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The electronic structure and magnetic behaviour in the Mn-containing cubic Laves-phase pseudobinary compound of YFe_2

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Abstract. The fully self-consistent discrete variational method within the local-spin-density framework has been employed to obtain the electronic structure and magnetic moments of the Mn-containing cubic Laves-phase pseudobinary compound of YFe_2 . The embedded-cluster model was used to simulate the local environments around Fe in this compound. The calculated results show that the substitution of Mn atoms on Fe sites weakens the ferromagnetism of this compound. With the change of the local environments around Fe, we find that when Fe has one or two Mn atoms in its nearest-neighbour sites, its magnetic moment decreases rapidly, while the Mn moment is $0.71\mu_B$, parallel to the Fe moment; when Fe has four or more than four Mn atoms in its nearest-neighbour sites, the moments of these Mn atoms are reversed and antiparallel to the Fe moments and meanwhile the Fe moments increase. In addition, calculations for the cluster with an Mn atom occupying a Y site indicates that such an Mn atom is in a high-spin state. Based upon our results, the various experimental data have been satisfactorily explained.

1. Introduction

For many years, the cubic Laves-phase compound YFe_2 and its pseudobinary compounds containing Al, Co, Mn etc have been subjected to intense experimental investigations [1–5], especially the Mn-containing pseudobinary compound of YFe_2 : quite a few experimental attempts have been made to establish its magnetic properties [5–11]. Because YMn_2 is an antiferromagnet with Mn magnetic moment $2.7\mu_B$ [12], the ferromagnet YFe_2 can form complete solid solutions with it while sustaining the cubic Laves-phase structure [3]. Magnetization measurements [8] and Mössbauer data [11] show the consistent result that $Y(Fe_{1-x}Mn_x)_2$ remains ferromagnetic until the breakdown of the magnetic order at $x = 0.7$. As to the magnetic moments of Fe and Mn in this pseudobinary compound, however, contradictory results have been reported. Schaafsma *et al* [11] suggested from Mössbauer experiments that Mn appears to carry either less than $0.1\mu_B$ or no magnetic moment at all; from the NMR spectra of ^{89}Y , Nagai *et al* [9, 10] drew the conclusions that Fe moments are hardly changed and there are two kinds of Mn moment: one is antiparallel to the Fe moments and about $0.6\mu_B$ and the other is parallel to the Fe moments and about $2.8\mu_B$; meanwhile Besnus *et al* [8] showed from magnetization, diffuse neutron scattering, Mössbauer measurements, and NMR studies that Mn atoms possess magnetic moments, which are ferromagnetically coupled with Fe moments, and that the mean Fe moments decrease

strongly with increasing Mn content while the Mn moments appear to be less concentration dependent.

Various workers also carried out a large number of electronic structure calculations to explain the magnetic properties of YFe_2 and its pseudobinary compounds containing Al and Co. A few satisfactory results have been obtained [13–17]. However, the problem of the pseudobinary compound $\text{Y}(\text{Fe}_{1-x}\text{Mn}_x)_2$ has so far been put aside by theorists. In recent years, the Mn substitution effect on the magnetic properties of cubic Laves-phase compounds RFe_2 has been more attractive for its merits in improving the giant magnetostriction properties of these compounds [18]. Therefore a theoretical investigation on the magnetic properties of the Mn-containing cubic Laves-phase pseudobinary compound of YFe_2 is valuable.

In this paper we present calculations of charge, spin, and DOS for the Mn-containing pseudobinary compound of YFe_2 using the fully self-consistent discrete variational method within the local-spin-density framework. For transition metals and intermetallic compounds, it is now well recognized that the local magnetic properties and electronic structures are mostly determined by the nature of the atoms involved and the local environments of these atoms. So several embedded clusters are chosen to simulate the local environments of atoms in the Mn-substituted YFe_2 compound, and spin-polarized calculations on these clusters are performed to study the magnetic behaviour of the Mn-containing pseudobinary compound of YFe_2 . Such a self-consistent cluster calculation of local magnetic properties has been applied to a significant number of cases and has been proved to be a powerful technique for studying the local effect [19–23].

The paper is organized as follows. A brief outline of the theoretical approach is given in section 2. Our results are present and discussed in section 3. A summary of our conclusions is contained in section 4.

2. Theoretical approach

We have used the self-consistent-field-linear-combination-of-atomic-orbitals-molecular-orbital (SCF-LCAO-MO) method within the density-functional formalism to perform electronic structure calculations of clusters. The Rayleigh-Ritz secular equation $(H - ES)C = 0$ was solved using the discrete variational method (DVM) [24]. The computational procedure has been documented in detail elsewhere [21], and we only give a brief description. In the one-electron Kohn-Sham equation, the non-local Hartree-Fock exchange potential is replaced by an exchange-correlation potential depending only on the local density. The *von Barth-Hedin form for the exchange-correlation potential* [25] was used in the calculations. The numerical atomic orbitals of Fe, Mn, and Y were employed to construct MOs. The secular equation was then solved self-consistently using matrix elements of the Hamiltonian and overlap obtained by a weighted summation over a set of discrete Diophantus points. About 600 points per atom for larger clusters and 1000 points for smaller clusters were found to be sufficient for convergence in the eigenvalue spectrum to within 0.01 eV. The effect of the rest of the bulk was simulated through an embedding scheme [26].

3. Results and discussion

Since there have been numerous theoretical results for YFe_2 , a cluster calculation on the host compound YFe_2 is carried out first for comparison. The cubic Laves-phase compound YFe_2

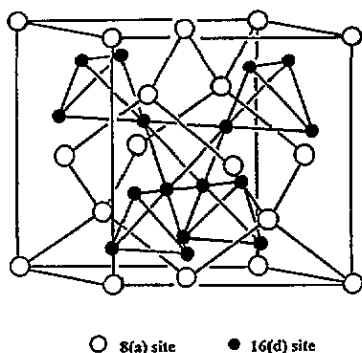


Figure 1. A unit cell of a cubic Laves phase (C15 structure).

Table 1. The local magnetic moments in the different atomic sites of the clusters $Fe_4Y_4Fe_{12}Y_6$ and $Mn_4Y_4Fe_{12}Y_6$.

Cluster			$Fe_4Y_4Fe_{12}Y_6$	$Mn_4Y_4Fe_{12}Y_6$
M(inner)	3d	(μ_B)	1.84	0.85
	4s + 4p	(μ_B)	-0.19	-0.14
	total	(μ_B)	1.65	0.71
Y(inner)	4d	(μ_B)	-0.42	-0.32
	5s + 5p	(μ_B)	-0.16	-0.13
	total	(μ_B)	-0.58	-0.45
Fe(outer)	3d	(μ_B)	3.46	2.92
	4s + 4p	(μ_B)	0.34	0.17
	total	(μ_B)	3.80	3.09
Y(outer)	4d	(μ_B)	-0.51	-0.36
	5s + 5p	(μ_B)	-0.12	-0.10
	total	(μ_B)	-0.63	-0.46

has the cubic $MgCu_2$ C15 structure (see figure 1). There are eight YFe_2 formula units per simple cubic unit cell in this structure. The larger Y atoms occupy a cubic diamond lattice. Regular tetrahedra built of four smaller Fe atoms are centred at the fourfold-coordinated interstitial sites of the diamond structure. So the 26-atom cluster $Fe_4Y_4Fe_{12}Y_6$, which consists of two distinct pairs of Fe and Y atoms, is chosen to represent the host compound YFe_2 . Table 1 lists the calculated magnetic moments of all atomic sites. It is noted that the magnetic moments of Fe atoms are large and coupled ferromagnetically with small negative moments for Y atoms, which is consistent with the conclusion of the band calculation [15].

By analysing the result of the cluster $Fe_4Y_4Fe_{12}Y_6$ in table 1, one can see that the moments for both Fe and Y tend to increase outwardly from inner sites to outer sites due to the surface effect, which results from the fact that the truncation of the cluster does not allow sufficient delocalization of the wave-function in the solid to take place on the cluster surface. The surface effect is unavoidable for the present cluster calculation method; however, the atoms toward the central site for a large cluster can reproduce the properties of the bulk solid [22]. In the present case, the calculated magnetic moment for the inner Fe atoms is $1.65\mu_B$, which is in fairly good agreement with the value of the band calculation [15], while the moment of the inner Y atoms is $-0.58\mu_B$, a bit larger than the band calculated result,

$-0.45\mu_B$; this difference is also attributed to the surface effect. It has been confirmed by many calculations that the cluster model tends to the same limit as band-structure methods when the cluster size increases; however, computation is too expensive for a larger cluster. For most physical properties, it has been observed that a three-to-four-atom-shell cluster is sufficient [19–23].

The atoms of Y in the compound YFe_2 were assumed to be non-magnetic before spin-polarized calculations of its band structure. The cluster and band-theory calculations on YFe_2 both show that the Y atoms are spin polarized with a small negative moment, which can be attributed to the hybridization between Fe 3d and Y 4d states. According to the band-structure calculation, the majority of the 4d bands for Y are just above the Fermi level [27], while most of the states just above the Fermi level for Fe are the 3d minority-spin states. So the 4d states of Y mainly hybridize with the minority-spin 3d states of its neighbour Fe, which results in the minority spin dominating for the occupied 4d bands of Y and hence a negative moment develops on the Y atoms.

Now we study the effect of Mn on the magnetic properties of the pseudobinary compound $Y(Fe_{1-x}Mn_x)_2$. We would like to point out that Mn atoms occupy the 16(d) sites of the C15 structure in the pseudobinary compound $Y(Fe_{1-x}Mn_x)_2$ in a disorderly fashion. However, if the Fe atoms of the cluster $Fe_4Y_4Fe_{12}Y_6$ are substituted arbitrarily with Mn atoms, calculations cannot be made for those clusters without any geometric symmetry. Thus the simple cluster $Mn_4Y_4Fe_{12}Y_6$ is plausible to represent the pseudobinary compound $Y(Fe_{1-x}Mn_x)_2$ with low Mn concentration, since for each Fe atom of the cluster $Mn_4Y_4Fe_{12}Y_6$, there is one Mn atom in its nearest-neighbour sites. We give the result for the cluster $Mn_4Y_4Fe_{12}Y_6$ also in table 1.

From table 1, it is noted that the moments of Mn and Fe are both positive for the cluster $Mn_4Y_4Fe_{12}Y_6$, which shows that Mn moments are coupled ferromagnetically with Fe moments in the pseudobinary compound $Y(Fe_{1-x}Mn_x)_2$ with low Mn concentration. Furthermore, one can see that the magnetic moment of Mn is $0.71\mu_B$ and the Fe moment, $3.09\mu_B$, is much less than that of the corresponding Fe atom in the host cluster, $3.80\mu_B$. The calculated Mn magnetic moment is in excellent agreement with the value obtained by polarized neutron scattering and NMR studies for the pseudobinary compound with low Mn concentration [8], while the Fe moment decreases rapidly with Mn substitution for Fe, which is also in accord with the experimental results [8]. In addition, the Y magnetic moment also decreases. The Mn magnetic moment deduced by Nagai *et al* [9, 10] is opposite to our calculated result, which may result from their oversimplified assumptions that Y atoms in the pseudobinary compound have no magnetic moment and that the hyperfine field at ^{89}Y is strictly proportional to the average magnetic moments of its nearest-neighbour atoms.

The DOS of the cluster $Mn_4Y_4Fe_{12}Y_6$ is depicted in figure 2 with a solid line. For comparison, we also show the DOS of the host cluster $Fe_4Y_4Fe_{12}Y_6$ with a dashed line in figure 2, which roughly resembles the band-structure calculations [28] except for some subtle features due to the total DOS for cluster model consisting of the contributions from all cluster atoms including surface atoms. One can consider it reasonable to concentrate on the changes when Mn atoms are introduced. From these two curves, one can find that there is not a large change in the shape of the DOS when Mn substitute at Fe sites of YFe_2 ; however, the positions of the peaks vary. For majority-spin states, the main peaks below the Fermi level move in the direction of high energy and meanwhile the peaks for minority-spin states move in the low-energy direction; thus the exchange splitting decreases with Mn diluting the Fe sublattice. As is well known, the origin of magnetism can be attributed to intra-atomic and interatomic exchange interactions, and the Curie temperature is proportional to the exchange splitting, so the reduction of the exchange splitting gives rise

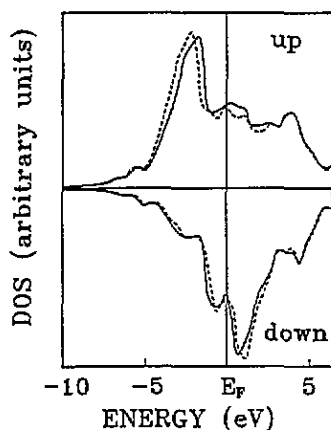


Figure 2. The total DOS for the clusters $Mn_4Y_4Fe_{12}Y_6$ (solid line) and $Fe_4Y_4Fe_{12}Y_6$ (dashed line). The spin-up and spin-down bands are normalized to the same scale.

to the decrease of the Curie temperature. Both magnetization measurement and Mössbauer data show that the Curie temperature decreases almost linearly with the Mn concentration in the pseudobinary compound $Y(Fe_{1-x}Mn_x)_2$ [8, 11], which is consistent with the above conclusion deduced from the electronic structure.

From the results for the cluster $Mn_4Y_4Fe_{12}Y_6$, some aspects of the magnetic properties of the pseudobinary compound $Y(Fe_{1-x}Mn_x)_2$ with low Mn concentration have been well explained. However, with the increase of the Mn concentration, there must be more than one Mn atom in the nearest-neighbour sites of Fe. In order to fully understand the magnetic behaviour of $Y(Fe_{1-x}Mn_x)_2$, several clusters with more than one Mn atom in the nearest-neighbour sites of Fe must be considered. It may be noted here that when more Mn atoms are introduced into the host cluster $Fe_4Y_4Fe_{12}Y_6$, the symmetry of the cluster is reduced. This lack of symmetry makes computations too difficult to execute. As is known, in the compound YFe_2 , an Fe is surrounded by six Fe atoms in its nearest-neighbour (NN) shell and by six Y atoms in its next-nearest-neighbour (NNN) shell. Thus the comparatively small clusters, $FeFe_6Y_6$, $Fe(Mn_2Fe_4)Y_6$, $Fe(Mn_4Fe_2)Y_6$, and $FeMn_6Y_6$, can be chosen to simulate the different local environments in this pseudobinary compound. Of course, the cluster-size effect will increase; nevertheless, one can focus on trends instead of absolute values for magnetic moments. For a reliable comparison, all input parameters, such as the atomic basis functions, the sample points, the crystal potentials, and the initial conditions before the self-consistent procedure are kept fixed for all these clusters.

Table 2. The electron occupation numbers and magnetic moments for clusters representing distinct atomic environments.

Cluster	Central Fe					NN Mn		
	n_{3d}	n_{4s+4p}	μ_{3d} (μ_B)	μ_{4s+4p} (μ_B)	μ_{Fe} (μ_B)	μ_{3d} (μ_B)	μ_{4s+4p} (μ_B)	μ_{Mn} (μ_B)
$FeFe_6Y_6$	6.32	1.63	2.72	-0.24	2.48	—	—	—
$Fe(Mn_2Fe_4)Y_6$	6.29	1.71	1.10	-0.33	0.77	3.91	0.13	4.04
$Fe(Mn_4Fe_2)Y_6$	6.24	1.78	2.16	0.28	2.44	-3.82	-0.31	-4.13
$FeMn_6Y_6$	6.22	1.83	2.05	0.33	2.38	-3.53	-0.17	-3.70

Table 2 shows the local magnetic moments and electron occupation numbers of the central Fe and the NN Mn for the clusters FeFe_6Y_6 , $\text{Fe}(\text{Mn}_2\text{Fe}_4)\text{Y}_6$, $\text{Fe}(\text{Mn}_4\text{Fe}_2)\text{Y}_6$, and FeMn_6Y_6 . Apparently, the central Fe magnetic moment of the cluster FeFe_6Y_6 is larger than the inner Fe moment of the cluster $\text{Fe}_4\text{Y}_4\text{Fe}_{12}\text{Y}_6$ in table 1 due to the cluster-size effect as noted above. From table 2, it can be found that the Mn moments are ferromagnetically coupled with Fe moments while the Fe magnetic moment decreases greatly when there are two NN Mn atoms; the same tendency is observed above in the cluster $\text{Mn}_4\text{Y}_4\text{Fe}_{12}\text{Y}_6$ where one Mn atom is present in the first shell of Fe; with more NN Mn atoms, the Mn moments are reversed and coupled antiferromagnetically with Fe moments, and meanwhile the Fe moment almost reverts to the value for no NN Mn atoms. Besides, it may be seen in table 2 that the magnitudes of the NN Mn moments, either positive or negative, change little with variation of the number of Mn atoms in these clusters.

Based upon the above results, it can be easily understood that the magnetization of the compound $\text{Y}(\text{Fe}_{1-x}\text{Mn}_x)_2$ decreases with increasing Mn concentration. Besnus *et al* [8] observed from NMR studies that in the pseudobinary compound $\text{Y}(\text{Fe}_{1-x}\text{Mn}_x)_2$, the nuclear spectra of Mn at Fe sites are shifted towards lower frequencies in an applied magnetic field when the Mn concentration is less than 20%; however, the Mn spectra broaden strongly when the Mn concentration is above 20%, which can also be explained from our calculated results. When the Mn concentration is low, almost all Mn magnetic moments are coupled ferromagnetically with Fe moments, so the nuclear spectra of Mn are shifted towards lower frequencies in an applied field; however, when Mn concentration increases, some of the Mn atoms have positive magnetic moment and the others have negative moment, and thus the Mn spectra broaden.

It is worth pointing out that charging effects are important to the formation of alloys and intermetallic compounds. From table 2, we can notice that the $4s + 4p$ electron occupation numbers of the central Fe atom increase as there are more and more NN Mn atoms, while its 3d electrons decrease. The former is consistent with the difference between the electronegativities of Fe, 1.8, and Mn, 1.4. Watson and Bennett [29] used a renormalized atom model to suggest that the charge flow in transition-metal alloys and compounds is such that the d-electron flow is in the opposite direction to the non-d-electron flow. This is the case in our present results.

Now we turn to the 3d partial DOS at the central Fe atom in the four distinct clusters, which are depicted in figure 3. As compared with the Fe 3d partial DOS when there is no NN Mn atom, one can find that the Fe 3d partial DOS with two NN Mn atoms exhibits greatly changed multipeak structures, i.e. the main peak for the majority-spin states moves to high energy and lies in the Fermi level; meanwhile the minority-spin states show multipeak structures of an increased peak just below the Fermi energy and reduced magnitude above the Fermi level. As a result, some of the majority-spin electrons flow to the minority-spin bands and the local magnetic moment of Fe decreases. However, the cases for the Fe 3d partial DOSs with four and six NN Mn atoms are completely different. In figures 3(c) and (d), the main peak of majority spin moves to low energy and the two greater peaks of minority spin tend to collapse into a single sharp peak lying in the Fermi level, which shows that the magnetic coupling between the central Fe and its environment is reduced. All these features may be understood from the different hybridizations of the Fe 3d and Mn 3d states. The width of the minority-spin 3d band is well known to be greater than that of the majority-spin 3d band; when the Mn moment is positive, the Mn minority-spin 3d band is higher than the majority-spin 3d band. This means that the interactions of the Fe 3d minority-spin states and Mn 3d minority-spin states are stronger than those of the majority-spin states. Such a strong hybridization results in the lowering of the Fe minority-spin 3d band, so the

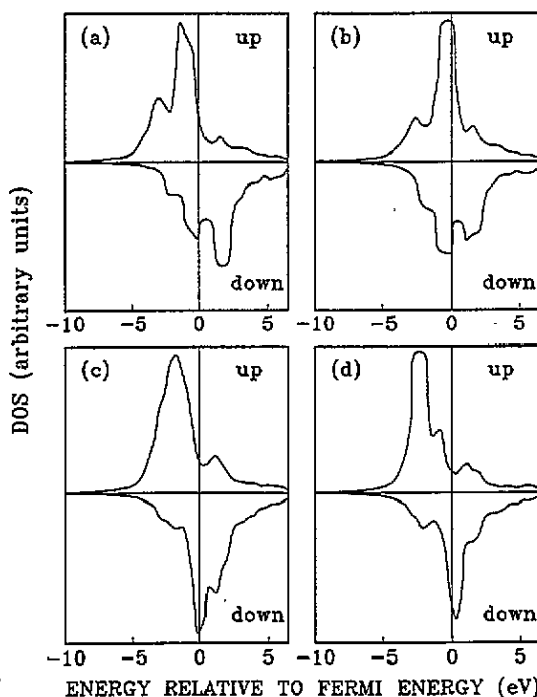


Figure 3. The partial DOS for central Fe 3d majority spin (up) and minority spin (down): (a) $FeFe_6Y_6$, (b) $Fe(Mn_2Fe_4)Y_6$, (c) $Fe(Mn_4Fe_2)Y_6$, and (d) $FeMn_6Y_6$.

majority-spin electrons flow to minority-spin states and the Fermi level moves toward the majority-spin 3d peak. However, when the Mn moment is negative, the Mn minority-spin 3d band is lower than the majority-spin 3d band; thus the hybridizations between Fe 3d states and Mn 3d states reduce greatly, and the Fe magnetic moment increases.

Finally, we consider the Y–Mn disorder effect, i.e. Mn atoms occupying the Y sites. A few percent of Y sites were found, by experimental analysis, to be replaced by Mn atoms in the Mn-containing pseudobinary compound of YFe_2 [8]. The magnetic moment of these Mn atoms was estimated to be $2.8\mu_B$. As is known from the crystalline structure of the cubic Laves-phase compound, the arrangement of near neighbours around a Y atom, in the compound YFe_2 , is composed of 12 Fe and four Y atoms, so the clusters $YFe_{12}Y_4$ and $MnFe_{12}Y_4$ are chosen to represent the ‘perfect YFe_2 ’ and the ‘doped YFe_2 ’ with Mn occupying Y sites, respectively, and the calculated results are given in table 3.

Table 3. The calculated magnetic moments for clusters $YFe_{12}Y_4$ and $MnFe_{12}Y_4$ representing the ‘perfect YFe_2 ’ and the doped YFe_2 with Mn occupying a Y site.

Cluster			$YFe_{12}Y_4$	$MnFe_{12}Y_4$
Central	d	(μ_B)	−0.46	4.23
	sp	(μ_B)	−0.19	0.05
	total	(μ_B)	−0.65	4.28
NN Fe	3d	(μ_B)	3.20	3.33
	4s + 4p	(μ_B)	−0.03	0.02
	total	(μ_B)	3.17	3.35

We notice from this table that the magnetic moment for the central Mn atom is very large. There is no doubt that the Mn atom is in a high-spin state. Of course, there is a cluster-size effect for these two 17-atom clusters, which can be seen from the moment of the central Y atom, $-0.65\mu_B$, larger than the band result, $-0.45\mu_B$. Assuming that the cluster-size effect on the central sites of these two clusters is the same, we calculate the Mn moment multiplied by a factor and its value is $2.96\mu_B$, which is inconsistent with the estimated value from the Mn hyperfine field [8]. It is noted from table 3 that when Mn occupies a Y site, the Mn effect on its NN Fe is very slight. In the compound YFe_2 , the NN distances between Fe and Fe and between Y and Fe are 2.603 \AA and 3.052 \AA , respectively. The latter is much larger than the former. So the Mn atom occupying a Y site hardly affects its NN Fe. Naturally, the Mn atom in such a local environment is more atomic like and its magnetic moment is in the high-spin state. The 3d partial DOS for an Mn atom occupying a Y site is shown in figure 4. Clearly, the main peaks of majority spin and minority spin are both very sharp, which is an 'isolated-atom' behaviour. The atomic-like nature would account for its enhanced magnetic moment.

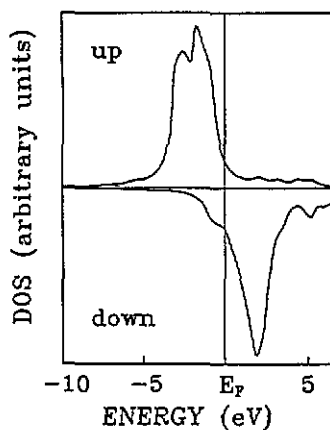


Figure 4. The 3d partial DOS for an Mn atom occupying a Y site.

4. Conclusions

We have performed first-principles SCF calculations on a number of embedded clusters representing the Mn-containing cubic Laves-phase pseudobinary compound of YFe_2 . Several possible environments of atoms around Fe have been considered to study the magnetic behaviour of this pseudobinary compound. Our calculated results for the first time provide an insight into its complex magnetic properties. The following is a summary of our results.

(i) In the compound YFe_2 , the magnetic moments of Fe atoms order ferromagnetically and cause small antiparallel moment at Y sites. Substitutions of Mn atoms on Fe sites reduce the exchange splitting of this compound and hence weaken its ferromagnetism.

(ii) When an Fe atom has one or two NN Mn atoms, its magnetic moment decreases rapidly, while the Mn moment is $0.71\mu_B$, parallel to the Fe moments; when an Fe atom

has four or more than four NN Mn atoms, the moments of these Mn atoms are reversed and antiparallel to the Fe moments, and meanwhile the Fe moment almost reverts to the value for no NN Mn atoms due to the reduction of the hybridization between the Fe 3d states and the Mn 3d states.

(iii) The Mn occupying a Y site has a very large magnetic moment. It is in the high-spin state, which is in consistent with the value estimated from the hyperfine field.

From our studies, we conclude that, when treating the magnetic properties of transition metals and intermetallic compounds with impurities, representation of the system by a small embedded cluster is not only computationally attractive but also physical reasonable. The cluster size may somewhat affect the absolute values of the calculated properties but the relative trend can be obtained quite accurately.

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