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# Magnetic states in mixed Fe$X$ ($X=3d$) clusters on the Ag(001) surface

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We apply the local approximation of the density-functional theory and Korringa-Kohn-Rostoker Green's-function method to investigate magnetic properties of Fe$X$ ($X=3d$)clusters on Ag(001). Mixed dimers, impurities in small Fe clusters, plain islands, and cluster sandwiches are considered. In many cases we find both ferromagnetic and antiferromagnetic solutions with large magnetic moments. In particular, we discuss FeCr and FeMn supported clusters. Total-energy calculations show that the energy difference between magnetic configurations in these systems is small; therefore, magnetic fluctuations are possible in FeCr and FeMn nanostructures. [S0163-1829(98)06220-1]

The magnetic coupling of Fe with 3$d$ elements has been intensively studied in the past few years, in part because of the discovery of oscillatory interlayer exchange coupling and the giant magnetoresistance in Fe/Cr multilayers.[1] Experimental investigations of 3$d$ layers on the Fe(001) surface demonstrated a complicated and contradictory picture of the magnetic coupling, and indicated that the structure of the surfaces and interfaces plays an important role in forming of magnetic states.[2] For example, the very large ($>4\mu_B$) magnetic moment for Cr atoms at the Cr/Fe(001) interface for submonolayer thicknesses, and a decreased moment of $M_{\mathrm{Cr}}=3\mu_B$ after completion of the first monolayer, have been found by means of *in situ* magnetometer measurements.[3] Spin-resolved photoemission and energy-loss spectroscopies of Cr give smaller moments for Cr at the interface with Fe ($M_{\mathrm{Cr}}=1.83\ \mu_B$) (Ref. 4) or a moment similar to bulk Cr.[5] Soft-x-ray magnetic circular dichroism measurements have indicated a small moment of Cr ($0.6\mu_B$) for a submonolayer level of coverage on Fe(001).[6]

A curious magnetic behavior was also found in experiments on Mn/Fe interfaces. Mn is of great interest as a possible high-magnetic-moment material. With a half-filled $d$ shell, the free Mn atom possesses the large magnetic moment of $5\mu_B$. In the bulk Mn is antiferromagnetic with a small magnetic moment of $0.65\mu_B$. There has been a constant search for a suitable environment where Mn could be found in a phase with a magnetic moment close to its value in the free atom. Investigations of Mn on Fe(001) by spin-polarized electron-energy-loss spectroscopy detected antiparallel coupling between 1 ML of Mn and Fe, but for low coverage a parallel coupling was found.[7] The study of ultrathin Mn films on Fe(001) by soft-x-ray magnetic circular dichroism showed that up to 2 ML the Mn/Fe interfacial coupling is ferromagnetic, and Mn has a magnetic moment about $1.7\mu_B$.[8] The most recent experiments on Mn/Fe(001), with the magnetic circular dichroism method, revealed that for a small level of monolayer coverage the magnetic moment of Mn is very large (more than $4\mu_B$) and antiparallel to the Fe substrate.[9] Antiferromagnetic coupling within the Mn monolayer was found in these experiments. Experiments with FeMn particles[10] demonstrated a ferromagnetic coupling, but alloys of the same compositions are antiferromagnetic.

First-principles calculations based on the density-functional theory[11] predicted that Fe layers in FeCr with $B2$ structure are ferromagnetically aligned with neighbouring Cr atoms, but the antiferromagnetic configuration becomes more stable for thicker Fe layers. The full-potential augmented-plane-wave method calculations[12] for Cr monolayers on Fe(001) showed that two magnetic states are nearly degenerate, and at the middle of the series the magnetic coupling changes from antiferromagnetic to ferromagnetic. Similar results have recently been found in the framework of the tight-binding (TB) approach,[13] and the possibility of various magnetic configurations in CrFe monolayers was found in TB calculations.[14] The complicated character of magnetic states was also pointed out in Fe$X$ alloys. For example, in ordered FeV compounds, the calculated local moments of Fe and V are antiparallel at large volumes and parallel at small ones.[15] Recent TB linear-muffin-tin-orbital coherent potential approximation (CPA) calculations of FeV alloys[16] showed that the magnetic moment of Fe approaches zero with an increasing number of V neighbors, while, in the Cr matrix, the moment of Fe does not change so dramatically and decreases linearly with an increasing number of Cr neighbors to a value of $1.85\mu_B$ Korringa-Kohn-Rostoker (KKR)-CPA calculations for FeMn and FeCr disordered bcc alloys indicated the transition from ferromagnetic to antiferromagnetic coupling with the concentration of Cr(Mn).[17] The calculations for Fe clusters embedded in antiferromagnetic

Cr[18] revealed that the order within Fe clusters changes from antiferromagneticlike to ferromagneticlike with increasing cluster size.

The local behavior of 3*d* impurities in the Fe host is different from those in Ni and Co hosts. Magnetic moments of 3*d* impurities in Fe change sharply from negative values for Cr to the positive one for Mn, but in Ni and Co such a transition takes place in a relatively large region of the coexistence of two solutions.[19] Investigations in the framework of KKR for 3*d* adatoms and dimers on the Fe(001) surface[20] predicted the transition from an antiferromagnetic state for Mn as an impurity in the surface layer to a ferromagnetic ground state for the Mn adatom. It was also found that ferromagnetic and ferrimagnetic solutions are degenerated for the Mn dimer. Thus experimental results and calculations by different theoretical methods lead to the conclusion that a rich variety of magnetic states is possible in Fe*X* systems. A small energy difference between magnetic configurations was found (20–100 meV/atom). Transitions between different states take place with a changing of the level of coverage in the monolayers. Therefore, investigations of magnetic states in small Fe*X* clusters are highly desirable. This can shed light on the physics of the very complicated character of magnetic states in Fe*X* systems. Also, one should note that recent results in atomic manipulation show that very small clusters of only a few atoms can be produced on metal surfaces.[21] The progress in new magnetic materials is connected to the possibility of creating magnetic systems on metal surfaces.

In this paper we investigate the magnetic states in small Fe*X* clusters on the Ag(001) surface. This surface is very often used in experiments, and plays an important role as an optimal substrate which allows two-dimensional (2D) magnetism to occur. Its influence on magnetic states in clusters, and monolayers comes mainly from an interaction between the $sp$ states of Ag and the $d$ states of supported clusters. We concentrate mainly on FeCr and FeMn clusters and show that different magnetic states are possible in these systems. To our knowledge this is the first *ab initio* calculation of supported small Fe*X* clusters. Our calculations are based on the density-functional theory in the local-spin-density approximation (LSDA). The LSDA has been used with great success in order to determine the structure and geometries of solids and molecules, and their vibrational properties and elastic constants, and in particular to describe the itinerant magnetism in solids composed of transition-metal elements. Lattice constants, bond lengths, and magnetic moments can be calculated within typical errors of some percent in comparison to experiments. A recent publication by Cheng and Wang[22] demonstrated that the LSDA is applicable to antiferromagnetic Cr clusters. As regards possible effects of involving generalized gradient corrections (GGA's), we have to note that although the GGA gives the correct bond length for some systems, it overcorrects LSDA predictions for some other systems.[23] In particular, it has been reported that the LSDA gives a more correct lattice constant for bulk Rh compared to the GGA, and that the GGA corrects the LSDA by just a little bit (0.2%) for the interlayer spacing of a clean Rh surface.[24] It is questionable which approximation (GGA or LSDA) gives more correct in-plane and out-of-plane lattice constants for Rh/Cu(001), investigated in Ref. 25. LSDA and GGA calculations of Singh[11] for magnetic transitions in FeCr multilayers[11] yielded similar results. Recently, Asada and Blügel investigated the energetics of Cu-3$d$ surface alloys using LSDA and GGA approximations.[26] They found that if the experimental lattice constant is used in the calculations, the results, obtained in the LSDA are almost equivalent to the GGA results. In our calculations we use the experimental lattice constant for the Ag ($a=7.73$ a.u.).[27]

The KKR Green's-function method for impurities and clusters on metal surfaces, developed in Ref. 28, is used. By removing the atomic potentials of a few monolayers (5-7) of a crystal, we create two half-crystals, which are not coupled due to the work-function barrier. A surface is treated as a 2D perturbation of a bulk. Multiple-scattering theory is used to obtain the Green's function of the surface using the Dyson equation. The structural Green's function of an ideal surface is used as the reference Green's function for calculations of clusters on metal surfaces. The atoms of the clusters studied here occupy ideal lattice sites (hollow sites). The nearest-neighbor distance of atoms in the cluster is the nearest-neighbor distance of the Ag lattice. The relaxation of the Ag surface has been found experimentally to be fairly small.[29] We allow the potentials of all adatoms and all reference sites adjacent to the adatoms to be perturbed. The full charge density is taken into account by a multipole expansion up to an angular momentum of $l=6$. Coulomb and exchange-correlation energies are calculated using $l=12$. The local potential of Ref. 30 is used in our calculation. The potential is assumed to be spherically symmetric inside the Wigner-Seitz spheres. The spherical symmetric potential is only used to generate the wave functions and the charge densities, whereas the full anisotropic charge density is used in the calculations of the total energies.[31] This approximation for the total energy calculations takes into account nonsphericity in the charge distribution at the surface, and leads to sufficiently accurate interaction energies. Our previous investigations showed that the spherical approximation for the potentials does not strongly influence magnetic moments of transition-metal impurities and supported clusters, because the contribution of $s$ electrons in magnetic moments (and energies) is very small. Moments and energies are mainly determined by well-localized $d$ electrons.

Our method has been successfully applied to various systems in the past.[28] For example, the prediction of 4*d* magnetism for adatoms on metal surfaces has just been verified experimentally.[32] Technical details of the method can be found elsewhere.[28]

First, to understand the main tendency in magnetic coupling in Fe*X* supported clusters, we discuss the mixed Fe*X* dimers which are the simplest supported clusters showing the influence of interatomic interactions on the magnetism. The general trend in electronic states of mixed Fe*X* supported dimers can be seen in Fig. 1, where the local density of states (LDOS) of a Fe, Mn, and Cr atom in FeFe, FeMn, and FeCr dimers are shown for ferromagnetic coupling. In FeFe and FeMn, the majority bands are filled and practically unchanged. At the same time the minority LDOS on Mn is shifted to higher energies compared to the LDOS of the FeFe. This shift arises because of the local Coulomb potential for Mn is less attractive. For the majority states the Coulomb and exchange potentials act at opposite directions;

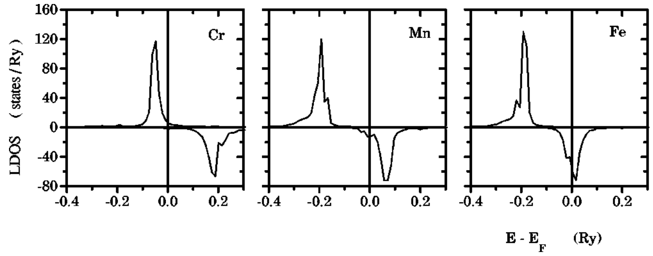

FIG. 1. LDOS (*d* component) on Cr, Mn, and Fe atoms in FeCr, FeMn, and FeFe dimers at the Ag(001) surface for the ferromagnetic configuration.

therefore in FeFe and FeMn the majority states are similar. For Cr in FeCr the exchange potential is not compensated for by the Coulomb potential, which is weaker than for Mn in FeMn; as a result, for Cr the majority states move to the Fermi level and become slightly depopulated. This effect destabilizes the ferromagnetic state in FeCr, and one can expect a transition to antiferromagnetic coupling in FeCr. Our total-energy calculations show that FeCr has antiferromagnetic ground state, but the energy difference between ferromagnetic and antiferromagnetic states is very small, 20 meV/atom. The ferromagnetic state for FeMn is more stable than the antiferromagnetic one, with the same order of the energy difference 50 meV/atom. A similar result was found for Cr monolayers on Fe(001).[12] Calculations for Mn impurities in Fe (Ref. 19) also indicate that Mn is a very critical case, and different magnetic solutions were reported for this system.

Magnetic moments of Fe*X* dimers are shown in Fig. 2. The largest moments are found for ferromagnetic FeMn and antiferromagnetic FeCr. For all mixed dimers, except FeSc and FeNi, the two solutions are found. For Sc we do not find the ferromagnetic solution. Ni shows only ferromagnetic coupling with Fe. The magnetic moments for antiferromagnetic and ferromagnetic states are very close. For example, for FeMn the following moments are obtained: $3.23\mu_B$ (Fe) and $4.50\mu_B$ (Mn) for the ferromagnetic state; and $3.35\mu_B$ (Fe) and $-4.40\mu_B$ (Mn) for the antiferromagnetic state. For FeCr the moments for both configurations are also very close: $3.35\mu_B$ (Fe) and $4.40\mu_B$ (Cr) and $3.25\mu_B$ (Fe) and $-4.50\mu_B$ (Cr). A similar tendency was found for 3*d* monolayers on Fe(001).[12]

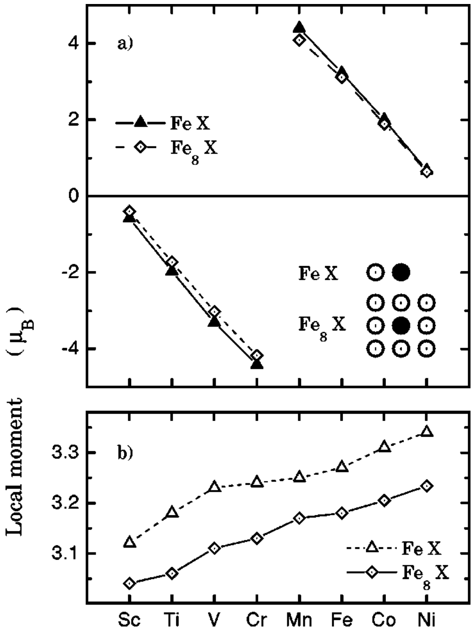

FIG. 2. (a) Magnetic moments on *X* (3*d*) atoms in mixed dimers and in ferromagnetic Fe clusters of eight atoms. The coupling is antiferromagnetic from Sc to Cr, and ferromagnetic from Mn to Ni. (b) Magnetic moments of Fe atom in dimers and Fe atoms as the nearest neighbors of impurities in clusters. Magnetic moments are given in Bohr magnetons.

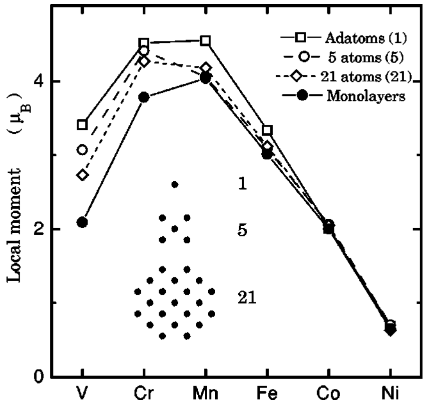

FIG. 3. Comparison of magnetic moments of adatoms and ferromagnetic islands with monolayer results. Moments of central atoms of clusters are presented. Results for clusters of nine atoms are similar to the 21-atom clusters.

In the last years considerable progress has been made concerning the local behavior of impurities in metals. Impurities in low-dimensional systems (clusters and monolayers) present a class of systems which can exist at surfaces due to the interdiffusion of atoms. Therefore, it is important to investigate properties of such systems. We have calculated magnetic states of 3*d* impurities in the ferromagnetic Fe clusters, as shown in Fig. 2(a). One can see that values of moments of 3*d* impurities are close to the dimer results, and that the character of magnetic coupling of impurities with Fe is the same: the transition from an antiferromagnetic to a ferromagnetic configuration is obtained for the Mn impurity in the Fe cluster. The inner atoms in the plain islands of nine atoms look like atoms in monolayers; therefore, one can expect that single 3*d* impurities in Fe monolayers show a similar behavior. To support this prediction, we have calculated ferromagnetic clusters of five and 21 atoms, and compared magnetic moments for the central atoms with monolayer results[33] (cf. Fig. 3). Since the 3*d* wave functions are well localized for the elements on the right side of the 3*d* series, the local magnetic moments at central atoms of clusters are very close to monolayer moments. In contrast, for the early elements (V, Cr) which exhibit a stronger hybridization due to the more extended 3*d* wave functions, the moments of the central atoms in clusters are not saturated. Therefore, we expect that magnetic moments of 3*d* impurities in small clusters are close to those in monolayers. For example, the magnetic moments of Cr and Mn impurities in an Fe cluster of 21 atoms ($-4.13\mu_B$ for Cr and $4.16\mu_B$ for Mn) are nearly the same as in a cluster of nine atoms. It is important to note that, in all clusters, the magnetic moments of Fe atoms as the nearest neighbors of impurities are close, but an interesting tendency is observed [cf. Fig. 2(b)]: for early 3*d* impurities the moment of neighboring Fe atoms show a decreased value

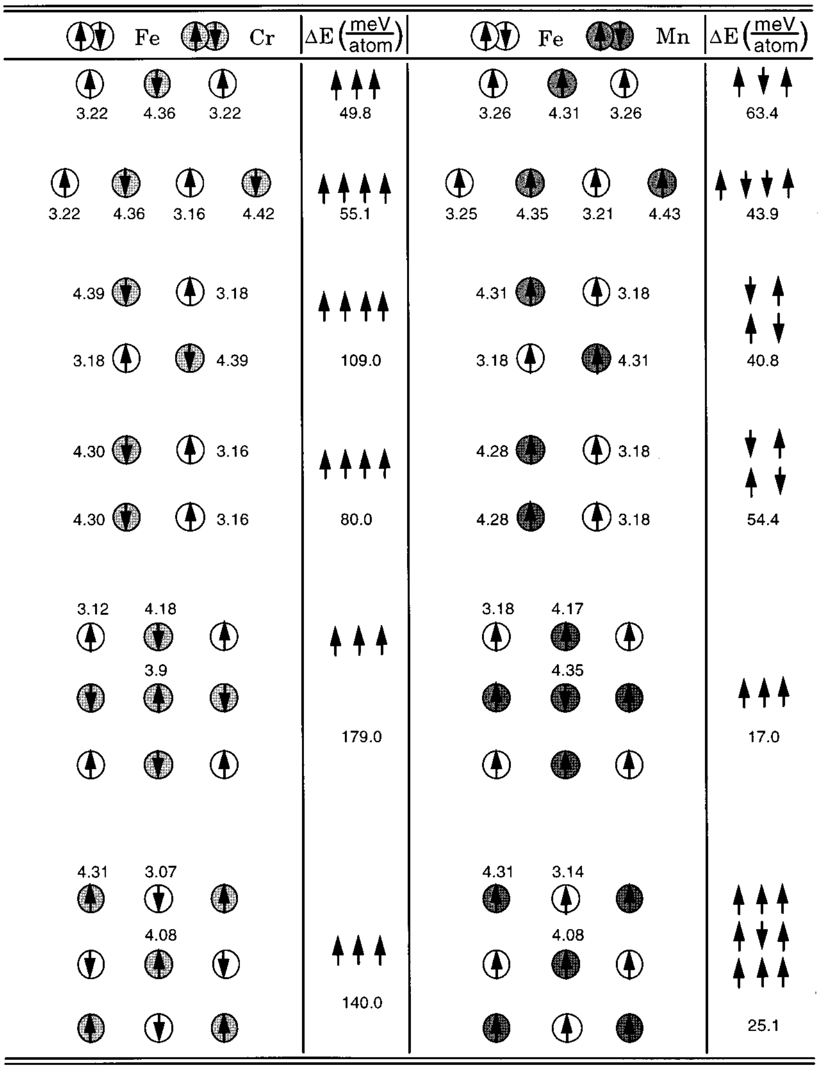

FIG. 4. Magnetic configurations in mixed clusters and energy differences between these states and metastable ones (in meV per atom). We do not present moments for metastable configurations because they are very close to those in Fig. 1.

compared to pure Fe clusters, whereas for late 3*d* impurities the moment is enhanced. This behavior is similar to what is found for 3*d* impurities in Fe,[19] and for 3*d* monolayers on Fe(001).[34]

We consider results for FeCr and FeMn clusters of different geometries and sizes in more detail. We performed calculations for linear chains and plain islands of these clusters. Although first-principles calculations of all the possibilities of intermixing are out of reach, we believe that the main results found in our investigations remain the same for clusters of different sizes and geometries. In Fig. 4 we show the most stable magnetic configurations for some cluster shapes and compositions. Energy differences between ground states and metastable configurations are also presented. Despite their different geometries, nearest-neighbor coordination, and composition, the magnetic moments of atoms in clusters are large and similar in magnitude. This is because the majority *d* states are practically filled for these elements, and *sp* contributions to the magnetic moments are small. It is useful to recall again the most recent publications for Fe/Cr (Ref. 3) and Fe/Mn (Ref. 9) interfaces. Large moments for Cr and Mn have been found experimentally. In all FeCr clusters, Fe and Cr adatoms have an antiferromagnetic coupling, while for FeMn ferromagnetic configurations are the most stable, except the cluster of nine atoms with Mn atoms as next-nearest neighbors. The energetic balance between the magnetic states in all clusters is very delicate. Transitions between these states could be caused by small variations in experimental conditions. We have investigated many different magnetic configurations for FeCr and FeMn clusters, and in all cases the energy differences between states are small. As an example, we present results for FeCr and FeMn systems with a sandwich structure (cf. Fig. 5). Ferromagnetic Fe clusters of 21 atoms are covered by Cr(Mn) clusters of 16 atoms.[35] The following magnetic configurations are calculated: (1) Cr(Mn) clusters being ferromagnetic, have a ferromagnetic coupling with Fe clusters; and (2) moments of Cr(Mn) and Fe clusters are antiparallel. The magnetic moments for the central part of the clusters for all configurations are shown in Fig. 5. The energy differences between magnetic states are also presented in this figure. One can see that, in cluster-cluster interfaces, the magnetic moments are large. Ferromagnetic and antiferromagnetic states for Fe/Cr sandwiches are degenerate. The ferromagnetic configuration for Fe/Mn is more stable than the antiferromagnetic one.

Our previous calculations for spin-polarization energies showed that, in most cases, these energies are large (about 1 eV and more). At the same time typical energies for lattice

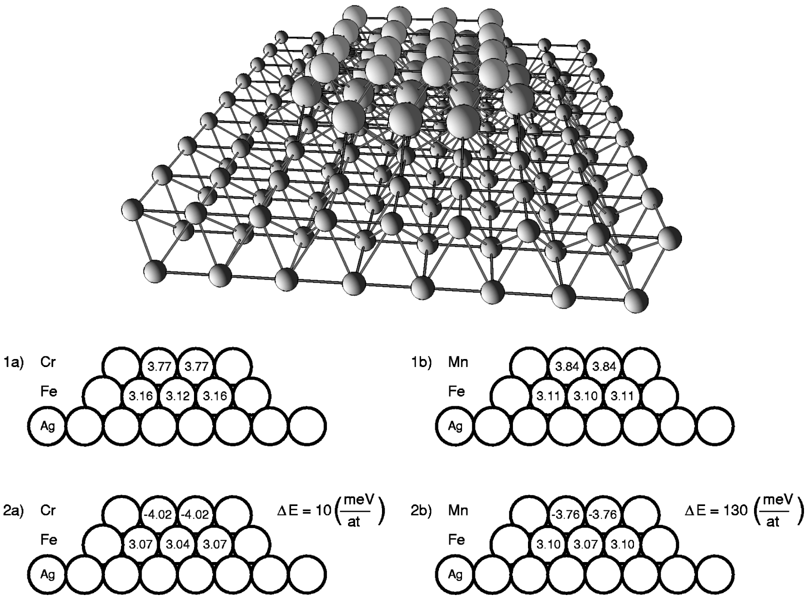

FIG. 5. Sandwiches of FeCr and FeMn clusters on an Ag(001) surface. Magnetic moments of the central part in the cluster-cluster interfaces are presented for two configurations, as explained in the text. (a) Ferromagnetic and antiferromagnetic interfaces for Cr/Fe cluster. (b) Ferromagnetic and antiferromagnetic interfaces for Mn/Fe cluster. The first configurations have lower energies.

relaxations are less than 0.1 eV. Therefore, in most cases, calculated moments cannot be seriously affected by relaxation.[36] The central result of our work is the small energy difference between magnetic configurations in FeCr and FeMn clusters. This result is obtained by ignoring any monolayer and cluster relaxations. A first-principles study of the relaxation of clusters on surfaces is difficult and, to our knowledge, has not yet been performed for transition-metal clusters. However, one of the dominant effects of surface relaxation is the change in the interatomic distance of the atoms in the cluster as well as on the surface. To examine the influence of the changes in bond lengths on the stability of various magnetic states, we calculate FeCrFe and FeMnFe linear chains of three atoms on the Cu(001) surface. The lattice constant of Cu is about 10% shorter than the lattice constant of Ag, which strongly increases the hybridization in clusters and with the substrate. We found that the energy difference between ferromagnetic and antiferromagnetic states is also small (58 meV for FeCr, and $-90$ meV for FeMn). We recall again recent calculations of Handschuh and Blügel for Cr monolayers on the Fe(001) surface.[12] Using the full-potential linearized augmented-plane-wave method, and taking into account interlayer relaxations, they found no switch from one magnetic coupling to any other one during the interlayer relaxation.

From the present results, one can expect that magnetic states in FeCr and FeMn clusters will be very sensitive to the structural and chemical environment, as it takes place for Fe/Cr and Fe/Mn interfaces and alloys. The changes in bond length in FeCr and FeMn caused by external conditions or relaxations can lead to different ground states in these clusters. One can speculate that these systems can be driven from one state to another by applying magnetic field or temperature.

In summary, we have performed first-principles calculations of magnetic states in Fe$X$ ($X=3d$) clusters on an Ag(001) surface. The transition from antiferromagnetic to ferromagnetic coupling is found in the middle of the $d$ series. Different magnetic structures with large local magnetic moments and with close energies are expected for FeCr and FeMn nanostructures. The small energy difference between magnetic configurations found in our calculations is in line with similar findings for monolayers. Therefore, different magnetic states should be found in future experiments with FeCr(Mn) nanostructures, and results might be very sensitive to the experimental growth conditions. We hope that this work will also stimulate research on magnetic bistability in supported FeCr and FeMn clusters.

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