First Principle Study of ScAgC

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Abstract

Half-Heusler compounds have unusual behavior because of metallic as well as semi-metallic nature. These compounds have XYZ nomenclature where two of three atoms belong from transition metal atom and one from p-block. We have done first principle study of ScAgC by rearranging atomic position. The optimized lattice parameter of ScAgC is found to be 4.9Å. The numbers of K-points are 1000 with RMT value 2 under PBE parameterization. It has been observed that out of three structural arrangement only one show half-metallic natures. That can be used in semiconducting application.

KEYWORDS

Half-heusler, semiconductor, thermoelectric, solar cell, spin polarization.

INTRODUCTION

Half-heusler compounds are the impressive class of materials with a huge potential for different applications. We present first principle study of Density Functional Theory based (DFT) calculations of the electronic and band structure of ScAgC [1]. We made an structural analysis of given compound by interchanging their atomic arrangements using Wien2k platform. This compound contains 18 valance electrons making semi metallic in nature [2]. This compound has unique property of spin polarization. Due to the unique property of this compound it can be used in solar applications. ScAgC compound is used in thermoelectric devices because of good conversion efficiency parameter (ZN) [3]. Their band gaps can readily be tuned by adding the impurity into the compound.

COMPUTATIONAL DETAILS

We perform the structural analysis of compound (ScAgC) by inter changing the atomic position using wien2K software. The space group number for this structure 216 F-43m is predicted by wien2k. The value of muffin-tin radius is 2 with 1000 k-points in full Brillouin zone. The energy convergence criteria are $0.0001Ry_0$. The exchange correlation potential treatment is done by generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof (PBE). We observe XYZ type atomic positioning of compound ScAgC as shown in figure1.

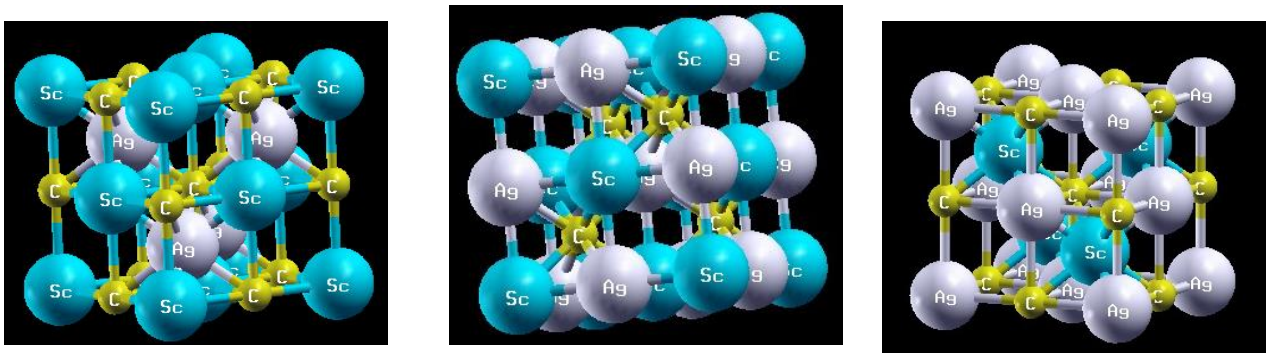


Figure 1.XYZ type atomic positioning of compound ScAgC.

Type-1 Sc at (0, 0, 0), C at (0.5, 0.5, 0.5), and Ag at (0.25, 0.25, 0.25)

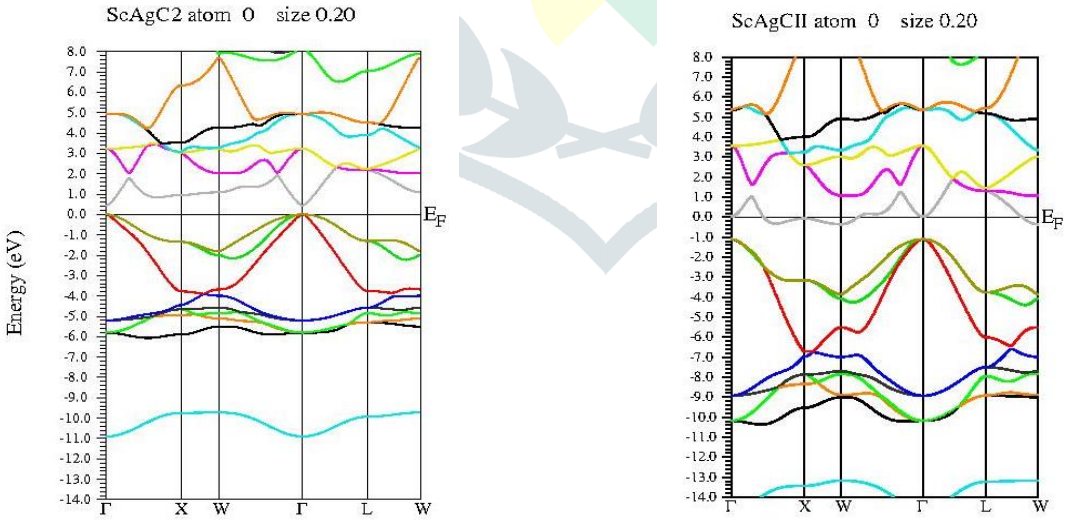
Type-2 Sc at (0, 0, 0), C at (0.25, 0.25, 0.25), and Ag at (0.5, 0.5, 0.5)

Type-3 Sc at (0.25, 0.25, 0.25), C at (o.5, 0.5, 0.5), and Ag at (0, 0, 0)

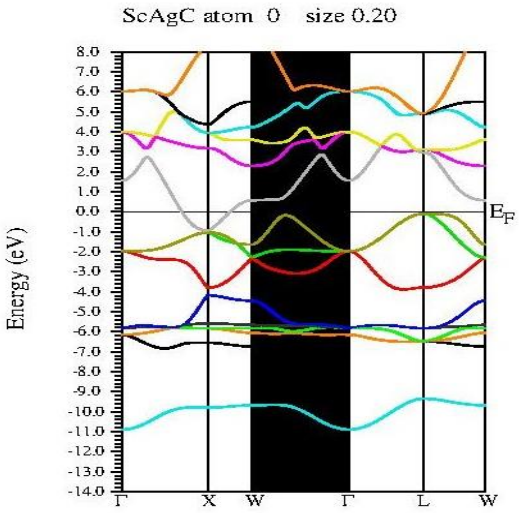
Result and Discussion

The band structures of all three types of structure are studied.

Only Type-I shows half metallic nature with a band gap of about 0.6eV but Type-III shows conducting behavior as compared to Type-II. The entire Band structure diagrams are plotted below:



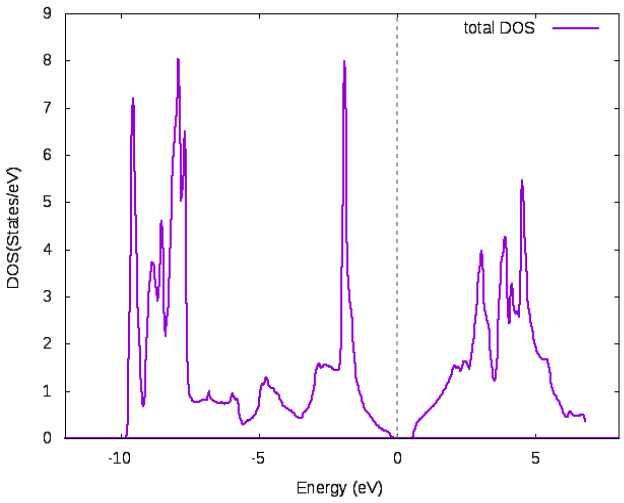
Type-I Type-II



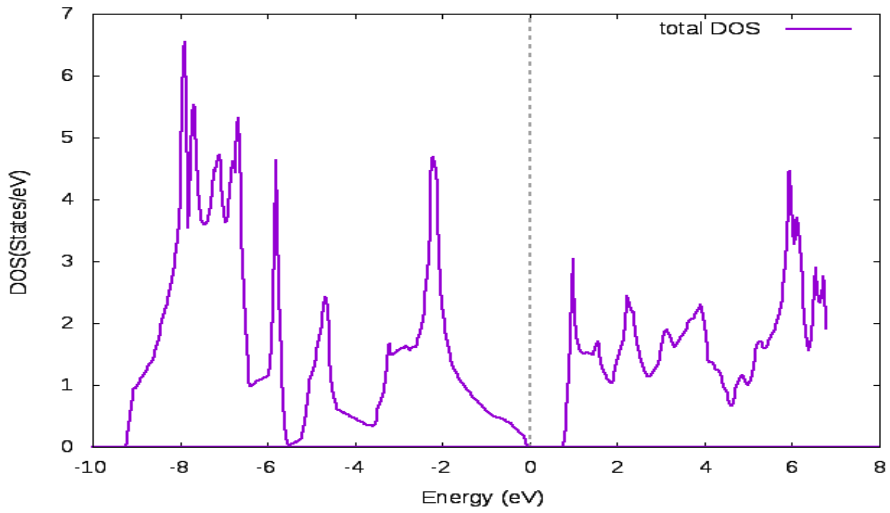
Type-III

The contribution of different electronic states can be shown by Density of state. Thus, we observe the Density of state (DOS) which are given below:

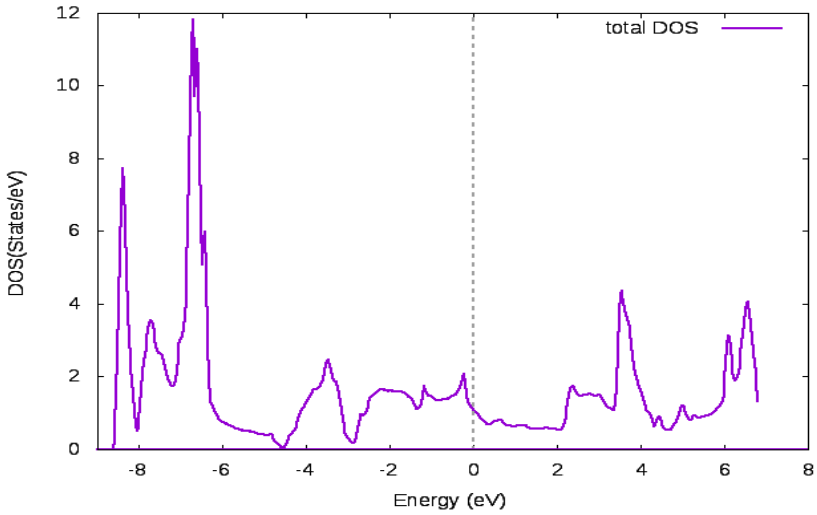
In Type-I the Sc d-state has greater contribution and the highest peak of total Density of state of Sc is observed at (-2eV) but in Type-II the highest peak of Sc is observed at (-8eV) while in Type-III peak is observed nearly at (-7eV) and Ag d-state has also greater contribution.



Type-I



Type-II



Type-III

CONCLUSION

We conclude that the alloy ScAgC has semiconducting behavior in Type-1. This can use in solar cell application because of its tunable band gap by mixing appropriate impurity. This compound will also be used in thermoelectric converters for power generation. The observed density of state is high due d-state of Sc and Ag. A high DOS at a specific energy level means that there are many states available for occupation.

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REFERENCES

[1] Felser C, Fecher G H and Balke B 2007 Angew. Chem. Int. Ed. **46 668-99**

[2] Juza R and Hund F 1946 Naturwissenschaften **33 121**

[3] Shutoh N and Sakurada S 2005 J. Alloys Compounds **38 204-8**