Research Article

Electronic Structure, Electronic Charge Density, and Optical Properties Analysis of GdX_3 ($\text{X} = \text{In}, \text{Sn}, \text{Tl}, \text{and Pb}$) Compounds: DFT Calculations

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The electronic properties of magnetic cubic AuCu_3 type GdX_3 ($\text{X} = \text{In}, \text{Sn}, \text{Tl}, \text{and Pb}$) have been studied using first principles calculations based on density functional theory. Because of the presence of strong on-site Coulomb repulsion between the highly localized 4f electrons of Gd atoms, we have used LSDA + U approach to get accurate results in the present study. The electronic band structures as well as density of states reveal that the studied compounds show metallic behavior under ambient conditions. The calculated density of states at the Fermi level $N(E_F)$ shows good agreement with the available experimental results. The calculated electronic charge density plots show the presence of ionic bonding in all the compounds along with partial covalent bonding except in GdIn_3 . The complex optical dielectric function's dispersion and the related optical properties such as refractive indices, reflectivity, and energy-loss function were calculated and discussed in detail.

1. Introduction

The rare earth based intermetallics, REX_3 ($\text{X} = \text{In}, \text{Sn}, \text{Tl}, \text{and Pb}$), have been investigated extensively because they show a variety of interesting physical properties: magnetism, de Haas-van Alphen (dHvA) effect, and thermal, transport, and electronic properties [1, 2]. They have cubic $L1_2$ (AuCu_3) crystal structure, space group $Pm\bar{3}m$. Electron-transport properties of GdIn_3 in the paramagnetic range are similar to those for other REIn_3 compounds and its Fermi surface is almost the same as that of the nonmagnetic compound LaIn_3 [3, 4]. Grechnev et al. [5] have studied GdM ($\text{M} = \text{Cu}, \text{Ag}, \text{and Mg}$) and RIn_3 ($\text{R} = \text{Gd}, \text{Tb}, \text{and Dy}$) with LMTO method within the atomic sphere approximation. They have done investigations of RM and RM_3 compounds in CsCl and AuCu_3 -type structures, in which the R sublattice is simple cubic and in which the energy band occupancy can be varied. They have chosen the position of Gd at (0, 0, 0) and M at (0.5, 0.5, 0.5) in the case of GdM and R at (0, 0, 0) and In at

(0, 0.5, 0.5) in the case of RIn_3 compounds. Magnetic neutron studies at pressures above 40 GPa have been used for GdX ($\text{X} = \text{As}, \text{Sb}, \text{and Bi}$) compounds by Goncharenko et al. [6]. They have reported that these compounds are stable up to 40 GPa in antiferromagnetic ordering. Duan et al. [7] have studied the magnetic ordering in Gd monopnictides using Heisenberg model. They have reported that the magnetic ordering in GdN undergoes a transition from ferromagnetic to antiferromagnetic state among the Gd monopnictides. The hyperfine fields in ferromagnetically ordered cubic Laves phase compounds of gadolinium with nonmagnetic metals (GdX_2 : $\text{X} = \text{Al}, \text{Pt}, \text{Ir}, \text{and Rh}$) have been investigated by Dormann and Buschow [8]. Pressure-induced structural phase transition of gadolinium monopnictides GdX ($\text{X} = \text{As and Sb}$) has been studied theoretically using interionic potential theory as reported by Pagare et al. [9]. Magnetic measurements have been performed for cubic Laves phase compounds RFe_2 ($\text{R} = \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Er}, \text{and Y}$) and $\text{R}_x\text{Y}_{1-x}\text{Fe}_2$ ($\text{R} = \text{Gd}, \text{Tb}, \text{and Er}$) in fields up to 30 kOe

TABLE 1: Density of states $N(E_F)$ of GdX_3 compounds in both spins at ambient conditions.

Solids	Approximation	E_F	$N(E_F)$ (states/eV)		γ
			Spin-up	Spin-down	
GdIn_3	LSDA + U	0.53511	1.14	1.47	2.69
	Expt.	—	1.59 ^a	—	—
GdSn_3	LSDA + U	0.58873	1.01	1.23	2.82
	Expt.	—	2.51 ^a	—	—
GdTl_3	LSDA + U	0.54759	0.56	1.25	1.32
GdPb_3	LSDA + U	0.52437	0.77	1.82	4.30

^aThe paper [5].

and for temperatures between 4.2° and 1000°K by Buschow and Van Stapele [10]. The structural and elastic properties of GdX ($X = \text{Bi, Sb}$) using FP-LMTO have been studied by Boukhari et al. [11]. The experimental data and results of *ab initio* calculations of the volume derivatives of the band structure and the exchange parameters for the corresponding series of compounds have been used to analyze the nature of the f-f interactions. Possibility of Kondo effect in Gd intermetallic compound has been studied by Yazdani and Khorassani [12]. They also showed that, with increasing electron concentration, Gd experiences electronic and magnetic instability, and these behaviors point to the appearance of the Kondo Lattice. The electronic structure of the intermetallic compound Gd_3Pd has been studied by Punkkinen et al. [13] using the local spin-density approximation (LSDA) and the LSDA + U approximation to the exchange-correlation potential of the spin-density functional theory. They found that the “5d” states of Gd play an important role in a correct description of the magnetic state of the Gd_3Pd . They also suggested that the crystal and magnetic structure of the Gd_3Pd is more complicated at low temperatures than at temperatures just below the transition temperature.

It is revealed from the literature that no efforts have so far been made to study the electronic and optical properties of GdX_3 ($X = \text{In, Sn, Tl, and Pb}$) compounds either theoretically or experimentally. In the present paper, we therefore aim to study theoretically the electronic structure and optical and magnetic properties of the above class of compounds using density functional theory within LSDA + U method. This method explicitly includes on-site Coulomb interaction term in the conventional Hamiltonian and influence of electronic and magnetic properties of such systems [14, 15].

2. Crystal Structure and Computational Details

The crystal structure of GdX_3 is stable in cubic AuCu_3 structure ($Pm\bar{3}m$). The ground state calculations were carried out using the full-potential linearized augmented plane wave (FP-LAPW) method [16] as implemented in the WIEN2k code [17]. The exchange-correlation effects were described with LSDA + U [18] approximation. In the calculations reported here, we have used the parameter $R_{\text{MT}} \times K_{\text{max}} = 7$ to determine the matrix size (convergence), where K_{max} is the plane wave cut-off and R_{MT} is the smallest atomic sphere

radius. Within these spheres, the charge density and potential are expanded in terms of the crystal harmonics up to an angular momentum of $L = 10$. A plane wave expansion has been used in the interstitial region. G_{max} was set to 14 (a.u.)⁻¹, where G_{max} is defined as the magnitude of the largest vector in the charge density Fourier expansion. Brillouin zone sampling was performed by the Monkhorst-Pack scheme [19] with $10 \times 10 \times 10$ mesh based on Hohenberg and Kohn theorems [20, 21]. The values of the kinetic energy cut-off and the grid were determined by ensuring the convergence of total energies within an accuracy of 1 meV/atom. Due to the strong on-site Coulomb repulsion between the highly localized 4f electrons of RE atoms, the local spin-density approximation (LSDA) with additional Hubbard correlation terms (LSDA + U approach) [18] is also used to calculate the accurate results. Thus, we present LSDA + U approach in order to obtain the appropriate results. In the LSDA + U calculations we have used an effective parameter $U_{\text{eff}} = U - J$, where U is the Hubbard parameter and J is the exchange parameter. We set $U = 6.70$ eV and $J = 0.70$ eV. We have optimized the atomic positions taken from XRD data [22] by minimization of the forces acting on the atoms. From the relaxed geometry, the electronic structure, electronic charge density, and the optical properties are determined. The optimized geometry along with the experimental values [22] is listed in Table 1.

3. Result and Discussion

3.1. Electronic Band Structure and Density of States. The electronic band structures of AuCu_3 -type GdX_3 ($X = \text{In, Sn, Tl, and Pb}$) intermetallic compounds have been calculated along the principal symmetry directions in both spins within LSDA + U approximation with the Fermi level at zero. Since the 4f orbital of Gd is half filled, the LSDA + U correction for GdX_3 is very essential. We have employed $U = 6.70$ eV and $J = 0.70$ eV for Gd atoms. We find that the four studied GdX_3 compounds have similar band structures except in the position of Gd “f” states, as shown in Figures 1(a)–1(h). It is clear from the band profiles that the valence and conduction bands overlap considerably and there is no band gap at the Fermi level for these compounds, which confirms the metallic nature of these compounds. The total density of states (TDOS) along with partial density of state (PDOS) at equilibrium lattice constants for cubic GdX_3 compounds is

FIGURE 1: Continued.

FIGURE 1: Electronic band structures of GdX_3 compounds in LSDA + U approach in both spins.

computed using LSDA + U approach, as shown in Figures 2(a)–2(h), respectively.

The lowest lying bands observed in the investigated compounds are due to “ s -like” states of X (In, Sn, and Pb) except for GdTl_3 in both spins. The lowest dense flat bands in GdTl_3 are due to “ d -like” states of Tl in both spins. The electronic configuration of Gd is $[\text{Xe}] 4f^7 5d^1 6s^2$. It is clearly seen from Figures 1(a)–1(h) and 2(a)–2(h) that the band structures of majority spin are similar to those for minority spin except that the half filled Gd- f bands are occupied and lie well below the Fermi level (near -8.0 eV) and the minority spin Gd- f bands are unoccupied and lie above the Fermi level. The half filled Gd- f bands in minority spin hybridize with the Gd- p , Gd- d , and In/Sn/Tl/Pb “ p ” spin-down states while the spin-up “ f ” bands remain unhybridized in all these compounds. The dominating character in GdX_3 at the Fermi level is due to Gd “ d ” states, with a significant hybridization with X “ p ” states, whereas in GdSn_3 significant contribution is due to Sn “ p ” states with a significant hybridization with Gd “ d -like” states in both spins. It is seen from Figures 1(a)–1(f) that a cluster of bands observed in the energy range between 1.5 and 3.0 eV above Fermi level in GdX_3 is mainly due to Gd “ d ” states.

The U parameter that acts on Gd “ $4f$ ” states pushes them further from the Fermi level as compared with the LSDA approach, and the intensities of Gd $4f$ states above the Fermi level show a decrease. It should be pointed out that the obtained profile of Gd $4f$ states is similar to the results by Pang et al. [23, 24]. The obtained values of the density of states at Fermi level $N(E_F)$ from LSDA + U approach for GdIn_3 , GdSn_3 , GdTl_3 , and GdPb_3 are given in Table 1 for both spins, which indicates their metallic nature.

3.2. Electronic Charge Density. Electron density denotes the nature of the bond among different atoms. In order to predict

the chemical bonding and the charge transfer in GdX_3 compounds, the charge-density behaviors in 2D are calculated in the (100) plane for these compounds and have been depicted in Figures 3(a)–3(d). Large difference in electronegativity (X) is responsible for charge transfer among different atoms resulting in ionic bond nature. Small electronegativity (X) difference results in charge sharing and is responsible for covalent bond nature. Electronegativity values for Gd, In, Sn, Tl, and Pb are 1.2, 1.78, 1.96, 2.04, and 2.33, respectively. The plot shows there is ionic and partial covalent bonding between Gd and In/Sn/Tl/Pb atoms in all compounds except in GdIn_3 . The calculated electron density shows that charge density lines are spherical in some areas of the plane structure which shows the sign of ionic bond of Gd and In/Sn/Tl/Pb atoms in all the studied compounds.

3.3. Optical Properties. The complex dielectric function is directly related to the energy band structure of solids. The optical spectroscopy analysis is a powerful tool to determine the overall band behavior of a solid. Therefore, precise FP-LAPW calculations are desirable to figure out the optical spectra. GdX_3 compounds have a cubic symmetry; it is sufficient to compute only one component of the dielectric tensor, which can completely determine the linear optical properties [25, 26]. Neither theoretical nor experimental literature has been found regarding the optical properties of these compounds. We denote the dielectric function by

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega), \quad (1)$$

where ω is the frequency and $\epsilon_2(\omega)$ is its imaginary part which is given by the relation

$$\epsilon_2(\omega) = \int \sum_{\nu, \sigma} |M_{\sigma\nu}(k)|^2 \delta(\omega - \omega_{\sigma\nu}(k)) d^3k, \quad (2)$$

FIGURE 2: Continued.

FIGURE 2: Total and partial density of states of GdX_3 in both spins in LSDA + U scheme.

FIGURE 3: Electronic charge density plots of GdX_3 at ambient conditions.

where the integral is taken over the first Brillouin zone. The momentum dipole elements

$$M_{\sigma\nu}(k) = \langle u_{\sigma k} | A \cdot \nabla | u_{\nu k} \rangle \quad (3)$$

are the matrix elements for direct transitions between the valences for direct transitions between the valence state $u_{\nu k}(r)$ and the conduction band state $u_{\sigma k}(r)$, A is the potential vector defining the electromagnetic field, and the energy $\hbar\omega_{\sigma\nu} = E_{\sigma k} - E_{\nu k}$ is the corresponding transition energy. The real part $\epsilon_1(\omega)$ of the dielectric function can be deduced from the imaginary part using the Kramers-Kronig relation [27, 28]:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega', \quad (4)$$

where P is the principal value of the integral. Once the real and imaginary parts of the dielectric function are determined,

we can calculate important functions such as optical refractive index $n(\omega)$ and electrical conductivity $\sigma(\omega)$ [28]:

$$\begin{aligned} \sigma(\omega) &= \sigma_1(\omega) + i\sigma_2(\omega), \\ \sigma_1(\omega) &= \frac{\omega}{4\pi} \epsilon_2(\omega); \\ \sigma_2(\omega) &= \frac{\omega}{4\pi} [1 - \epsilon_1(\omega)]. \end{aligned} \quad (5)$$

Figures 4(a)–4(d) show the spectrum of the real and imaginary parts of the complex dielectric function versus the photon energy of GdIn_3 , GdSn_3 , GdTl_3 , and GdPb_3 . The interpretation of this spectrum in terms of electronic structure, presented in Figures 1(a)–1(h), reveals the manner by which these compounds absorb the incident radiation. As shown in Figures 4(a)–4(d), the optical spectra of GdIn_3 and GdTl_3 as well as GdSn_3 and GdPb_3 appear to be almost similar. We noticed a sharp increase in the imaginary part of the electronic dielectric function $\epsilon_2(\omega)$ of GdX_3 compounds below 1.0 eV. This sharp rise in the optical spectral structure of these compounds is mainly due to Drude term [29]. The effect of the Drude term is more prominent for energies less than

FIGURE 4: Calculated imaginary and real part of GdX_3 with the incident photon energy.

1.0 eV. We can see two significant peaks in $\epsilon_2(\omega)$ spectrum for all compounds except $GdIn_3$, in which the first peak lies at 0.48 eV, 0.31 eV, 0.94 eV, and 0.18 eV and second peak occurs at 1.32, 1.18, 1.54, and 0.80 eV for $GdIn_3$, $GdSn_3$, $GdTi_3$, and $GdPb_3$, respectively. An additional third peak is observed at 1.86 eV for $GdIn_3$.

Knowing the imaginary part of the complex dielectric function, we have calculated its real part using Kramers-Kronig relations and then computed various optical constants which characterize the propagation of the electromagnetic wave through the material [30]. The real part of dielectric function shows ability of a material to allow the external electromagnetic field to pass through it. It is observed from Figures 4(a)–4(d) that as we go along the period from $GdIn_3$ to $GdSn_3$ the peaks get increased. Similar behavior is observed as we move from $GdTi_3$ to $GdPb_3$. This rise in

the peak values is due to the increase in the number of $5p$ electrons of X in all the GdX_3 compounds. If the Gd “ $4f$ ” electrons play a role in determining the optical properties, the interband transitions should occur between the occupied Gd $5d$ bands and the unoccupied Gd $4f$ bands. Since the majority-spin Gd “ $4f$ ” bands are located around -7 eV below the Fermi level in all the studied compounds, it is not possible for them to contribute to the optical spectra in the lower energy range. The occupied Gd $5d$ bands are mostly spin-up bands, while the unoccupied Gd “ $4f$ ” bands are spin-down bands. Since the spin-up optical transition is very unlikely, there is hardly a significant contribution from the Gd $5d-4f$ interband transitions. The lowest peak of $\epsilon_1(\omega)$ lies at 0.23 eV, 0.12 eV, 0.29 eV, and 0.07 eV for $GdIn_3$, $GdSn_3$, $GdTi_3$, and $GdPb_3$, respectively. The second peak is observed at 1.0 eV for $GdIn_3$ and $GdSn_3$ and at 1.4 eV and 0.6 eV for $GdTi_3$ and

FIGURE 5: Variation of refractive index of GdX₃ compounds with the incident photon energy. FIGURE 6: Calculated reflectivity spectra of GdX₃ compounds.

GdPb₃, respectively. The calculated values of static dielectric $\epsilon_1(0)$ of these compounds are found to be 48.72, 115.25, 58.65, and 144.46, respectively. This data explains inverse relation between the band gap and static dielectric function which means a larger $\epsilon_1(0)$ value yields smaller energy gap, which again confirms the studied GdX₃ compounds metallic nature.

The most important constant among the other evaluated optical properties is the refractive index $n(\omega)$, which is related with the linear electrooptical coefficient that in turn determines the photorefractive sensitivity of GdX₃ compounds. The dispersion curves of refractive index for GdX₃ compounds depicted in Figures 5(a) and 5(b) show a similar behavior. These compounds in low energy show a maximum value of refractive indices. It is observed that the refraction index reaches maximal values for the energies near

the absorption threshold of the material. The extinction coefficient (k) is significant in metals, which shows absorption of energy on surface of the material.

The frequency dependent reflectivity $R(\omega)$ spectrum for all the GdX₃ compounds is displayed in Figures 6(a) and 6(b). Figure 6(a) shows that the maximum reflectivity is at 7.74 eV for GdIn₃, 7.20 eV for GdSn₃, 4.88 eV for GdTl₃, and 6.98 eV for GdPb₃. Rapid decrease in reflectivity can be observed at 20 eV for all these studied compounds, which may be due to collective plasma resonance. $\epsilon_2(\omega)$ can be used to find out the depth of plasma minimum and is a measure of the degree of overlapping between interband absorption regions [31]. In the present work, the reflectivity at zero frequency is obtained as 0.55 for GdIn₃, 0.69 for GdSn₃, 0.73 for GdTl₃, and 0.60 for GdPb₃, respectively.

FIGURE 7: Calculated energy-loss spectra of GdX_3 compounds.

Added to the dielectric function, the energy-loss function $L(\omega)$ is also calculated at ambient conditions. Energy-loss function $L(\omega)$ is large at plasma energy and determines the energy lost in traversing of a fast moving electron [31]. The collective oscillation of valence electron causes plasmon loss. In the interband transitions, the scattering probability for volume is directly related to $L(\omega)$. We have calculated the spectrum of frequency related to plasma resonance and displayed in Figures 7(a) and 7(b). The maximum peaks are situated at 11.77 eV for GdIn_3 , 13.45 eV for GdSn_3 , 32.20 eV for GdTl_3 , and above 35 eV for GdPb_3 , respectively.

4. Conclusion

In this work, we have investigated the electronic band structure, density of states, electronic charge density, and optical properties of GdX_3 ($X = \text{In, Sn, Tl, and Pb}$) compounds using FP-LAPW method, within LSDA + U as exchange-correlation scheme. The electronic band structure calculations show that all the studied compounds have zero band gap value and show metallic nature. The electronic charge density plots reveal the presence of ionocovalent bonding in all the compounds along with partial covalent bonding except in GdIn_3 . The linear optical response of these compounds is also studied and discussed in detail. Additionally, the maximum peak values of the imaginary part of dielectric function $\epsilon_2(\omega)$ and the energy-loss function $L(\omega)$ and the zero frequency limit of real part of dielectric function $\epsilon_1(\omega)$ and reflectivity function $R(\omega)$ are calculated for all the investigated GdX_3 compounds. Our calculated results on optical properties reveal the possibility of their use as infrared optoelectronic materials as well as good dielectric materials, which will be tested in the future experimentally as well as theoretically.

Disclosure

Sankar P. Sanyal is a coauthor.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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