Spin-Orbit Coupling's Effect on the Electronic Properties of Heavy Elements-Based Compounds

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Abstract. The topological insulating is the topic studied in the last days, these compounds have a lot of properties as electronics, optics and till superconducting, among compounds that will be a topological insulating or topological semimetals are: the semi-Heuslers that contain heavy elements of general formula XYZ, this study was about one of them is: ScPdBi. We studied its structural properties to investigate its crystallographic phase: ferromagnetic (FM) or anti-ferromagnetic (AFM), we found that it is an AFM compound and we classified its structural properties parameters. After that, we studied its electronic properties (band structure and DOS) without spin-orbit coupling (SOC) where we found that this compound has a metallic character. Finally, we applied the SOC where we found different results according the electronic properties where the inversion band appeared so the topological non-trivial nature appeared; this compound is from the most important candidate for the superconducting applications found by an external effect about it as hydrostatic pressure. The calculations were by the first principle based in DFT implemented in ELK code; the exchange potential calculated by general gradient approximation (GGA).

Keywords: Heavy fermions · Topological insulating · Semi-Heuslers · Spin-orbit coupling

1 Introduction

The spin-orbit coupling (SOC) [1] effect is more important because give us a different characters specially in electronic properties as we will show in this work, our study was about one of the important compounds in industry and intelligent materials actually [2, 3], that is the heavy elements compounds that can be appeared as a semi-Heusler compound of general formula XYZ, in this work we studied the structural properties of one of these compounds: ScPdBi and we will show its crystallographic phase if it is a ferromagnetic or anti-ferromagnetic, then we did an electronic calculations: band structure and DOS without SOC for compare with those are with and the appearance of topological insulating (Ti) character [4, 5]. Finally; we applied the SOC where we showed a different character according the band structure, the DOS confirmed the result. We used the first principle based by the density functional theory (DFT) [6] with general gradient approximation (GGA) [7, 8] implemented in ELK code. Our results are compatible with literature.

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Finally, we can confirm after interpreting results found that the effect of spin-orbit coupling is more important to specify a topological insulating character of heavy fermion-based compounds that it is a good candidate for the superconducting applications. We did the spin-orbit coupling because our compound has heavy atoms that have a grand electronic correlation.

2 Compound Studied

2.1 Details

The compounds studied is ScPdBi, it is a semi-Heuslers compound, with space group 216 (P $\overline{4}$3m) (Fig. 1).

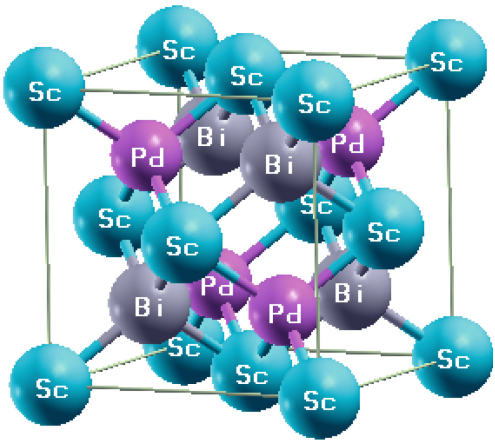


Fig. 1. ScPdBi mesh.

2.2 Calculations Methods

The study was carried out by a first principle calculation based on the density functional theory (DFT) implemented in the ELK code, and using the linear potential augmented linear waveform method (FP- LAPW). The exchange and correlation potential is processed by the generalized gradient approximation (GGA).

3 Results and Discussion

3.1 Structural Properties

We made many calculations about different mesh parameter in the both phases: ferromagnetic (FM) and anti-ferromagnetic (AFM), then we plotted the volume-energy

curve (Fig. 2), where we find that the most stable phase is AFM; so it is AFM compounds. The structural properties parameters are is Table 1.

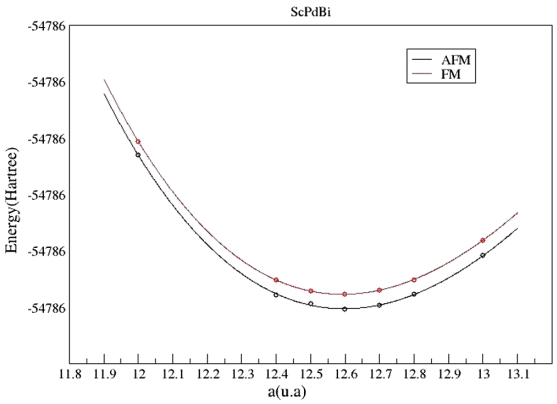


Fig. 2. Volume-Energy curve of ScPdBi

Table 1. Structural properties parameters of ScPdBi

Compounds	A(A°)	B_0(GPa)	B'_0
ScPdBi AFM	6,664	66,914	4,452

3.2 Electronic Properties

We calculated the band structure and DOS for the AFM compounds without Spin-Orbit Coupling, we found that ScBiPd AFM has a metallic character; where the spin up (a) and spin down (b) of band structure (Fig. 3) are the same.

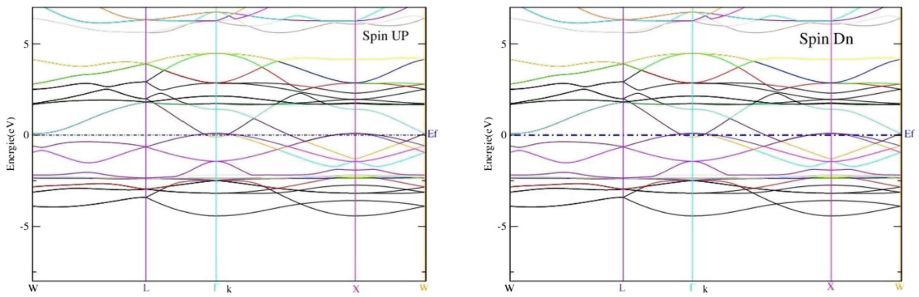


Fig. 3. Band structure (a): spin Up, (b): spin Dn of ScPdBi

The results found by band structure are confirmed by TDOS (Fig. 4), where we show that is the same character in spin Up and spin Dn because the compound is antiferromagnetic.

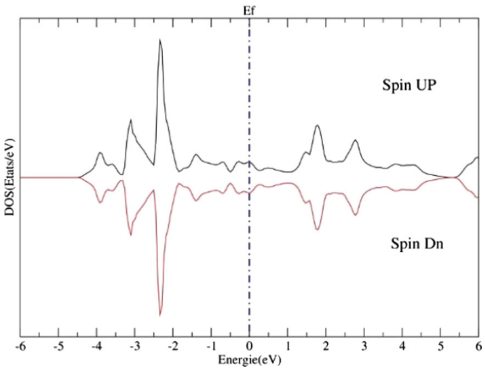
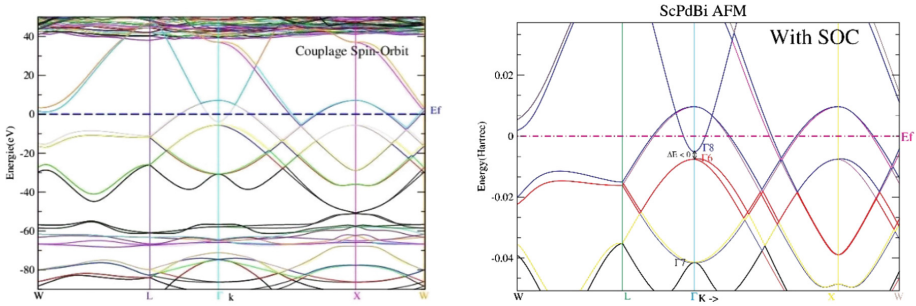


Fig. 4. Total DOS (spin (Up and Dn)) of ScPdBi

3.3 Spin-Orbit Coupling Effect

We did the same study about ScPdBi previous but we aplied the SOC, so we found that the topological nature appeared in band structure (Fig. 5) as a topological non-trivial with $\Delta E = E(\Gamma 6) - E(\Gamma 8) = -0.21$ eV (Fig. 5b). As we show that is a band inversion and states surface because the spin Up and spin Dn of band here gave different results; so this compound can be as topological insulating or topological semimetal.



(a) (b)

Fig. 5. Band structure (spin (Up and Dn)) with SOC of ScPdBi, (a): general band structure, (b) specify band structure of Γ states: Γ8 in blue, Γ6 in red and Γ7 in black.

The previous results found by band structure are confirmed by the TDOS with a spin-orbit coupling (SOC) where we show that in spin Up and spin Dn of TDOS aren't the same but there is a band inversion appeared (Fig. 6).

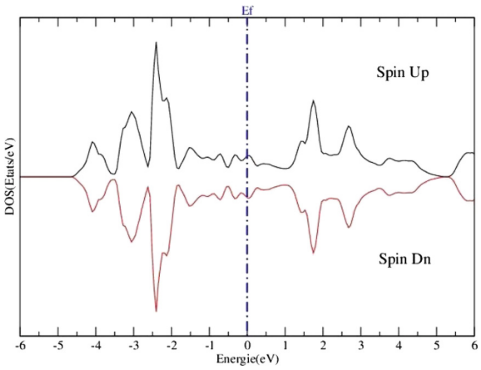


Fig. 6. Total DOS (spin (Up and Dn)) with SOC of ScPdBi

4 Conclusion

The study of structural stability has shown us that this compound is antiferromagnetic. We then adjusted the mesh parameter variation curve as a function of energy by a Murnaghan state equation [9], which allowed us to calculate the mesh parameter of this compound. Our results found are in good agreement with the literature.

The study of the electronic properties shows us that this material is as topological insulating or topological semimetal compound with a topological nature non-trivial appeared by SOC effect that give us a supply fuel to investigate the band structure. Under the effect of hydrostatic pressure and therefore a good candidate for superconducting applications [10].

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