The Magnetic and Electronic Properties of $Ce_{1-x}Pr_xIn_3$ Compounds

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ABSTRACT

The ab initio total energy calculations have been performed to investigate the structural, magnetic, and electronic properties of the Pr doped $CeIn_3$ compound in $AuCu_3$ structure. Spin-polarized electronic band structure and density of states (DOS) were calculated and interpreted. The magnetic moments of the Pr doped $CeIn_3$ compound was calculated. The obtained data were compared with the available experimental and theoretical work.

1. INTRODUCTION

The rare earth intermetallic compound $ReIn_3$ have attracted attention due to their interesting properties [1-3]. Magnetic interaction is important in the appearance of these properties [1]. Among the $ReIn_3$ compounds, $CeIn_3$ is key compound for understanding characteristics of strongly correlated systems [2]. $CeIn_3$ shows Kondo-type as well as superconducting behavior when pressure is applied [2].

İlkhani et al. have studied the impacts of pressure on the structural and electronic properties of $CeIn_3$ [3]. The low temperature heat capacity of $(R_xEr_{1-x})In_3$ (R = Y, Ce, Pr, and Dy) has been studied by Hale et al. [4]. Knebel et al. have studied the phase diagram of the antiferromagnetic Kondo-lattice compound $CeIn_3$ under pressure up to 100 kbar by the resistivity measurements [5]. The pressure dependency of localization degree in heavy fermion $CeIn_3$ using density functional theory have been studied [1]. The magnetic structure of $CeIn_3$ with Neutron diffraction measurements has been studied by Benoit et al. [6]. Kletowski has studied the transverse and longitudinal magnetoresistances of $LaIn_3$, $CeIn_3$, $PrIn_3$ and $SmIn_3$ in magnetic fields up to 32 T [7].

The diverse experimental and theoretical studies have been carried out to determine the magnetic and electronic properties. To our best knowledge, the structural, magnetic, and electronic properties of the Pr doped $CeIn_3$ compound are not studied. Therefore, in this paper the first-principles calculations of Pr doped $CeIn_3$ have been performed.

2. THE CALCULATION METHOD

All calculations were carried out using the Vienna Ab initio Simulation Package (VASP) [8-11] and performed for cubic $AuCu_3$ structure in 2 × 2 × 2 supercell. The exchange and correlation terms are described in the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) [12] and the electron-ion interaction is considered in the form of the projector-augmented-wave (PAW) method [10, 13]. The kinetic energy cutoff was set at 425 eV. 9 x 9 x 9 k-point grid were used to sample the Brillouin zone [14]. The optimization was performed until the total energy tolerance and maximum force tolerance was below 1.0 x 10^{-7} eV and 1.0 x 10^{-5} eV/Å, respectively. Also, spin-polarization effects have been included in the calculations.

2. RESULTS AND DISCUSSION

$ReIn_3$ rare earth intermetallic compounds are crystalized in $AuCu_3$-type structure (Space Group: Pm-3m, No: 221) and crystal view of Pr doped $CeIn_3$ compound are given in Figure 1 for the interested concentrations. The calculated lattice constants are given in Table 1 for $Ce_{1-x}Pr_xIn_3$ compound.

Table 1. The calculated lattice constant (a in Å) and magnetic moment (M in μ_B/atom) values of $Ce_{1-x}Pr_xIn_3$ compound with available values.

x	***a***	M_{Ce}	M_{Pr}	***Ref.***
0.00	4.7122	0.690	-	Present
	4.689	0.48±0.08		Exp. [6]
	4.6894			Exp.[4]
		0.65±0.1		Exp. [15]
	4.691	0.658		AFM [3]
	4.702	0.713		AFM+SOC [3]
	4.707	0.855		AFM+SOC+GGAU [3]
0.25	4.7117	0.706	2.134	Present
0.50	4.7048	0.058	2.150	Present
0.75	4.7103	0.726	2.149	Present
1.00	4.7096	-	2.149	Present
	4.6717			Exp. [4]

It is seen that the present lattice parameters do agree with the other available experimental values. The calculated lattice parameter is about %1 larger than the available values. This is expected for GGA-PBE calculations. Also, the calculated magnetic moment values of $Ce_{1-x}Pr_xIn_3$ compound are given in Table 1. The calculated magnetic moment value for Ce and Pr is agreement with the experimental and theoretical values. The total magnetic moment increases as the Pr contribution increases.

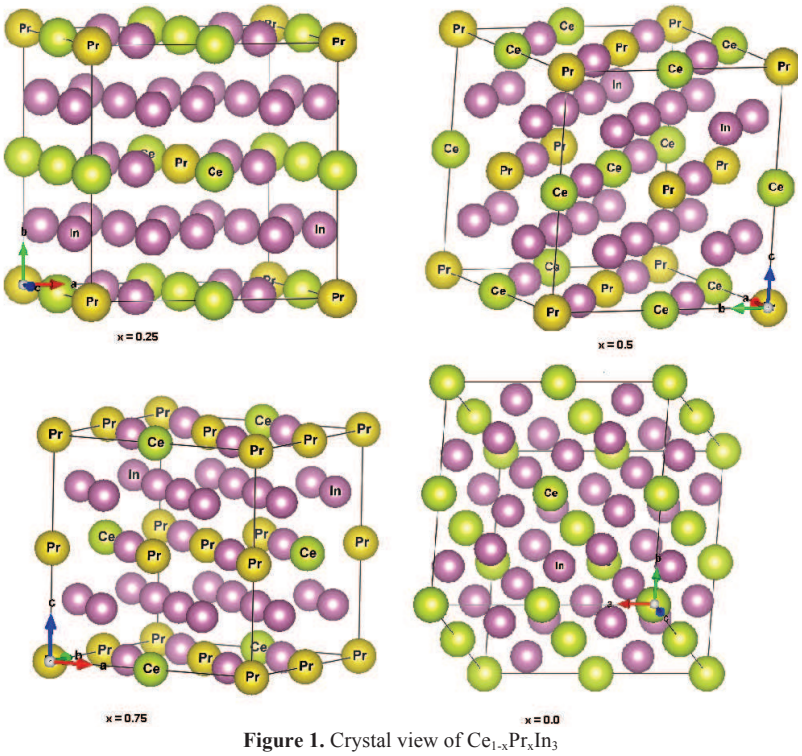

Figure 1. Crystal view of $Ce_{1-x}Pr_xIn_3$

The total density of states (TDOS) of $Ce_{1-x}Pr_xIn_3$ compounds along the high symmetry directions are calculated and given in Figure 2. The energy shift between the spin up and spin down causes the occurrence of the magnetic polarization. It seen that $Ce_{1-x}Pr_xIn_3$ compounds exhibit metallic character.

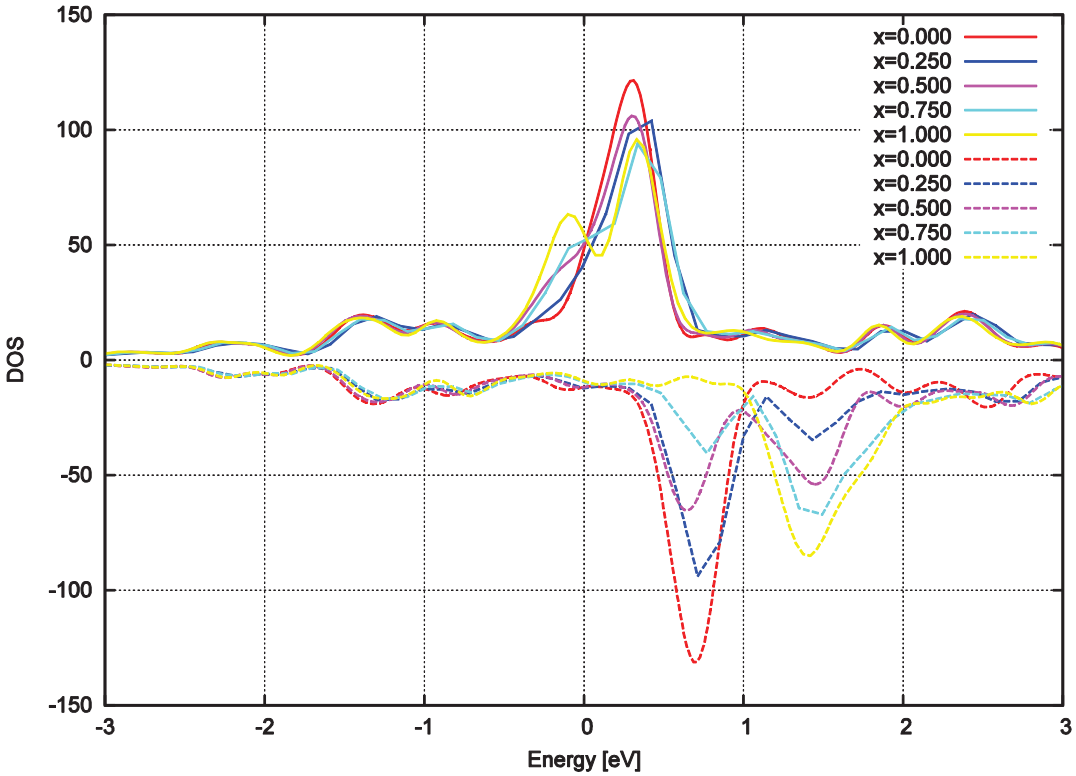

Figure 2. The calculated TDOS of $Ce_{1-x}Pr_xIn_3$

3. CONCLUSION

The structural, magnetic, and electronic properties of the Pr doped CeIn3 compound are calculated using density functional theory. The calculated lattice constant and magnetic moment values for $Ce_{1-x}Pr_xIn_3$ compound are accord with the other available experimental and theoretical values. The DOS of $Ce_{1-x}Pr_xIn_3$ reveals the metallic character.

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