# Electronic and magnetic structures of V-doped zinc blende $Zn_{1-x}V_xN_yO_{1-y}$ and $Zn_{1-x}V_xP_yO_{1-y}$

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Electronic and magnetic structures of zinc blende ZnO doped with V impurities are studied by first-principles calculations based on the Korringa–Kohn–Rostoker (KKR) method combined with the coherent potential approximation (CPA). Calculations for the substitution of O by N or P are performed and the magnetic moment is found to be sensitive to the N or P content. Furthermore, the system exhibits a half-metallic band structure accompanied by the broadening of vanadium bands. The mechanism responsible for ferromagnetism is also discussed and the stability of the ferromagnetic state compared with that of the paramagnetic state is systematically investigated by calculating the total energy difference between them by using supercell method.

**Keywords:** *ab initio* calculations, density of states, magnetic moment doping, diluted magnetic semiconductors

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## 1. Introduction

Ferromagnetism in diluted magnetic semiconductors (DMSs), i.e. non-magnetic semiconductors (or insulator) doped with a small concentration of a magnetic element, has aroused great interest in fundamental research in view of their important potential applications in the spintronics field.[1−3] The interplay between the charge carriers and the electron spins of a ferromagnetic metal doped into the semiconductor, which is the basis of the spintronic, can be used for many magneto/spin-electronic devices. The big challenge to successful applications of spintronic materials is to find a semiconductor material that is a half-metal ferromagnet or exhibits a ferromagnetic state at room temperature. Ohno *et al.*[4] showed that Mn-doped GaAs is a ferromagnetic semiconductor with Curie temperature $T_c$ ∼110 K. Such a discovery has aroused increasing interest in DMS. Magnetic impurities, like transition metals, can make the semiconductor half-metallic: the majority spin bands are metallic while the minority spin bands are semiconducting. As a result, the compound presents a fully (100%) spin polarized density of states (DOS) at the Fermi energy, a property that is required by the electronic industry in order to build spintronic devices.

Half-metallic ferromagnetism (HMF), especially in diluted magnetic semiconductors,[5,6] has attracted more and more attention since it was first discovered by De Groot *et al.* in 1983.[7−9] To explore the possible spintronic applications of the HMFs to semiconductor devices, there have been a great many studies where the half metallicity in the binary compounds of zinc-blende (ZB) structure is used,[10−12] whose structure is simple and compatible with existing III–V and II–VI semiconductors.

In DMS materials, transition metal (TM) or rare earth metal ions are substituted onto cation sites of the host semiconductor and coupled with free carriers to introduce ferromagnetism.[13] Dietl *et al.*[14] and Sato Katayama-Yoshida[15] have predicted that among the DMSs, ZnO doped with transition metal impurities is one of the most promising spintronic materials. There is considerable interest in the develop-

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ment of zinc oxide based (ZnO:TM) diluted magnetic semiconductors because of their high Curie temperature, which is essential for spintronic devices.[14]

A number of experiments have revealed magnetic properties of ZnO thin films doped with a transition metal at room temperature.[16−19] ZnO thin films can be deposited by several physical and chemical deposition techniques, such as laser-molecular-beam-epitaxy,[20] chemical vapour deposition,[21] pulsed laser deposition,[22] and sputtering.[23] Among these depositing techniques, the sputtering technique presents some important advantages and improved technological possibilities.[24−26] The (Zn,V)O obtained by metallorganic vapour-phase epitaxy (MOVPE) with *in situ* incorporation of the V atoms or by aqueous chemical growth (ACG) in combination with an ion-implantation process has been studied by Schlenker *et al.*[27] Recently, Fukumura *et al.*[28] and Jin *et al.*[29] showed experimentally that 3d transition metal atoms were soluble up to 35% in ZnO. Therefore, ZnO is very promising at this point. Indeed, it was proposed by experimental studies that such a high solubility may result in the phase separation that occurs in TM-doped ZnO, in which the phase containing the magnetic impurity is coherently embedded into the non-magnetic host.[30] However, TM-doped ZnO without a secondary phase has also been observed experimentally for low TM concentrations.[31]

It has been considered that the II–VI semiconductors are not suitable for the fabrication of functional DMS because of the difficulty in carrier control. Moreover, by using the co-doping method, Yamamoto and Katayama-Yoshida[32] proposed the materials designed for the fabrication of low-resistivity p-type ZnO, while Joseph *et al.*[33] successfully prepared p-type ZnO thin films. Therefore, it is worthwhile investigating carrier-induced ferromagnetism in the ZnO-based DMSs.

On the other hand, *ab initio* calculations based on the local density approximation by Sato Katayama-Yoshida[15] showed a ferromagnetic ordering of ZnO doped with V, Cr, Fe, Co, and Ni without any additional charge carriers. However, some investigations revealed that other factors, like the crystalline quality[34−38] or annealing temperatures,[39] also have a strong effect on the magnetic behaviour.

In the present paper, the electronic and magnetic properties of the zinc-blende ZnO co-doped with V and N or P, each as a function of impurity and carrier concentrations, are studied. We present our calculation methods in Section 2. The obtained results are discussed in Section 3 and the conclusion is given in Section 4.

## 2. Calculation methods

The electronic structure and magnetic properties of zinc-blende structure based on the Korringa–Kohn–Rostoker coherent potential approximation (KKR-CPA)[40] with the parameterization of Moruzzi, Janak, and Williams (MJW),[41] have been studied. The KKR-CPA method[42,43] is one of the most efficient band structure calculation methods for treating disordered systems like DMS. To solve the density functional theory (DFT) one-particle equations, one uses multiple-scattering theory, i.e. the KKR Green's function (KKR-GF) method and the KKR-CPA for low impurity concentration.

The relativistic effects are taken into account by employing the scalar relativistic approximation. The form of the crystal potential is approximated by a muffin-tin potential, and the wave functions in the respective muffin-tin spheres are expanded in real harmonics up to $l = 8$, where $l$ is the angular momentum quantum number defined at each site. 350 K points in the irreducible part of the first Brillouin zone are used in our calculations. For the present KKR-CPA calculations, we use the package MACHIKANEYAMA2000 coded by Akai.[44] The calculated lattice parameter of the zinc-blende ZnO is 4.533 Å (1 Å = 0.1 nm), which is only 0.7% larger than that of the experimental parameter of 4.5 Å.[45] The calculated ZnO density of states is given in Fig. 1. The band gap of about 2.70 eV for bulk ZnO is around the experimental value of 3.3 eV.

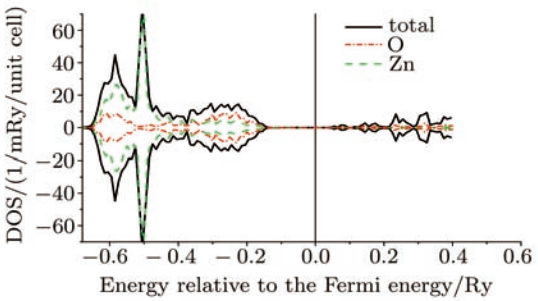



**Fig. 1.** Total and partial densities of states (DOSs) of ZnO.

The systems with impurities are treated by the supercell method. The V-doped ZnO is based on the $2 \times 2 \times 2$ supercell containing 32 ZnOs. We consider a variety of configurations with 1, 2, and 4 V atoms, corresponding to concentrations of 3.125%, 6.25%, and 12.5%, respectively. The ferromagnetic state in which

all of the V magnetic moments are parallel to each other is written as (Zn,$V_x^{up}$ )O, where $x$ is the concentration of the V atoms. The paramagnetic state in which the V magnetic moments are pointed randomly at each other is written as (Zn,$V_{x/2}^{up}$; $V_{x/2}^{down}$)O. Therefore, the system has no magnetization. The disordered local moment approach (DLM)[46] has been used to calculate the paramagnetic state energy.

The difference in energy per unit cell (two formula units) between the ferromagnetic and the paramagnetic states, in the V-doped ZnO, as a function of the carrier concentration, has been calculated. The studied compounds are $Zn_{28}V_4O_{32}$ (V content: 12.5%), $Zn_{30}V_2O_{32}$ (V content: 6.25%), and $Zn_{31}VO_{32}$ (V content: 3.125%) separately. For 3.125%-V atom concentration $\Delta E = E_{para} - E_{FM} = 0.0235$ mRy (1 Ry = 13.605 eV) showing that the ferromagnetic state is more stable than the paramagnetic one. Hole carriers are introduced into this system by substituting O atoms with N or P atoms, and electron carriers are introduced by putting V atoms instead of Zn atoms. A fixed impurity concentration of 12.5% and discrete carrier concentrations of $Zn_{28}V_4O_{28}N_4$ (12.5%: N), $Zn_{28}V_4O_{24}N_8$ (25%: N), and $Zn_{28}V_4O_{20}N_{12}$ (37.5%: N) are studied.

## 3. Results and discussion

Recently, some new DFT calculations with LDA approximation were proposed[46–48] for high-$T_c$ DMS. New functional DMS with magnetic properties depending on the external field or the carrier concentration is a promising candidate for future spintronic applications.

The current study focuses on $Zn_{1-x}V_xN_yO_{1-y}$ and $Zn_{1-x}V_xP_yO_{1-y}$ materials. The (Zn,V)O system, when co-doped with N or P, could turn into a ferromagnet as nitrogen and phosphorus introduces hole carriers. These in turn could mediate the ferromagnetic coupling between V spins. The strong p–d exchange interaction mediated by holes is thought to be the origin of ferromagnetism. Our *ab initio* calculations show a decreasing V spin magnetic moment with the N or P concentration increasing.

The calculated total density of states (TDOS) and partial density of states (PDOS) of $Zn_{1-x}V_xO$, $x = 3.125\%$, 6.25%, and 12.5% are given in Figs. 2(a)–2(c), respectively. We note that the O 2s states are not included in these figures; the lowest conduction band and the highest valence band originate mainly from V 3d, and O 2p states. Fully occupied impurity states are generated close to the mid-band gap. The spin magnetic moment increases from 2.29 $\mu_B$ for 3.125% V concentration to 2.35 $\mu_B$ for 6.25% V, and to 2.39 $\mu_B$ for 12.5% V.

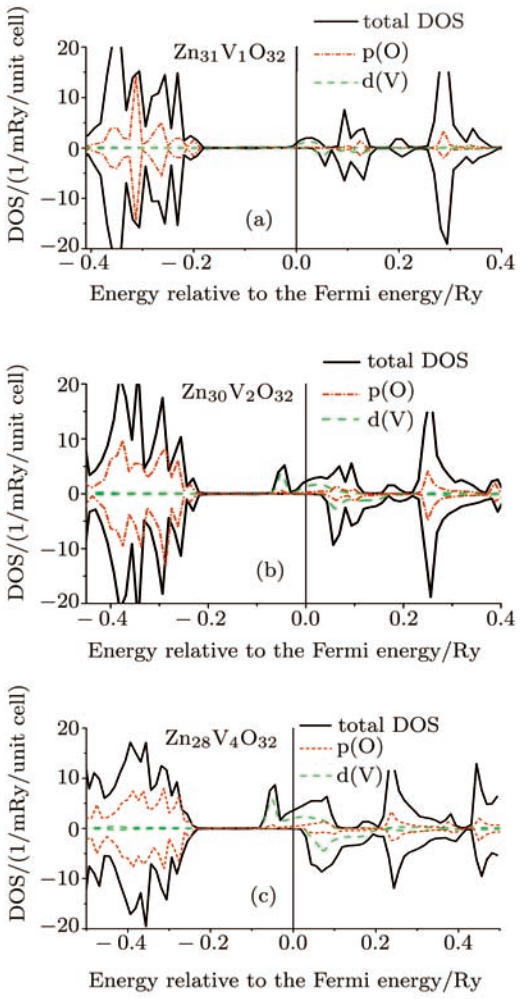



**Fig. 2.** Total and partial DOSs for the ferromagnetic $Zn_{1-x}V_xO$ with $x = 0.03125$ (a), 0.0625 (b), and 0.125 (c), for spin up and spin down, showing total DOS (solid black line), d(V) state (dashed green line), and p(O) state (dotted red line).

The ferromagnetic state is more stable than the paramagnetic one in $Zn_{1-x}V_xO$. Indeed, the total energy difference, $\Delta E$, between the DLM system with 50% V moments up and that with 50% down, is distributed randomly, i.e., $Zn_{1-x}V\uparrow_{x/2}V\downarrow_{x/2}O$, and the ferromagnetic system, e.g., $Zn_{1-x}V\uparrow_xO$, is positive (Table 1). This stability is enhanced by increasing the V concentration. Moreover, the hole concentration introduced due to the substitution of O by N or P ($Zn_{1-x}V_xN_yO_{1-y}$ or $Zn_{1-x}V_xP_yO_{1-y}$) enhances stability, except for $x = 0.125$ and $y = 0.375$, where the paramagnetic state is more stable than the ferromagnetic one. This may be explained by the charge neutrality. Indeed, each V substituting Zn in ZnO gives

three extra electrons compared with the host cation, while each N (P) substitution anion gives one hole. Thus when the V:N composition is 1:3, this formally maintains the charge neutrality. For $x = 12.5$ at% V, the neutrality corresponds to $y = 37.5$ at% N(P).

**Table 1.** Fermi energy ($E_F$), and relative energy of ferromagnetic and paramagnetic states ($\Delta E = E_{DLM} - E_{FM}$ ) for various $Zn_{1-x}V_xN_yO_{1-y}$ and $Zn_{1-x}V_xP_yO_{1-y}$ systems. The ferromagnetic phase is stable for $\Delta E > 0$.

| | $E_F$/Ry | $\Delta E = (E_{para} - E_{FM})$/mRy |
|---|---|---|
| $Zn_{30}V_2O_{32}$ | 0.4520762 | 0.4898 |
| $Zn_{28}V_4O_{32}$ | 0.4653023 | 0.8683 |
| $Zn_{28}V_4O_{28}N_4$ | 0.4683221 | 1.0211 |
| $Zn_{28}V_4O_{24}N_8$ | 0.5152023 | 1.2116 |
| $Zn_{28}V_4O_{20}N_{12}$ | 0.4851013 | −0.0002 |
| $Zn_{28}V_4O_{28}P_4$ | 0.4699113 | 1.1801 |
| $Zn_{28}V_4O_{24}P_8$ | 0.4703111 | 1.2141 |
| $Zn_{28}V_4O_{20}P_{12}$ | 0.4633421 | −0.0012 |

Figures 2(a)–2(c) show that the conduction bands of $Zn_{1-x}V_xO$ consist mainly of V states. The V 3d states, exhibiting a large exchange splitting, are observed near $E_F$. Because of this situation, a portion of carriers occupies V-3d states when V atoms are doped into this system. The electronic structure of $(Zn_{0.875}V_{0.125})O$ is characterized by an impurity band in the gap, and $E_F$ (Table 1) is in the upper part of this band, leaving one state empty per V. Moreover, the increase in vanadium content enhances the half metallic behaviour. For this reason, we will investigate in the following the effects of N and P co-doping on the 12.5%-V concentration.

In the case of hole doping, figures 3(a)–3(c) show that the hybridization between V 3d states and N 2p states is large, but the hole states still consist mainly of V 3d states. The overlap is observed between V 3d , N 2p, and O 2p states in the spin-up bands, which leads to important DOS at the Fermi energy and hence to the half-metallic character of N co-doped $Zn_{1-x}V_xN_yO_{1-y}$ system. The DOS given in Figs. 3(a) and 3(b) exhibits a double-exchange interaction, which stabilizes the ferromagnetic phase, with the introduction of hole concentration by N co-doping, $y = 0.125$ and 0.25, while for $y = 0.375$, the paramagnetic phase is more stable (Table 1). Moreover, one observes that the gap decreases with increasing N concentration. This shows that ferromagnetism, observed in the $Zn_{1-x}V_xN_yO_{1-y}$, is induced by carriers. Our results are in agreement with experimental ones, which give a strong indication of ferromagnetism.[27] Our discussion does not necessarily mean that the paramagnetic behaviour should be observed in the high carrier concentration region of the diluted magnetic semiconductor. It should be noted that our discussion has been restricted to the ground state properties. It is rather likely that the system is paramagnetic down to a very high carrier concentration. The paramagnetic state is realized because there is no itinerant carrier and there is no contribution of the double-exchange interaction with the ferromagnetism (Fig. 3(c)).

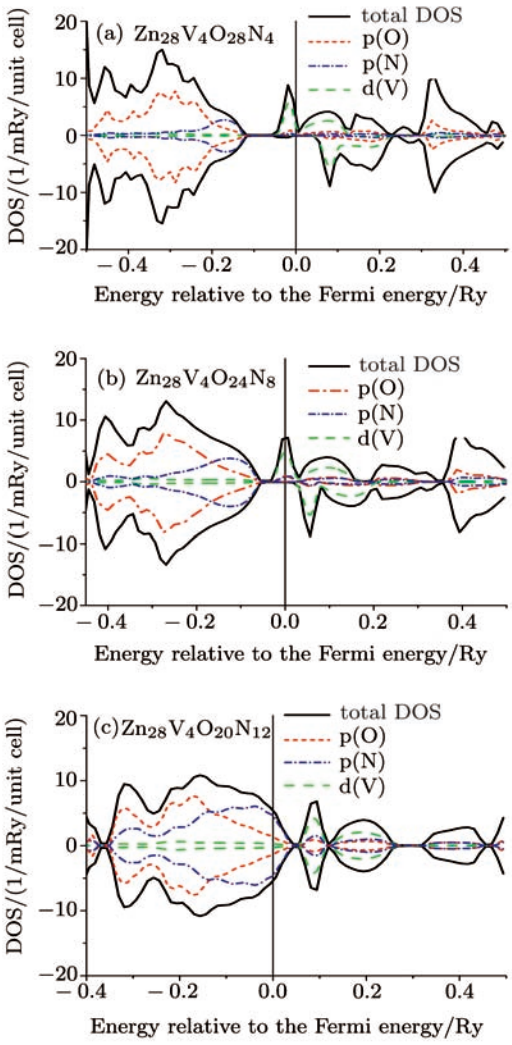



**Fig. 3.** Total and partial DOSs for the ferromagnetic $Zn_{1-x}V_xN_yO_{1-y}$ with $x = 0.12$ and $y = 0.125$ (a), 0.25 (b), and 0.375 (c) for spin up and spin down, showing total DOS state (solid black line), d(V) state (dashed green line), p(O) state (dotted red line), and p(P) state (short dashed-dotted blue line).

Figures 4 (a) and 4(b) show a half-metallic behaviour, in $Zn_{1-x}V_xP_yO_{1-y}$, in the sense that the Fermi level state density is finite for the spin-up. This half-metallicity is due to the V-3d states well hybridized with the P-2p and O-2p states. Due to this hybridization with the V-3d states, holes are itinerant

with keeping their d-character. Therefore, the kinetic energy is lowered so efficiently that the ferromagnetic state is stabilized by the double-exchange mechanism (Table 1).

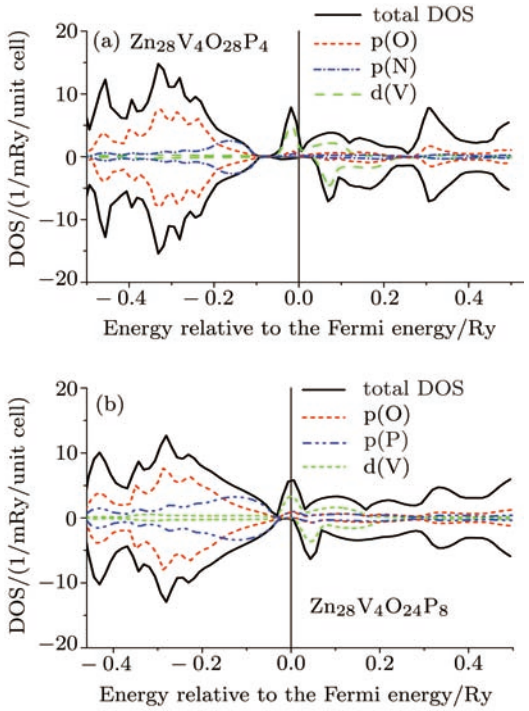



**Fig. 4.** ((a) and (b)) Total and local DOS for the ferromagnetic $Zn_{1-x}V_xP_yO_{1-y}$ with $x = 0.125$ and $y = 0.125$ and 0.25 for spin up and spin down, showing total DOS state (solid black line), d(V) state (dashed green line), p(O) state (dotted red line), and p(P) state (short dashed-dotted blue line).

The nature of the hybridization of the V 3d states and host p-states depends strongly on their relative position in the conduction band or valence band. This hybridization gives rise to the exchange interaction between the localized 3d spins and the carriers in the host conduction band. The d band is divided into spin-up and spin-down sub-bands, and the up and down states are displaced in energy with respect to one another, so that the spin-up band is filled first, while the spin-down states are filled by the remaining electrons, if any. Moreover, one observes that a gap decreases with P concentration increasing. The main characteristic near the Fermi energy is the determination of the magnetic property. It is clearly seen from Figs. 3 and 4 that when N or P changes from 0.125 to 0.25, a smooth change in DOS is observed for both the total DOS and the partial DOS for each kind of atom except near the Fermi level where the changes are significant. By changing the valence number, the electron configuration of magnetic ions differs from $d^5$. But, with P-doped ZnVO, the half metallic character is ensured since there are carriers to mediate the double exchange interactions (p–d exchange).

We also discussed the carrier concentration ($y$) dependence of the V spin magnetic moment (Fig. 5). Doping by N or P atoms introduces carriers, while doping by V atoms introduces local magnetic moments. We find that the ferromagnetic state is the result of N 2p or P 2p and V 3d interaction. Therefore, our calculations show a decrease in the spin magnetic moment with N or P concentration increasing. Indeed, for $y = 37.5\%$-N (P) and $x = 12.5\%$-V concentrations, the paramagnetic phase appears. As indicated above, this corresponds to the charge neutrality.

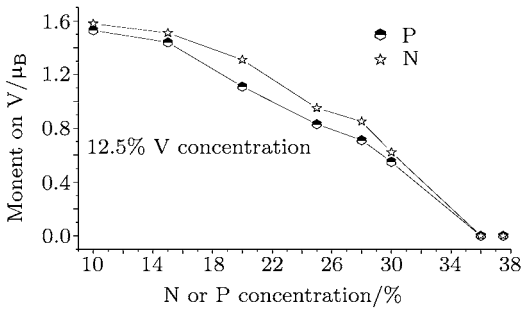



**Fig. 5.** Magnetic moments versus N or P concentration.

## 4. Conclusion

In this work, we report the results of first-principles theoretical calculations of magnetic properties of the zinc-blende ZnO co-doped with V and N or P. The effects of various N and P concentrations on the electronic structures in $Zn_{1-x}V_xN_yO_{1-y}$ and $Zn_{1-x}V_xP_yO_{1-y}$ are studied using the supercell method. The results, obtained within the local density approximation, suggest that the two compounds are likely to order half-metallicity, leading to a magnetically ordered state. We have shown that the V doping atom is the main contributor to the magnetic moment of the structure for both compounds $Zn_{1-x}V_xN_yO_{1-y}$ and $Zn_{1-x}V_xP_yO_{1-y}$. But in the $Zn_{1-x}V_xN_yO_{1-y}$ structure the magnetic moment of V is slightly bigger than that in $Zn_{1-x}V_xP_yO_{1-y}$, which is due to the spin delocalization. The roles of N and P atoms in stabilizing ferromagnetism are studied on the basis of the density of states in N- or P-doped ZnVO.

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