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Effects of spin-orbit coupling on the spin structure of deposited transition-metal clusters

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The influence of the spin-orbit coupling on the magnetic structure of deposited transition-metal nanostructures has been studied by fully relativistic electronic-structure calculations. The interplay of exchange coupling and magnetic anisotropy was monitored by studying the corresponding magnetic torque calculated within *ab initio* and model approaches. We find that a spin-orbit-induced Dzyaloshinski-Moriya interaction has a profound effect on the spin structure of such complex magnetic systems and that in combination with magnetic anisotropies and isotropic exchange this can result in peculiar magnetic properties.

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I. INTRODUCTION

The rapid progress in the field of nanostructured magnetic materials has led in recent years to the emergence of a "second generation" of nanometer-sized magnetic units having usually more than just one constituent.[1–3] Apart from simple alloyed particles or clusters one can find examples of core-shell systems in the literature as well as the very popular approach of depositing structures containing magnetic 3*d* elements on various 5*d* metal substrates.[2,4] In this way, experimental scientists succeeded in assembling surface supported single-domain particles where the magnetic moments of all atoms form a so-called macrospin and it is commonly believed that the special magnetic characteristics of such structures are mainly due to their exposed low-coordinated edge atoms.[2,5] For some of these novel systems, however, unexpected low anisotropies or reduced magnetic moments are observed which makes it difficult to find promising candidates for real-life technical applications.[1] Due to the complex correlations between atomic composition and magnetism within these systems a quantitative theory to describe them should be based on a fully relativistic *ab initio* description of their electronic structure. By this means a correct account of the subtle role played by spin-orbit coupling (SOC) that links the magnetic moments with their spatial environment is guaranteed. Therefore theoretical frameworks based on relativistic density-functional theory (DFT) (Ref. 6) are applied to a large extent in computational simulations to support these experimental efforts.

In this paper we set out to disentangle the complicated SOC-induced magnetic interactions within deposited clusters and other bimetallic nanostructures by explaining them in simpler terms of a model Hamiltonian for the individual magnetic moments associated with different atomic sites. In this context the mapping of energetic properties obtained from first-principles calculations onto a classical Heisenberg model (HM) Hamiltonian has proved to be a very robust and successful scheme.[7,8] Moreover, for many systems the results concur with those from an *ab initio* disordered local-moment theory in which no prior mapping to a HM is assumed.[9,10] An extensively used approach to calculate the isotropic exchange-interaction parameter J_{ij} for two magnetic moments on sites i and j for use in a HM was worked out by Lichtenstein *et al.* using perturbation theory and the so-called Lloyd formula.[7] A corresponding fully relativistic approach was later introduced by Udvardi *et al.* producing an exchange-interaction tensor $\mathcal{J}_{ij}$ for use in a prescribed extended HM.[8] This scheme generates in particular a Dzyaloshinski-Moriya (DM)-type interaction,[11,12] which may explain many interesting phenomena including the magnetic ground-state configuration of magnetic thin films and other extended nanostructures.[13–16] By a detailed study of its building blocks we show here what form an effective HM should have when applied to low-dimensional *finite* nanostructures. For this we determined the electronic structure for Fe, Co, and Ni dimers deposited on a Pt(111) surface (seen as most simple examples) within the local-density approximation of DFT,[17] using the spin-polarized relativistic Korringa-Kohn-Rostoker multiple-scattering formalism.[18] In this scheme, the Dirac Green's function was calculated self-consistently for the dimers assuming pseudomorphic deposition on a 38-layer Pt slab having the experimental lattice constant (3.924 Å). Furthermore we applied the atomic sphere approximation to the potentials and neglected lattice relaxations (see Ref. 19 for more details). For Fe_2 and Co_2 we identify strong DM-type interactions as well as an additional substrate-generated effect in Ni_2. The conclusions of our results can then be applied straightforwardly to larger clusters and nanostructures.

II. THEORETICAL APPROACH

We start by considering the magnetic torque vector $\vec{T}_i^{(\hat{e}_i)}$ acting on an atomic magnetic moment on a site i (for dimers $i=1,2$) and aligned along direction $\hat{e}_i$. $\vec{T}_i^{(\hat{e}_i)}$ is defined in terms of the change in energy $E(\{\hat{e}_k\})=E(\hat{e}_1,\hat{e}_2)$ of the system when changing the orientation of the magnetic moment

$\hat{e}_i$ on site i, i.e., $\vec{T}_i^{(\hat{e}_i)} = -\partial E(\{\hat{e}_k\})/\partial \hat{e}_i$. The component

$$T_{i,\hat{u}}^{(\hat{e}_i)} = -[\partial E(\{\hat{e}_k\})/\partial \hat{e}_i] \cdot (\hat{u} \times \hat{e}_i) \tag{1}$$

of $\vec{T}_i^{(\hat{e}_i)}$ with respect to the axis $\hat{u}$ can be determined from first principles using an expression derived by Staunton *et al.*[20] Following on from this the derivative $\partial^2 E/\partial \hat{e}_i \partial \hat{e}_j$ describing the change in energy upon changing the orientation of two magnetic moments on sites i and j can also be obtained.[7,8] By making use of the rigid spin approximation[21] this approach leads then to a fitting of the magnetic-energy landscape $E(\{\hat{e}_k\})$ obtained from first-principles calculations onto a HM. Including SOC an anisotropy in the exchange interaction may occur and we then use these quantities in an extended HM for the magnetic moments $\{\hat{e}_k\}$ of the following form:[8,22]

$$H = -\frac{1}{2}\sum_{i,j(i\neq j)} J_{ij}\hat{e}_i \cdot \hat{e}_j - \frac{1}{2}\sum_{i,j(i\neq j)} \hat{e}_i \mathcal{J}_{ij}^S \hat{e}_j - \frac{1}{2}\sum_{i,j(i\neq j)} \vec{D}_{ij} \cdot [\hat{e}_i \times \hat{e}_j] + \sum_i K_i(\hat{e}_i). \tag{2}$$

Here the exchange-interaction tensor $\mathcal{J}_{ij}$ has been split into its conventional isotropic part J_{ij}, its traceless symmetric part $\mathcal{J}_{ij}^S$, and its antisymmetric part $\mathcal{J}_{ij}^A$ which is represented in terms of the DM vector $\vec{D}_{ij}$ with $D_{ij}^{\gamma} = \epsilon^{\alpha\beta\gamma}(J_{ij}^{\alpha\beta} - J_{ij}^{\beta\alpha})/2$ and $\epsilon^{\alpha\beta\gamma}$ being the Levi-Civita symbol. Finally, the anisotropy constants $K_i(\hat{e}_i)$ account for the on-site magnetic anisotropy energy (MAE) associated with each individual moment oriented along $\hat{e}_i$.

From our *ab initio* calculation of $T_{i,\hat{u}}^{(\hat{e}_i)}$ we can test whether such a HM is justified and also find the values for the J_{ij}, K_i, $\mathcal{J}_{ij}^S$, and $\vec{D}_{ij}$ parameters. For the HM in Eq. (2) $T_{i,\hat{u}}^{(\hat{e}_i)}$ can be partitioned into the following contributions:

$$T_{i,\hat{u}}^{(\hat{e}_i)} = T_{i,\hat{u}}^{\mathrm{iso}} + T_{i,\hat{u}}^{\mathrm{S}} + T_{i,\hat{u}}^{\mathrm{DM}} + T_{i,\hat{u}}^{K}, \tag{3}$$

where $T_{i,\hat{u}}^{\mathrm{iso}}$ and $T_{i,\hat{u}}^{\mathrm{S}}$ correspond to the isotropic and traceless symmetric terms in Hamiltonian Eq. (2), respectively. The term of $T_{i,\hat{u}}^{(\hat{e}_i)}$ arising from the DM coupling is given by

$$T_{i,\hat{u}}^{\mathrm{DM}} = \sum_{j\neq i} (\vec{D}_{ij} \cdot \hat{u})(\hat{e}_i \cdot \hat{e}_j) - \sum_{j\neq i} (\vec{D}_{ij} \cdot \hat{e}_i)(\hat{u} \cdot \hat{e}_j). \tag{4}$$

The last term derives from the single-site anisotropy term, i.e.,

$$T_{i,\hat{u}}^{K} = [\partial K_i(\hat{e}_i)/\partial \hat{e}_i] \cdot (\hat{u} \times \hat{e}_i). \tag{5}$$

III. RESULTS AND DISCUSSION

By focusing on nanoclusters having a collinear arrangement of the magnetic moments the MAE terms can be determined. Note that the last term in Eq. (4) does not contribute to $T_{i,\hat{u}}^{(\hat{e}_i)}$ in the case of a collinear magnetic structure and also the sum of the DM contributions $T_{i,\hat{u}}^{\mathrm{DM}}$ from all sites in a nanocluster vanishes in this case. However, the anisotropy of the exchange interaction, represented by the symmetric tensor $\mathcal{J}_{ij}^S$ can give rise to a finite contribution to $T_{i,\hat{u}}^{(\hat{e}_i)}$ and thus to the total MAE of a nanocluster.

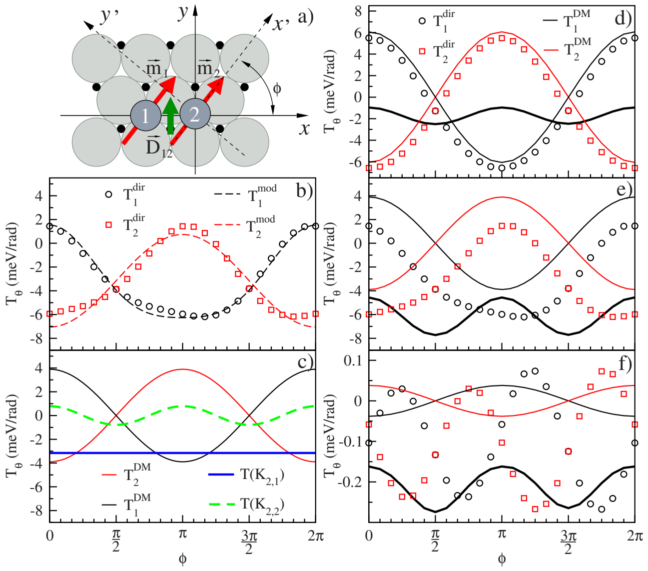

FIG. 1. (Color online) Magnetic torque results for Fe, Co, and Ni dimers on Pt(111) for $\theta = \pi/4$ as a function of the azimuth angle ϕ. (a): magnetic configuration of the transition-metal dimers deposited on a Pt(111) substrate. The large (small) spheres present Pt surface (subsurface) atoms. The medium size spheres represent the dimer atoms with the projection of their magnetic moments onto the surface (xy plane) represented by arrows. The projection of the DM-vector $\vec{D}_{12}$ onto the surface is represented by a short arrow. (b): *ab initio* T_i^{dir} compared with HM T_i^{mod} for Co_2 on Pt(111). (c): T_i^{DM} and T_i^{K} contributions to T_i^{mod} for Co_2 on Pt(111). [(d)–(f)]: *ab initio* T_i^{dir} for the two atoms of (d) Fe_2, (e) Co_2, and (f) Ni_2. T_1^{dir} and T_2^{dir} are presented by circles and squares, respectively, and their sum by the thick solid line. The thin solid lines give the DM contributions according to Eq. (4).

We now see how well our *ab initio* results for the deposited Fe, Co, and Ni dimers fit such model torques. First, we find that the dimers when constrained to be magnetically collinear exhibit a pronounced out-of-plane MAE. The collinear magnetic moments $\hat{e}_1$ and $\hat{e}_2$ have been assumed to be orientated at an angle to the surface normal (z axis) being expressed in terms of polar and azimuth angles θ and ϕ, respectively, i.e., $\hat{e}_1 = \hat{e}_2 = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. Figure 1(a) shows the atomic configuration together with the projection of the moments onto the surface (xy plane). In parallel to the fixed frame of reference (x,y,z) we use a second one (x', y', z') rotated by ϕ with respect to the fixed one with $z = z'$. In all calculations the torque component $T_{i,\hat{u}}^{(\hat{e}_i)}$ is taken around the y' axis, i.e., $\hat{u} = \hat{y}' = (-\sin\phi, \cos\phi, 0)$, for θ fixed to $\pi/4$ as a function of the azimuth angle ϕ (i.e., we can now write $T_i \equiv T_{i,\hat{y}'}^{(\hat{e}_i)}$). From the HM an expansion of the MAE term $K(\hat{e}_i)$ in terms of spherical harmonics up to $\ell = 2$ gives the single-site contribution to the torque in the present configuration to be

$$T^K = -2(K_{2,1} + K_{2,2}\cos 2\phi + K'_{2,2}\sin 2\phi) \tag{6}$$

whereas T_i^{DM} deduced from the HM has a $\cos\phi$ or $\sin\phi$ variation when $\vec{D}_{12}$ lies in the yz or xz plane, respectively.

In Fig. 1(b) the *ab initio* results T_i^{dir} are compared with T_i^{mod} deduced from the HM for $\mathrm{Co_2}$ on Pt(111). As one notes, T_1 and T_2 are different but are related with respect to their ϕ dependence according to the C_s symmetry of the system. On comparing T_i^{dir} and T_i^{mod} of the two Co atoms we find the symmetric part of the exchange-interaction tensor T_i^S to be negligible. The contributions T_i^{DM} and T^K are shown in Fig. 1(c). Clearly, T_1^{DM} and T_2^{DM} vary with cos ϕ and are opposite in sign being in accordance with symmetry and forcing the DM vector $\vec{D}_{12}$ to lie in the yz plane [see Fig. 1(a)]. For T_i^K we find $K'_{2,2}$ to be very small and the dominating terms $K_{2,1}$ and $K_{2,2}$ to be practically the same for both atomic sites leading to $T_1^K \approx T_2^K$. The contribution to T_i^K connected with $K_{2,1}$ does not depend on ϕ while that connected with $K_{2,2}$ varies with cos 2ϕ. As one can see, T_i^{mod} reproduces the results T_i^{dir} rather well. The remaining deviations are primarily due to the limitations of the HM with respect to the dependency of the magnetic energy on the magnetic-moment orientations $E(\{\hat{e}_k\})$. From the decomposition of T_i via the HM it becomes clear that its ϕ dependence is dominated by the DM contribution while the $K_{2,2}$ contribution gives rise to a minor additional modulation. Owing to the large positive value of $K_{2,1}$ for both atoms an out-of-plane MAE results for the total system. This can also be seen from Fig. 1(e) where $T_{\mathrm{tot}}^{\mathrm{dir}} = T_1^{\mathrm{dir}} + T_2^{\mathrm{dir}}$ for $\mathrm{Co_2}$ on Pt(111) is shown together with the individual contributions T_i^{dir} and the corresponding DM terms T_i^{DM}. Once more one can see that the ϕ dependence of T_i is determined by T_i^{DM} while that of $T_{\mathrm{tot}}^{\mathrm{dir}}$ is set by the $K_{2,2}$ on-site MAE terms. This also holds for $\mathrm{Fe_2}$ in Fig. 1(d) for which the DM terms are even more dominant, i.e., the ϕ dependence of T_i is nearly exclusively due to T_i^{DM}.

A further change in the occupation of d states leads to a noticeably different situation for $\mathrm{Ni_2}$ on Pt(111) as shown in Fig. 1(f) for which the DM terms give only minor contributions to T_i. In contrast to $\mathrm{Fe_2}$ and $\mathrm{Co_2}$ the difference between T_1 and T_2 cannot be attributed to DM coupling as the period of oscillation is varying with sin 2ϕ. Clearly, this effect is not represented by the exchange-interaction terms in the HM of Eq. (2) and must derive from interactions of the Ni moments with those induced in the Pt substrate. As a DM-type interaction can produce only torques of the type $T_1 = -T_2$ a sin 2ϕ variation would arise if a term of the form $(\vec{A}\cdot\hat{e}_1)(\vec{B}\cdot\hat{e}_1) - (\vec{A}\cdot\hat{e}_2)\cdot(\vec{B}\cdot\hat{e}_2)$ were added to Eq. (2), with $\vec{A}$ pointing along $\hat{x}$ and $\vec{B}$ along $\hat{y}$. These Ni dimer results indicate that an HM must be used with caution for systems where the magnetic structure of a nanocluster is strongly influenced by the spin polarizability of the substrate.

For $\mathrm{Fe_2}$ and $\mathrm{Co_2}$, however, the HM works very well. For our chosen geometry $\theta = \pi/4$ and $\phi = 0$ and using the symmetry properties of the elements in the exchange tensor, one finds for $\mathrm{Co_2}$ on Pt(111) with $T_1^K \approx T_2^K$ the total torque

$$T = T_1 + T_2 = -\left(J_{12}^{Szz} - J_{12}^{Sxx}\right) + 2T_1^K. \tag{7}$$

Finally, the MAE of the dimer being the difference in energy when the magnetic moments are both oriented along $\hat{e}_b$ and $\hat{e}_a$, is given by the integral $-\int_{\hat{e}_a}^{\hat{e}_b} \vec{T}(\hat{e})d\hat{e}$. Obviously, this has no contribution from the DM interaction. For $\mathrm{Co_2}$ on Pt(111) we find the exchange parameters J_{12}^{xx}, J_{12}^{yy}, and J_{12}^{zz} to be nearly identical implying that the total MAE of the dimer is nearly exclusively due to the on-site contributions. The values $K_{2,1} = 1.5$ meV and $K_{2,2} = 0.39$ meV for $\mathrm{Co_2}$ on Pt(111) lead as mentioned above to a pronounced out-of-plane MAE, i.e., in the ground state the total magnetization points along the surface normal. Taking the difference between T_1 and T_2 one arrives at the relation $D_{12}^y = (T_1 - T_2)/2$ allowing D_{12}^y to be deduced directly from the T_i^{dir}. Table I shows the corresponding results for all three dimers in comparison with data derived from a mapping to our HM.

TABLE I. Components D_{12}^{α} of the DM vector $\vec{D}_{ij}$, the isotropic exchange constant J_{ij} (in meV), and the tilt angle α (in degrees) for the Fe, Co, and Ni dimers on Pt(111). The *ab initio* data is compared with the data obtained via mapping onto the HM.

	Ab initio	Model				
	D_{12}^y	D_{12}^x	D_{12}^y	D_{12}^z	J_{12}	α
$\mathrm{Fe_2}$	6.04	0.00	6.07	−3.34	138.0	2.52
$\mathrm{Co_2}$	3.69	0.00	3.89	−3.84	108.0	2.07
$\mathrm{Ni_2}$	−0.02	0.00	−0.04	−0.24	30.4	0.07

The closeness of agreement justifies once more the use of the HM for $\mathrm{Fe_2}$ and $\mathrm{Co_2}$ and one notes that D_{12}^y has an appreciable value when compared to the isotropic exchange constant J_{12}. Fixing the azimuth angle ϕ to be $\pi/2$ and performing similar steps one finds D_{12}^x to be zero while D_{12}^z may take a nonzero value and is found to be comparable to D_{12}^y (see Table I). Thus, the above analysis shows that T_1 and T_2 may differ even if the total torque is zero, i.e., if the moments are aligned collinearly along the easy axis (surface normal). The difference between T_1 and T_2 is caused exclusively by the D_{12}^y term leading to a rotation around the y axis. Minimizing the magnetic energy $E(\{\hat{e}_k\})$ of the two atoms leads to an outward tilting of the magnetic moments by an angle α given by $\alpha = \mathrm{atan}\,(D_{12}^y/J_{12})$. The corresponding results given in Table I show that the DM interaction causes the deposited Fe and Co dimers to have an appreciable deviation from collinear configurations in spite of the pronounced ferromagnetic exchange coupling. This SOC effect is completely in line with the findings of Sandratskii[23] and Kübler for bulk systems while the substrate clearly plays a crucial role in the DM interaction. First, hybridization with the substrate breaks the inversion symmetry for the dimers leading to a nonzero DM vector. This symmetry effect is also confirmed by test calculations for free dimers and for dimers embedded in a bulk Pt matrix. Second, the hybridization with the substrate also allows the SOC effects of the substrate to be transferred to the magnetic $3d$ transition-metal dimer. We have confirmed this by further calculations in which the SOC of the substrate and the dimer atoms were manipulated separately. Enhancing the SOC for $\mathrm{Co_2}$ only leads primarily to an increase in the on-site anisotropy constant $K_{2,2}$. However, enhancing the SOC for the Pt substrate atoms leads to a strong increase in the anisotropy constant $K_{2,1}$ as well as to a larger difference in T_1 and T_2, reflecting an increase in the DM interaction. This behavior is in line with Levy's model of the indirect DM interaction between two spin moments, which is

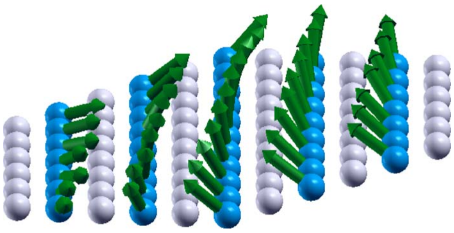

FIG. 2. (Color online) Magnetic structure of a 91-atom FePt (2×1) 2D alloy cluster deposited on a Pt(111) surface determined via MC simulations for $T=0.1$ K. The arrows denote the orientation of the magnetic moments associated with the iron atoms.

mediated by nearby atoms.[24] As a consequence, the magnitude of the DM interaction is essentially determined by the SOC strength of the neighboring atoms.

The effect of anisotropic exchange is even more spectacular in more complex magnetic nanostructures, where for example magnetic atoms are separated by nonmagnetic atoms with large SOC. This can be demonstrated for a FePt (2×1) two-dimensional (2D) alloy cluster deposited on a Pt(111) surface pertinent to experimental studies by Honolka *et al.*[1] Our *ab initio* torque results show the clear trend that the magnetic structure of this cluster is noncollinear and Fig. 2 displays the outcome of a Monte Carlo (MC) simulation based on our effective HM for $T=0.1$ K. The noncollinearity between the Fe chains is essentially caused by the nearest-neighbor Fe-Fe interchain DM interaction $(|\vec{D}|=4.6$ meV) being of similar magnitude when compared to the isotropic-exchange coupling $(J=8.8$ meV). Within a Fe chain, however, the DM interaction is more than 1 order of magnitude smaller when compared to the isotropic exchange leading only to a slight screwing of the Fe magnetic moments along the chain. Intriguingly, this system shows a strong in-plane MAE of 1.1 meV per Fe atom and the magnetic easy axis being perpendicular to the chains but with the total magnetic moment pointing along the surface normal due to the peculiar interplay between MAE, exchange coupling, and DM interactions leading to an unexpected hysteresis behavior.[1]

IV. SUMMARY

In summary this work shows that *ab initio* magnetic torque calculations enable the impact of SOC on magnetic interactions within finite nanostructures to be monitored in a very detailed way revealing subtle anisotropic effects. The further analysis of such results within a HM gives further insights and identifies the role of various contributions as well as the limitations of such models. For Fe_2 and Co_2 on Pt(111) the DM interaction was found to be pronounced owing primarily to the SOC of the substrate leading to noncollinear magnetic configurations for the dimers in spite a pronounced ferromagnetic coupling and out-of-plane MAE. These SOC-induced effects can be quite profound in more complex systems where for example magnetic atoms are separated by nonmagnetic spacers having large SOC as this allows the isotropic exchange to become comparable in size with the DM couplings. In particular we infer that the magnetic structure around the edges of magnetic nanoparticles is likely to be significantly affected by these interactions.

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