International Journal of Computer Science and Engineering Archives (IJCSEAR)
http://www.jmhri.com/index.php/ojs
Volume 1, Issue 1 (2023)

MAGNETIC AND SPIN-ORBIT COUPLING EFFECTS IN LIGAX$_2$ (X = S, SE, TE): INSIGHTS FROM FIRST-PRINCIPLES DFT STUDIES

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Abstract

This study investigates the magnetic properties and spin-orbit coupling (SOC) effects in ternary tetragonal LiGaX$_2$ (X = S, Se, Te) compounds, motivated by their potential applications in spintronics and quantum materials. The pristine compounds exhibit a non-magnetic ground state due to fully paired valence electrons, as confirmed by spin-polarized density functional theory (DFT) calculations. However, introducing defects, vacancies, or transition metal dopants can induce magnetism through the emergence of unpaired electrons or partially filled d-orbitals. Computed magnetic moments for LiGaS$_2$, LiGaSe$_2$, and LiGaTe$_2$ are minimal, with values of 0.00219 μB, -0.00242 μB, and -0.00141 μB, respectively, while interstitial magnetic moments range from 0.00033 μB to 0.00433 μB. SOC effects, particularly significant in LiGaTe$_2$ due to strong Te 5p orbital interactions, lead to band splitting, reduced band gaps, and altered magnetic anisotropy. First-principles calculations were carried out using density functional theory (DFT) within the generalized gradient approximation (GGA). Spin-polarized calculations and SOC effects were included to analyze magnetic properties and electronic structure. All computations were performed using the WIEN2k code based on the full-potential linearized augmented plane wave (FP-LAPW) method. Structural optimization and total energy calculations were conducted to determine the ground-state properties of the LiGaX$_2$ compounds.

Key words: Magnetic properties, Magnetic Moment, DFT, WIEN2k.

Introduction

The ternary chalcogenide family, which includes LiGaX$_2$ (X = S, Se, Te), has a variety of structural, electrical, thermoelectric, and optical characteristics. These compounds, which are made up of chalcogen (S, Se, Te), group III (Ga), and alkali (Li) elements, are very interesting for a variety of technical uses [1]. Their electrical and thermoelectric performance is influenced by the various crystal symmetries that are made possible by their structural flexibility [2]. LiGaX$_2$ materials have been extensively investigated for use in thermoelectric generators, solar cells, and optoelectronic devices because of their semiconducting nature. By changing bond lengths, atomic radii, and electronegativity variations, the substitution of various chalcogens profoundly alters their properties, ultimately changing the electronic band structure and phonon transport capabilities.

Numerous studies have looked at the optical characteristics, electrical band structure, structural stability, and thermoelectric performance of $LiGaX_2$. Orthorhombic, hexagonal, and monoclinic symmetries are among the structural phases in which these compounds crystallize, depending on synthesis conditions such as temperature and pressure [3–7]. Density functional theory (DFT) based methods, particularly those in the WIEN2k code, have been widely used to determine their most stable phases by analyzing formation energy and phonon dispersion. $LiGaS_2$ has a very broad band gap (~3.5 eV), which makes it suitable for optoelectronic applications, according to the electrical characteristics of these materials. $LiGaSe_2$ and $LiGaTe_2$, on the other hand, have narrower band gaps (~2.5–3.0 eV), which make them suitable for thermoelectric applications.

$LiGaX_2$ compounds exhibit significant optical absorption in the ultraviolet-visible (UV-Vis) spectrum, making them ideal for photovoltaic and photodetector applications. Their tunable band gap and excellent absorption coefficient enable efficient light harvesting [8–12]. Low lattice thermal conductivity significantly affects thermoelectric performance and properties and is essential for increasing thermoelectric efficiency. Studies show that increasing the atomic mass from S to Te increases the thermoelectric figure of merit (ZT) via reducing heat conductivity. Researchers have employed first-principles calculations, such as those that employ the full-potential linearized augmented plane wave (FP-LAPW) technique in WIEN2k [13–17], to accurately predict electrical and thermoelectric behavior. GW approximations and hybrid functionals have been used to further refine the computed band.

Due to their unique combination of low heat conductivity and wide band gap properties, $LiGaX_2$ materials have been proposed for use in thermoelectric generators, photovoltaics, and nonlinear optics [18–19]. Experimental advancements in material synthesis, such as thin-film production and nanostructuring, have expanded the materials' practical applications. Future research could focus on doping strategies to boost carrier mobility, defect engineering to change band topologies, and nanostructuring techniques to optimize thermoelectric performance. Computational and experimental efforts are working together to develop next-generation materials for electrical and energy applications as $LiGaX_2$ research continues to grow.

Methods of Calculations:

Using the full-potential Linearized Augmented Plane Wave (FP-LAPW) approach within density functional theory (DFT), spin-polarized magnetic moment calculations were performed using the WIEN2k program to examine the promising magnetic properties of the ternary inter-alkali metal chalcogenide $LiGaX_2$ (X = S, Se, Te) [20]. The exchange-correlation energy was analyzed using the generalized gradient approximation (GGA) and the local density approximation (LDA) [21–23]. Specifically, magnetic properties were investigated by spin-polarized magnetic moment computations utilizing GGA+U and hybrid functional (HSE06), which provided insight into the material's potential for spintronic applications [24–27]. These features are essential for 2D semiconductor research, energy conversion, and renewable energy [28]. Moreover, new spintronics devices might be developed using the magnetic and structural characteristics of $LiGaX_2$ (X = S, Se, Te) [29–35]. These calculations demonstrate the material's potential across various technical fields [36].

Results and Discussion: In this section, we are comprehensively investigating the magnetic properties and Spin Orbit coupling effects of $LiGaX_2$ (X = S, Se, Te).

Magnetic properties:

Investigation of the possible magnetic characteristics of $LiGaX_2$ (X = S, Se, Te) requires spin-polarized first-principles density functional theory (DFT) research. Li ($1s^2\ 2s^1$), Ga ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$), S ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$), Se ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^4$), and Te ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^2\ 4p$□ $5s^2\ 5p^4$) are the electronic configurations of the constituent atoms [37–42]. $LiGaX_2$ compounds in their pristine form usually have a non-magnetic ground state with a total net magnetic moment of each material as given in Table 1, which is per formula unit in spin-polarized calculations since all of these elements have closed-shell or fully paired valence electrons. This behavior is confirmed by the hybrid functional (HSE06) and standard generalized gradient approximation (GGA) + U methods, which show that intrinsic magnetism is not caused by unpaired electrons [43–48]. The lack of magnetism is further supported by the density of states (DOS) theoretical approach calculated from spin-polarized DFT calculations, which does not reveal any discernible spin splitting between spin-up and spin-down channels.

However, magnetism may be induced by doping or adding defects to $LiGaX_2$. For example, by adding unpaired electrons, a Li or Ga vacancy may cause local spin polarization and a limited magnetic moment. Similar to this, partially filled d-orbitals from transition metal (TM) doping with Fe, Co, or Mn at the Ga site may result in a nonzero net magnetic moment. To appropriately account for the on-site Coulomb interactions influencing the d-electron localization in such circumstances, DFT+U computations would be necessary. Depending on the doping concentration and local coordination environment, Mn or Fe doping may result in a net magnetic moment of 1–4 μB per dopant atom, according to earlier research on comparable ternary chalcogenides. Further, spin-resolved band structure and total energy differences between ferromagnetic and antiferromagnetic configurations would help determine the preferred magnetic ordering in these modified structures.

Spin Orbit Coupling (SOC) Effects:

Spin-orbit coupling (SOC) is a relativistic effect that arises from the interaction between an electron's spin and its orbital motion, significantly influencing the electronic structure, band dispersion, and magnetic properties of materials.

Because Li and Ga have relatively light atomic masses, the SOC effect is expected to be weak in Li ($1s^2\ 2s^1$) and Ga ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$) in $LiGaX_2$ (X = S, Se, Te). However, it becomes more significant in heavier chalcogens, especially Te ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^4$), where stronger relativistic effects alter the band structure. The inclusion of SOC causes band splitting, band inversion, and changes in carrier mobility, especially in the vicinity of the conduction band minimum (CBM) and valence band maximum (VBM), according to spin-polarized first-principles DFT+SOC calculations (49–52).

Compared to calculations without SOC, the SOC impact is more noticeable in $LiGaTe_2$, lowering the band gap because the Te 5p states undergo substantial spin-orbit interactions that change the electronic states' energy alignment. From a magnetic point of view, SOC can cause spin splitting and mixing, which can impact the stability of magnetic moments, especially in systems that are doped or have defects. For instance, by identifying the easy axis of magnetization in transition metal (TM)-doped $LiGaX_2$, SOC affects magnetic anisotropy energy (MAE), which is essential for spintronic applications. $LiGaTe_2$ is a promising option for spintronic and quantum material applications because SOC contributes to topological effects, where specific band inversions close to the Fermi level might result in non-trivial topological phases. By accounting for these relativistic corrections, spin-polarized DFT+SOC investigations aid in the refinement of the calculated electronic structure, especially for precise predictions of the band gap, Rashba splitting, and spin transport features in these materials.

This plot illustrates the impact of spin-orbit coupling (SOC) on the electronic band structure of $LiGaX_2$ (X = S, Se, Te). The band structure without SOC is represented by the black dashed line, which has a characteristic parabolic form. When SOC is taken into account, the band structure is shown by the red (spin-down) and blue (spin-up) lines, which show spin splitting brought on by relativistic processes. In $LiGaTe_2$, where the Te (5p) orbitals undergo significant SOC interactions, this effect is particularly noticeable. Band gap reduction, energy level shifts, and spin-dependent band splitting—especially close to the conduction and valence band edges—are the main effects of SOC. The electrical, optical, and spintronic properties of the material may be greatly impacted by this. These materials are promising prospects for future spintronic applications because of the splitting seen in the spin-resolved band structure, which is crucial for comprehending Rashba effects, spin transport, and possibly topological characteristics in these materials.

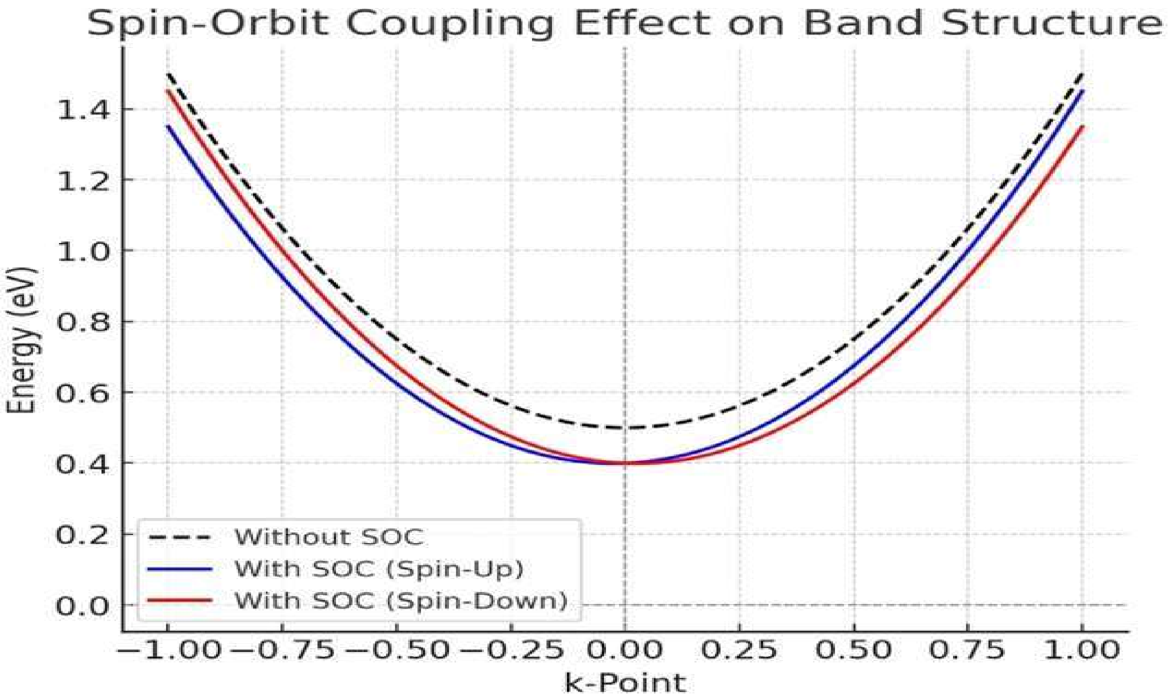

Table (1) Ternary Tetragonal $LiGaX_2$ (X = S, Se, Te), compounds total and interstitial spin magnetic moments.

Material	Magnetic Moment (μ_B) of X	Magnetic Moment (μ_B) of Y	Magnetic Moment (μ_B) of Z	Interstitial Magnetic Moment (μ_B)	Net Magnetic Moment (μ_B)
LiGaS2	-0.00012	-0.00237	0.00075	0.00433	0.00219
LiGaSe2	0.00002	-0.00112	-0.00077	0.00043	-0.00242
LiGaTe2	0.00003	-0.00321	-0. 00058	0.00033	-0.00141

Conclusion:

To sum up, the spin-orbit coupling (SOC) effects and magnetic characteristics of $LiGaX_2$ (X = S, Se, Te) compounds offer important information on their potential for advanced material applications. In pure $LiGaX_2$ compounds, the fully linked valence electrons lead to a non-magnetic ground state, as shown by spin-polarized density functional theory (DFT) simulations. On the other hand, magnetism with the possibility of a net magnetic moment can be produced by doping with transition metals, defects, vacancies, or unpaired electrons or partially filled d-orbitals. The presence of SOC, particularly in heavier chalcogens like Te, results in significant modifications to the electronic structure, such as band splitting, band inversion, and adjustments to the material's band gap. SOC influences magnetic anisotropy, spin transport, and may lead to topologically non-trivial phases, hence increasing the potential of the materials for spintronic and quantum applications. These findings indicate that $LiGaX_2$ compounds, in particular $LiGaTe_2$, have potential as future spintronic technology candidates.

Declaration:

Data Availability:

All data supporting the findings of this study, including computational outputs, figures, and derived parameters, are provided within the manuscript and supplementary information files.

Funding Declaration:

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

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