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Ab-initio Investigation of Structural, Electronic and Topological Properties of Half- Heusler Compounds: TiRhz (Z=Sb,Bi).

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Introduction

Topological insulator (TI) is a new class of materials discovered recently, which has a insulating gap in thebulk and metallic surface states [1]. In recent years, TIs have generated a great interest in view of their great potential technological for spintronic and quantum computing applications [1,2]. Currently, the search for TIs isextended to the Heusler family [3,4] due to their various interesting physical properties such as magnetism, spintronics, superconductivity, half-metallicity and thermoelectricity. In this work, we have investigated the structural, electronic and topological properties of half- Heusler compounds TiRhZ(Z=Sb,Bi) in order to discuss the topological band structure behavior.

Computational Details

In this study, we perform our calculations using FP- LAPW method implemented in Elk code [5] with the exchange and correlation energy of GGA-PBE. Spin-orbit coupling is essential for calculating the electronic band structure, is included in our calculations by second- variational procedure. The SCF calculations is achieved by demanding the convergence of the total energy is smaller than 10^{-6} eV.

Results and Discussion

Structural Optimization

Generally, the half-Heusler compounds crystallize in a face-centered cubic (cfc) with space group F43m (no.216). There are three different configuration: α-phase,ϐi- phase and γ- phase. According to Gautier et al.[6], α-phase is more stable.

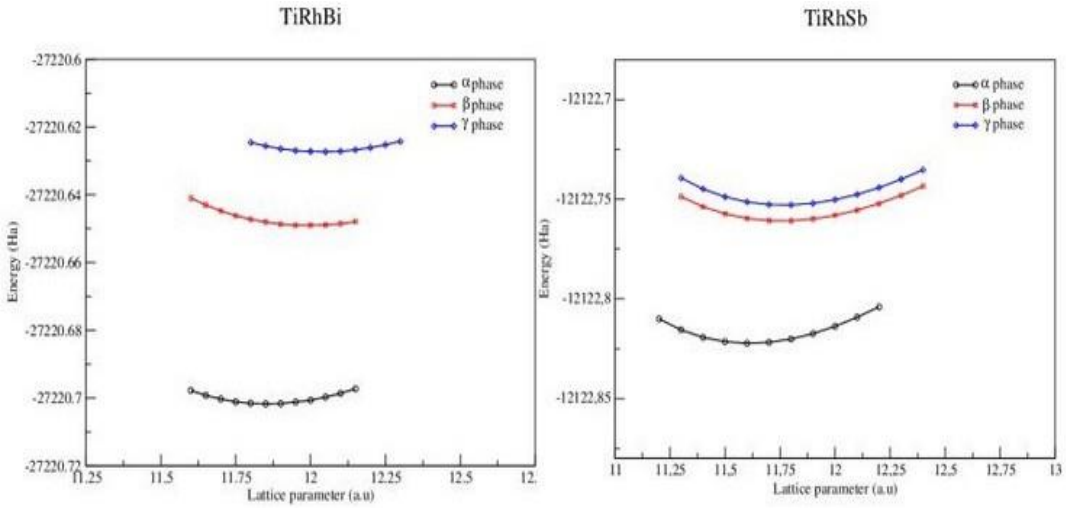

Figure 1: Structural optimization of half-Heuslercompounds TiRhBi and TiRhSb in three configurations.

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Table 1: Parameters optimization of stable phase; i.e; α-phase.

Compounds	a_0 (A)	E (Ha)	B_0(GPa)	B_0'
TiRhSb	6.143	-12122.822	142.879	4.811
TiRhBi	6.273	-27220.701	123.628	4.791

ELECTRONIC AND TOPOLOGICAL PROPERTIES

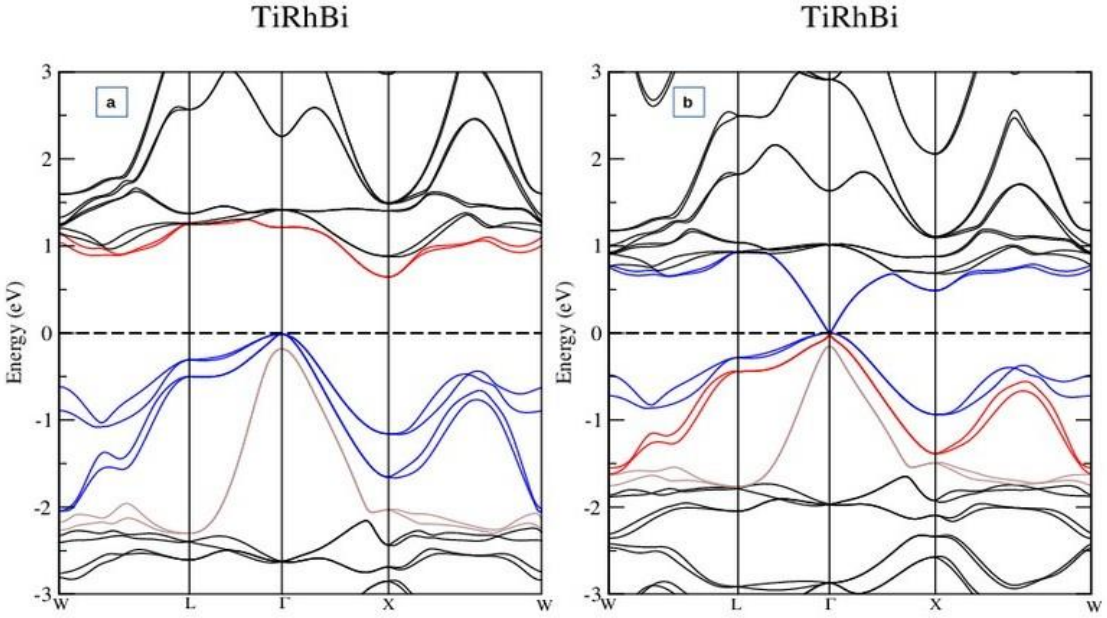

Figure 2: Band structure of TiRhBi, (a) at equilibrium lattice parameter and (b) with hydrostatic strain in order to find a topological semimetal.

Conclusion

In this work, we have study the topological band structure of new half-Heusler and we summarize in few points:

- Our half-Heusler compounds TiRhZ are more stable in α-phase and we have a good agreement with others results.
- The two compounds are trivial semiconductors withindirect band gap, that means they used in severalapplications.
- In this study, we have confirmed that the band topology is sensitive with lattice parameter that made us apply a hydrostatic strain to find a new topological material with inverted band structure[7].

Acknowledgments

Part of the calculations were conducted on ENPO UCI Al- Farabi Supercomputer

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