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First Principal Study of MgCuSb with Different Atomic Arrangements

Vijay
M. Sc (Physics), NET-JRF

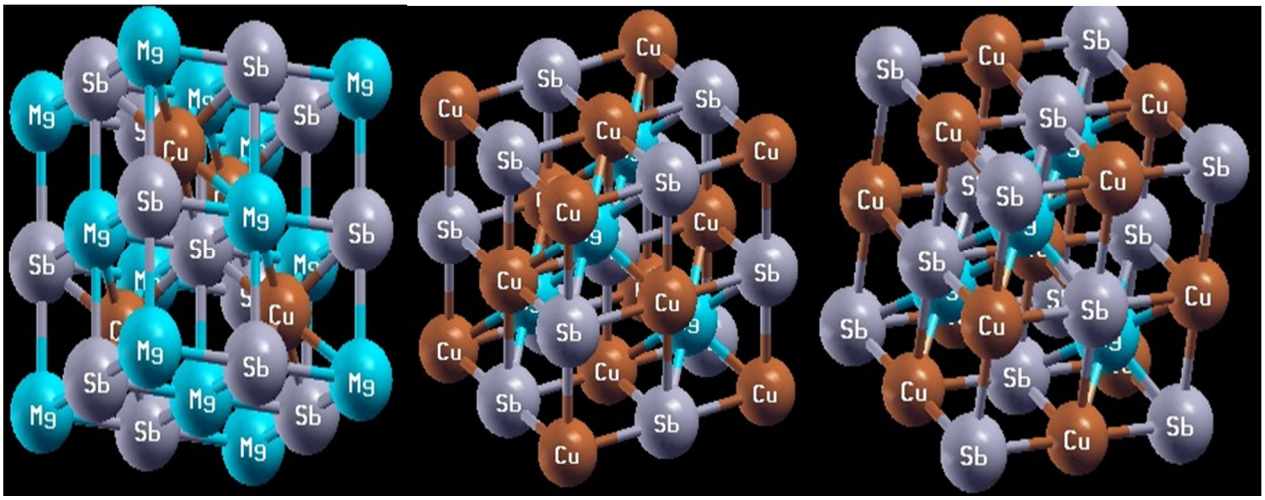
Abstract: ***In this paper we analyze the different structural arrangement of MgCuSb and studied the corresponding band structures and density of states. We predicted that by interchanging atomic positions of all three atoms we can tune the band gap. After studying these properties the compound MgCuSb shows that, it has both metallic and semi metallic nature according to different atomic arrangement that we have studied in this paper. We kept same RMT, number of K-points and Exchange-correlation potential Perdew-Burke-Ernzerh of (PBE) in all the structures. We predicted that out of six possible arrangements only two shows band gap of 0.2 eV.***

Keywords: Band structure, PBE, Exchange Correlation potential, DoS

I. INTRODUCTION

The scientific study of the compound having low energy band gap has latest trends in various technological sectors. These types of compounds has comparatively small band gap as compare to that of silicon at room temperature. The semiconductors with low energy band gap can be used as thermoelectric materials. MgCuSb is a multifunctional compound can have application in nanoscale spin filters and infrared detectors. In this paper we investigated the structural stability, band structure and density of state (DoS) based upon total energy calculation. All the properties and parameters are calculated using Wien2k software. The crystalline structure of MgCuSb is intermixing of rock salt type and Zinc blend type structure with space group 216_F-43m. The structural arrangement of MgCuSb is given in table: 1. The cubic crystal structure of all the six arrangement is shown in fig: 1.

Structure Type	Mg	Cu	Sb	Metallic and Half - metallic
Type 1	(0,0,0)	(0.5,0.5,0.5)	(0.25,0.25,0.25)	Metallic
Type 2	(0,0,0)	(0.25,0.25,0.25)	(0.25,0.25,0.25)	Metallic
Type 3	(0.25,0.25,0.25)	(0.5,0.5,0.5)	(0,0,0)	Metallic
Type 4	(0.25,0.25,0.25)	(0,0,0)	(0.5,0.5,0.5)	Half -metallic
Type 5	(0.5,0.5,0.5)	(0,0,0)	(0.25,0.25,0.25)	Half -metallic
Type 6	(0.5,0.5,0.5)	(0.25,0.25,0.25)	(0,0,0)	Metallic



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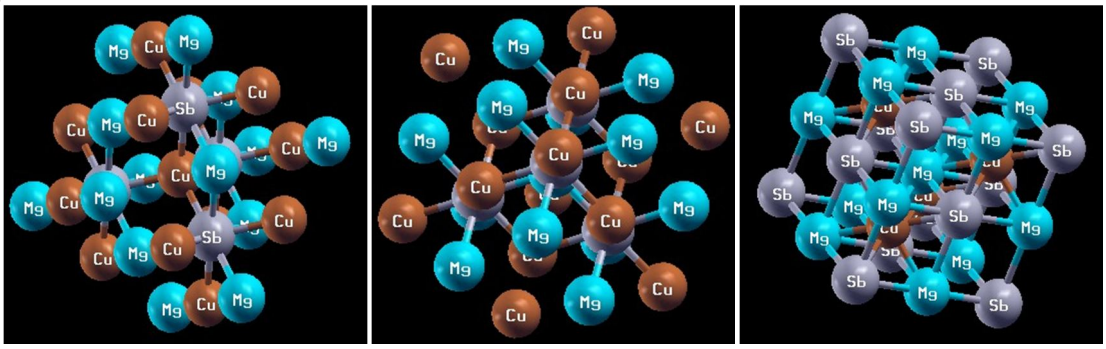


Type: 4 Type: 5 Type: 6

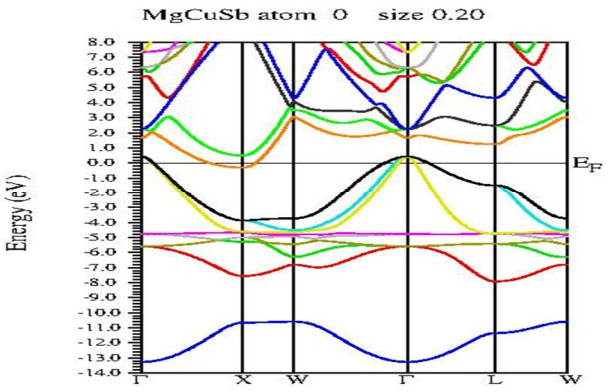
Figure 1: Possible Structural arrangements of MgCuSb under space group F-43m (216)

A. Computational Details

We have used WIEN2k code to simulate given compound. By using density functional theory (DFT) the structural and electronic properties of MgCuSb have been evaluated. To examine the exchange correlation effect Perdew-Burke-Ernzerhof (PBE) in Generalized gradient approximation (GGA) approach is used. The optimized lattice parameter 5.8 A^o is considered. The muffitin radius is taken to be 2 with R-kmax value 7.Energy separation between core and valence electrons is -6.0 Ry. The number of k points in brillouin zone is 1000 for all six type structure whereas for density of state calculation we prepared denser k mesh of about 1500 k-points.

B. Result

After optimization the calculated band structure diagram of all possible arrangements shows that out of six only two shows a narrow band gap of 0.2 eV, which is similar for two structures. The band structure and density of states plots for all structures are shown in figure: 2 and figure: 3, respectively.



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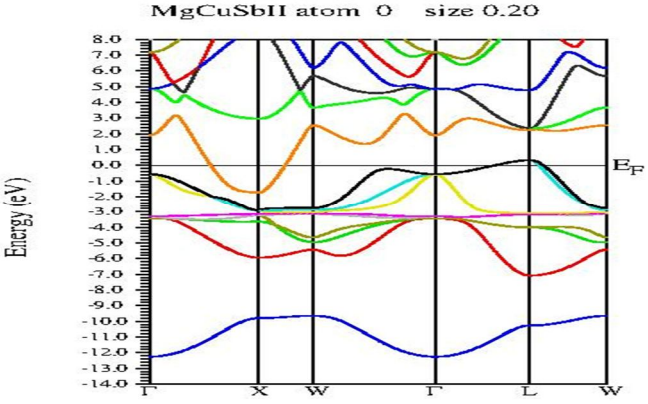

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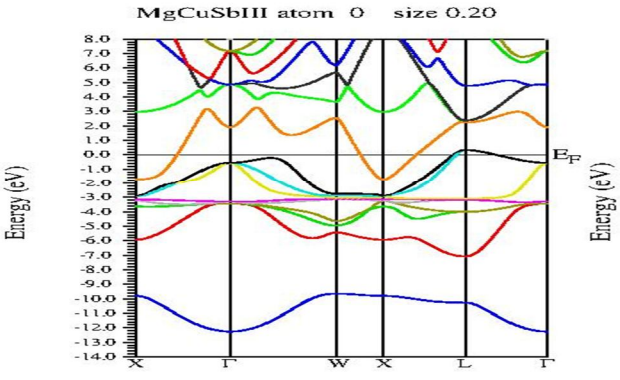

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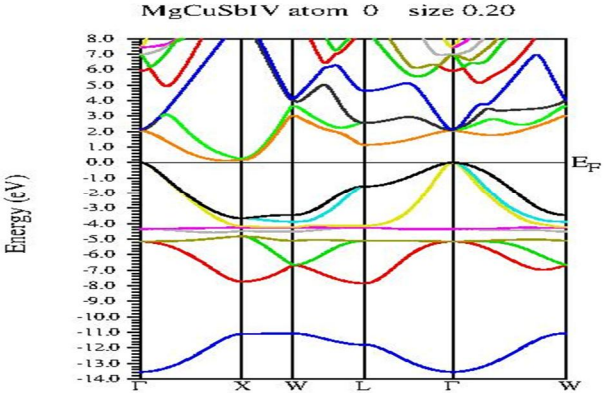

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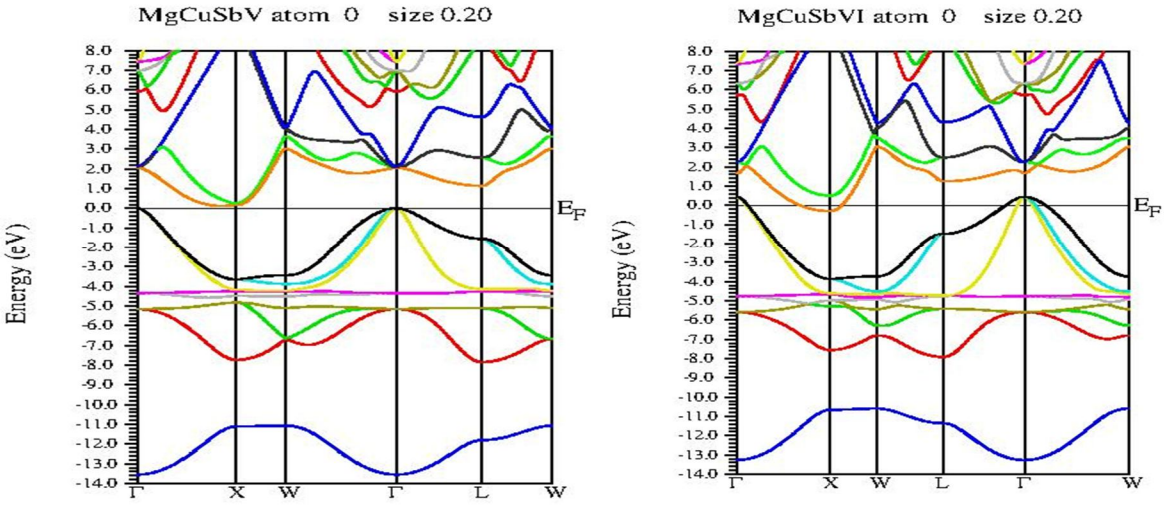

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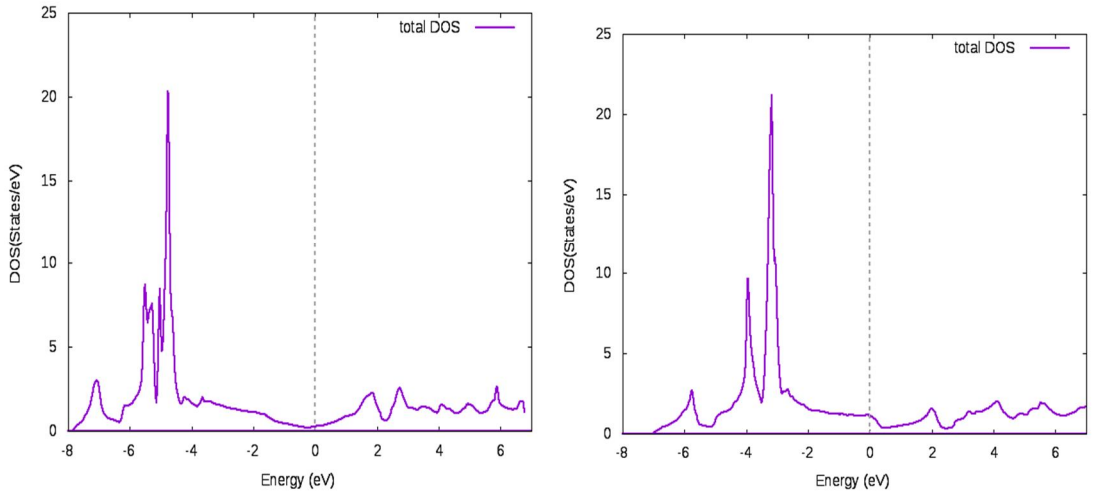
Figure 2: Band Structure diagrams of studied atomic arrangements.

It has been seen from Density of States (DoS) plots that the contributions to total DOS were from Mg-d & Sb-6p electron states.



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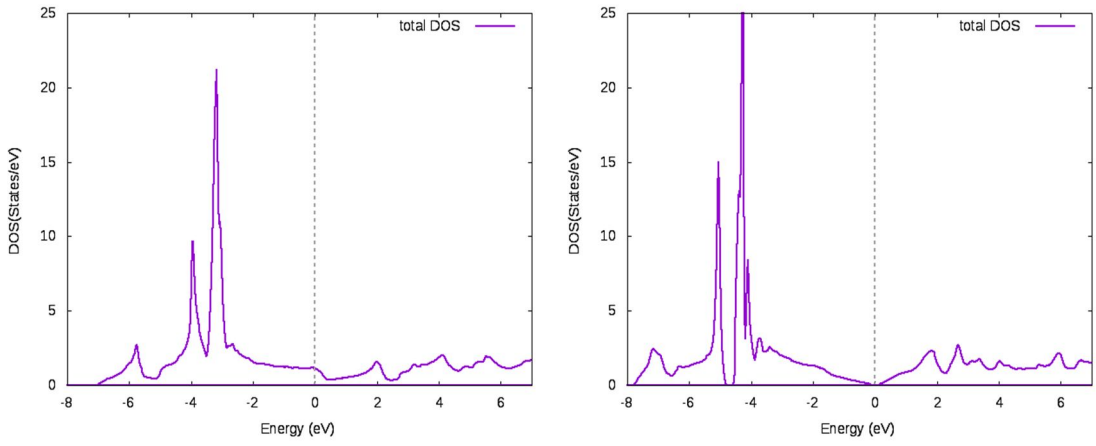

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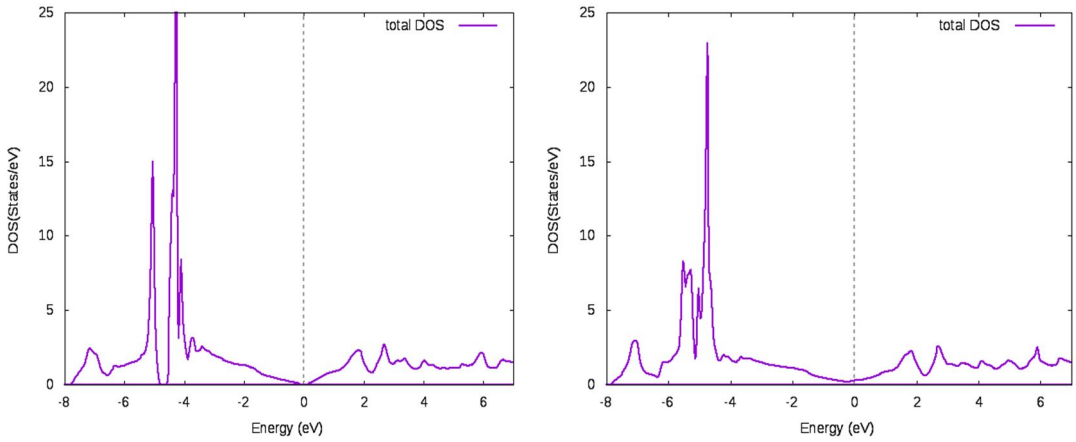

Type: 5 Type: 6

Figure 3: DoS plots of MgCuSb for different atomic positions.

II. CONCLUSION

The band structructure of two states having same band gap can be considered as equivalent. MgCuSb has 18 valence electrons in its outermost shell because of which type 4 and 5 shows an band gap of approx 0.2eV. Generally compounds having ABX type structure where A & B belongs to transition metal atoms whereas X represent p- block elements with 18 valence electrons shows semiconducting behavior in a particular atomic arrangement. With this narrow band gap this alloy can be used in many applications like thermoelectric devices, I.R detectors etc.

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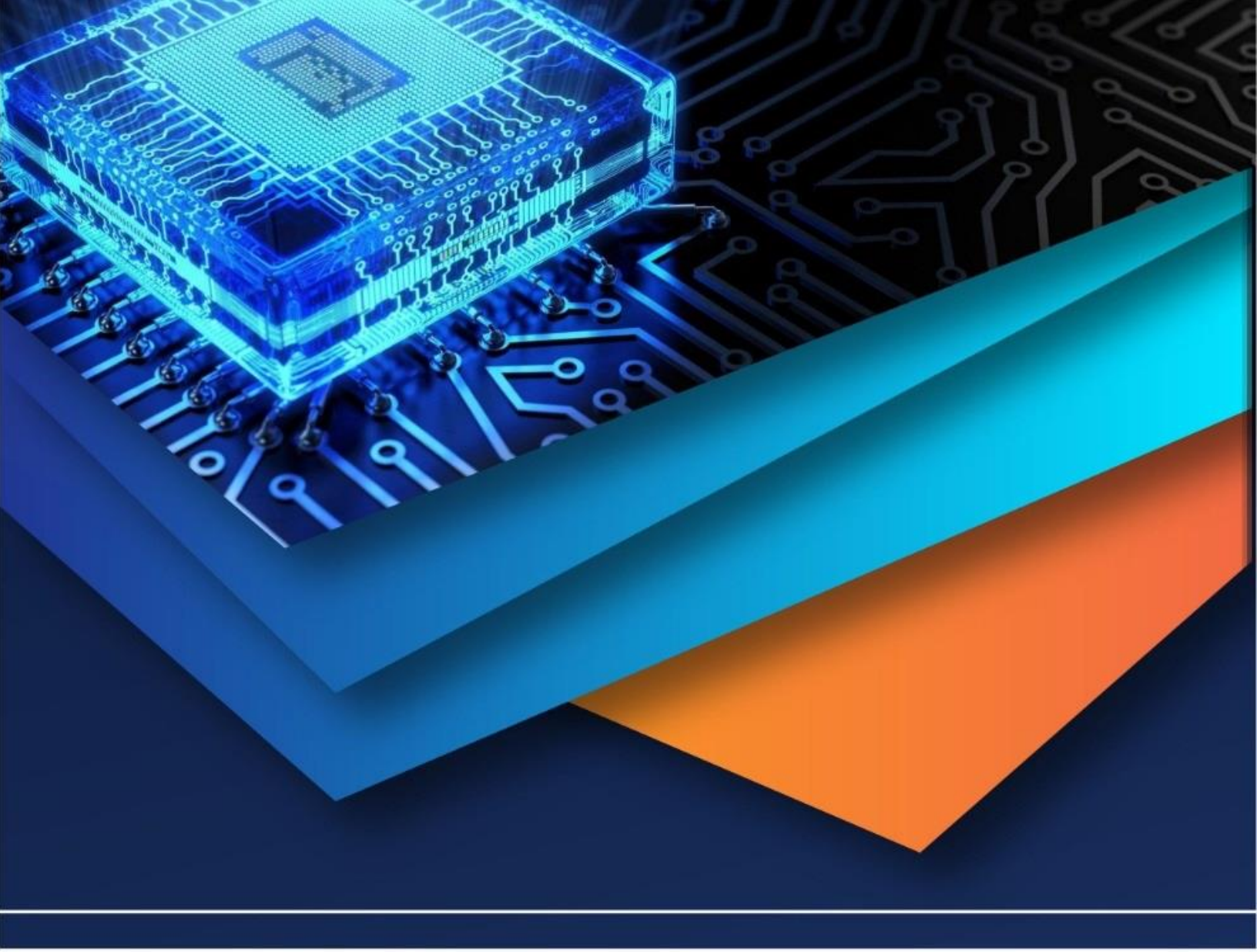

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