Tuning exchange interactions in antiferromagnetic Fe/W(001) by 4d transition-metal overlayers

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We use first-principles calculations based on density functional theory to study how the magnetic properties of an Fe monolayer on a W(001) surface – exhibiting a c(2 × 2) antiferromagnetic ground state – can be modified by an additional 4d transition-metal overlayer. To obtain an overview of how the 4d-band filling influences the exchange interactions in the Fe layer we have calculated the energy dispersion of spin spirals for 4d/Fe/2W unsupported quadlayers, in which the W(001) substrate is represented by only two atomic layers. Hybridization with the overlayer leads to a reduced ferromagnetic nearest-neighbor exchange interaction and the next-nearest neighbor exchange gains in strength. Surprisingly, we find that the c(2 × 2) antiferromagnetic state is unfavorable for all systems with a 4d overlayer. For 4d overlayers from the beginning (Nb) or end (Pd) of the series we find a ferromagnetic ground state. As one moves to the center of the series there is a transition via a spin spiral (Mo, Rh) to a p(2 × 1) antiferromagnetic ground state (Tc, Ru). We have studied the Mo, Ru, and Pd overlayer on Fe/W(001) representing the surface by a sufficiently large number of W layers to obtain bulk like properties in its center. The energy dispersion of spin spirals show qualitatively the same results as those from the 4d/Fe/2W quadlayers. The Dzyaloshinskii-Moriya interaction calculated upon including spin-orbit coupling shows significant strength and considerable frustration effects. The calculated magnetocrystalline anisotropy energy is large as well. All 4d/Fe/W(001) films are potential candidates for complex non-collinear spin structures.

I. INTRODUCTION

Iron is the prototypical ferromagnetic element with a high Curie temperature. However, its magnetic structure can be drastically modified into a non-collinear spin spiral state upon changing its bulk crystal structure from bcc to fcc. In ultrathin Fe films the diversity of observed magnetic structures is even larger. An antiferromagnetic (AFM) checkerboard structure was suggested based on density functional theory (DFT) and discovered for an Fe monolayer (ML) on the W(001) surface. Based on DFT calculations it has been predicted that a Ta_{x}W_{1−x} (001) surface alloy allows to tune the state from ferro- to antiferromagnetic. It has been demonstrated that the nearest-neighbor exchange interaction in an Fe monolayer can be tuned from ferro- to antiferromagnetic by reducing the band filling of a 4d or 5d transition-metal surface. This can lead to non-collinear magnetic ground states such as the Néel state observed for an Fe monolayer on Re(0001).

In ultrathin Fe films with a small nearest-neighbor exchange interaction intriguing magnetic ground states can occur due to the interplay with other magnetic interactions. For example an Fe ML on Rh(111) exhibits a double-row wise AFM (or ↑↑↓↓ state). Even more complex and on a nanometer scale is the nanoskyrmion lattice which has been found in an Fe ML on Ir(111). Atomic overlayers of 4d transition-metals allow to tune the magnetic structure into other states. A Pd overlayer on Fe/Ir(111) leads to a spin spiral ground state that turns into a skyrmion lattice upon applying an external magnetic field. Depending on fcc or hcp stacking of a Rh overlayer on Fe/Ir(111) either a spin spiral ground state or a canted ↑↑↓↓ state occurs. Such a change in the magnetic ground state is driven by higher-order exchange interactions as shown for a Pd/Fe bilayer on Re(0001). In all of these examples there is a subtle interplay of different magnetic interactions. Besides Heisenberg and higher-order exchange interactions, the Dzyaloshinskii-Moriya interaction (DMI) plays a key role for non-collinear magnetic structures.

The c(2 × 2)-AFM ground state of Fe/W(001) is stabilized by a strong antiferromagnetic nearest-neighbor exchange interaction and a large magnetocrystalline anisotropy favoring an out-of-plane magnetization. Experimentally no evidence for a deviation from a collinear AFM state has been observed. The DM interaction which results from spin-orbit coupling (SOC) and can occur at surfaces due to the broken inversion symmetry, is apparently not strong enough in this system in comparison with exchange interaction and anisotropy to induce a non-collinear magnetic ground state. The strength of the DMI in Fe/W(001) has been obtained based on density functional theory (DFT) calculations. It is only a little smaller than that of Fe/Ir(111) but considerably weaker than for Mn/W(001) in which it induces a spin spiral ground state.

The exchange interaction can favor collinear magnetic states, such as the FM or the AFM state or non-collinear spin structures such as spin spirals. It can also stabilize two-dimensionally modulated non-collinear spin structures such as non-chiral skyrmions. Chiral skyrmions, on the other hand, are stabilized in ultrathin films due to the interfacial DMI. It has been proposed that the DMI can induce skyrmions in two-dimensional antiferromagnets and favorable trans-
port properties have been predicted. Since DFT provides a good description of the electronic and magnetic properties of transition-metal interfaces which can host skyrmions, it can guide experimental efforts to realize antiferromagnetic skyrmions.

Here we discuss the effect of 4d transition-metal (TM) overlayers on the magnetic interactions in Fe/W(001) using DFT. We have applied the full-potential linearized augmented plane wave (FLAPW) method as implemented in the FLEUR code. Fe/W(001) has been chosen since a checkerboard AFM ground state has been observed and a significant DMI has been predicted based on DFT calculations. However, the exchange interaction and the magnetocrystalline are apparently too strong to allow for complex non-collinear spin structures such as skyrmions. Based on previous studies of ultrathin Fe films we anticipate that the hybridization with a 4d TM overlayer can weaken both interactions.

We first present the total energy difference between the FM and the c(2 × 2) AFM state for 4d TM overlayers on Fe/W(001) varying the 4d TM from Nb to Pd. As expected the energy difference between the FM and the AFM state is much reduced compared to Fe/W(001). Unexpectedly, the FM state is favorable for all considered overlayers.

In order to scan a larger part of the magnetic phase space we have performed spin spiral calculations. We start by discussing calculations for films of four layers, denoted as quadlayers, consisting of the 4d TM layer, the Fe layer, and two layers of the W(001) substrate. These model systems allow to obtain the trend of magnetic interactions and ground states. Surprisingly, we find that the $p(2 \times 1)$ AFM (row-wise AFM) state is favorable in the middle of the 4d series which is linked to a large next-nearest neighbor antiferromagnetic exchange interaction. We have calculated the energy dispersion of spin spirals for Ru, Mo, and Pd overlayers on Fe/W(001) using a tungsten substrate consisting of eight atomic layers. Qualitatively, we obtain the same results as for the corresponding quadlayers. Ru/Fe/W(001) exhibits a $p(2 \times 1)$ AFM ground state, but the DMI is significant and a local spin spiral minimum is only slightly higher in total energy. For Mo we find an extremely small nearest-neighbor exchange interaction and a spin spiral ground state driven by competing exchange interactions. For Pd/Fe/W(001) the FM state is the lowest in total energy amongst all considered magnetic configurations. However, the energy dispersion of spin spirals is very shallow and reminiscent to that of Fe/Ir(111) in which a nanoskyrmion lattice has been discovered.

This paper is structured as follows. We begin with a description of the computational details and the methods which we used. In section III we discuss the results of our calculations. We start with the structural relaxations and the energy difference between the FM and c(2 × 2) AFM state. Then we present the spin spiral calculations for the 4d/Fe/2W quadlayers. Finally, we present detailed studies for a Ru, Mo, and Pd overlayer on Fe/W(001) including the effects of spin-orbit coupling, i.e. DMI and magnetocrystalline anisotropy.

### II. COMPUTATIONAL DETAILS

We applied DFT as implemented in the full-potential linearized augmented plane wave method (FLAPW) in film geometry. The structural, electronic, and magnetic properties of 4d transition-metal (TM) overlayers on Fe/W(001) were calculated using the Jülich DFT code FLEUR. The linearized augmented plane wave basis for the valence states was extended by local orbitals to describe the 4s and 4p orbitals of the 4d TM atoms and the 5p orbitals of the W atoms. For all types of atoms we used a muffin-tin radius of 2.25 a.u. (1 a.u. = 0.529 Å). The energy cutoff for the basis functions was $k_{\text{max}} = 4.1$ a.u. $^{-1}$ unless stated otherwise. The experimental lattice constant of W was used ($a_{\text{W}} = 3.165$ Å) which is only by 0.5 % smaller than the value obtained within the generalized gradient approximation of DFT.

#### A. Structural relaxations

We used a symmetric film to calculate the relaxed interlayer distances for all 4d/Fe/W(001) systems and for Fe/W(001). We considered the ferromagnetic (FM) and the c(2 × 2)-antiferromagnetic (AFM) state. The substrate was represented by nine tungsten layers. An
atomic layer of iron and an overlayer of the 4d transition metal was added on both sides of the film. For the inner seven tungsten layers we fixed the interlayer distances to the experimental values. All other interlayer distances were calculated by minimizing the forces to less than \(10^{-5}\) hartree/a.u. acting on the atoms. We chose the general gradient approximation (GGA) of the exchange-correlation potential. In the FM state, we used one atom per layer in the two-dimensional unit cell and 840 \(k\)-points in the full two-dimensional Brillouin zone (2D-BZ). For the \(c(2 \times 2)\) AFM state we used a two atomic two-dimensional unit cell and 400 \(k\)-points in the full 2D-BZ. Since we found the FM state to be energetically more favorable than the \(c(2 \times 2)\) AFM state for all 4d overlayers we have chosen the relaxed interlayer distances for the FM state in all subsequent calculations (see Table I for values).

B. Spin-spiral calculations

We have calculated the energy dispersion \(E(q)\) of flat spin spirals characterized by a vector \(q\) from the 2D-BZ. The magnetic moment \(M_i\) on lattice site \(R_i\) is given for a flat spin spiral by 
\[
M_i = M \left( \cos (qR_i), \sin (qR_i), 0 \right).
\]
We first performed self-consistent calculations without spin-orbit coupling applying the generalized Bloch theorem. Based on these calculations we obtained the energy contribution due to spin-orbit coupling, i.e. from the DM interaction, for cycloidal spin spirals in first order perturbation theory as described in Ref. [36] and [39].

Spin spiral calculations were performed for freestanding quadlayers consisting of a 4d TM layer, an Fe layer and two layers of the W(001) surface (denoted as \(4d\text{-Fe}/2W\) below) as well as for asymmetric films of a Mo, Ru, or Pd overlayer on an Fe layer and eight layers of the W(001) surface (denoted as \(4d/Fe/W(001)\) below). For the later we have checked that increasing the thickness of the W substrate does not qualitatively change our results. The relaxed interlayer distances given in Table I have been used. For all freestanding quadlayers we used 1156 \(k\)-points in the full 2D-BZ. For Mo/Fe/W(001) and Ru/Fe/W(001) we also used 1156 \(k\)-points and for Pd/Fe/W(001) 2304 \(k\)-points were chosen in the full 2D-BZ. Calculations were performed in local density approximation (LDA).

The total energies of spin spiral calculations can be mapped to the classical Heisenberg model on the two-dimensional atomic lattice of the Fe layer:

\[
H_{ex} = - \sum_{ij} J_{ij} \left( m_i \cdot m_j \right),
\]
where the exchange constants \(J_{ij}\) denote the strength of the exchange interaction between the magnetic moments \(m_i\) and \(m_j\) located on lattice sites \(i\) and \(j\). Here \(m_i = M_i / M\) is the unit vector of the magnetic moment. Upon

including spin-orbit coupling the Dzyaloshinskii-Moriya (DM) interaction arises

\[
H_{DM} = - \sum_{ij} D_{ij} \cdot \left( m_i \times m_j \right),
\]
where \(D_{ij}\) is the DM vector that denotes the strength and direction of the pairwise DM interaction between magnetic moments on the lattice. The exchange constants \(J_{ij}\) can be obtained by fitting the energy dispersions of spin spirals calculated via DFT without spin-orbit coupling to the model given by Eq. (1). The energy contribution of spin spirals due to spin-orbit coupling was used to determine the parameters \(D_{ij}\) of the DM interaction. To describe the interaction of a given magnetic moment with the \(i\)-th shell of its nearest neighbours we introduce the shell resolved values \(J_{i}\) and \(D_i\). The directions of the DM vectors are given by symmetry (see e.g. Ref. [41] for (001) bcc surface), while the magnitude and sign depend on the electronic structure.
C. Magnetocrystalline anisotropy

The magnetocrystalline anisotropy energy (MAE), i.e. the energy difference between a state with a magnetization perpendicular to the film and with an in-plane magnetization, has been calculated for Mo/Fe/W(001), Ru/Fe/W(001), and Pd/Fe/W(001) applying the force theorem. We have used asymmetric films with 12 tungsten layers for the W(001) substrate in order to obtain converged values of the MAE. First we performed a self-consistent scalar-relativistic calculation in LDA with $k_{\text{max}} = 4.1$ a.u.$^{-1}$ and 1156 $k$-points in the full 2D-BZ. Then we applied the force theorem$^{42}$ to evaluate the MAE. We performed calculations for a magnetization along the out-of-plane ($\perp$) and the in-plane ($\parallel$) direction based on the second variation method$^{43}$ Here, we used $k_{\text{max}} = 4.3$ a.u.$^{-1}$ and 1936 $k$-points. The obtained energy difference $K = E_{\perp} - E_{\parallel}$ can be included in the atomistic spin model by an uniaxial anisotropy term

$$H_{\text{MAE}} = -\sum_i K (m_i^z)^2.$$ (3)

III. RESULTS

A. Structural relaxations

Figure 2 shows the relaxed interlayer distances between the four uppermost layers of both sides of the symmetric 4$d$/Fe/W(001) films. Both the FM (orange curve) and the c(2×2) AFM state (red curve) of the Fe layer have been considered. Overall the differences in relaxations for these two magnetic configurations are small. The interlayer distances between the 4$d$ transition-metal overlayer and the Fe layer show a parabolic curve with respect to the 4$d$ band filling. Starting from Nb, the bonding orbitals are first filled until at the middle of the series anti-bonding states are also occupied. The distance between the Fe and the W layer [Fig. 2(b)] slightly decreases from Nb to Rh. It is larger than the relaxed interlayer distance of 2.44 and 2.58 a.u. reported for the FM and c(2×2) AFM state of Fe/W(001)$^{22}$ leading to a reduced Fe-W hybridization in 4$d$/Fe/W(001). A sharper drop is observed between Rh and Pd due to the complete filling of the 4$d$ shell for Pd. The variation of the distance between the upper two tungsten layers is small [Fig. 2(c)] and very close to the perfect unrelaxed value (green line with $a_{\text{W}}/2$).

Since the differences of the structural relaxations between the FM and the c(2×2)-AFM state are small, we performed all subsequent calculations only for the interlayer distances obtained for the FM state (cf. Table II) which is energetically lower than the c(2×2)-AFM for all 4$d$ overlayers (cf. section III.B). For Fe/W(001) the c(2×2)-AFM state is the ground state and its interlayer distances were used.

FIG. 3. (a) Calculated energy differences $E_{\text{AFM}} - E_{\text{FM}}$ between the c(2×2)-AFM and the FM state for 4$d$/Fe/W(001) films. In (b-d) the corresponding magnetic moments are shown for the upper three layers of the films, i.e. the 4$d$ overlayer, the Fe layer, and the upper W layer, in the FM (blue filled circles) and in the c(2×2)-AFM state (red filled circles).

B. FM vs. c(2×2) AFM state

Next we study how the 4$d$ transition-metal overlayer affects the energy difference between the FM and the c(2×2)-AFM state for 4$d$/Fe/W(001) films as shown in Fig. 3(a). A positive sign of $\Delta E = E_{\text{AFM}} - E_{\text{FM}}$ indicates that the FM state is favorable while the AFM state is preferred for a negative value. If one restricts the Heisenberg model to nearest neighbors $\Delta E$ is directly proportional to $J_1$, i.e. the exchange constant between nearest neighbor atoms. However, as we will see in the following sections in these systems exchange interactions beyond nearest neighbors need to be taken into account to describe the magnetic states.

In agreement with previous studies we find that Fe/W(001) prefers the c(2×2)-AFM state by a large value of 125 meV/Fe atom. In contrast for all considered 4$d$/Fe/W(001) films the FM state is lower in total energy than the c(2×2)-AFM state. However, the absolute value of the energy difference is relatively small. Hybridization with the 4$d$ transition-metal layer leads to lower energy differences, where Pd/Fe/W(001) has the largest energy
FIG. 4. Spin-resolved local density of states in the ferromagnetic state for the topmost layers of (a-c) Mo/Fe/W(001), (d-f) Ru/Fe/W(001), (g-i) Pd/Fe/W(001), and (j-k) Fe/W(001). Red and blue curves show the majority and minority spin channel, respectively. The magnetic moments of the different layers are given in the lower part of each panel.

difference with 65 meV/Fe atom and Mo/Fe/W(001) the smallest with 15 meV/Fe atom. These results show that one can reduce the energy difference between the two magnetic states and thereby of the exchange interaction by an overlayer. For the Pd overlayer this shift to a FM state is consistent with the expectation from DFT calculations of 3d TM monolayers on Pd(001) which showed a FM ground state for Fe/Pd(001).

Since GGA tends to overestimate the AFM state the calculations shown in Fig. 3 have been performed in LDA using the relaxed interlayer distances obtained for the FM state (cf. Table I). Note, that we find qualitatively the same trend as a function of the 4d transition-metal overlayer in GGA.

The magnetic moments of the 4d-transition metal, the Fe, and the W atoms of the topmost layers are shown in Fig. 3 (b-d). As expected, Fe has the largest magnetic moment. Its size depends significantly on the 4d-transition metal due to hybridization between the 3d and 4d states. At the beginning of the 4d series it is about 1.5 \( \mu_B \) in both magnetic states while it rises above 2 \( \mu_B \) for the Rh and Pd overlayers. In the c(2 \times 2)-AFM state the adjacent 4d and W layers obtain no induced magnetic moments due to symmetry. In the FM state the induced moments in the 4d layer change from negative to positive with 4d band filling due to the change of their spin susceptibility. For Rh the largest magnetic moment of about 0.4 \( \mu_B \) is found. The induced magnetic moment of the W atoms at the interface is opposite to that of the corresponding 4d atoms.

To obtain more insight into the influence of the 4d overlayer on the electronic and magnetic properties of the films, we present in Fig. 4 the local density of states (LDOS) of the topmost three layers for the Mo, Ru, and Pd overlayer on Fe/W(001). Compared to Fe/W(001) in all 4d/Fe/W(001) systems the LDOS of Fe becomes broader and flatter due to the increased coordination and strong hybridization of 3d and 4d states. This leads to the strongly reduced exchange splitting and magnetic moment at the beginning of the 4d series. The shape of the LDOS for all the 4d transition-metal overlayers is similar and shows the filling of the 4d band. The LDOS narrows and increases due to the reduction of the extent of the 4d orbitals from Nb to Pd. The hybridization with the Fe 3d states induces a small magnetic moment in the 4d overlayer. One can see a number of peaks in the vicinity of the Fermi energy which appear in both the overlayer and the Fe layer, prominently in the majority spin channel for
Mo and Fe (Figs. 4a,b) and Ru and Fe (Figs. 4d,e), indicating the pronounced 3d-4d hybridization. The LDOS of the W surface layer is rather flat due to the larger extent of the 5d states resulting in a larger band width. The LDOS of the W layer also displays a hybridization with the Fe layer which shows most clearly in the absence of an overlayer, i.e. for Fe/W(001) (Figs. 4j,k). Some of the hybrid states show peaks in the 4d, Fe, and W LDOS which is therefore also affected by the 4d overlayer.

C. Spin spirals in unsupported quadlayers

So far, we have studied only two collinear magnetic states, the FM and the c(2×2) AFM state. To understand the effect of the hybridization with the 4d overlayer on the exchange interactions in the Fe layer we need to expand our investigation to non-collinear magnetic states such as spin spirals. From their energy dispersion we can obtain the exchange constants as discussed in the method section. However, spin spiral calculations are computationally very demanding and time consuming. Therefore, we focus in this section on model systems consisting of only four layers: the 4d overlayer, the Fe layer, and two layers of the W(001) substrate which we denote as unsupported quadlayers 4d/Fe/2W. Our studies show that two W layers are already sufficient to obtain qualitatively the correct trends concerning the magnetic ground state as long as we neglect spin-orbit coupling. To obtain even a qualitatively reasonable description of the Dzyaloshinskii-Moriya interaction or the magnetocrystalline anisotropy more W layers are needed. Film calculations for selected overlayers are discussed in section III D.

The calculated energy dispersion $E(q)$ of spin spirals for the quadlayers are shown in Fig. 5(a). The solid circles are the energies obtained from DFT without SOC and the lines are fits to the Heisenberg model, Eq. (1). At the high symmetry points collinear states are obtained: the $\Gamma$ point ($q = 0$) corresponds to the FM state, the $\bar{M}$ point to the c(2×2) AFM state, and the $\bar{X}$ point to the p(2×1) AFM state (cf. Fig. 1).

As a general trend we note from Fig. 5(a) that as the 4d overlayer is varied the energy of the p(2×1)-AFM state first decreases from Nb ($\approx +20$ meV) to Ru ($\approx -70$ meV) and then rises again up to a value of $\approx +65$ meV for Pd. The energy of the c(2×2)-AFM state, on the other hand, shows no change of sign in qualitative agreement with the observation from the film calculations presented in Fig. 3. These trends for the energy difference between the collinear magnetic states are summarized for the 4d/Fe/2W quadlayers in Fig. 5(a). Quantitative discrepancies with the film calculations are not surprising since the thickness of the substrate certainly influences the result of the calculations. Importantly, we find that it is the p(2×1)-AFM state which is most influenced by the hybridization between Fe and the 4d overlayer.

The shape of the dispersion curves $E(q)$ as well as the global energy minima (summarized in Table I) strongly varies with the 4d transition-metal overlayer and its band filling. For Nb and Mo overlayers we observe extremely flat energy dispersion curves compared to all other quadlayers. In Nb/Fe/2W the energy minimum is at the FM state, while a spin spiral with a period of $\lambda = 0.96$ nm along $\overline{\Gamma M}$ is the lowest state for Mo/Fe/2W. Interestingly, there is no minimum in the other high symmetry direction $\overline{\Gamma M}$ for Mo/Fe/2W. This suggests a strong directional anisotropy of spin spirals in Mo/Fe/W(001).

The energy dispersion for Tc/Fe/2W and Ru/Fe/2W exhibit a larger energy scale and the FM and c(2×2) AFM are unfavorable. The global energy minimum for these two systems is at the p(2×1)-AFM state. In addition, there is a local minimum for a spin spiral along the $\overline{\Gamma M}$ direction with a period of about 0.9 nm (Tc) and 1 nm (Ru). For the Ru overlayer the minimum at the p(2×1)-AFM state is much lower than for Tc indicating a stronger antiferromagnetic exchange interaction.

Rh/Fe/2W has two spin spiral minima with nearly the same energy. One minimum lies in $\overline{\Gamma X}$- and the other one...
in \( \Gamma \)-direction, the latter being energetically slightly deeper. The spin spirals have periods of \( \lambda_{\text{Fe}} = 1.62 \) nm and \( \lambda_{\text{TM}} = 1.41 \) nm. Finally, in Pd/Fe/2W the global minimum is at the FM state as at the beginning of the 4\( d \) series for Nb. However, the energy rises much more quickly in the vicinity of the \( \Gamma \) point of the Brillouin zone.

The magnetic moments of the Fe layer in the unsupported quadlayers [Fig. 5(b)] show a similar rise with increased band filling of the 4\( d \) overlayer as observed previously in the film calculations [Fig. 3(c)]. However, as a function of spin spiral vector (or period) we find only a relatively small variation of the moment. This underlines that a fit to the Heisenberg model, which rests on the assumption of constant magnetic moments, to extract exchange constant is reasonable.

From the energy dispersion \( E(\mathbf{q}) \) of spin spirals [Fig. 3(a)] we have obtained the exchange interactions by fitting to the Heisenberg model, Eq. (1). The values of the first three exchange constants are shown in Fig. 5(b). The behavior of the energy differences between the collinear states is also reflected in the exchange constants. The curve showing \( J_1 \) is qualitatively analogous to the energy difference between the FM and the c(2 \( \times \) 2)-AFM state. It indicates that all systems are characterized by a small ferromagnetic nearest-neighbor interaction. For example, we note that \( J_1 \approx -22 \) meV for an unsupported Fe monolayer on the W(001) lattice constant and \( J_1 = -26 \) meV for Fe/W(001). Interestingly, we do not find a change of sign of \( J_1 \) with band filling of the overlayer as has been reported previously for Fe monolayers on transition-metal surfaces.

The trend of \( J_2 \) follows the energy of the p(2 \( \times \) 1) AFM state, i.e., it is "v"-shaped [cf. Fig. 6(a)] and becomes strongly antiferromagnetic in the center of the 4\( d \) series. For Nb, Mo, Rh, and Pd overlayers the exchange constants for the first three neighbors are of similar magnitude but vary in sign characteristic of exchange frustration. For \( J_3 < 0 \) this can lead to spin spiral ground states (cf. phase diagrams shown in Ref. 6) as observed for Rh/Fe/2W and Mo/Fe/2W. For quadlayers with Tc and Ru the exchange constant between second nearest neighbors, \( J_2 \), is negative and dominates resulting in the collinear p(2 \( \times \) 1) AFM state being lowest.

The magnetic moments of the Fe layer rise in the quadlayers from low values of about 1\( \mu_B \) for a Nb overlayer to about 2.4\( \mu_B \) for the Rh overlayer [Fig. 6(c)]. The trend with the 4\( d \) overlayer as well as the order of magnitude of the magnetic moments is very similar to that observed for the Fe layer in the film systems discussed in Fig. 3(c).

Based on the results presented in this section and in the previous section we conclude that one can significantly tune the energy difference between the FM state and the c(2 \( \times \) 2)-AFM state via hybridization with a 4\( d \) transition-metal overlayer as discussed in the introduction. However, the spin spiral calculations for quadlayers demonstrate that the variation of the energy difference between the FM state and the p(2 \( \times \) 1)-AFM state is influenced much more strongly, even displaying a transition, which is reflected in the exchange constant between second nearest neighbors becoming negative and dominant in the middle of the 4\( d \) series.

It is remarkable that we can obtain quite a variety of magnetic properties of the Fe layer in terms of the global

| Material       | \( q \) in 2\( \pi/a \) | Magnetic State       |
|----------------|------------------------|----------------------|
| Nb/Fe/2W       | (0.00,0.00)            | FM                   |
| Mo/Fe/2W       | (0.23,0.23)            | spin spiral (\( \lambda = 0.96 \) nm) |
| Tc/Fe/2W       | (0.50,0.00)            | p(2 \( \times \) 1)-AFM |
| Ru/Fe/2W       | (0.50,0.00)            | p(2 \( \times \) 1)-AFM |
| Rh/Fe/2W       | (0.16,0.16)            | spin spiral (\( \lambda = 1.41 \) nm) |
| Pd/Fe/2W       | (0.00,0.00)            | FM                   |

FIG. 6. (a) Energy of the p(2 \( \times \) 1)- and the c(2 \( \times \) 2)-AFM states with respect to the FM state for 4\( d \)/Fe/2W unsupported quadlayers, i.e. obtained from the energy dispersion of spin spirals shown in Fig. 3(a). A positive (negative) sign denotes that the FM (AFM) state is more favorable. (b) First three exchange constants obtained from fitting the energy dispersion of spin spirals and (c) magnetic moments of the Fe layer in the three collinear magnetic states at the high symmetry points of the Brillouin zone (cf. Fig. 5(a)).

TABLE II. Global energy minima extracted from the energy dispersion of spin spirals for unsupported 4\( d \)/Fe/2W quadlayers. The spin spiral vector \( q \) of the minimum and the associated magnetic state are given.
energy minima, the magnetic moments, and the exchange constants. Due to the strong frustration in the exchange interaction, the systems with Nb, Mo, Rh, and Pd overlayers are promising candidates for the stabilization of complex non-collinear magnetic states, so further investigation in a more realistic film structure is worthwhile. The system with Ru is also interesting in this context, although the frustration is smaller. However, this system can be considered as a candidate for the stabilization of skyrmions in a p(2 × 1)-AFM background.

D. Film calculations

All 4d/Fe/W(001) systems seem to be suitable candidates for the stabilization of non-collinear magnetic states based on the results within the approximation of quadlayers presented in the previous section. Here we focus on three representative systems for a detailed study: Mo/Fe/W(001), Ru/Fe/W(001) and Pd/Fe/W(001).

Note, that we have not studied Rh/Fe/W(001) since our key interest lies in finding spin spiral minima in the vicinity of the antiferromagnetic states or with magnetic properties distinctively different from other film systems studied previously. The results on Rh/Fe/2W quadlayers strongly suggest that the corresponding film system will exhibit small period spin spirals stabilized by frustrated exchange interactions. In this respect, this system is similar to fcc-Rh/Fe/Ir(111) for which such a spin spiral ground state has been observed by spin-polarized scanning tunneling microscopy experiments.

As we will see below the system with the Mo overlayer displays the smallest value of the nearest-neighbor ferromagnetic exchange constant. Due to exchange beyond nearest neighbors a spin spiral ground state is stabilized. For the Ru overlayer the nearest-neighbor ferromagnetic exchange is enhanced, however, a row-wise antiferromagnetic next-nearest neighbor exchange. Finally, the nearest-neighbor ferromagnetic exchange dominates for the Pd overlayer system and we find the ferromagnetic state to be lowest among all considered states. However, exchange beyond nearest-neighbors is significant and higher-order exchange interactions may lead to a non-collinear spin structure. In none of the systems, the Dzyaloshinskii-Moriya interaction is large enough to enforce a non-collinear ground state.

The calculated energy dispersions of spin spirals without and with spin-orbit coupling for the three film systems are displayed in Fig. 7. The magnetocrystalline anisotropy energy has been calculated for the collinear magnetic state with the lowest total energy. We discuss the systems in detail below one by one.

1. Mo/Fe/W(001)

From the quadlayer calculations we anticipate for Mo/Fe/W(001) that the energy scale of spin spirals is very small and that the energy landscape is anisotropic (cf. Fig. 7(a)). The result for the film calculation with a W(001) substrate with 8 layers shown in Fig. 7(a) is qualitatively in agreement with this expectation. We observe a deep spin spiral energy minimum along the ΓM direction with a short period of \( \lambda = 0.90 \) nm, similar to that of the quadlayer (cf. Tab. I), while the dispersion is almost flat along the other high symmetry direction. The Fe magnetic moment is about 1.4 \( \mu_B \) and varies only little as a function of spin spiral vector (not shown) as in the quadlayer calculations. This provides further evidence that the quadlayers are a good approximation to obtain the general trends concerning the change of the
exchange interaction due to the 4$d$ overlayer.

Upon including spin-orbit coupling the energetic degeneracy between clockwise (cw) and counterclockwise (ccw) rotating spin spirals is lifted due to the Dzyaloshinskii-Moriya interaction. By symmetry of the DMI cycloidal spin spirals are preferred and for Mo/Fe/W(001) the counterclockwise rotational sense is favorable (denoted as ccw DMI in Fig. 7(a)). The spin spiral energy minimum becomes slightly deeper due to the effect of the DMI.

Spin-orbit coupling further results in the magnetocrystalline anisotropy which leads to a preference of collinear magnetic states over spin spiral states. The magnetocrystalline anisotropy energy, i.e. the energy difference between an out-of-plane and an in-plane magnetization direction, denoted as $K$ shifts the total energy of spin spirals by $K/2$ in the limit of large spin spiral periods, i.e.

$$\frac{E_{\text{MAE}}}{N} = -\frac{1}{N} \sum_{i=1}^{N} K \left( \hat{e}_z \cdot \hat{S}_i \right)^2 \approx \left| \frac{K}{2} \right|. \quad (4)$$

$N$ is the number of magnetic moments averaged over and $\hat{e}_z$ a direction vector that is perpendicular to the surface. We have calculated the magnetocrystalline anisotropy energy in the FM state which is the energetically lowest among the collinear magnetic states. Note that the magnetocrystalline anisotropy energy depends on the electronic structure and therefore it can be sensitive to the considered magnetic state. For Mo/Fe/W(001) we obtain an in-plane anisotropy with $K = 1.1$ meV per Fe atom. The shift of the spin spirals with respect to the FM state is marked by an open circle at the $\Gamma$ point (FM state) in Fig. 7(a).

The calculated energy dispersion $E(q)$ of flat spin spirals is used to determine the parameters of the atomistic spin model. The corresponding fits are shown as lines in Fig. 7. The energies without spin-orbit coupling, are used to find the parameters of the exchange constants (Tab. IV). Nine shells of the nearest neighbors are considered. The energy contribution to spin spirals due to spin-orbit coupling $\Delta E_{\text{DMI}}(q)$ is used to determine the parameters of the DM interaction. For these it is sufficient to consider four nearest neighbor shells to obtain a good fit (Tab. IV).

The exchange interaction is frustrated (Tab. IV), i.e. a positive value of the nearest- and next-nearest-neighbor exchange $J_1$ and $J_2$ preferring ferromagnetic alignment compete with a much larger negative value of $J_3$ which favors an antiferromagnetic alignment. The relative strengths and signs of the exchange constants are consistent with those obtained from the quadlayer calculations (cf. Fig. 3(b)). The absolute values of all exchange constants are very small compared to the nearest-neighbor exchange constant $J_1 = -26$ meV reported for Fe/W(001). The DM interaction also shows considerable frustration (Tab. IV). The largest contribution comes from the second shell of the neighbors $D_2 < 0$. However, there are quite large competing contributions from the first and third shell of neighbors.

Our results for Mo/Fe/W(001) demonstrate how drastically the magnetic interactions in the Fe monolayer can be modified due to the hybridization with a 4$d$ overlayer. An experimental study therefore seems worthwhile. Given the strong exchange frustration and the small absolute values of the exchange constants, it is likely that higher-order exchange interactions such as the 4-spin or the biquadratic interaction could lead to the stabilization of a two-dimensional non-collinear magnetic state.

2. Ru/Fe/W(001)

The spin spiral energy dispersion of Ru/Fe/W(001) [Fig. 7(b)] shows that the ground state is the p($2 \times 1$) row-wise antiferromagnetic state in agreement with the expectation from the quadlayer calculations (cf. Fig. 5). We obtain a magnetic moment for Fe of about 1.7$\mu_B$ at the FM state which varies with the spin spiral vector as observed in the quadlayer.

We map the total energy calculations from DFT to the atomistic spin model to obtain further insight into the magnetic interactions. For the exchange interaction we need to take six shells of neighbors into account (Tab. IV). The exchange interaction is dominated by $J_2 \approx -13$ meV, which favors an antiferromagnetic alignment of next-nearest-neighbor magnetic moments and leads to the p($2 \times 1$) row-wise antiferromagnetic ground state. This term has to compete with the ferromagnetic nearest-neighbor exchange $J_1 = 3.6$ meV which is already much larger than for Mo/Fe/W(001), however, still extremely small compared to that of e.g. a free-standing Fe monolayer on the tungsten lattice constant ($J_1 \approx 22$ meV). We also observe frustration of the DMI as seen from the values given in Table IV.

Due to the large in-plane magnetocrystalline anisotropy of $K = 1.8$ meV the p($2 \times 1$) row-wise antiferromagnetic state is also favorable with respect to a local spin spiral minimum at $q = 0.477 \cdot 2\pi/a$ ($\lambda \approx 13.8$ nm). However, the spin spiral which gains energy due to the DMI is in total only 0.5 meV/Fe atom higher in energy as seen from the inset Fig. 7(c). Therefore, an experimental study would be very interesting.

In principle, higher-order exchange interactions could also stabilize a more complex non-collinear state at the superposition of two spin spirals at the two $\text{M}$ points of the 2D-BZ a so-called 2Q state. However, we have calculated the 2Q state for Ru/Fe/W(001) and found that it is energetically unfavorable by 14 meV/Fe-atom with respect to the row-wise AFM state.
Table III. Calculated magnetocrystalline anisotropy energy for 4d overlayers on Fe/W(001). For each system the value of $K$ is given in meV per Fe atom, the easy magnetization axis, and the corresponding magnetic state for which the calculation was performed. As a reference the value for Fe/W(001) is given from Ref. [3].

| System          | $K$  | preferred direction | magnetic state |
|-----------------|------|---------------------|----------------|
| Mo/Fe/W(001)    | $-1.1$ | in-plane            | FM             |
| Ru/Fe/W(001)    | $-1.8$ | in-plane            | p(2×1)-AFM     |
| Pd/Fe/W(001)    | $2.1$  | out-of-plane        | FM             |
| Fe/W(001)       | $2.4$  | out-of-plane        | c(2×2)-AFM     |

Table IV. Exchange constants $J_i$ for $i$-th nearest neighbors obtained from fits to the energy dispersion of spin spirals without spin-orbit coupling obtained from DFT calculations. All values are given in meV.

| System          | $J_1$ | $J_2$  | $J_3$  | $J_4$  | $J_5$  | $J_6$  | $J_7$  | $J_8$  | $J_9$  |
|-----------------|-------|--------|--------|--------|--------|--------|--------|--------|--------|
| Mo/Fe/W(001)    | 0.92  | 0.43   | $-3.09$ | 0.06   | 1.17   | 0.14   | 0.02   | 0.13   | $-0.43$ |
| Ru/Fe/W(001)    | 3.60  | $-13.11$ | 0.47   | 0.85   | 0.44   | 0.57   |        |        |        |
| Pd/Fe/W(001)    | 6.44  | $-0.42$ | $-2.48$ | 0.10   | 0.41   | $-0.18$ | 1.01   | $-0.06$ |        |

3. Pd/Fe/W(001)

For Pd/Fe/W(001) we conclude from the energy dispersion in Fig. 7(d) that the ferromagnetic state (Γ point) is lowest among all spin spiral states even upon including spin-orbit coupling. For the ferromagnetic state the magnetocrystalline anisotropy energy of $K = 2.1$ meV/Fe atom is quite strong and favors an out-of-plane magnetization direction. The energy contribution due to DMI is relatively small for spin spiral states in the vicinity of the Γ-point. However, the overall energy scale of the energy dispersion is small compared to an unsupported Fe ML indicating the strong influence of the hybridization of the Fe layer with the adjacent Pd and W layers. The energy dispersion is surprisingly very similar to that of an Fe ML on Ir(111) which exhibits a nanoskyrmion lattice.

The atomistic spin model is used to describe the interactions. It turns out that both the energy dispersion without and with spin-orbit coupling around the FM state (Γ-point) has a curvature that can not be perfectly described by the model. Even increasing the number of adjacent neighbors to as many as thirteen shells does not lead to a significant improvement. However, the energy scale is extremely small. As best solution for the exchange interaction seven shells of the nearest neighbors are taken into account (Tab. IV) and for the DM interaction five shells (Tab. IV).

Compared to Mo/Fe/W(001) and Ru/Fe/W(001) the nearest-neighbor ferromagnetic exchange further increases to $J_1 \approx 6.5$ meV and is the dominating exchange constant (see Tab. IV). However, $J_1$ is still small enough such that exchange beyond nearest-neighbors can compete which is reflected in the complex shape of the energy dispersion curve (Fig. 7(d)). In particular, $J_3 \approx -2.5$ meV is of a similar order of magnitude. The DMI is similarly dominated by the nearest-neighbor interaction, but there is also some competition with terms beyond nearest neighbors.

As expected from the similar energy dispersion curves the exchange constants of Pd/Fe/W(001) are quite similar to those obtained for an Fe monolayer on Ir(111) ($J_1 = 5.7$ meV, $J_2 = -0.84$ meV, $J_3 = -1.45$ meV, values from Ref. [10]). Fe/Ir(111) also possesses an out-of-plane magnetocrystalline anisotropy, albeit with a significantly smaller value of $K = 0.8$ meV/Fe atom, and a strong DM interaction of $D = 1.8$ meV. Although the different lattice structure – square vs. hexagonal – makes a one-to-one comparison difficult it is still intriguing to see the similarities which suggest that Pd/Fe/W(001) could also exhibit a complex magnetic ground state. Therefore, an experimental determination of the ground state of this film system appears to be worthwhile.

4. Extrapolated exchange energy landscape

As discussed in the previous section it is in particular the exchange interaction in the Fe layer which can be strongly tuned by the 4d overlayers. Therefore, it is interesting to compare the exchange interaction in Mo/Fe/W(001), Ru/Fe/W(001) and Pd/Fe/W(001) by calculating the energy landscape $E(q)$ for flat spin spirals in the Brillouin zone [Fig. 8] based on the determined exchange constants of Table IV.

From Fig. 8(a) the strong anisotropy in the exchange energy is clearly recognizable for Mo/Fe/W(001). Also in the two-dimensional BZ, the energy minimum lies on the high-symmetry line between Γ and M point consistent with the spin spiral energy dispersions shown in Fig. 7(a). In contrast $E(q)$ is isotropic in the vicinity of the Γ point for Ru/Fe/W(001) and Pd/Fe/W(001) as seen from the contour lines in Fig. 8(b,c).

The directional anisotropy increases with the length of
TABLE V. Dzyaloshinskii-Moriya interaction constants $D_i$ for $i$-th nearest neighbors obtained from fits to the energy dispersion of spin spirals including spin-orbit coupling obtained from DFT calculations. All values are given in meV.

|       | $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ |
|-------|-------|-------|-------|-------|-------|
| Mo/Fe/W(001) | −0.40 | −0.97 | 0.40  | 0.10  |       |
| Ru/Fe/W(001)   | 0.18  | 1.44  | −0.51 | −0.13 | −0.35 |
| Pd/Fe/W(001)   | −1.38 | −0.34 | 0.31  | 0.17  | −0.01 |

FIG. 8. Energy dispersion of flat spin spirals $E(q)$ in one quarter of the 2D BZ obtained based on the atomistic model with the exchange constants determined via DFT (cf. Table IV) for (a) Mo/Fe/W(001) (a), Ru/Fe/W(001) (b) and Pd/Fe/W(001). High symmetry points of the 2D BZ are indicated.

IV. CONCLUSIONS

We have demonstrated that it is possible to drastically change the magnetic interactions and the magnetic order in Fe/W(001) by hybridization with a 4$d$ transition-metal overlayer. Since the nearest-neighbor exchange interaction is relatively small in all studied systems a frustration of exchange and DM interaction occurs. As a result one must go beyond the nearest-neighbor interactions within the atomistic spin model to describe the energy landscape accurately. We have studied three systems in detail: Mo/Fe/W(001), Ru/Fe/W(001), and Pd/Fe/W(001) which are all interesting candidates for future experimental studies.

In Mo/Fe/W(001) the nearest-neighbor exchange and the Fe magnetic moment is very small and a spin spiral energy minimum is obtained due to a dominating third nearest-neighbor exchange constant. In Ru/Fe/W(001) the antiferromagnetic next-nearest exchange dominates and a row-wise antiferromagnetic state is predicted to be the ground state, however, a spin spiral driven by DM interaction is very close in energy.

Surprisingly, Pd/Fe/W(001) is similar to the Fe monolayer on Ir(111) in terms of the exchange interactions and strength of DM interaction only the magnetocrystalline anisotropy energy is significantly larger. Therefore, it would be extremely interesting to find out experimentally whether it shows a conventional ferromagnetic ground state or a similarly intriguing spin structure as the nanoskyrmion lattice reported for Fe/Ir(111). While we have not performed explicit calculations for Rh/Fe/W(001) our results from the Rh/Fe/2W quad-layer strongly suggests a spin spiral ground state with a period on the order of 1.5 nm in this system.

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