

# Electronic and Structural Properties of $\text{Li}_{1-x}\text{K}_x\text{MgN}$ Half Heusler Alloy

Metin Aslan

Sakarya University, Department of Physics, Esentepe Kampus Serdivan, 54187, Sakarya, TURKEY

Tel.: +90 264 295 6800

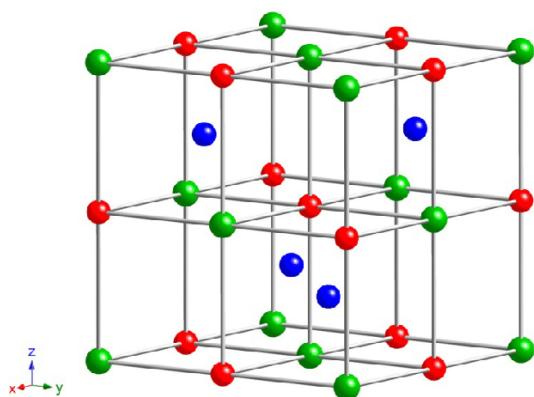
E-mail address: [maslan@sakarya.edu.tr](mailto:maslan@sakarya.edu.tr)

**Abstract:** I have performed the first-principles method to determine the electronic properties of cubic  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  Half-Heusler semiconductor alloy using density functional theory with  $x=0, 0.25, 0.75, 1$ . The exchange and correlation effects are treated using a generalized gradient approach based on Perdew et al. I have used modified Becke-Johnson potential to obtain accurate band gap results. From the electronic band gap calculation, I have found that the direct band gap of the alloy varies from 1, 39 eV to 3, 07 eV. Because of the bandgap range,  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  can be a good candidate for visible and IR optoelectronic applications. From the structural calculation, I have found that the lattice parameter of cubic  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  varies from 4.97 Å to 5.91 Å. This range allows the alloy to grow on many common substrates like Si, GaAs, Ge, InP. Finally, I have also calculated the density of states in order to understand some properties of the materials, such as the band structure, bonding characters, and dielectric functions.

**Keywords:** Half-Heusler, Semiconductors Alloys, Density Functional Theory, Electronic Properties, Structural Properties

## 1. Introduction

The search for materials suitable for changing application areas has been ongoing for many years. Especially in optoelectronics, materials ideal for many application areas has been developed with III-V and II-VI group semiconductors and their alloys. However, the search for the most suitable material still continues. Apart from the III-V and II-VI groups of semiconductors, many kinds of research are carried out on Half-Heusler (HH) compounds whose chemical composition is in the form of XYZ. Where X represents the first group, Y the second group, and Z represents the fifth group element. The Half-Heusler has the composition 1:1:1 and C1b structure, formed by three interpenetrating FCC-lattices as shown in Fig. 1.



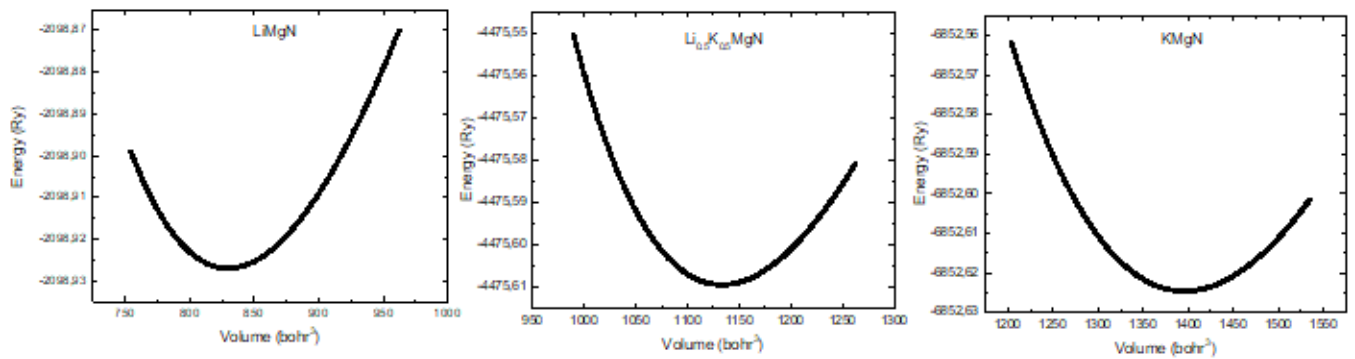
**Fig. 1.** The crystal structure of a typical Half-Heusler compound XYZ.

Half-Heusler alloys have recently shown great promise as thermoelectric materials. They have high power factors as well as resistance to high temperatures. However, the figure

of merit (ZT) of Half-Heusler alloys is restricted by their considerable thermal conductivity [1, 2]. The lattice parameters, band gaps, and dielectric constants of Half-Heusler compounds at different pressure are investigated as new candidates for the optoelectronic devices by Mehnane et al. [3]. The structural, electronic, and optical properties of Half-Heusler compounds are studied on several types using first-principles calculations based on the density functional theory by Kacimi et al. [4]. In this study, I have investigated the electronic and structural properties of  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  ternary and quaternary Half-Heusler alloys with the help of the density functional theory.

## 2. Method of Calculation

In the present work, the first-principles calculation for  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  alloys is performed using the full-potential linearized augmented plane wave (FP-LAPW) [5] method based on density functional theory (DFT) as applied in Wien2K [6] computer package program. The exchange and correlation interactions are taken into account using the generalized gradient approach (GGA) [7] proposed by Wu and Cohen [8]. For the electronic properties, modified Becke-Johnson (mBJ) potential [9] was chosen. This potential is used to improve the band gap obtained by the conventional DFT-based methods. Volume optimization of  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  alloys is performed with symmetry P1 with 8-atom  $1 \times 1 \times 1$  simple cubic supercell. To get the total energy convergence, the Kohn-Sham wave functions are expanded up to  $\text{RMTKmax} = 6$  (RMT is the plane wave radii, and  $\text{Kmax}$  is the maximum reciprocal lattice vector). Partial waves inside atomic spheres have been expanded up to  $\text{lmax} = 10$ .



(a) (b) (c)

Figure 2: Volume Optimization graphs of  $Li_{1-x}K_xMgN$  alloys for a)  $x=0$ , b)  $x=0.5$ , and c)  $x=1$

### 3. Results and Discussions

1	5, 914	56, 1732	----	6.01[13]
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#### 3.1 Structural Properties

In this section, I have presented the structural properties of quaternary alloys  $Li_{1-x}K_xMgN$  for the composition of  $x=0, 0.25, 0.5, 0.75$ , and  $1$ . In order to get the most valid lattice constant, I have made volume optimization processes for cubic  $Li_{1-x}K_xMgN$  alloys. In Fig. 2, I have shown the energy versus volume graph of studied  $Li_{1-x}K_xMgN$  with  $x=0, 0.5$ , and  $1$  as an example on the Birch-Murnaghan equation of state.

The calculated total energies were fitted to the Murnaghan's equation of state [10] in order to obtain the ground-state properties such as equilibrium lattice constant ( $a_0$ ) and bulk modulus ( $B_0$ ). I have summarized the calculated lattice parameter and bulk modulus of  $Li_{1-x}K_xMgN$  alloys with other theoretical and experimental data in Table 1.

Table 1: Calculated the lattice parameters and bulk modulus of  $Li_{1-x}K_xMgN$  with other theoretical and experimental results

x	This Work		Other Works	
	$a_{Wien2k} (A^\circ)$	B (GPa)	$a_{exp.} (A^\circ)$	$a_{theo.} (A^\circ)$
0	4, 9723	101, 8	4, 96 [11]	5.01[12]
0.25	5, 2695	83, 2127	----	----
0.5	5, 5172	71, 0802	----	----
0.75	5, 7311	64, 7666	----	----

The calculated lattice parameter for  $LiMgN$  and  $KMgN$  are found to be  $4.9723$  and  $5.914$ , respectively. The results show that the equilibrium lattice parameter of considered ternary compounds are in excellent agreement with the experimental [11] and other theoretical [12, 13] data. The obtained theoretical result over estimated the experimental lattice parameter by only more than  $0.25\%$ . These results indicate the reliability of the present calculations. As seen from the table, the compressibility denoted by bulk modulus of the studied alloys increased when Li concentration increased as expected. On the other side, the lattice parameter of the unit cell is decreased when Li concentration is increased. The treatment of lattice parameters of quaternary alloys can be defined as a linear combination of the lattice constant of the two forming ternary compounds. Therefore it is assumed that the atoms are located at the ideal lattice sited. The lattice constant varies linearly with composition  $x$  according to the so-called Vegard's Law [14] as shown in Fig. 3. Unfortunately, there is no experimental and theoretical data for  $x=0.25, 0.5$ , and  $0.75$  of  $Li_{1-x}K_xMgN$  alloys. So it is hoped that the obtained results can be used to cover the lack of data in the literature for  $Li_{1-x}K_xMgN$  alloys.

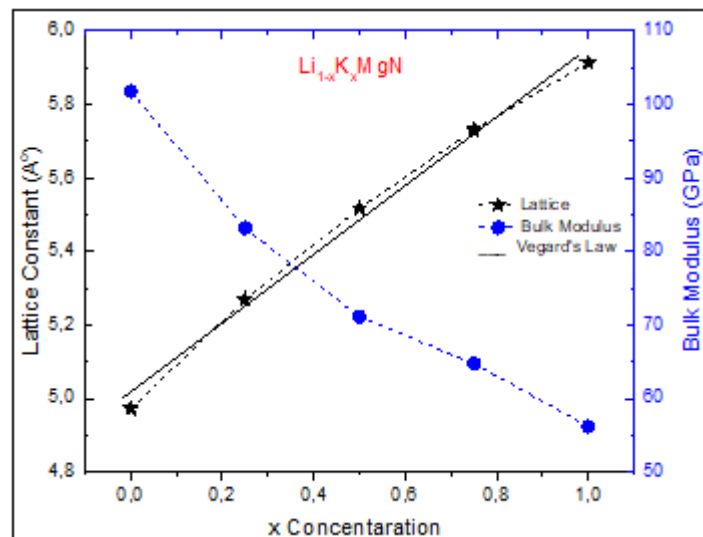


Figure 3: Lattice constant and bulk modulus graph of studied  $Li_{1-x}K_xMgN$  alloys.

### 3.2 Electronic Properties

It is well known that the standard density functional calculation of both GGA and the local density approximation (LDA) [15] underestimates the band gap energy [16, 17] of semiconductors. This underestimation is mainly based on simple model assumptions, which are not sufficiently flexible to accurately reproduce the exchange-correlation energy and its charge space derivative. To overcome this drawback, I have used mBJ approach, which brings the calculated gap close to the measured one. The

electronic band structure of the studied alloys was obtained using the computed lattice constants at the equilibrium. Fig. 4 presents the electronic band structures of the ZB phase of LiMgN and KMgN Half Heusler along with the high symmetry directions. The band structure of  $Li_{1-x}K_xMgN$  ternary semiconductor Half Heusler alloys that are given in Fig. 5 is for  $x=0.25, 0.5,$  and  $0.75$ . Fig. 4 and 5 show that Half Heusler compounds are direct bandgap semiconductors with the minimum conduction band at  $\Gamma$  symmetry point at the center of the Brillouin zone.

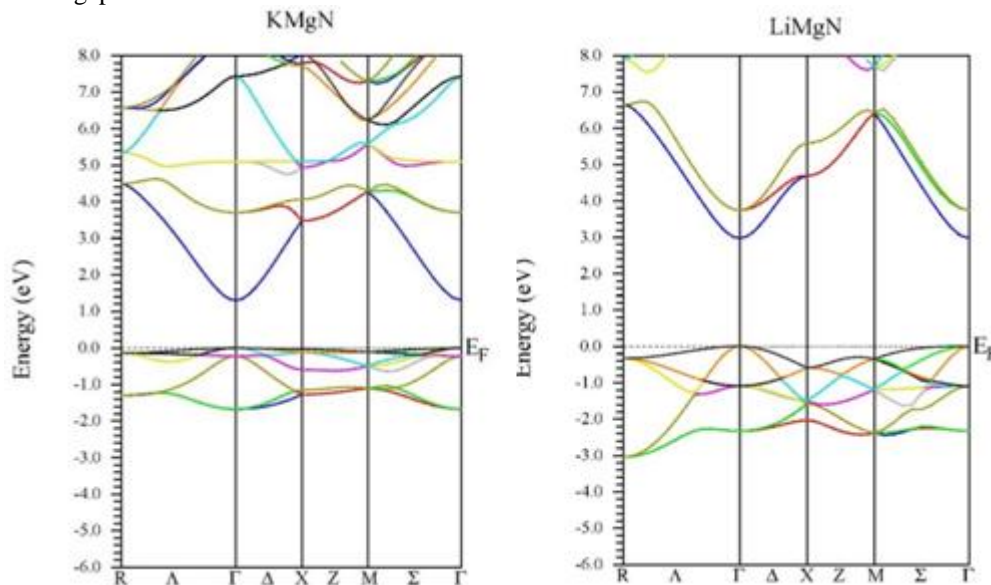


Figure 4: Electronic bandstructure of KMgN and LiMgN. The Fermi level is adjusted as the zero energy level

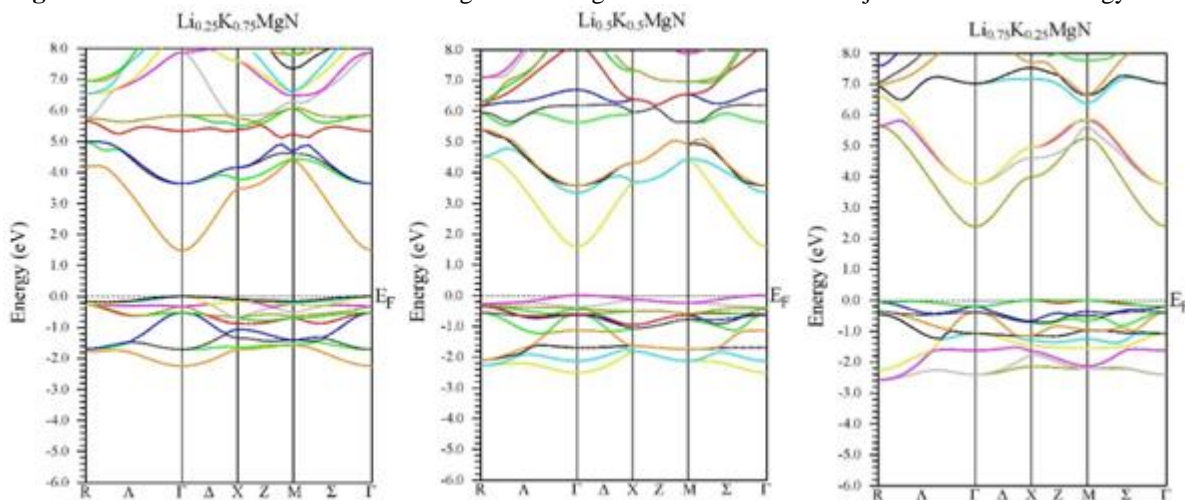


Figure 5: Electronic band structure of  $Li_{0.25}K_{0.75}MgN$ ,  $Li_{0.5}K_{0.5}MgN$  and  $Li_{0.75}K_{0.25}MgN$ . The Fermi level is adjusted as the zero energy level

The calculated band gap energies of  $Li_{1-x}K_xMgN$  alloys are summarized in Table 2. together with other theoretical [18, 19, 20 ] and experimental [11 ] works. The results show that the band gap energy of considered ternary compounds are in excellent agreement with the experimental and other theoretical works. Unfortunately, there is no data for  $x=0.25, 0.5,$  and  $0.75$  of  $Li_{1-x}K_xMgN$  alloys. The band gap energy decreases as the K atom in the alloy increases. The band gap energy value obtained between the range of 3.07 eV and 1.39 eV indicates that these alloys are a good candidate for visible and near IR region applications.

Table 2: Calculated three band gap energy ( $E_g$ ) of  $Li_{1-x}K_xMgN$  with other theoretical and experimental results

x	ThisWork	Other Works	
	$E_g$ (eV)	$E_g$ (eV) exp	$E_g$ (eV) theo
0	3.07	3.23 [21]	3.67 [18]
0.25	2.46	----	----
0.5	1.68	----	----
0.75	1.56	----	----
1	1.39	----	3.44 [19] 1.38 [20]

I have also calculated density of states (DOS) of the alloy presented in Fig. 6 only for  $x=0, 0.5,$  and  $1$  composition to

save some places. It's obvious to see that the Nitrogen (N) atom has a dominant character near the valance band maximum and near the conduction band minimum.

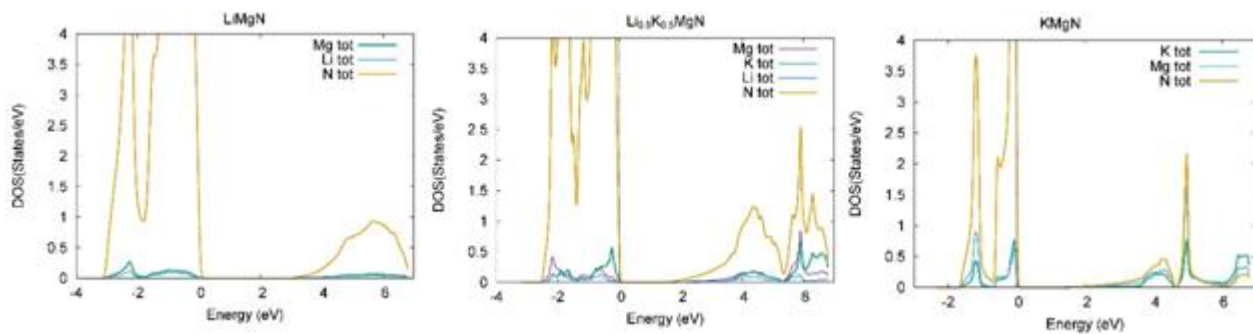


Figure 6: Calculated DOS calculated of  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  for  $x=0, 0.5, \text{ and } 1$ .

#### 4. Conclusions

In conclusion, from the structural calculation, I have found that the lattice parameters of cubic  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  vary from  $4.97 \text{ \AA}$  to  $5.91 \text{ \AA}$ . From the density of states, I investigated that the nitrogen atom has a very dominant effect near the valance band maximum and the conduction band minimum. From The electronic band gap calculation, I have found that the direct band gap of the alloy varies from  $1.39 \text{ eV}$  to  $3.07 \text{ eV}$ .

Because of the bandgap range,  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  can be a good candidate for visible and near IR optoelectronic applications. The most common substrates used world wide for opto electronic applications are Si, GaAs, InP. As seen in Fig. 7, the results I get from structural and electronic calculations allow growing the alloys on many common substrates like Si, GaAs, Ge, InP for optoelectronic applications.

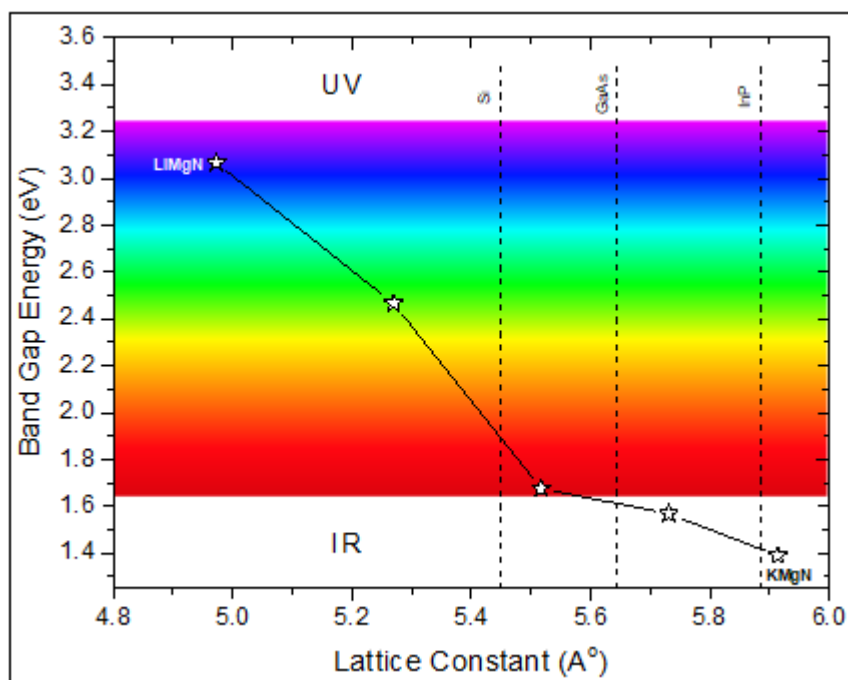


Figure 7: Band gap energy versus lattice constant graph of  $\text{Li}_{1-x}\text{K}_x\text{MgN}$  Half-Heusler semiconductor alloy

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