Half-metallicity in Rhodium doped Chromium Phosphide: An ab-initio study

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Abstract

By the theoretical approach using full potential linearized augmented plane wave (FP-LAPW) method, the electronic and half-metallic properties of CrP doped with Rh are investigated by the electronic band structure calculations. CrP at its equilibrium lattice constant of 5.35 Å is observed to exhibit conducting characteristics in the undoped state. CrP exhibits metallic character due to the crossing of the electronic bands at the Fermi level (E_F). Doping Rh in the supercell of Cr_8P_8 in 12.5% doping concentration, the compound $Cr_{0.875}PRh_{0.125}$ is formed. The compound $Cr_{0.875}PRh_{0.125}$ is predicted to exhibit half-metallicity in the minority spin channel. It is observed that $Cr_{0.875}PRh_{0.125}$ exhibits 100% spin polarization at the E_F.

Keywords: ***First principle calculations; DFT; Electronic properties; Half-metallicity.***

1. Introduction

By utilizing the spin of an electron other than its charge characteristic, the field of technology has been revolutionized by the crafting of multi-functional devices. Groot et al first predicted the half-metallicity in Heusler alloys in 1983 [1,2]. At the Fermi level (E_F), half-metals have an energy band gap in one of the spin channels exhibiting semiconducting properties whereas in the other spin channel they exhibit conducting properties. The half metals are used in the field of spintronics. This property makes them potential candidates to be used in high-tech electronic devices, basic computer units, data storage devices and to enhance the efficiency of the devices [3-5]. Half-metallic ferromagnetism (HMF) has been predicted theoretically in oxides of some transition metals like CrO_3,Fe_3O_4 [6,7], dilute magnetic semiconductors [DMS] [8], Full Heusler and Half Heusler alloys [9,10].

Transition metal pnictides are a class of compounds that are known to exhibit half-metallic ferromagnetism (HMF). Galanikis et al. studied binary transition metal pnictides and reported half-metallicity in the compounds [11]. Zhang *et al*. studied various transition metal pnictides and predicted CrBi to exhibit HMF [12]. A small spin polarization was predicted by Shirai *et al*. in CrP at its Fermi level (E_F) [13]. The studies done so far predict CrP to be a conductor at its equilibrium lattice constant of 5.35 Å [14, 15]. To study the effect of doping, Rh in 12.5% doping concentration is added as an impurity in Cr_8P_8 supercell formed at its equilibrium lattice constant. The compound $Cr_{0.875}PRh_{0.125}$ is predicted to exhibit half-metallicity due to the shifting of the bands at the E_F in the minority spin channel.

The work done in the paper is formulated as follows. Section 2 describes the methodology of the calculations. Section 3 presents volume optimization and electronic properties. The conclusion is reported in Section 4.

2. Methods of Calculation

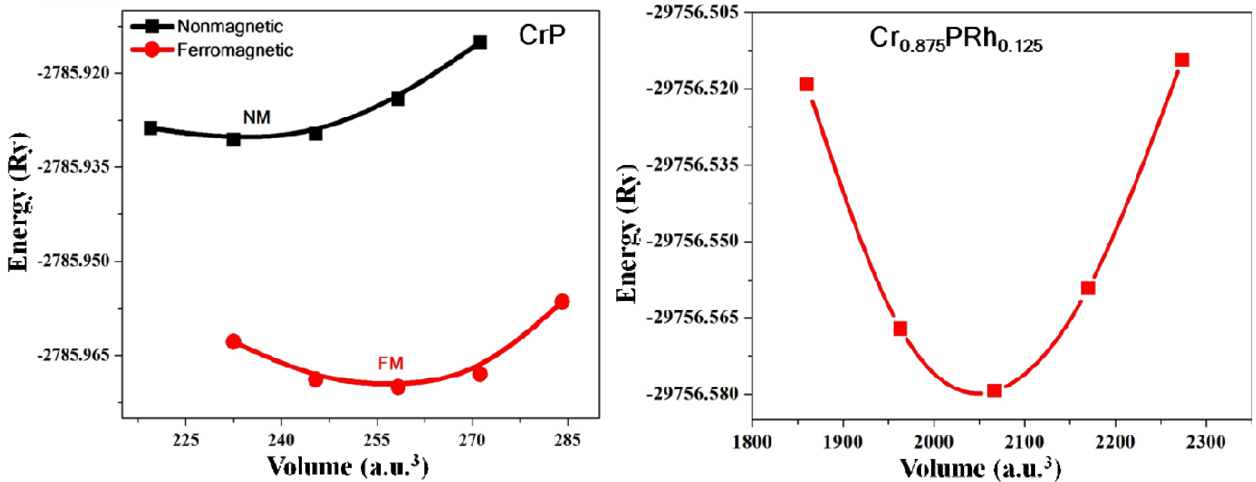
We use the full potential linearized augmented plane (FP-LAPW) method within the framework of density functional theory (DFT) [16,17] implemented in WIEN2k code [18-20] to perform the theoretical calculations for investigating the electronic and half-metallic properties of CrP doped with Rhodium. The generalized gradient approximation (GGA) [21] proposed by Perdew et al. [22-24] was used to solve the Kohn-Sham equations for exchange and correlation potential. For the irreducible Brillouin Zones, the integration was done on the grid of 1000 k points generated using the Monkhorst-Pack scheme [25]. The potential and charge density are treated without shape approximation, and core electrons are treated relativistically in order to exclude the interactions of spin-orbit coupling. Rk_{max}, the plane wave cut-off for the basis function was set to 7.0.

CrP having the lattice constant of 5.35Å is taken as the primitive unit cell in zb cubic crystal system. The supercell of Cr_8P_8 is created with 2 × 2 × 2 dimensions in which Rhodium is doped in 12.5% doping concentration to investigate the electronic and half-metallic properties. The R_{MT} values for Cr, P and Rh atoms are taken as 2.27, 1.86 and 2.27 a.u., respectively. The self-consistent calculations were found to converge when the total energy of the system is stable within 10^{-4} Ry.

3. Results and Discussions

3.1 Volume optimization and Electronic Structure.

CrP is a metallic compound stable in zinc blende zb cubic crystal system having the space group 216 (F-43m) in which Cr and P atoms are present at (0, 0, 0) and (½,½,½) positions respectively. Volume optimization run in both ferromagnetic and non-magnetic phases predict CrP to be stable in ferromagnetic phase by observing the Energy vs Volume curves given in Fig. 1 (a). The ferromagnetic curve is much lowered in energy than that of non-magnetic phase attributing to the stability of CrP in ferromagnetic phase.



(a) (b)

Fig. 1. Volume optimization of (a) CrP (b) $Cr_{0.875}PRh_{0.125}$

After the volume optimization was performed the lattice constant was calculated to be 5.349Å which is a near value to that of equilibrium 5.35Å. Table 1 presents the minimum equilibrium energy and lattice constant of CrP and $Cr_{0.875}PRh_{0.125}$. Cr_8P_8 is the supercell formed with 2 × 2 × 2 dimensions having 16 atoms as the basis. In the supercell Cr_8P_8, Cr atom at (0 0 0) is replaced by the Rh atom in 12.5% doping concentration forming the compound $Cr_{0.875}PRh_{0.125}$. In the supercell structure of $Cr_{0.875}PRh_{0.125}$, 64 atoms are found to be present. $Cr_{0.875}PRh_{0.125}$ after volume optimization yielded a lattice constant of 10.66 Å as shown in Fig. 1 (b).

Table 1. Minimum equilibrium energy and lattice constant of CrP and $Cr_{0.875}PRh_{0.125}$

Compound	**Phase**	**Equilibrium Energy (Ry)**	**Lattice Constant (Å)**
CrP	Non-magnetic Ferro-magnetic	-2785.9306 -2785.97002	5.165 5.349
$Cr_{0.875}PRh_{0.125}$	Ferro-magnetic	-29756.579	10.66

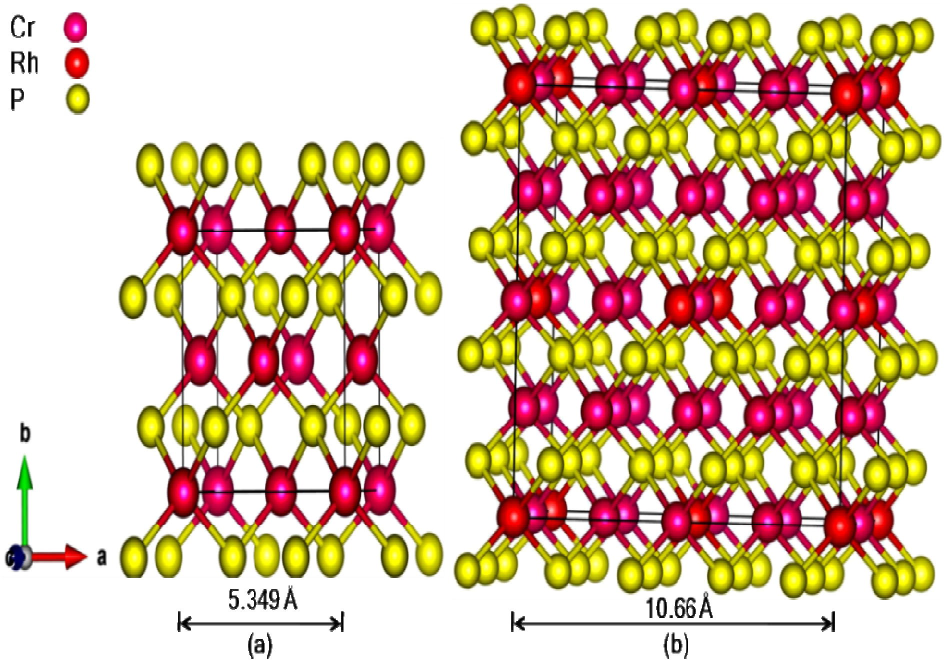


Fig. 2. Structure of (a) CrP (b) $Cr_{0.875}PRh_{0.125}$

The radius of Cr, P and Rh atoms were theoretically found out to be 1.29 Å, 1.10 Å and 1.34 Å respectively. The crystal structures of undoped CrP and doped $Cr_{0.875}PRh_{0.125}$ shown in Fig. 2 (a,b) are plotted using the VESTA software [26].

3.2 Band Structure and Density of States

To study the electronic band structure and density of states (DOS), spin-polarized calculations are performed. Fig. 3 representing the total DOS of CrP in the undoped state exhibits metallic behavior. The conducting characteristics of CrP arise due to the electronic bands that are crossing at the Fermi level (E_F) in both the majority spin and minority spin channels as observed in the band structure given in Fig. 4.

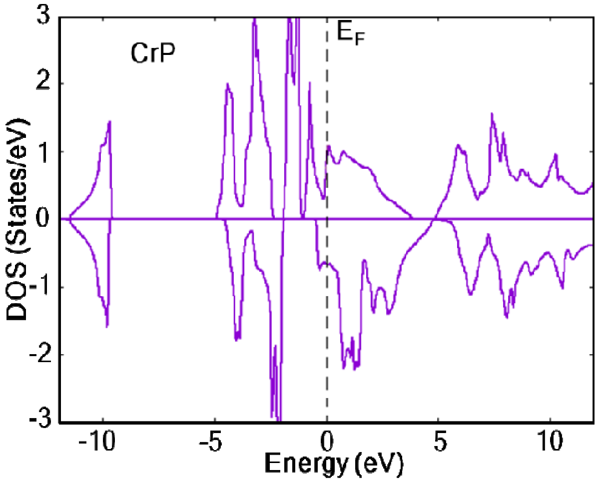


Fig. 3. Total DOS of CrP in both the spin channels.

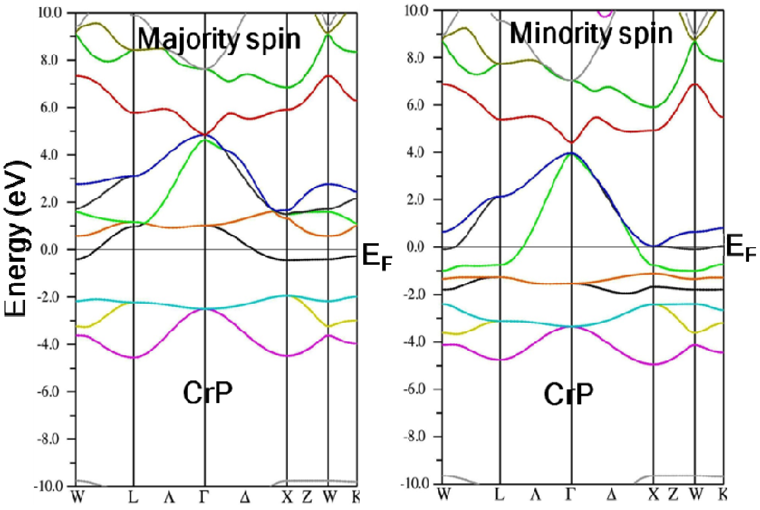


Fig. 4. Band structure CrP in both the spin channels.

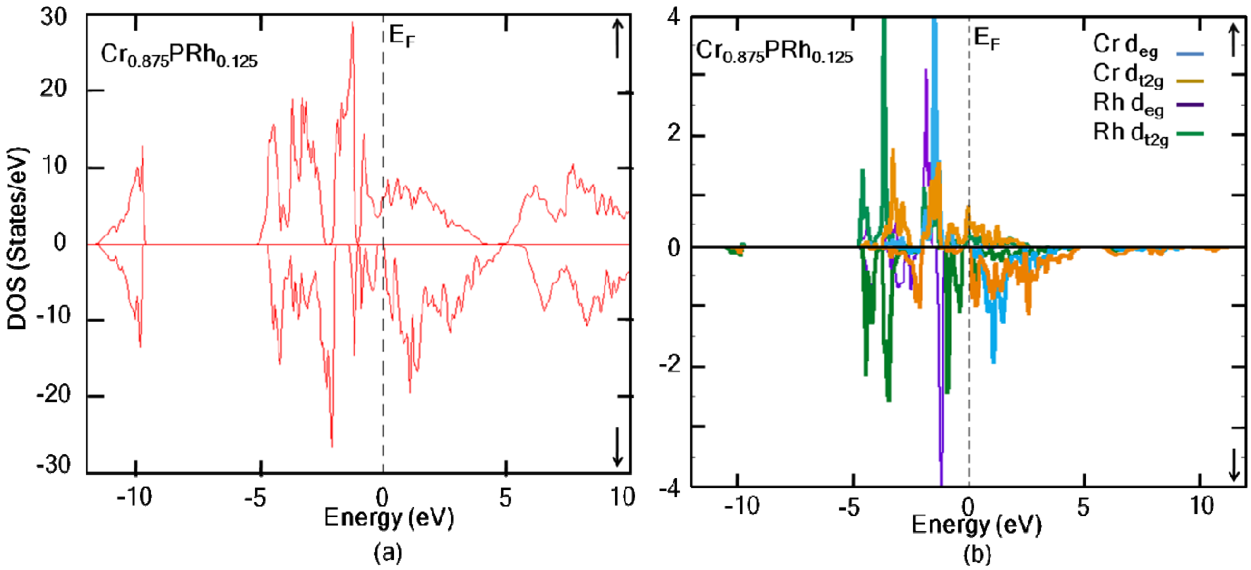


Fig. 5. (a) Total DOS of $Cr_{0.875}PRh_{0.125}$ (b) Partial DOS of $Cr_{0.875}PRh_{0.125}$ in both the spin channels.

$Cr_{0.875}PRh_{0.125}$ in which Rh is doped in 12.5% doping concentration exhibits half metallic properties as shown in the total DOS in Fig. 5 (a). The hybridization of Cr and Rh contribute much to the electronic bands in the compound. The d energy states of Cr and Rh are split up into t_{2g} and e_g states as observed in Fig. 5 (b). At -1.484 eV in the majority spin channel, a peak is observed due to e_g states of the Cr atom. The electronic bands at -3.20 eV and the bands having a width from -0.89 eV to 3.67 eV are the bands arising due to Cr t_{2g} states. The electronic bands observed at -3.59 eV and -4.53 eV are arising due to Rh t_{2g} states and the band observed at -1.84 eV is due to Rh e_g states. From the partial DOS, it is observed that the hybridized d-states of Cr and Rh atoms are crossing the E_F thus determining the metallic properties in the spin up channel of $Cr_{0.875}PRh_{0.125}$.

In the minority spin channel of $Cr_{0.875}PRh_{0.125}$, the electronic band at -0.94 eV and the bands having a width from -1.17 eV to -2.26 eV are observed due to Rh t_{2g} states. At about 0.04 eV beyond the E_F to 4.6 eV, are the hybridized bands with more contribution of the Cr t_{eg} and Cr t_{2g} states. The shifting of the bands at the E_F result in the bandgap of about 0.23 eV in the minority spin channel. The Rh t2g states are pushed below the EF whereas Cr t2g states are raised slightly above the EF resulting in the formation of a band gap at the EF. The small band gap is also observed in the band structure of $Cr_{0.875}PRh_{0.125}$ shown in Fig. 6.

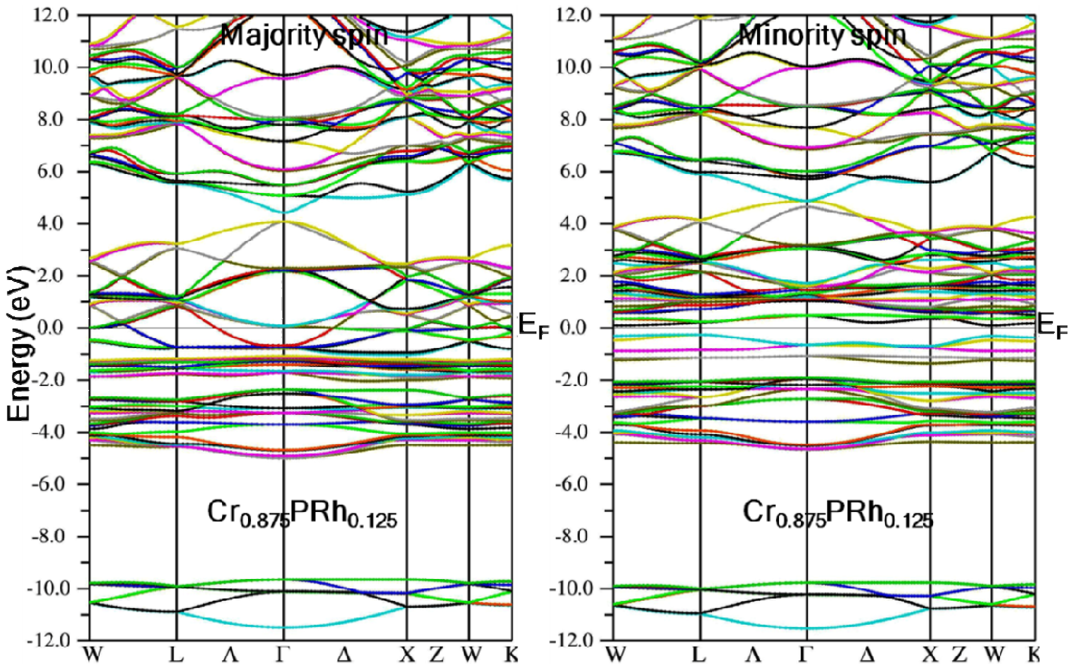


Fig. 6. Band structure of $Cr_{0.875}PRh_{0.125}$ in both the spin channels.

Thus $Cr_{0.875}Pd_{0.125}P$ having Rh in 12.5% doping concentration exhibits half-metallic properties in the minority spin channel having 100% spin polarization at the E_F whereas majority spin state exhibits conducting properties.

4. CONCLUSION

The half-metallic predictions in CrP doped with Rh in 12.5% doping concentration have been reported for the cubic zb structures by the first principle calculations using theoretical approach. CrP is found to be stable in ferromagnetic phase exhibiting metallic characteristics at its equilibrium lattice constant. $Cr_{0.875}Pd_{0.125}P$ having 12.5% doping concentration of Rh is predicted to exhibit Half-metallic properties (HMF) having a bandgap in the minority spin channel whereas in the majority spin channel it exhibits conducting properties. The compound $Cr_{0.875}PRh_{0.125}$ can be investigated experimentally due to its half-metallic properties to be used in the field of spintronics.

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