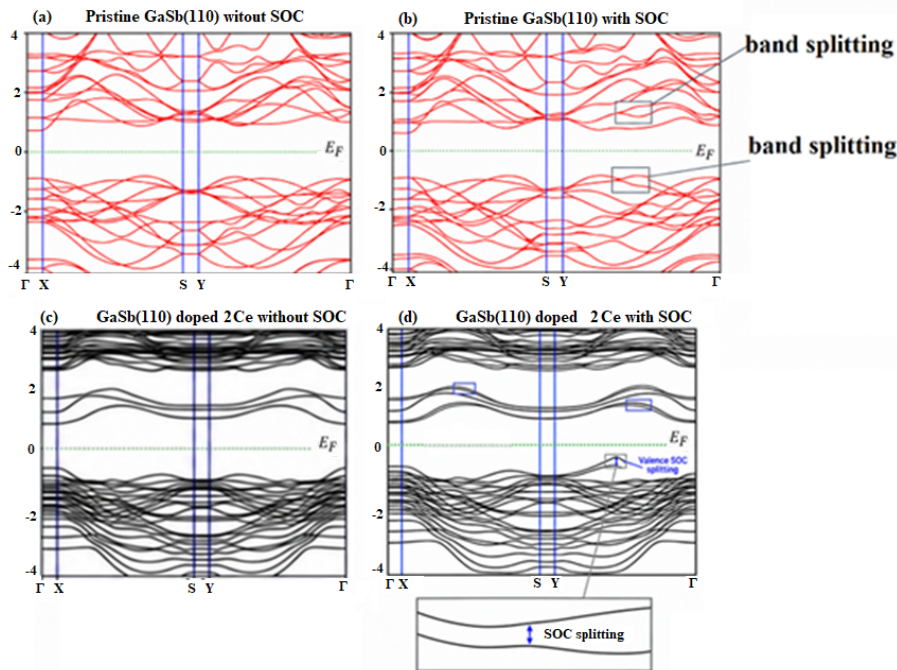


Fig. 7. Panels (a) and (b) show the pristine GaSb(110) slab without and with SOC, respectively, while panels (c) and (d) show the corresponding band structures of the Ce-doped GaSb(110) slab. The horizontal dashed line at $E_F=0$ eV denotes the Fermi level.

density of a hybridized doped slab, where the Ce 4f spin density is partly delocalized onto neighboring Sb/Ga orbitals and then partitioned by the Mulliken scheme. Thus, non-integer magnetic moments are expected when localized Ce states hybridize with the host lattice and when the spin density is not fully confined to isolated dopant ions. The total magnetic moment is slightly reduced to $2.01 \mu_B$ in the 2Ce+2Te system and is about $2.10 \mu_B$ in the 2Ce+3Te system. In all Ce+Te configurations, the dominant contribution remains associated with Ce, while Sb contributes only a minor induced moment and Te remains essentially nonmagnetic. Increasing Te concentration therefore modifies the Ce–host electronic environment but does not directly generate magnetism.

The calculated dielectric response of the doped GaSb(110) slabs was analyzed for light polarized along the two orthogonal in-plane crystallographic directions, $[1\bar{1}0]$ and $[001]$. The real and imaginary parts of the dielectric function, $\epsilon_1(E)$ and $\epsilon_2(E)$, respectively, are presented as functions of photon energy (Fig. 8). The $[110]$ direction corresponds to the surface normal and is therefore excluded from the in-plane optical response discussed here. We discuss the dielectric spectra of the Ce- and Te-doped slabs in terms of dopant-induced modifications to the electronic structure and density of states. Therefore, the present analysis focuses mainly on the spectral features and relative changes introduced by doping rather than on a direct correlation between dielectric amplitudes and slab thickness. In Ce-doped slabs, transitions involving occupied Ce 4f states and unoccupied states near the conduction-band edge may contribute to the low-energy optical response. This interpretation is consistent with the appearance of Ce-derived states in the calculated electronic structure. However, the band structure and density of states alone cannot uniquely identify individual optical transitions responsible for specific spectral features; therefore, these assignments should be considered as qualitative interpretations.

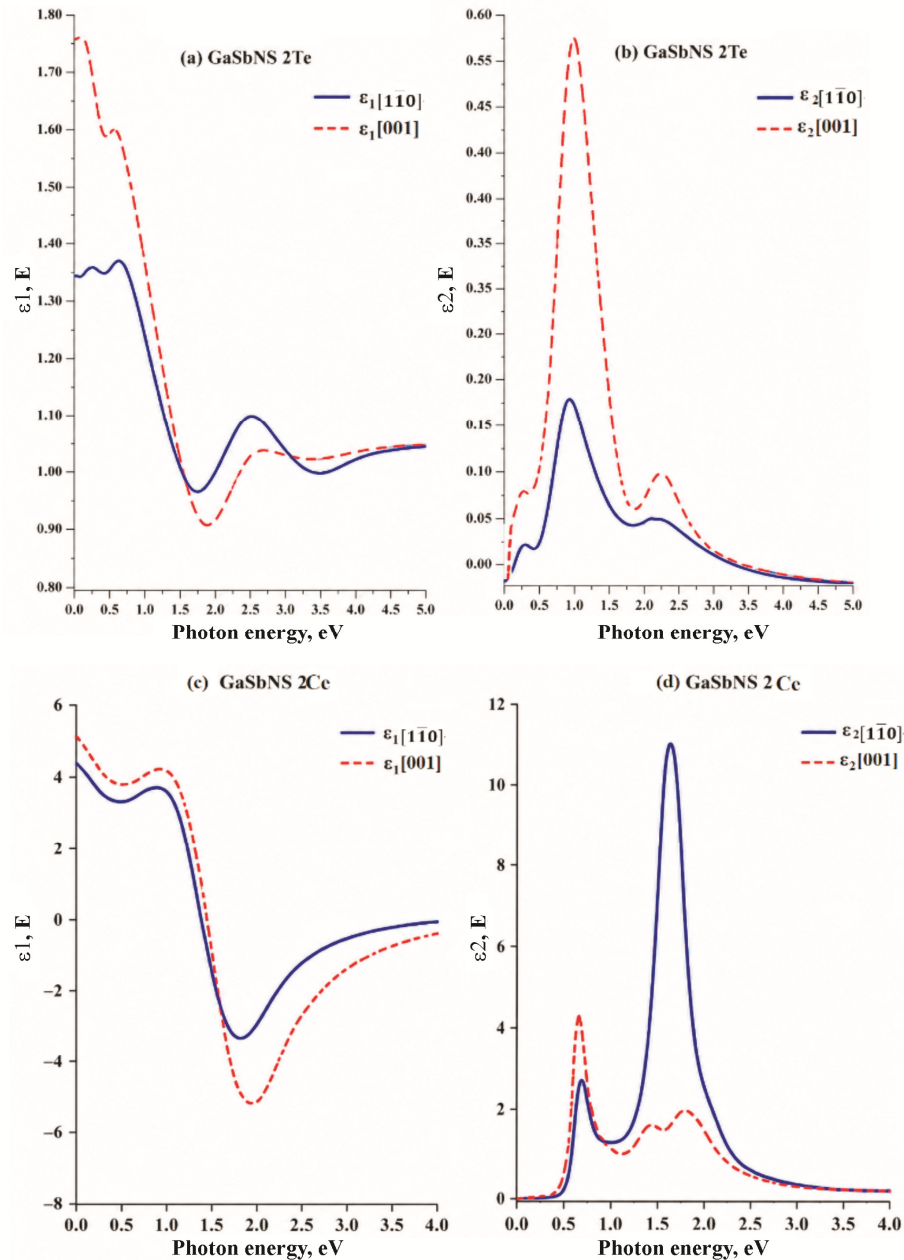


Fig. 8. Real $\varepsilon_1(E)$ and imaginary $\varepsilon_2(E)$ parts of the dielectric function of Te- and Ce-doped GaSb(110) slabs as a function of photon energy. Panels (a) and (b) show the real and imaginary parts, respectively, for the 2Te-doped GaSb(110) slab, while panels (c) and (d) show the corresponding results for the 2Ce-doped GaSb(110) slab. The blue solid and red dashed curves correspond to light polarized along the two orthogonal in-plane crystallographic directions $[1\bar{1}0]$ and $[001]$, respectively. The $[110]$ direction is normal to the GaSb(110) surface.

Figs. 9 and 10 show the photoluminescence (PL) spectra of GaSb and Ce-doped GaSb nanocrystals, respectively, measured under 785 nm laser excitation at 70 and 300 K. The excitation photon energy is approximately 1.58 eV, which is higher than the fundamental band-gap energy of GaSb and is therefore sufficient to generate electron-hole pairs. For both samples, the PL intensity decreases markedly as the temperature increases from 70 to 300 K, demonstrating a pronounced temperature dependence of the emission process.

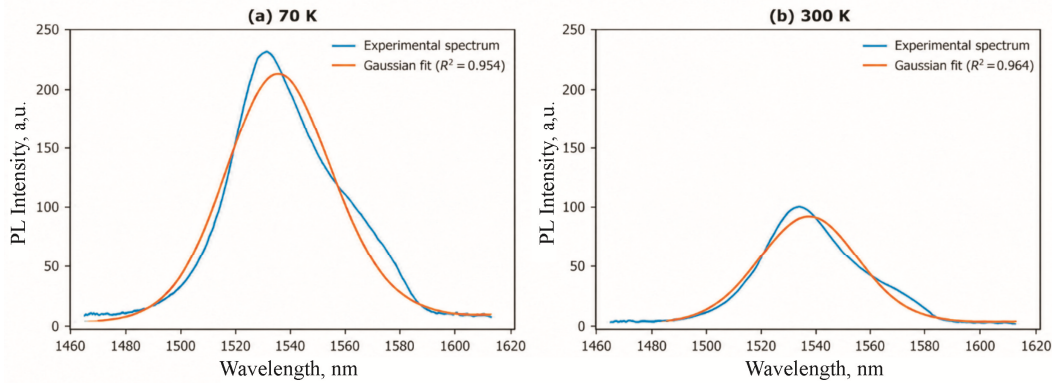


Fig. 9. Temperature-dependent photoluminescence spectra of GaSb nanocrystals under 785 nm excitation. The solid curves represent single-Gaussian fits to the dominant PL emission band.

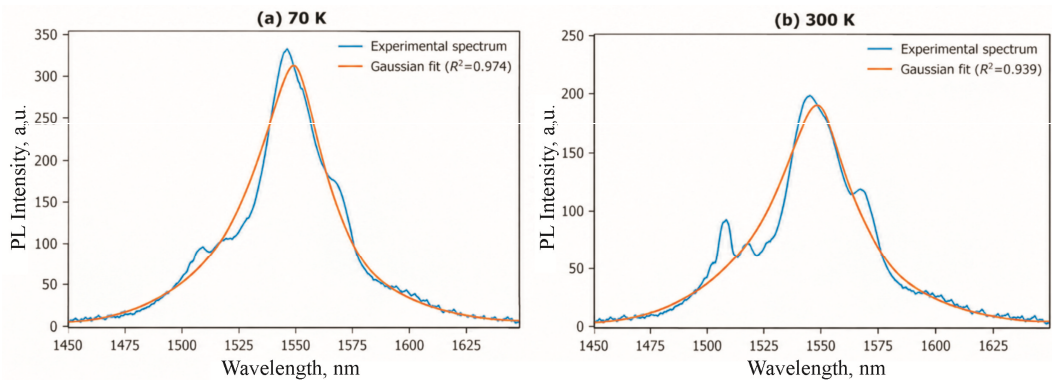


Fig. 10. Temperature-dependent photoluminescence spectra of Ce-doped GaSb nanocrystals under 785 nm excitation. The solid curves represent single-Gaussian fits to the dominant PL band; additional features are not fitted or assigned separately.

To obtain a more quantitative description of the PL response, the experimental spectra were fitted using Gaussian functions, and the corresponding coefficients of determination, R^2 , are shown in Figs. 9 and 10. For GaSb, the single-Gaussian fits yield $R^2=0.954$ at 70 K and $R^2=0.964$ at 300 K, indicating good overall agreement with the dominant emission band. Small deviations between the experimental spectra and the single-Gaussian fits are visible, particularly around 1570 nm. This additional feature was not included separately in the fitting because the analysis aimed to describe the principal emission band rather than assign individual weak spectral components. The available PL data cannot uniquely determine its origin. The main emission feature remains in the near-infrared region, centered at approximately 1530–1550 nm within the measured spectral range. Thus, the most pronounced temperature-dependent change is in the PL intensity rather than a clearly resolved shift of the main emission maximum. The Ce-doped GaSb nanocrystals exhibit a broader, more asymmetric PL profile than undoped GaSb. Noticeable deviations from the single-Gaussian profile appear around the main emission band, with additional features at approximately 1505, 1520, and 1575 nm. We did not include these features as separate Gaussian components because the available PL measurements cannot uniquely establish their origin. They may arise from overlapping recombination channels associated with dopant-related states, surface defects, local structural disorder, or a distribution of nanocrystal environments. Therefore, the single-Gaussian fit is used primarily as a

phenomenological description of the dominant emission band rather than as a decomposition of all individual spectral contributions. The corresponding single-Gaussian fits give $R^2=0.974$ at 70 K and $R^2=0.939$ at 300 K. The lower R^2 at 300 K reflects the more complex, asymmetric spectral profile and the presence of additional features not fully described by a single Gaussian function. The modification of the PL spectral shape upon Ce incorporation can be discussed in the context of the calculated electronic structure. The DFT results indicate occupied, localized Ce 4f states and empty acceptor-like states near the band gap in the Ce-doped system. These dopant-related states can modify the local electronic environment and carrier localization. In addition, surface defects, local structural disorder, nanocrystal size distribution, and dopant-induced potential fluctuations may produce a distribution of recombination energies. Together, these effects can account for the broader and more asymmetric PL profile observed after Ce incorporation. Nevertheless, the present PL data do not permit individual spectral components to be assigned uniquely to specific Ce-related electronic transitions. The reduction in PL intensity at 300 K can be qualitatively associated with thermally enhanced non-radiative recombination and carrier delocalization. As temperature increases, carriers localized at radiative states may more readily access non-radiative relaxation pathways, leading to PL quenching. Because PL measurements were performed only at 70 and 300 K, the available data are insufficient for a reliable quantitative determination of an activation energy. Therefore, this study does not attempt an activation-energy analysis.

Overall, the Gaussian fitting provides a quantitative assessment of the principal PL bands and complements the spectral analysis. The relatively high R^2 values for the GaSb spectra indicate that a Gaussian profile reasonably approximates their dominant emission feature, whereas the lower R^2 value for Ce-doped GaSb at 300 K reflects its more complex, asymmetric spectral shape. These results suggest that Ce incorporation modifies the local electronic environment and carrier recombination pathways of GaSb nanocrystals, primarily changing the spectral width and shape rather than producing a clearly resolved, separate Ce-related emission band.

5. Conclusions

This study analyzes the electronic, optical, and magnetic properties of finite-thickness GaSb(110) slabs doped with Ce and Te. Thickness-dependent band-structure calculations and phonon dispersion analysis confirm that the 7-layer GaSb(110) slab provides a dynamically stable host model with a bulk-like interior electronic structure. Ce doping introduces both occupied localized 4f states below the Fermi level and empty acceptor-like states near the gap, indicating a tendency toward p-type electronic behavior. Te doping introduces donor-like states near the conduction-band side, indicating a tendency toward n-type behavior. These assignments describe the calculated electronic structure and do not represent direct measurements of carrier transport properties. In Ce+Te co-doped slabs, donor-acceptor compensation governs the electronic structure. The co-doped systems should therefore be described as compensated electronic systems rather than as materials with simultaneous strong electron and hole conduction. Magnetism is dominated by Ce 4f states, while Te contributes negligibly to the magnetic moment. Fractional total magnetic moments arise from partial spin delocalization, Ce-host hybridization, and Mulliken partitioning of the spin density. The temperature-dependent PL response highlights the roles

of carrier localization and thermally enhanced non-radiative recombination in the optical behavior of GaSb-based nanocrystals. Gaussian fitting quantitatively describes the measured PL spectra, with R^2 values of 0.954 and 0.964 for GaSb and 0.974 and 0.939 for Ce-doped GaSb at 70 and 300 K, respectively. The poorer fit for Ce-doped GaSb at 300 K is consistent with its broader, more asymmetric spectral profile. The main emission feature remains in the near-infrared region around 1530–1550 nm, while Ce incorporation primarily modifies the spectral width and shape rather than producing a clearly resolved separate Ce-related emission band. Because we investigated only two temperatures, the present data do not support a reliable quantitative determination of an activation energy.

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Анотація. Ми дослідили електронні, оптичні та магнітні властивості пластин GaSb(110) скінченної товщини, легованих Ce-, Te- та Ce+Te, використовуючи розрахунки з перших принципів. Чиста 7-шарова пластинка GaSb(110) має розрахункову ширину забороненої зони 0,76 eV. Легування Ce звужує ширину забороненої зони до 0,64 eV та вводить зайняті локалізовані 4f-стани Ce нижче рівня Фермі разом з порожніми акцепторно-подібними станами поблизу щілини, що вказує на акцепторно-подібний електронний характер. Легування Te дає ширину забороненої зони 0,72 eV та зміщує рівень Фермі в бік зони провідності, що узгоджується з донорно-подібною поведінкою. Спільне легування Ce+Te модифікує електронну структуру шляхом донорно-акцепторної компенсації, тоді як магнітна поведінка в основному пов'язана зі станами, що походять від Ce. Оптичний відгук проявляє зміни, викликані легуванням, у спектральній області низьких енергій, які можуть бути пов'язані з електронними станами, що походять від легуючих домішок. Досліджена фотолюмінесценція нанокристалів GaSb та легованого Ce при збудженні 785 нм проявляє виражену температурну залежність, з вищою інтенсивністю фотолюмінесценції при 70 K, у порівнянні з 300 K. Гаусівська апроксимація спектрів фотолюмінесценції добре узгоджується для GaSb ($R^2=0,954$) при 70 K та ($R^2=0,964$) при 300 K, тоді як нижча якість апроксимації для легованого Ce GaSb при 300 K ($R^2=0,939$) відображає його більш складний та асиметричний спектральний профіль. Основні особливості випромінювання проявляються в ближній інфрачервоній області близько 1530–1550 нм, тоді як включення Ce переважно розширює та асиметризує смугу фотолюмінесценції. Ці зміни можуть бути

пов'язані з модифікаціями в процесах локалізації носіїв та рекомбінації, що виникають через стани, пов'язані з домішками, поверхневими дефектами та структурною неоднорідністю. Оскільки вимірювання фотолюмінесценції здійснювались лише при 70 та 300 K, кількісний аналіз енергії активації не проводився. Ці результати пояснюють, як спільне легування рідкісноземельними елементами та донорами може налаштувати електронну, магнітну та оптичну реакцію моделей плит GaSb(110) для оптоелектронних та спінтронних застосувань.

Ключові слова: магнетизм, розрахунки з перших принципів, оптоелектронні властивості, інженерія забороненої зони, спільне легування