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Density functional study of d^0 half-metallic ferromagnetism in a bulk and (001) nano surface of KP compound

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ABSTRACT

According to many applications of half-metals in the spintronics devices, we investigate half-metallic properties of KP compound in rock-salt (RS), zinc-blende (ZB), cesium chloride (CsCl) and wurtzite (WZ) structural phases by using density functional theory. Results indicate that KP compound is half-metal in RS, ZB and WZ structures, while in CsCl structure, due to small lattice constant and failure of Stoner criterion, KP compound doesn't have any magnetic properties. Half-metallic gap values obtained are 0.47, 0.95 and 0.91 eV for RS, ZB, WZ structures, respectively. Although KP compound in CsCl structure is more stable than RS structure energetically, but from dynamical point of view only RS structure is stable and other structures are unstable. Calculations corresponding to (001) surface of RS structure demonstrate the conservation of bulk half-metallic properties in this crystallographic direction. So nano-layers of KP compound in RS structure might be an appropriate candidate for application in near future spintronics devices.

1. Introduction

In conventional magnetic systems, magnetism is due to the presence of transition-metal or rare-earth atoms with partially occupied *d* or *f* shells [1]. The *p* orbitals are generally believed to be delocalized and magnetism is usually not expected [2]. This viewpoint was violated with the discovery of weak magnetism in CaB_6 compound [3], because this compound is lack of partially filled *d* or *f* orbitals. Coey selected d^0 ferromagnetism expression for magnetic systems without *d* orbitals or magnetic systems which their magnetic properties aren't due to *d* orbitals [4]. Geshi et al. discovered magnetic properties in calcium pnictides, i.e. CaP, CaAs and CaSb theoretically, which their magnetization is due to spin polarization of *p* orbitals and a new route opened in magnetic materials [5]. Since then *p* magnetization has been predicted in several binary I^A–III^A [6], I^A–IV^A [7], I^A–V^A [8], I^A–VI^A [9], II^A–IV^A [10] and II^A–V^A [11] compounds. Prominent property of these compounds is their half-metallic behavior in special structures. To successfully incorporate spins into existing semiconductor technology, one has to detection of spin polarization as well as spin-polarized currents [12]. Therefore half-metals have attracted considerable research attention because of 100% spin-polarization at the Fermi level. In this work, we make use of density-functional method to study KP compound for the rock-salt (RS), zinc-blende (ZB), cesium chloride (CsCl) and wurtzite (WZ) structures in order to find half-metallic ferromagnetic phases. However, investigate the dynamic stability is important for hypothetical compounds, but the previous studies on hypothetical binary ionic compounds with no transition metals are considered to this issue rarely. Nevertheless we studied the dynamic stability of KP compound in structures investigated. Finally we investigated the half-metallic properties of constructed KP nano-layers at [001] crystallography direction of RS structure.

2. Computational method

We have used the first-principles pseudopotential plane wave method based on the density-functional theory incorporated into the Quantum-Espresso package to calculate the electronic and magnetic properties of KP compound in bulk and surface (001). For exchange correlation correction the generalized gradient approximation (GGA) was employed. The plane-wave cutoff energy was assumed to be 80 Ry, while the Brillouin zone sampling mesh parameters for the *k*-point set were chosen as $10 \times 10 \times 10$ for RS, ZB and CsCl structures and $11 \times 11 \times 10$ for the wurtzite structure and $10 \times 10 \times 1$ for surface (001). The criterion of the energy convergence is set to 0.001 mRy. The atomic configurations used to generate the norm conserving pseudopotentials are $4s^1$ for K and $3s^2 3p^3$ for P. We obtain the theoretical equilibrium lattice con-

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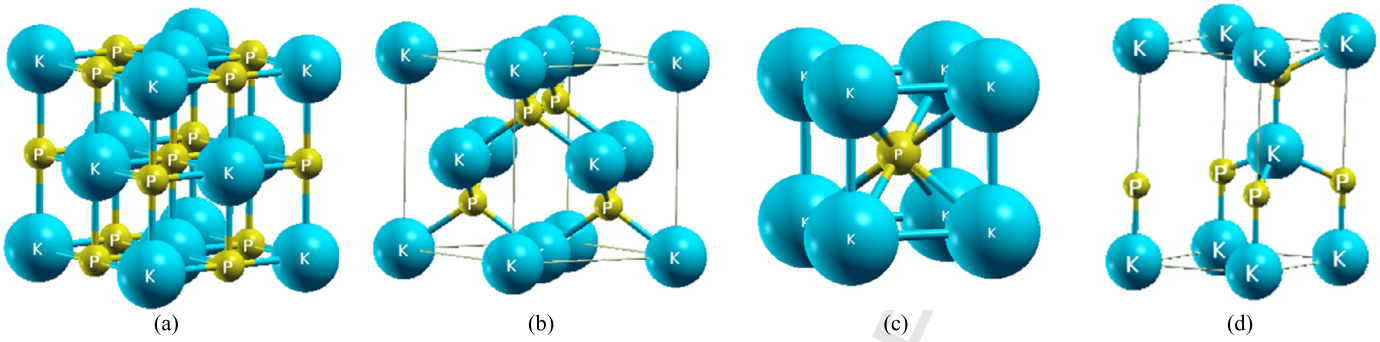

Fig. 1. (a) RS, (b) ZB, (c) CsCl and (d) WZ crystal structures of KP compound.

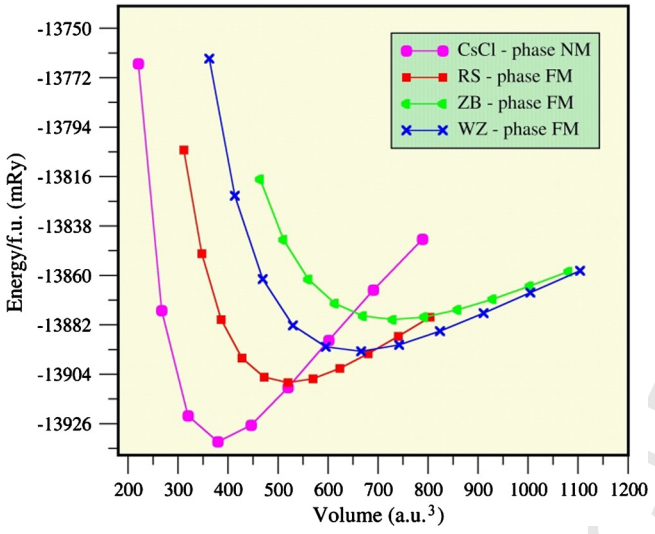

Fig. 2. Total energy per unit cell as a function of volume per formula unit for KP in crystal structures. FM and NM represent ferromagnetic and nonmagnetic states, respectively.

stant for KP compound in RS, ZB, CsCl and WZ the value of 12.766, 14.291, 7.244 and 10.922 ($c/a = 1.162$) Bohr, respectively.

3. Results and discussion

In this paper, we consider four hypothetical RS, ZB, CsCl and WZ structures for KP compound which are shown in Fig. 1. RS, ZB and CsCl structures have two atoms in their unit cell, while WZ structure has four atoms.

We will start our discussion from compute the primitive cell energy of all structures under study as a function of their primitive volume, in the ferromagnetic and nonmagnetic phases. The results indicate that the RS, ZB and WZ structures of KP are ferromagnetic around their equilibrium volume, while CsCl structure stabilized in a nonmagnetic ground state and among all structures under study, CsCl exhibits the lowest energy. But RS structure located less energy than the other two structures, among ferromagnetic structures (see Fig. 2). To determine the magnetic ground state of RS exactly, we also calculate the total energy of KP in the antiferromagnetic state of this structure by means of reference [13]. Total energy difference between the antiferromagnetic and ferromagnetic states is about +116 meV/f.u., which shows KP compound has a ferromagnetic ground state in the RS structure.

An integer value of the magnetic moment is a characteristic feature of half-metallic ferromagnets [14]. The total magnetic moments consist of three parts: the K atom, P atom, and the interstitial regions, and the total moments contain integer Bohr magnetons of $2\,\mu_B$ for RS, ZB and WZ structures and $0\,\mu_B$ for CsCl

Table 1
The calculated total and partial magnetic moments for the KP compound with all structures under study at their equilibrium lattice parameters.

	μ_{tot} (μ_B)	μ_K (μ_B)	μ_P (μ_B)	μ_{in} (μ_B)
RS	2.000	0.031	1.553	0.416
ZB	2.000	0.026	1.480	0.494
CsCl	0	0	0	0
WZ	2.000	0.025	1.470	0.505

structure. The calculated total and partial magnetic moments for the KP compound with all structures under study at their equilibrium lattice parameters listed in Table 1. The main contribution to the magnetic moment comes from the p states of P atoms.

Half-metallic ferromagnets exhibit the property of having a metallic density of electron states for the one spin direction, while there is a band gap around the Fermi level for states of the opposite spin [15]. According to this definition and total density of states provided in the Fig. 3, we can say that the KP compound is half-metal in RS, ZB and WZ structures. Because the Fermi level crosses density of states only in one spin channel. From density of states of CsCl structure in Fig. 3 we can see that, spin-up and spin-down density of states are quite the same and no spin polarization have been observed. Therefore KP compound is not half-metal in CsCl structure. We note that the SrC, BaC and NaN have a similar behavior like KP, which don't show half-metallicity behavior in CsCl structure [14,16]. In CsCl, metallic state is observed because the large spreading of density of states around the Fermi level which is more than 3.6 eV due to the small lattice constant of 7.244 Bohr compared with the other structure under study. Large lattice constant caused density of states localized around the Fermi level in RS, ZB and WZ structures (see Fig. 3). The obtained results corresponded with the results obtained for magnetic moment.

As mentioned in the introduction this magnetic materials is called p magnetization, because their anions p states are fully spin polarized. With regard to this issue, we have identified p orbitals of P atom contribution with blue areas for spin up and red areas for spin down in Fig. 3. As can be seen in Fig. 2, the main contribution to the total density of states comes from the p orbitals of P atom around the Fermi level. So we can say that, the origin of magnetism of KP compound in investigated structures comes from the spin polarization of the p states of P atom.

Because of the nonmagnetic property of KP compound in CsCl structure is due to a failure of Stoner criterion in this structure. In a simple issue of the Stoner criterion, the condition of the stability of the ferromagnetic state is as follows:

$$D(E_f)I \succ 1 \qquad (1)$$

Where I is the Stoner parameter and $D(E_f)$ is the nonmagnetic density of states at the Fermi level. From the equation (1), it is inferred that a large value of $D(E_f)$ or I favors the ferromagnetic

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