# First-principle investigation of magnetic and electronic properties of vanadium- and chromium-doped cubic aluminum phosphide

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A R T I C L E   I N F O

A B S T R A C T

We have investigated the half-metallic ferromagnetic and electronic properties of vanadium- and chromium-doped cubic aluminum phosphide ($Al_{1-x}TM_xP$; $TM=V$ or Cr, $x=0.0625$) in zinc-blende phase using the full-potential linearized augmented plane-wave method of density functional theory. The electronic structures show that $Al_{0.9375}V_{0.0625}P$ and $Al_{0.9375}Cr_{0.0625}P$ compounds are half-metallic ferromagnets with spin polarization of 100%. The half-metallic ferromagnetic behavior is confirmed by the integrals Bohr magneton of total magnetizations of $2\,\mu_B$ and $3\,\mu_B$ for $Al_{0.9375}V_{0.0625}P$ and $Al_{0.9375}Cr_{0.0625}P$, respectively. In these compounds, the ferromagnetic state is originated from double-exchange mechanism. We have found that the half-metallic gap is 0.674 eV for $Al_{0.9375}V_{0.0625}P$ and it is 0.523 eV for $Al_{0.9375}Cr_{0.0625}P$. Therefore, the V-doped AlP seems to be a better potential candidate than that of Cr-doped AlP for spintronic applications.

## 1. Introduction

Spintronics (spin transport electronics or spin-based electronics) is a new generation of microelectronics, which exploits the spin of charge carriers in the emerging field of promising materials for spin-based multifunctional devices [1–3]. The diluted magnetic semiconductors (DMSs) are main candidates for development of a new kind of this technology because they combine the magnetic and semiconductor transport properties. These materials are characterized by the Curie temperature higher than room temperature and half-metallic behavior [4]. These two important features make the DMSs to promising candidates for realizing spintronic devices. However, the expected advantage of spintronic devices over the conventional electronic ones would be non-volatility, increased data processing speed, increased transistor density and decreased power consumption [5]. Thence, the doping magnetic ions produced spin-polarized carriers in the DMSs, resulting in the variation of the density of states of majority-spin (up) and minority-spin (down) at the Fermi level ($E_F$), the spin polarization of a system at $E_F$ can be determined as [6]

$$P = \frac{N^{\uparrow}(E_F) - N^{\downarrow}(E_F)}{N^{\uparrow}(E_F) + N^{\downarrow}(E_F)} \tag{1}$$

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where $N^\uparrow(E_F)$ and $N^\downarrow(E_F)$ are the spin-up and spin-down densities at Fermi level ($E_F$), respectively. The concept of half-metallic ferromagnetism was discovered by de Groot et al. [7] as materials exhibiting a gap in one spin direction and metallic nature in the other, which yields a polarization $P=1$ when $N^\uparrow(E_F)$ or $N^\downarrow(E_F)$ equals zero, this leads to 100% carrier spin polarization at $E_F$ [8].

The DMSs based on III–V semiconductors are the most promising materials for spintronic device applications because they show the stability of the ferromagnetism at temperatures higher than the room temperature and half-metallic ferromagnetic behavior [9,10]. In the recent years, there are several theoretical reports [11–27] on the prediction of half-metallic ferromagnetism in (Ti, V, Cr, Mn, and Fe)-doped III–V semiconductors in order to estimate the possibility of their use in spintronics applications. The AlP is a wide-band gap semiconductor [28] that belongs to III–V group; it is an important material design of optoelectronic devices for industrial purpose [29]. However, several experimental methods have been realized in intention to discover the ferromagnetism in III–V doped with transition metal elements such as the GaP doped with Mn [30] has been obtained by using ferromagnetic resonance (FMR) and AC magnetization measurements, and Cr-doped AlN thin films have been grown successfully with a variety of techniques [31], for example a reactive sputtering [32,33], ion implantation [34], and molecular beam epitaxy [35,36]. The AlP doped with 5% Mn is considered a possible candidate as a DMS material according to a theoretical study of Katayama-Yoshida and Sato [37], as well the half-metallic ferromagnetism was predicted in the $Al_{1-x}Cr_xP$ [38], and Zhang et al. [39] estimated a Curie temperature higher than 600 K for Cr-doped AlP. Recently, the half-metallic ferromagnetism is investigated in the Mn-doped AlP [24], Cr-doped AlP [25], Ti-doped AlP [26], and Ca-doped AlP [40].

In the present work, we have investigated the half-metallic ferromagnetism and electronic properties of $Al_{1-x}TM_xP$ (TM=V and Cr) at concentration $x=0.0625$ based on simple ordered $Al_{15}VP_{16}$ and $Al_{15}CrP_{16}$ supercells of 32 atoms, using the first-principle full-potential linearized augmented plane-wave calculations with generalized gradient approximation functional proposed by Wu and Cohen [41]. We have predicted that $Al_{0.9375}V_{0.0625}P$ and $Al_{0.9375}Cr_{0.0625}P$ are ideal half-metallic ferromagnets and they are potential candidates for spintronic applications.

## 2. Detail of calculations

### 2.1. Method of calculations

This study is performed using density functional theory (DFT) calculations [42,43] within the framework of first-principle full-potential linearized augmented plane-wave (FP-LAPW) method as implemented in WIEN2K package [44]. The generalized gradient approximation functional proposed by Wu and Cohen (WC-GGA) [41] was used for the exchange correlation potential due to its better performance for structural optimization [4,22,24,45–48], resulting from the fourth-order gradient expansion of exchange-correlation functional [41,47]. This new functional

is more accurate for solids than any existing GGA and meta-GGA forms [48]. We have taken the averages of non-overlapping muffin-tin radii ($R_{MT}$) of Al, P, V and Cr in such a way that the muffin-tin spheres do not overlap. We have expanded the wave functions in the interstitial region to plane waves with a cut-off of $K_{max}=8.0/R_{MT}$ (where $K_{max}$ is the magnitude of the largest $K$ vector in the plane wave and $R_{MT}$ is the average radius of the muffin–tin spheres). The maximum value for partial waves inside the atomic sphere was $l_{max}=10$, while the charge density was Fourier expanded up to $G_{max}=12$ a.u.$^{-1}$, where $G_{max}$ is the largest vector in the Fourier expansion. The energy cutoff was chosen as $-6$ Ry, which defines the separation of valence and core states. For the sampling of the Brillouin zone, $4\times4\times2$ Monkhorst–Pack mesh [49,50] is used for both $Al_{0.9375}V_{0.0625}P$ and $Al_{0.9375}Cr_{0.0625}P$, where the self-consistent convergence of the total energy was at 0.1 mRy.

### 2.2. Optimization of crystal structures

The binary AlP has zinc-blende (B3) cubic structure with space group of 216 ($F\bar{4}3m$), where the Al atom is positioned at (0, 0, 0) and P atom at (0.25, 0.25, 0.25). The $Al_{1-x}TM_xP$ (TM=V and Cr) compounds with concentration $x=0.0625$ are obtained by substituted of one Al cation site at position (0, 0, 0) by one (TM=V and Cr) atom in supercell of 32 atoms. We get the $Al_{0.9375}V_{0.0625}P$ and $Al_{0.9375}Cr_{0.0625}P$ ($1\times2\times2$) supercells of 32 atoms with concentration $x=0.0625$ of tetragonal structure [12,14,22,24,46] with space group of 111 ($P\bar{4}2m$) as shown in Fig. 1. The formation energy is usually used to measure the phase stability in solid states [51–53], for determining the thermodynamic stability of the present $Al_{0.9375}TM_{0.0625}P$ (TM=V and Cr) in ordered ZB phase, the formation energies are estimated for these ternary compounds using the following expression [53]:

$$E_{form} = E_{total}\left(Al_{16-y}V_yP_{16}/Al_{16-y}Cr_yP_{16}\right)$$
$$-\frac{(16-y)E_{tot}^0(Al)}{32} - \frac{yE_{tot}^0(V/Cr)}{32} - \frac{16E_{tot}^0(P)}{32} \quad (2)$$

where the terms $E_{total}\left(Al_{16-y}TM_yP_{16}\right)$, $E_{tot}^0(Al)$, $E_{tot}^0(V/Cr)$ and $E_{tot}^0(P)$ are the total energy per atom of the $Al_{16-y}V_yP_{16}$ or $Al_{16-y}Cr_yP_{16}$, total energy per atom of each bulk Al, (V or Cr) and P, respectively, and the $y$ is the number of substitute V or Cr atom in supercell. For the concentration $x=0.0625$, the
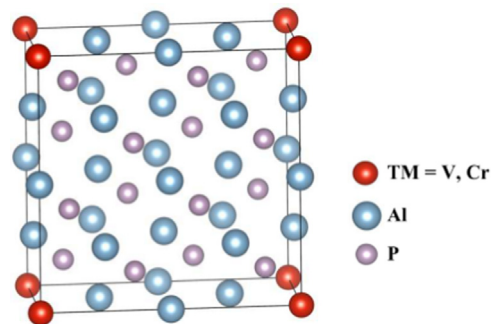


**Fig. 1.** The crystal structure of $Al_{1-x}TM_xP$ supercell of 32 atoms with (TM=V and Cr) and concentration $x=0.0625$.