Theoretical Study of the Structural Electronic Properties of half-Heusler RbInSn Alloy

Kara Ilham[1*], Mostefa Zahira[2] and Mahi fattima[2]

[1] Department of Physics, University of Oran1 Ahmed Ben Bella, theorical and simulation laboratory of materials

[2] Department of Physics, University Abd Hamid ben badis, Mostaganem, Laboratoire de Structure, Elaboration et Applicationdes Matériaux

*Corresponding author

Introduction

The aim of the searchers is to find multifunctional materials which combine many physical properties in order to assure a various technological functionality. All these characteristics can be found in half-Heusler with topological behavior [1]. We frequently concentrate on investigating the properties of previously reported compound RbInSn [2].

Experimental/Theoretical Study

Here we present ab initio study of RbInSn half Heusler alloy with 8-valence electrons in the quest to discover its thermoelectric skills. We use the full-potential linearised augmented plane-wave (LAPW) method, implemented in the WIEN2K code and the GGA exchange correlation functional including the spin orbit coupling (SOC) effect to predict its structural and electronic properties.

Results and Discussion

Our results show that this compound exhibit a topological behaviour signed by the inversion between the states s and p. The stability of our compound is confirmed by computing phonon dispersion and mechanical calculations. After having performing the elastic constants (Cij) we theoretically calculate the lattice thermal conductivity Kl its absolute value decreases rapidly with increasing temperature and reached 0.14 W/m°K at 1200 °K.

Conclusion

Our finding can be useful for tuning thermoelectricdevices.

Acknowledgments

Authors can acknowledge any person, or funding agencythat has made a significant contribution to the work.

References

1. Feng. W, Xiao. D, Zhang. D and Yao. Y, “Half-Heusler topological insulator: A first-principales study with the Tran-Blaha modified Becke- Johnson density functional,” Physical Review 2010 B 82, 235121.
2. Zhang. X.M, Xu. X.G, Du. Y, Liu. E. K, Liu. Z. Y and Wang. W. H, “A new class of topological insulators from I-II-IV half-Heusler compounds with strong band inversion strength,” Journal of Applied Physics, 2014 .115, 083704.
3. Feng. W, Xiao. D, Zhang. D and Yao. Y, “Half-Heusler topological insulator: A first-principales study with the Tran-Blaha modified Becke- Johnson density functional,” Physical Review 2010 B 82, 235121.

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5