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# Ab-initio Calculations of the Half-metallic Ferromagnetic New Variant Perovskites $Li_2CrO_6$ and $Li_2CuO_6$

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**Highlights**

- This paper includes half-metallic properties of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$.
- GGA-PBE exchange-correlation approximation was used for performing calculations.
- The magnetic moments of compounds were 4.00 $\mu_B$/f.u. and 5.00 $\mu_B$/f.u., respectively.

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**Abstract**

The half-metallic calculations of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were carried out by using WIEN2k computational code. First, the ferromagnetic (FM) and non-magnetic (NM) phases were compared, and FM phases were obtained energetically more stable. The equilibrium lattice constants were obtained as 7.63 Å and 7.66 Å for $Li_2CrO_6$ and $Li_2CuO_6$, respectively. Second, the electronic calculations were performed, and the semiconduction properties were seen in spin-up states while spin-down states showed metallic nature. The band gaps were obtained as 1.806 eV and 1.177 eV for $Li_2CrO_6$ and $Li_2CuO_6$, respectively. Since variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ showed 100% spin polarizations, these were obtained as true half-metallic ferromagnetic materials. Then the total magnetic moments were obtained as 4.00 $\mu_B$/f.u., 5.00 $\mu_B$/f.u. When both the electronic and magnetic properties of the compounds are examined, the variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ are suitable materials for spintronics applications.

## 1. INTRODUCTION

Spintronics is one of the branches of sciences that examines the technological systems of nano-sized devices that emerge by controlling spin currents [1,2]. This research area also includes sub-disciplines such as molecular spintronics, semiconductors and spintronics [3]. Spintronics science contains the basis of many technological products that are actively used today. Because there are ferromagnetic, ferrimagnetic, antiferromagnetic, and even non-magnetic material groups in spintronics applications. Non-magnetic materials are used by polarizing their spins with the help of spin injection. Therefore, the transmission and usage areas of these material groups under temperature or magnetic effects have made spintronics applications quite remarkable. Tunneling Magnetoresistance (TMR) [4], Giant Magnetoresistance (GMR) [5,6] and Johnson transistors [7] are the most used methods to polarize spins of a non-magnetic material. The most common usage areas of spintronic materials in recent years are magnetic sensors [8], magnetic random-access memories [9,10], spin-polarized light emitting diodes [11,12] and spin-polarized field effect transistors [13] can be given as examples.

NiMnSb alloy was explored as a half-metallic ferromagnetic material by de Groot [14]. Then half-metallic materials have become one of the materials that are frequently used in spintronic applications. They are quite distinctive from other materials with their 100% spin polarization properties around Fermi energy levels, since one of the spin-up or spin-down electron states cuts the Fermi energy level, the other does not [15-20]. Half-metallic properties of some half-full, quaternary Heusler alloys [21-26], diluted magnetic semiconductors [27-30], perovskite/double perovskite compounds [31,32] have been extensively studied in recent years. Different from simple or double perovskite groups, variant perovskite compounds have been

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studied intensively in recent years. In 1978, the chemical shift magnitudes of $L_{\alpha1,2}$ (Nb) X-ray spectra of Nb-Cl systems were investigated by Kostikova et al. [33]. In this study, variant perovskites $K_2NbCl_6$, $Rb_2NbCl_6$ and $Cs_2NbCl_6$ were used. In 2007, Jahn-Teller effects were investigated for the phase transition effects of variant perovskite $K_2NbCl_6$ and $Rb_2NbCl_6$ compounds by Henke [34]. In 2011, Brik et al. [35] performed lattice parameters and electronegativity estimations of 85 variants perovskite compounds. The used structure was $A_2XY_6$. Elements of A were determined as K, Cs, Rb, Tl, X elements as tetravalent cation and Y elements were chosen as F, Cl, Br, I. In 2018, Faizan et al. [36] carried out the structural, electronic, and magnetic properties of $A_2MnF_6$ alkali metal fluorites with ab-initio calculations. Here, the authors chose the A elements from the K, Rb and Cs elements, which were used most frequently in variant perovskite compounds. Ali et al. investigated the half-metallic properties of $Cs_2NpBr_6$ and $Rb_2TaZ_6$ (Z = Cl, Br) in 2020 and $A_2NbCl_6$ (A= K, Rb) and $Cs_2WX_6$ (X = Cl, Br) variant perovskite compounds were investigated in 2021 with the help of density functional theory and introduced new compounds that can be used in spintronics to the literature [37-40]. In addition, the structural, electronic, magnetic, and optical properties of $Cs_2NbI_6$ [41] and $K_2OsX_6$ (X = Cl, Br) [42], and bulk modulus calculations of $A_2BX_6$ variant perovskite compounds [43] were investigated by Ullah et al. In $Cs_2NbI_6$ compound, ferromagnetic (FM) phase was energetically more stable than non-magnetic (NM) and antiferromagnetic (AFM) phases. Additionally, total magnetic moment values were obtained as 1.0019 $\mu_B$, 0.9997 $\mu_B$, and 1.0003 $\mu_B$, and indirect band gaps were calculated as 1.38 eV, 1.88 eV, and 1.93 eV for GGA, GGA+U, and mBJ approximations, respectively. In $K_2OsCl_6$ and $K_2OsBr_6$, the compounds were stable in FM phase. The band gap and magnetic calculations were investigated with GGA and GGA+U. The direct band gap values for $K_2OsCl_6$ and $K_2OsBr_6$ compounds were obtained as 1.93 eV and 1.56 eV, and 2.69 eV and 2.1 eV at $E_{g(X-X)}$ symmetry in GGA and GGA+U, respectively. Then total magnetic moment values of $K_2OsCl_6$ and $K_2OsBr_6$ compounds were calculated as 2.00 $\mu_B$ with GGA and GGA+U [42]. Inspired by all these studies, new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were investigated via density functional theory. The structures of $Li_2CrO_6$ and $Li_2CuO_6$ compounds were formed in the Fm-3m symmetry group, and their atomic positions were determined from previous similar studies. It is noteworthy that the high magnetic moments of the variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ are quite distinctive when compared with the previous magnetic properties. In addition, the atomic structures of variant perovskite compounds are as different from the atomic structures of double perovskite compounds as a transition metal and their symmetry. Therefore, changes in magnetic and structural properties can be easily observed by doping these gaps in variant perovskite compounds with different materials. Since the number of atoms is higher compared to perovskite compounds, it can be expected that more contributions to magnetic properties and higher magnetic moments will be obtained on an elemental basis. Therefore, it is possible to mention different properties of variant perovskite compounds compared to perovskite and double perovskite compounds. Since the variant perovskite compounds used in this study have not been studied experimentally or theoretically before, the results cannot be compared. As a result, new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ are suitable materials that can be used in spintronic applications with their structural, electronic, high magnetic, and true half-metallic properties.

## 2. MATERIAL METHOD

The structural, magnetic, and half-metallic calculations of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were performed by WIEN2k computational code [44-46] with the framework FP-LAPW [47] in Generalized Gradient Approximation (GGA-PBE) method [48, 49].

While forming the compounds, Li, Cr/Cu and O atoms were located at 0.25/0.25/0.25, 0/0/0 and 0.233/0/0 points, respectively. Figure 1 showed the structural representations of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$. After constructing the structures in space number of 225 and symmetry group of Fm-3m, the volume-energy optimization calculations were performed for FM and NM phases to compare which phase was energetically more stable. In Figure 1, Li, Cr, Cu, and O atoms are seen. In order to calculate the total energy of the compounds, potential calculations of the atoms were performed separately. These potential calculations of each atom were performed within an imaginary sphere as called Muffin-Tin.

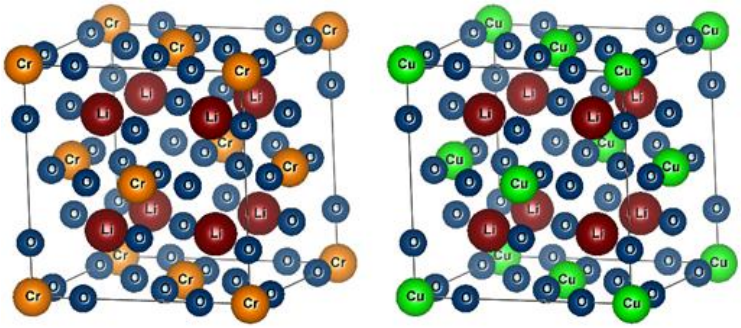


***Figure 1***. *The structural representations of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$. The structures were created in 225 space number*

Therefore, the radii of the atoms and radii of the Muffin-Tin spheres surrounding those atoms must be compatible. If the radius of the MT and the radius of the atom are incompatible, for example, if the radius of the atom is larger than the radius of the MT, potential deficiencies in calculations may be appeared. As a result of this situation, deficiencies in energy values may also occur. MT radii of Li, Cr/Cu and O atoms were selected as 2.10 a.u., 1.61 a.u./1.66 a.u. and 1.46 a.u., respectively. Here, the plane cut-off and smallest of atomic radii values were chosen as 7. The plane-wave expansion cutoff parameter $G_{max}$ was adjusted as 13 $(a.u.)^{-1}$, and cut-off energy value was determined as -6 Ry. The charge convergence parameters were selected as $10^{-4}$ e, and *1728* k-points were chosen in first Brillouin zone to calculate the charge density.

## 3. RESULTS AND DISCUSSION

The initial calculations and ground state values of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were determined with the help of Murnaghan's equation of states [50]

$$E = E_0(V) + \frac{BV}{B'(B'-1)}\left[B\left(1-\frac{V_0}{V}\right)+\left(\frac{V_0}{V}\right)^{B'}-1\right] \quad (1)$$

Figure 2 showed that the FM phases were energetically more stable. Table 1 gave the ground state values obtained in the case of the FM phase.

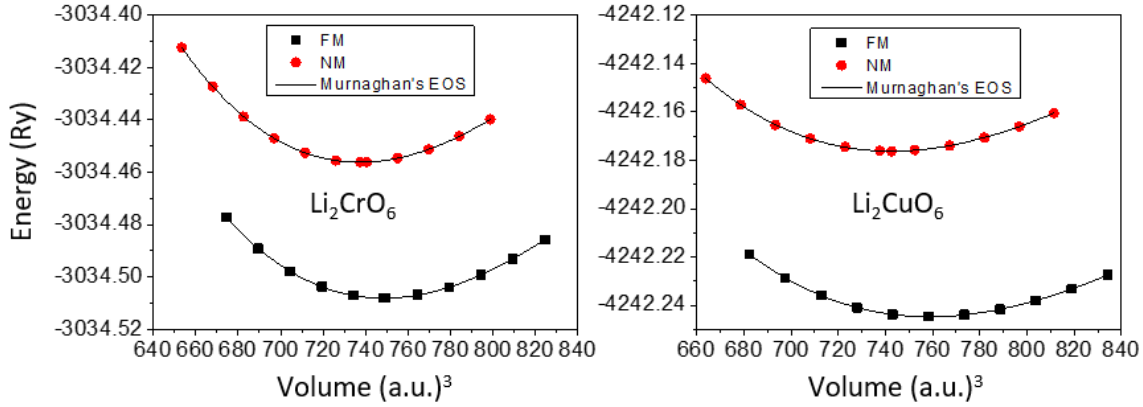


***Figure 2.*** *The FM and NM optimization curves of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$*

***Table 1.*** *The ground state, the spin-up, spin-down electron and polarization values of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$*

| Alloys | Lattice (Å) | Bulk Module (GPa) | B' | Volume $(a.u.)^3$ | $n_\uparrow$ | $n_\downarrow$ | Polarization (%) |
|---|---|---|---|---|---|---|---|
| $Li_2CrO_6$ | 7.63 | 101.89 | 4.43 | 748.587 | 0 | 4.381 | 100 |
| $Li_2CuO_6$ | 7.66 | 80.674 | 4.71 | 758.734 | 0 | 6.009 | 100 |

The transition metals of the compounds in this study were chosen differently. The equilibrium lattice parameters of the structures formed using different transition metals were quite close. Even though the atomic radius of copper is lower than that of chromium, the equilibrium lattice parameter of the cubic $Li_2CuO_6$ structure was obtained larger. Differences in these atomic radii were seen in bulk modules and equilibrium energy values. It is clear from results that $Li_2CrO_6$ compound have higher bulk modulus value than $Li_2CuO_6$ compound due to atomic radius. However, as seen in the Murnaghan's equation of state, the energy value depends on the volume, bulk modulus and its first pressure derivative. Therefore, the energy value was obtained bigger in $Li_2CuO_6$.

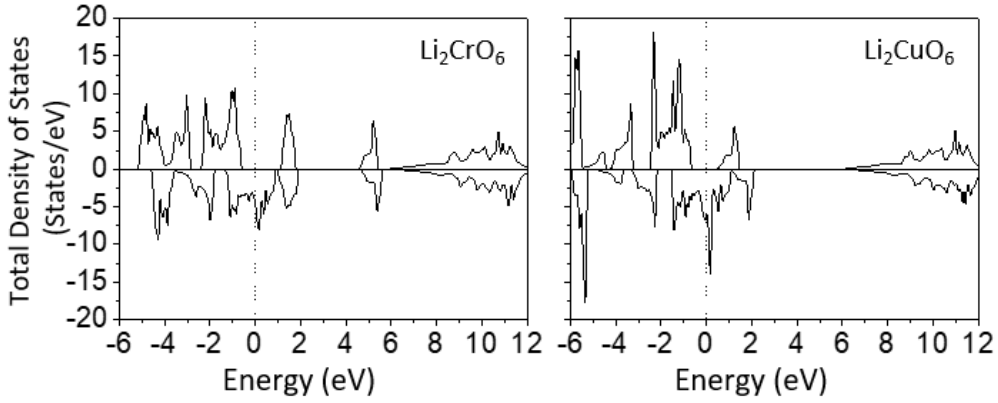


***Figure 3.*** *The obtained total density of states (TDOS) of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$*

The TDOS of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were given in Figure 3 to see the electron density contributions. To compare both compounds more clearly, the y-axis values were chosen with the same values in the range of -20 to +20 States/eV, and to observe all electron contributions, the energy values were arranged in the range of -6 to +12 eV. Positive and negative densities of states, and dotted lines at the zero-energy points represent the spin-up, spin-down states, and Fermi energy levels, respectively. Electron densities give information about the electronic properties of materials. In both compounds, the electron densities in the negative energy region were numerically higher than in the positive energy region. Especially in $Li_2CuO_6$ compound, the electrons distributions are denser than $Li_2CrO_6$ compound, considering the same energy ranges. In both $Li_2CrO_6$ and $Li_2CuO_6$ compounds, as they approach the Fermi energy levels, the spin-up electrons are not found at all in the energy regions close to the Fermi energy level. This means that there are energy gaps between the valence band and conduction band in the spin-up states, and the spin-up states show semiconductor properties. However, electron densities can be easily seen in the Fermi energy level in spin-down states. Intensities that start in the negative energy region can easily pass through the zero-energy region and pass into the positive energy region. This means that in spin-down states, electrons can pass from the valence band to the conduction band without spending any energy, that is, their spin-down states show metallic properties. This both semi-conductor and metallic characters proved that the variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ compounds were true half-metallic ferromagnets. Because this character provides 100% spin polarization, which is the most critical condition of half-metallic materials around the Fermi energy level. Both spin-up and spin-down electron density values and polarization amounts at Fermi energy levels were given in Table 1.

In Figure 4, the partial density of states (PDOS) was given to see the electron contributions to the total densities of states at the atomic level. When the TDOS and PDOS were compared, it can be easily seen that the contributions in the negative energy region and far positive energy regions belong to O and Li atoms, respectively. These contributions came from the p orbitals of Li and O atoms. Although the contributions from the d orbitals of the transition metals Cr and Cu atoms were numerically higher than the other atoms, the contributions around the Fermi energy level were quite small. Although electron densities for metallic characters came from all atoms in spin-down states, it can be said that the contributions from the p orbital of the O atom were greater than the others.

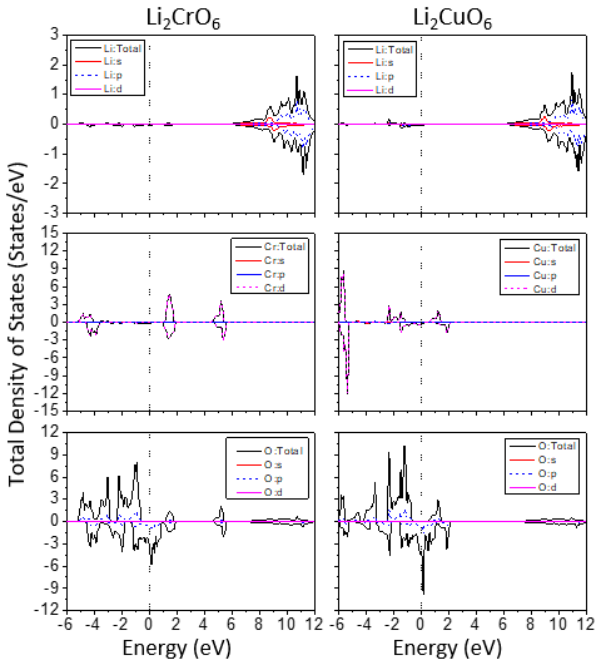


***Figure 4.*** *The PDOS of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ obtained with GGA method*

Interactions around the Fermi energy level were also investigated with the band structures plotted in Figure 5. In the TDOS, it was clearly seen from the band structures that the spin-up states were semiconductor, and the spin-down states were metallic. The band gaps in the spin-up states of variant perovskite compounds appear, while the horizontal dots represented Fermi energy levels. The valence band maximum (VBM) and conduction band minimum (CBM) values of variant perovskite $Li_2CrO_6$ were at Γ-points, while VBM and CBM values of variant perovskite $Li_2CuO_6$ were at Γ and X-points. Therefore, direct and indirect band gaps existed in $Li_2CrO_6$ and $Li_2CuO_6$ compounds, respectively. Here, the VBM values of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were -0.6377 eV and -0.6881 eV, respectively, while the CBM values were 1.1686 eV and 0.4889 eV.

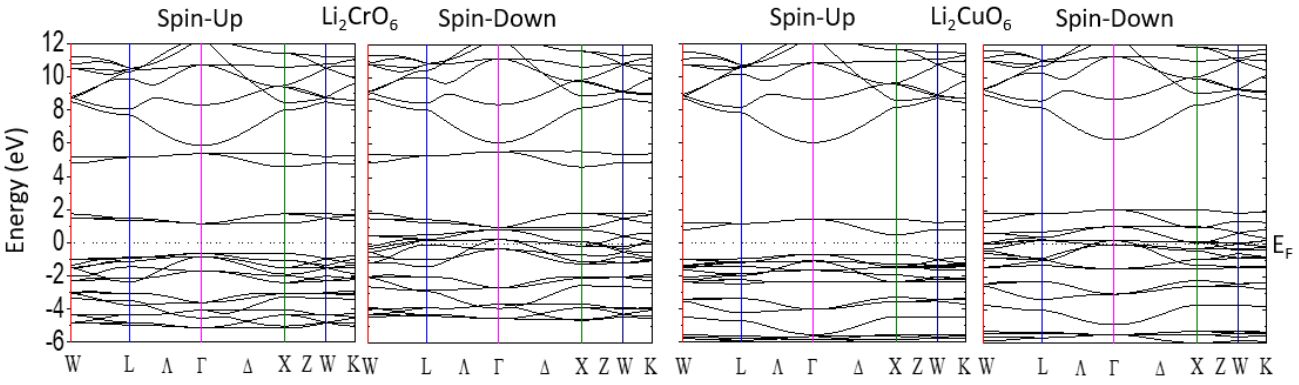


***Figure 5.*** *The spin-up and spin-down electronic band structures of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ obtained with GGA method*

The band gaps of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ obtained as true half-metallic ferromagnetic materials in GGA methods were 1.8063 and 1.1770 eV, respectively, as given in Table 2.

***Table 2.*** *The obtained VBM, CBM and total band gaps of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ for GGA method*

| Alloys | VBM (eV) | CBM (eV) | Gap (eV) |
|---|---|---|---|
| $Li_2CrO_6$ | -0.6377 | 1.1686 | 1.8063 |
| $Li_2CuO_6$ | -0.6881 | 0.4889 | 1.1770 |

The magnetic properties of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were investigated. In Figure 6, magnetic moments, and half-metallic band gap values of $Li_2CrO_6$ and $Li_2CuO_6$ compounds were given.

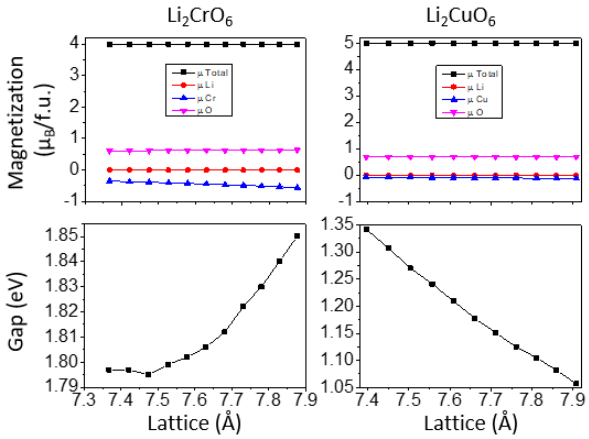


***Figure 6.*** *The obtained total, partial magnetic moments, and half-metallic band gaps of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$*

In the magnetic studies of variant perovskites $Rb_2TaZ_6$ [40], $Cs_2NbI_6$ [41], and $K_2OsX_6$ [42] compounds, the main contributions to the total magnetic moments came from the transition metals. In the total densities of states calculations of these studies, the asymmetric electron distributions between the spin-up and spin-down states of the transition metals can be easily seen. However, in this study, the most contribution to total magnetic moments came from O. This was an expected result. Because when the total electron densities were examined, the most contribution around the Fermi energy level was made from O atoms as numerical values. Also, when the TDOS were carefully examined, the spin-up and spin-down electrons of Li and transition metals of Cr/Cu were almost symmetrical. Therefore, these bonded electrons will cause neutralization and will greatly reduce the magnetic moment values. However, the asymmetries between the spin-up and down electron distributions in O atoms caused the net magnetic contributions to be higher. Therefore, the electronic properties shed light on the accuracy of the magnetic results. Total and partial magnetic moment values of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were given in Table 3.

***Table 3.*** *The obtained total and partial magnetic moments of $Li_2CrO_6$ and $Li_2CuO_6$ compounds*

| Alloys | $M_{Tot}$ ($\mu_B$/f.u.) | $M_{Li}$ ($\mu_B$/f.u.) | $M_{Cr}$ ($\mu_B$/f.u.) | $M_{Cu}$ ($\mu_B$/f.u.) | $M_O$ ($\mu_B$/f.u.) |
|---|---|---|---|---|---|
| $Li_2CrO_6$ | 4.000 | -0.0050 | -0.0447 | - | 0.6197 |
| $Li_2CuO_6$ | 5.000 | -0.0089 | - | -0.1065 | 0.6874 |

According to Figure 6, while half-metallic band gap values increase with increasing lattice parameter in variant perovskite $Li_2CrO_6$, gaps decrease in $Li_2CuO_6$. The band gap values given in Table 2 were for the obtained equilibrium lattice parameters of 7.63 Å and 7.66 Å. Finally, variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ compounds were obtained as true half-metallic ferromagnetic materials with magnetic moments of 4.00 $\mu_B$/f.u. and 5.00 $\mu_B$/f.u., respectively, and showed 100% spin polarizations demonstrated by spin-up electrons.

## 4. CONCLUSION

The density functional theory approaches of new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ compounds were performed by using WIEN2k computational code. First, FM phases were energetically more stable. Therefore, the variant compounds were ferromagnetic materials. Second, the semiconduction properties were seen in spin-up states for both variant perovskites. The compounds were obtained as true half-metallic ferromagnetic materials. Then the band gaps of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were calculated as 1.8063 eV and 1.1770 eV, respectively. Finally, the total magnetic moments of variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ were obtained as 4.00 $\mu_B$/f.u. and 5.00 $\mu_B$/f.u., respectively. The main magnetic contributions belong to O-atoms. Finally, the new variant perovskites $Li_2CrO_6$ and $Li_2CuO_6$ are quite remarkable materials for spintronic applications.

## CONFLICTS OF INTEREST

No conflict of interest was declared by the author.

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