

# Proximity effects on the magnetic behavior of Cr<sub>6</sub>-Cr<sub>9</sub> atomic clusters embedded in Fe Bulk

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The magnetic behavior of clusters Cr<sub>6</sub>-Cr<sub>9</sub> in bulk Fe is determined by using an electronic Hamiltonian which includes *s*, *p* and *d* electrons. The spin density distribution is calculated self-consistently in the unrestricted Hartree-Fock approximation. The local magnetic moments  $\mu(i)$  are obtained at various atoms *i* of Cr clusters and of the surrounding matrix. The local magnetic moments at Fe atoms and the magnetic moments of Cr atoms present an antiparallel coupling. The magnetic behavior of Cr clusters depends on two factors, the size of the cluster and the proximity between them. For Cr<sub>6</sub> the magnetic moments at Cr atoms are parallel whereas for Cr<sub>9</sub> the  $\mu_{Cr}(i)$  are antiparallel. The magnetic order in the matrix is not broken by the presence of the Cr atoms, but the local magnetic moments of Fe atoms in the interface cluster-matrix are reduced respect to Fe bulk magnetization. [v.g.  $\mu_{Fe}(5^*)=2\mu_B$  in Cr<sub>6</sub>;  $\mu_{Fe}(3)=1.8\mu_B$  in Cr<sub>9</sub>].

*Keywords:* Local magnetic moments; Magnetic order; Magnetic frustrations

## 1. Introduction

The physics of nanoscale magnetic materials is a current subject in magnetism research. This is partially due to the potential in modern data storage [1] but mainly due to the wide spectrum of novel effects found [2]. When one or more dimensions are reduced, surface and interface effects start to dominate the magnetic behavior; such effects are present in thin films, multilayers and atomic clusters.

The study of small magnetic particles continues to be of importance not only for recording technologies but also for other areas such as biological applications [3]. In particular magnetic nanostructures involving transition metals (TM) have been widely studied, because they exhibit interesting properties subordinated to the structure and of the chemical environment of the atoms. This behavior has motivated the production and experimental study of a large variety of complex magnetic materials involving TM in different geometrical arrangements, trilayers [4], superlattices [5], multilayers [6].

During the last 60 years the magnetism of small particles embedded in a nonmagnetic matrix has been a topic of interest, from both basic and applied points of view [7]. In the last few years, the appearance of new experimental techniques capable of generating samples with controlled nanostructures [8] has led to important advances in the understanding of the behavior of these systems.

One of the most studied systems is Fe-Cr due to the significant interest in exchange coupled Fe/Cr multilayers displaying a giant magnetoresistance effect [9]. Today, an extensive literature has evolved, which traces different aspects of the Cr magnetism in Fe/Cr systems [10], from

these studies it was concluded that the formation of spin density wave magnetism in thin Cr films is governed by a strong exchange coupling acting at the Cr/Fe interface on the hand and by the interface structure/disorder on the other hand [11]. Similar observations have also been made for the spin density wave behavior in other Cr/ferromagnet systems, such as Cr/Co and Cr/Ni [12].

In this paper, we study the magnetic behavior of Cr<sub>6</sub>-Cr<sub>9</sub> isolated embedded clusters and also interacting embedded clusters in a Fe matrix, the atoms of the clusters are located as substitutional impurities in the bulk bcc Fe. This specific problem has been chosen not only for its potential technological relevance but for the rich magnetic behavior of Fe/Cr interfaces. Our systems studied here are non-periodic and one distinction with periodic systems is the existence of local environment effects, in these non-periodic systems all the atoms of the same type present different magnetic behavior, therefore the competition between the antiferromagnetism of Cr and the ferromagnetism of the Fe matrix offers particularly interesting physical situations for studying the interplay between the magnetic properties of clusters and those of the environment. From the perspective of interface magnetism, our work provides additional information to investigations of Fe/Cr systems.

The remainder of the paper is organized as follows. In next section we present the details on how the electronic calculation was performed, which parameters were used, in section 3 we present the discussion of our results, and in section 4 the conclusions of our work are presented.

**Table 1.** Results for local magnetic moments to Cr<sub>6</sub> and Cr<sub>9</sub> atomic clusters embedded in bulk Fe. The upper panel correspond to Cr<sub>6</sub> and the lower panel correspond to Cr<sub>9</sub>. There are three rows; in the first row we give the kind of atoms in each shell, Fe or Cr, in the second row the value of the local magnetic moments  $\mu(i)$  in atomic sites of shell  $i$ , and in the third row the number NN Cr (Fe) atoms in shell  $i$ .

Cr <sub>6</sub>	1'	2'	3'	4'	5'	6'
	Cr	Cr	Fe	Fe	Fe	Fe
	-0.4	-1.39	2.14	2.24	2.0	2.14
	4 Fe	6Fe	1 Cr	0Cr	2 Cr	1 Cr
Cr <sub>9</sub>	1	2	3	4	5	6
	Cr	Cr	Fe	Fe	Fe	Fe
	0.92	-1.76	1.8	2.05	2.27	2.14
	0 Fe	7 Fe	4 Cr	2 Cr	0 Cr	1 Cr

## 2 Model

In order to study the magnetic and electronic properties, we consider a tight binding scheme within the Hubbard Hamiltonian in the unrestricted Hartree-Fock approximation, details for the Hamiltonian used here can be found in Ref. [13]. The diagonal elements of the Hamiltonian can be written as:

$$\mathcal{E}_{i\alpha\beta} = \mathcal{E}_{i\alpha 0} + \sum_{\beta} (U_{\alpha\beta} \Delta v_{i\beta} - \frac{1}{2}\sigma J_{\alpha\beta} \mu_{i\beta}) + z_i \Omega_{\alpha} \quad (1)$$

where  $\mathcal{E}_{i\alpha 0}$  stands for the energy level of the orbital  $\alpha$  of atom  $i$  in the paramagnetic solution of the bulk (e.g. V or Fe). The second term in eq. (1) takes into account the level shifts due to the redistribution of the spin polarized density and to the resulting intra-atomic Coulomb interactions.  $\Delta v_{i\beta} = v_{i\beta} - v_{i\beta 0}$  where  $v_{i\beta} = \langle n_{i\beta\uparrow} + n_{i\beta\downarrow} \rangle$  is the average electronic occupation of the orbital  $i\beta$  and  $v_{i\beta 0}$  the corresponding average occupation in the bulk.  $\mu_{i\beta} = \langle n_{i\beta\uparrow} - n_{i\beta\downarrow} \rangle$  refers to the spin polarization of the orbital  $i\beta$ . The intra-atomic direct and exchange Coulomb integrals are denoted by  $U_{\alpha\beta}$  and  $J_{\alpha\beta}$  respectively. Finally, the last term in eq. (1) takes into account the environment dependent energy level shifts due to non-orthogonality effect and to the crystal-field potential of the neighboring atoms [14], which are approximately proportional to the local coordination number  $z_i$ . The average occupations,  $v_{i\alpha}$  and the local magnetic moments  $\mu_{i\alpha}$  at site  $i$  are determined self-consistently by requiring

$$\langle n_{i\alpha\sigma} \rangle = \int_{-\infty}^{\epsilon_f} \rho_{i\alpha\sigma}(\epsilon) d\epsilon \quad (2)$$

where  $\rho_{i\alpha\sigma} = \text{Im}G_{i\alpha\sigma, i\alpha\sigma}(\epsilon)$  refers to the local density of states (LDOS) at the spin-orbital  $i\alpha\sigma$ . In the case of finite embedded clusters, the Fermi energy ( $\epsilon_f$ ) is given by the matrix (in the present case Fe). The local Green's functions

are calculated by using the recursion method. The number of levels  $M$  of the continued fraction expansion of  $\text{Im}G_{i\alpha\sigma, i\alpha\sigma}(\epsilon)$  is chosen large enough so that the calculated orbital occupations and magnetic moments are independent of  $M$ , in our calculations we used  $M=17$ . All the recursion effects are determined exactly without spurious effects. Therefore a large number of atoms, (about 25000-40000) is involved in the real-space expansion.

The parameters used in the calculations are determined as follows. The hopping integrals  $t(i\alpha, j\beta)$  represent the amplitude for transferring an electron from the orbital  $i\alpha$  to the orbital  $j\beta$  and are given by  $t(i\alpha, j\beta) = \langle i\alpha | H | j\beta \rangle$ , where  $H$  is the Hamiltonian of the system [13].

For atoms of the same element, these  $t(i\alpha, j\beta)$  are fitted to band-structure calculations for the pure elements. The heteronuclear hoppings at the clusters-matrix interface are obtained as the geometric average of the corresponding homonuclear hoppings, this procedure has been proved to be a very good approximation in calculations for alloys and multilayers of TM [15], in the study of the magnetic properties of free TM clusters [16] and in embedded TM clusters in TM matrix [17], whose results are in good agreement with experimental and theoretical results. In this study, the  $d$ -electron exchange integrals are chosen to yield the proper magnetic moment and exchange splittings in the bulk at  $T=0$ ,  $J_{dd}(\text{Fe})=1.05$  eV and  $J_{dd}(\text{Cr})=0.86$  eV. For simplicity we ignore the differences between  $s$  and  $p$  integrals (i.e.  $U_{ss} = U_{sp} = U_{pp}$ ) and take the ratios between the direct Coulomb integrals  $U_{ss}:U_{sd}:U_{dd}$  from atomic Hartree-Fock calculations [18].

The Cr atoms are located as substitutional impurities in the Fe bcc lattice, occupying the full shell of neighbors. We neglect the lattice relaxations around the impurities by fixing the neighboring host atoms at the Fe lattice positions, because both Fe and Cr have the same bcc structure and approximately the same lattice constant 2.87 Å and 2.88 Å for Fe and Cr respectively.

**Table 2.** Results for local magnetic moments to Cr<sub>6</sub>-Cr<sub>9</sub> interacting clusters embedded in bulk Fe, see Fig. 2, there are three rows; in the first row we give the kind of atoms in each shell, Fe or Cr, in the second row the corresponding value of the local magnetic moment is given, in the third row the number of NN Cr (Fe) atoms to Fe(Cr) in shell *i*. The upper panel correspond to Cr<sub>6</sub> and the lower panel correspond to Cr<sub>9</sub>.

Cr <sub>6</sub>	1'	1''	2'	3'	4'	5'	6'
	Cr	Cr	Cr	Fe	Fe	Fe	Fe
	-0.26	0.78	-1.45	2.15	2.27	2.01	2.15
	4Fe	0 Fe	6 Fe	1 Cr	0 Cr	2 Cr	1 Cr

Cr <sub>9</sub>	1	2	2''	3	3''	4	4''	5	5''	6
	Cr	Cr	Cr	Fe	Fe	Fe	Fe	Fe	Fe	Fe
	0.89	-1.75	-1.49	1.80	1.80	2.01	1.80	2.27	2.27	2.15
	0 Fe	7 Fe	6 Fe	4 Cr	4 Cr	2 Cr	4 Cr	0 Cr	0 Cr	1 Cr

The structure around Cr isolated clusters is illustrated in Fig. 1, and the structures around Cr interacting clusters are shown in Fig. 2 and Fig. 3. In all the figures, the numbers label the different non-equivalent atomic sites at which the spin density distribution is calculated self-consistently.

### 3 Results and discussion

In all the cases studied local charge neutrality is imposed at each site *i*. The self-consistent calculations include all the Cr cluster atoms and the Fe matrix atoms at least up to the sixth shell away from the interface between the cluster and the Fe matrix; beyond this shell the spin-density is taken to be the same as in pure Fe. From the figures we can notice that the cluster-matrix interface is not uniquely defined because depends strongly of the number of Cr atoms and their geometrical arrangement. We recall that the total number of NN is eight.

Results for the local magnetic moments of the isolated clusters are given in Table 1, and for interacting clusters are in Table 2 and Table 3.

We found that  $\mu_{Fe}(i)$  and  $\mu_{Cr}(i)$  of the atoms in the cluster-matrix interface present an antiparallel (AP) coupling, which agrees with experimental studies [19] and theoretical calculations [20-22]. The AP alignment at the interface cluster-matrix was explained in terms of the hybridizations between Fe and Cr *d* orbitals [21]. These hybridizations between Fe and Cr *d* orbitals tends to shift the minority (up) *d* levels of Cr to higher energies and the majority (down) Cr *d* levels to lower energies. This reduces the energy and stabilizes the antiferromagnetic solution, this AP alignment rules the magnetic behavior into Cr clusters.

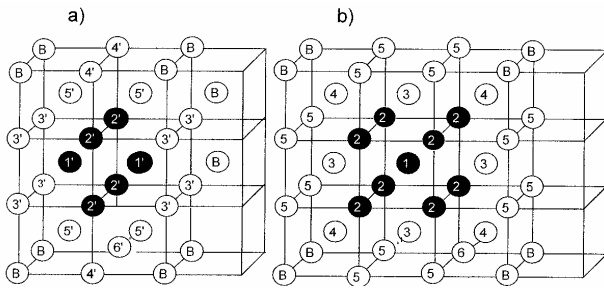
For Cr<sub>6</sub>, the Cr atoms are located at the interface, see Fig. 1; and their local magnetic moments are AP to Fe bulk magnetization giving a parallel (P) coupling between the local magnetic moments at Cr atoms. These atoms have different local environment; therefore the value of the  $\mu_{Cr}(i)$  are different among them, the atomic site 1' has 4 NN Cr atoms and 4 NN Fe atoms, whereas the site 2' has 2 NN Cr atoms and 6 NN Fe atoms. The hybridizations between Fe matrix and the Cr atoms produce a different effect on the *d* the band width at Cr atoms, for atomic site 1' these hybridizations increase the *d* band width at Cr atoms

resulting in a low value of  $\mu_{Cr}(1')$  (the magnetization of bulk Cr is  $0.6\mu_B$ ), whereas for  $\mu_{Cr}(2')$ ; the opposite effect is retained leading to an enhancement of the local magnetic moment. In the Fe matrix only those atomic sites that have Cr atoms into their NN shell present magnetic moments slightly reduced respect to Fe bulk magnetization ( $\mu(Fe)=2.22\mu_B$ ), these reductions are about 3%-10%. From Table 1, we can notice that  $\mu_{Fe}(3')$  and  $\mu_{Fe}(6')$  are equal, due both atomic sites have 1 NN Cr atom; whereas the atomic 5' has 2 NN Cr atoms and present the lowest value ( $\mu_{Fe}(5')=2\mu_B$ ).

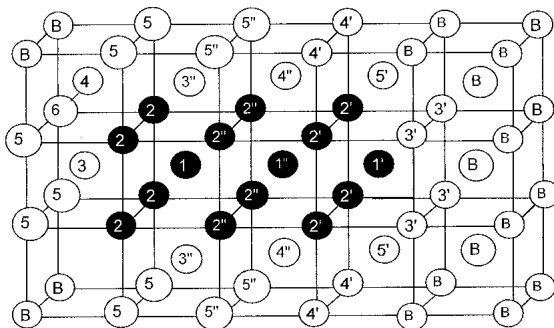
For Cr<sub>9</sub>, not all the Cr atoms are located at the interface cluster-matrix, in this arrangement exist one internal atom and eight interface Cr atoms, see Fig. 1. A change in the magnetic order into the cluster is observed, their local point in opposite direction but the AP coupling at the interface cluster-matrix is not broken. We must notice that the local magnetic moments of Cr atoms at the interface are enhanced by the Fe atoms which are present in their first NN shell, see Table 1.

In both cases, the value of the local magnetic moments of Fe atoms presents a dependence with the number of Cr NN atoms; when the number of Cr NN atoms increases the  $\mu_{Fe}(i)$  are diminished respect to Fe bulk magnetization. From Table 1, we can notice that  $\mu_{Fe}(3)$  is the most reduced, about 19%; this reduction is due to the presence of 4 Cr NN atoms and 4 Fe NN atoms in the NN atomic shell, see Fig. 1; this atomic site can not satisfy an AP coupling with the Cr atoms and a P coupling with the Fe matrix at the same time; this result is known as a magnetic frustration.

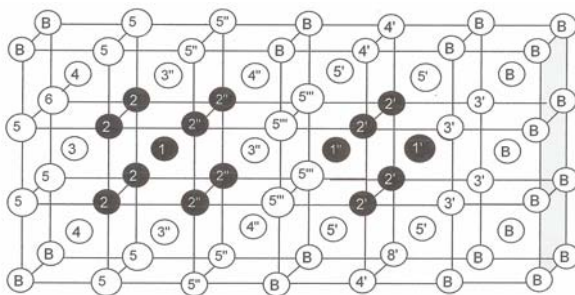
The reductions in the value of  $\mu_{Fe}(i)$  can be qualitatively understood as the result of hybridizations between majority (minority) Fe *d* orbitals and the corresponding minority (majority) *d* orbitals of Cr, which increase the effective local *d* band width at the Fe atoms of the interface. These magnetic frustrations indicate that this system is a candidate to exhibit non-collinear magnetism, and have been found in free Fe<sub>5</sub> cluster [23] and in small Cr clusters [24]. In all these works, the atoms where are present the magnetic frustrations have geometrical arrangements with triangular faces, in our calculations the atoms (Fe or Cr) that present magnetic frustrations have this same



**Figure 1.** Illustration of the lattice structure of Cr<sub>6</sub> and Cr<sub>9</sub> isolated clusters embedded as substitutional impurities in bulk Fe (bcc structure). The cluster atoms are represented by filled circles and the Fe host atoms are represented by open circles. The numbers label the non-equivalent atomic sites *i*. The a) and b) correspond to Cr<sub>6</sub> and Cr<sub>9</sub> respectively, in both cases we show only few atoms, due to the symmetry the other atoms can be inferred.



**Figure 2.** Illustration of the lattice structure of Cr<sub>6</sub> and Cr<sub>9</sub> interacting clusters embedded in bulk Fe, this case correspond when the separation between clusters is the shortest one. The Cr atoms are represented by filled circles and the Fe atoms by open circles. The numbers label the non-equivalent atomic sites, we show only few atoms, due to the symmetry the other atoms can be inferred.



**Figure 3.** Illustration of the lattice structure around of Cr<sub>6</sub> and Cr<sub>9</sub> interacting clusters, this case correspond when the separation between the clusters is increased. The Cr atoms are represented by filled circles and the Fe atoms by open circles.

geometrical arrangement; therefore from the point of view of non-collinear magnetism this system is interesting [25].

For the case of interacting clusters, see Fig. 2, the presence of another Cr cluster modifies the local environment of some atoms (Cr or Fe) and for the sake of comparison we have tried to maintain the same enumeration that for the isolated clusters cases, for example for Cr atoms corresponding to Cr<sub>6</sub>, the atoms labeled with 2' have the same NN atomic shell as in the

isolated case, whereas the atoms located at the vertices only one of them (1') has the same local environment and the other one present now 8 NN Cr atoms, therefore is enumerated 1''; this same situation is present for Cr atoms corresponding to Cr<sub>9</sub>, mainly in the 8 atoms located at the interface cluster-matrix, only 4 atoms present a different NN atomic shell and they are numerated like 2''.

We can see from Fig. 2, that for some Fe atoms their NN atomic shell has been modified too, for example the atomic sites located at the third NN atomic shell (4, 4'').

The first case to consider is when the closest distance between the clusters exist, the lattice structure around the clusters is shown in Fig. 2. From Table 2, we can notice that for Cr<sub>6</sub> the magnetic order is not well defined, the local magnetic moments  $\mu_{Cr}(1'')$  and  $\mu_{Cr}(2')$  are AP among them, whereas  $\mu_{Cr}(1')$  and  $\mu_{Cr}(2')$  are P. This behavior is due that both 1' and 2' are located at the interface cluster-matrix and prefer an AP coupling with Fe matrix, whereas 1'' does not belong to the interface, now the atomic site is surrounded by 8 Cr NN atoms, see Fig. 2, and prefer the AP coupling with these Cr atoms. We can notice that all the Cr atoms in Cr<sub>6</sub> have changed the modulus of their  $\mu(i)$  (with respect to isolated Cr<sub>6</sub>), see Table 2. For the atoms located at the interface cluster-matrix, the largest change correspond to  $|\mu(1')|$  this change is about 35%, and for internal atoms the largest change correspond to the site 1''.

For Cr<sub>9</sub>, the magnetic order is not broken, the coupling between Cr atoms is keeping AP. But the modulus of  $\mu_{Cr}(1)$  and  $\mu_{Cr}(2'')$  are different respect to the Cr<sub>9</sub> isolated cluster, they are reduced; for atomic site 1, its local magnetic moment has diminished about 3%, whereas  $|\mu_{Cr}(2'')|$  present a change about 27%, and  $|\mu_{Cr}(2)|$  does not present a significant change, takes almost the same value that  $\mu_{Cr}(2)$  in Cr<sub>9</sub> isolated cluster, because this atomic site presents the same local environment.

When the distance between the Cr clusters is increased, Fig. 3, we can notice that the local environment for each cluster is the same that the corresponding isolated cluster, see Fig. 1, *i.e.* for Cr<sub>6</sub>, the Cr atoms are located at the interface cluster-matrix and the  $\mu_{Cr}(i)$  are aligned P and the magnetic coupling with the Fe atoms is AP, the local magnetic moments in Cr and Fe atoms take the same value that for Cr<sub>6</sub> isolated cluster.

For Cr<sub>9</sub>, the different  $\mu(i)$  take the same value as for Cr<sub>9</sub> isolated cluster and the AP coupling is not broken, see Table 3.

For the next distance, our results shown the same values for  $\mu(i)$  and magnetic behavior than for the corresponding isolated clusters, these results allow us conclude that the interaction between Cr clusters is of short order. One perspective for this work, is consider larger interacting clusters in order to study the role of the geometry of them in the local magnetic moments of the Fe atoms, because in some cases the AP coupling between Fe and Cr atoms can be broken as is shown by [26].

In all the cases studied the ferromagnetic order in Fe matrix is not broken by the presence of Cr clusters, the

main changes are in the modulus of  $\mu_{\text{Fe}}(i)$  with Cr atoms into their NN atomic shell.

Comparing the results for different Fe atoms, one observes that the  $\mu_{\text{Fe}}(i)$  decreases as the number of NN Cr atoms ( $z_{\text{Cr}}(i)$ ) increases. For  $z_{\text{Cr}}(i) = 4$ , the  $\mu_{\text{Fe}}(i)$  takes the lower value ( $\approx 1.88\mu_{\text{B}}$ ), in this case this results can be interpreted like a magnetic frustration as was discussed above, for  $z_{\text{Cr}}(i) = 2$  the  $\mu_{\text{Fe}}(i) = 1.98\mu_{\text{B}}$  and for  $z_{\text{Cr}}(i) = 1$ , the  $\mu_{\text{Fe}}(i) \approx 2.08\mu_{\text{B}}$ , see Table 1, Table 2 and Table 3.

#### 4 Conclusions

The proximity effects on the magnetic properties of bcc  $\text{Cr}_6$  and  $\text{Cr}_9$  clusters embedded in a Fe matrix have been determined by solving a Hubbard-like Hamiltonian in the unrestricted Hartree-Fock approximation, this model includes *spd* electrons. The competition between the ferromagnetic order of Fe matrix and the tendency of Cr clusters to an AP alignment in their  $\mu_{\text{Cr}}$ , results in a remarkable dependence of the environment and of the chemical composition of the atoms. The main conclusions are summarized as follows.

- a) The AP coupling between the magnetic moments of the atoms at the cluster-matrix interface rules the magnetic coupling into Cr atoms; for  $\text{Cr}_6$  the local magnetic moments  $\mu_{\text{Cr}}(i)$  points in the same direction, whereas for  $\text{Cr}_9$  the local magnetic moments are antiparallel.
- b) The magnetic behavior into Cr atoms for  $\text{Cr}_6$  is not well established, *i.e.*, the P coupling as AP coupling between  $\mu_{\text{Cr}}(i)$  coexist due to the presence of another Cr cluster, whereas for Cr atoms in  $\text{Cr}_9$  the AP alignment is keeping.
- c) When the distance among the clusters is increased the coupling alignment between  $\mu_{\text{Cr}}(i)$  in  $\text{Cr}_6$  is P, as a  $\text{Cr}_6$  as in  $\text{Cr}_6$  isolated cluster but  $\mu_{\text{Cr}}(1'')$  presents a slightly variation on its modulus, whereas for  $\text{Cr}_9$  the behavior is the same as in the isolated cluster case. These results show that the interaction between Cr clusters is a short range type.
- d) The presence of another cluster, modifies the local environment of some Cr atoms leading a strong variation in the corresponding magnetic moments, for  $\text{Cr}_6$ ,  $\mu_{\text{Cr}}(1'') = 0.78\mu_{\text{B}}$ ; besides the interaction modifies the local magnetic moment of Cr atoms where the local environment does not change,  $\mu_{\text{Cr}}(1') = -0.26\mu_{\text{B}}$  see Fig. 2 and Table 2.
- e) In all the cases studied here, the ferromagnetic order in Fe matrix is not broken, although the magnetic moments of Fe atoms close to Cr clusters are diminished respect to Fe bulk magnetization ( $\mu_{\text{Fe}} = 2.22\mu_{\text{B}}$ ); when the number of Cr atoms  $z_{\text{Cr}}(i)$  increases,  $\mu_{\text{Fe}}(i)$  decrease, and present the lowest value when  $z_{\text{Cr}}(i) = 4$ .

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