Current induced switching in Mn$_2$Au from first principles

Severin Selzer,¹ Leandro Salemi,² András Deák,³ Eszter Simon,³
László Szunyogh,³,⁴ Peter M. Oppeneer,² and Ulrich Nowak¹

¹Fachbereich Physik, Universität Konstanz, DE-78457 Konstanz, Germany
²Department of Physics and Astronomy, Uppsala University, P. O. Box 516, S-751 20 Uppsala, Sweden
³Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Múegyetem rkp. 3., HU-1111 Budapest, Hungary
⁴MTA-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Múegyetem rkp. 3., HU-1111 Budapest, Hungary

(Dated: February 1, 2022)

It is well established that it is possible to switch certain antiferromagnets electrically, yet the interplay of Néel-spin-orbit torques (NSOT) and thermal activation is only poorly understood. Combining ab initio calculations and atomistic spin dynamics simulations we develop a multiscale model to study the current induced switching in Mn$_2$Au. We compute from first principles the strength of thermal activation is required to help overcoming the relevant energy barrier.

Here, we combine ab initio calculations with atomistic spin dynamics simulations to develop and employ a multi-scale model of the current induced switching in Mn$_2$Au. The three ingredients for this multi-scale model are ab initio calculations of the exchange interactions and anisotropies (section II), first-principles calculations of the current induced magnetic moments (section III), and atomistic spin model simulations (section IV), that include the results from the first-principles calculations and investigate the switching mechanism and its dynamics. We show that the switching is fast, on a time scale of some tens of picoseconds, but not purely deterministic, requiring some degree of thermal activation to overcome the anisotropy energy barrier during the switching process.

I. INTRODUCTION

Antiferromagnets (AFMs) are promising materials for spintronic devices. Among the advantages over ferromagnets (FMs) are the lack of stray fields, the very low susceptibility to magnetic fields, the abundance of materials and much faster spin dynamics [1,3]. However, the antiferromagnetic order parameter in AFMs is difficult to read and to control because of a lack of macroscopic magnetization, a fact which is strongly related to some of their advantages. A major step in the field of antiferromagnetic spintronics [1,3] was the discovery of electrically induced NSOT [4,8] in specific antiferromagnetic materials. These torques are a result of a special magnetic structure, where, for the magnetic state, global inversion symmetry is broken but one sublattice forms the inversion partner of the other, in combination with the inverse spin-galvanic or (Rashba–)Edelstein effect [4], which is the generation of a nonequilibrium spin polarization by electrical currents. Currently, CuMnAs and Mn$_2$Au are the two known materials that provide antiferromagnetic order at room temperature and possess the specific crystal structure required for NSOT. The latter is the more promising material as its critical temperature is about 950 K, where the material decomposes [9]—and it is easier to handle due to the lack of toxic components.

II. DERIVATION OF THE SPIN MODEL FROM AB INITIO CALCULATIONS

We employ the fully relativistic screened Korringa–Kohn–Rostoker (SKKR) method [13] to determine the electronic structure and magnetic interactions of Mn$_2$Au. Mn$_2$Au crystallizes in the MoSi$_2$ structure with the lattice constants $a_{2d} = 3.328$ Å and $c = 8.539$ Å [9,14]. The MoSi$_2$-type lattice geometry is depicted in Fig. 1. The potentials were treated within the atomic sphere approximation (ASA) with an angular momentum cutoff of $\ell_{\text{max}} = 2$ to describe the electron scattering. For energy integrations we used 15 energy points on a semicircular contour on the upper complex semiplane, and up to 7260 $k$-points in the irreducible wedge of the Brillouin zone near the Fermi energy for the calculation of spin model parameters.

We perform self-consistent calculations for the layered
AFM state shown in Fig. 4 which has been identified as the magnetic ground state by neutron diffraction experiments [9], but also for the FM state. We find the layered AFM state lower in energy than the FM state by 25.8 mRy/atom, which compares fairly well to the value reported in Ref. [16] (21.5 mRy/atom). Also in agreement with Ref. [16] we obtain a larger magnetic moment for the Mn atoms in the layered AFM state (3.74 μB) than in the FM state (3.70 μB). For the description of the switching process we consider the following spin model:

\[ \mathcal{H} = - \frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i d_{1z} S_{i,z}^2 - \sum_i d_{2z} S_{i,z}^4 - \sum_i d_{xy} S_{i,x}^2 S_{i,y}^2, \]  

(1)

where the isotropic exchange interactions \( J_{ij} \) are obtained from the Relativistic Torque Method (RTM) [17], while the anisotropy parameters \( d_{1z}, d_{2z}, \) and \( d_{xy} \) are derived from band energy calculations in the spirit of the magnetic force theorem [13].

The isotropic exchange interactions calculated from the layered AFM state as reference are plotted in Fig. 1 as a function of the interatomic distance. We can identify three dominant Heisenberg couplings: antiferromagnetic ones for the two nearest neighbors, \( J_1 = -43.84 \) meV and \( J_2 = -81.79 \) meV, but a ferromagnetic one for the third nearest neighbor, \( J_3 = 39.28 \) meV. These values show good qualitative agreement with those calculated in Ref. [10] also in terms of the KKR-ASA method, but using a cutoff of \( \ell_{\text{max}} = 3 \) for the partial waves, \( J_1 = -68.30 \) meV, \( J_2 = -91.70 \) meV and \( J_3 = 19.86 \) meV. Since the interactions \( J_1 \) and \( J_2 \) act between sublattices (layers), while \( J_3 \) is the leading interaction within a sublattice (cf. Fig. 1), these couplings clearly favor the layered AFM state as the ground state of the system.

It turns out that taking into account only the first three nearest neighbor interactions is not sufficient for a precise determination of the inter- and intra-sublattice interactions. In our simulations we, hence, consider interactions up to a distance of \( 2.7 a_{2d} \), resulting in an inter-sublattice exchange interaction of \( J_{\text{inter}} = -371.13 \) meV and an intra-sublattice exchange interaction of \( J_{\text{intra}} = 182.36 \) meV. Considering exchange interactions only in the first three shells yields \( J_{\text{inter}} = 4J_1 + J_2 = -257.15 \) meV and \( J_{\text{intra}} = 4J_3 = 157.12 \) meV, being thus 30 and 14% smaller in magnitude than the ones calculated with a spatial cutoff of \( 2.7 a_{2d} \).

Experimental values for the effective inter-sublattice exchange coupling, \( J_{\text{eff}} = -J_{\text{inter}}/4 \) [19], were previously provided based on susceptibility measurements for Mn_2Au powder [9] and thin films [19], \( J_{\text{eff}} = 75 \) meV and \( J_{\text{eff}} = 22(5) \) meV, respectively. The corresponding values from our calculations, \( J_{\text{eff}} = 92.8 \) meV, and the one derived from the exchange interactions in Ref. [10] \( J_{\text{eff}} = 90 \) meV, compare remarkably well and are also in good agreement with the experimental result for the powder sample [9].

From our spin dynamics simulations we obtain a Néel temperature of 1680(3) K, which is in good agreement with the value of 1610(10) K calculated in Ref. [10] via Monte-Carlo simulations using nine nearest neighbor shells (the numerical values of which, however, were not provided beyond the first three shells). Note that due to a peritectic temperature of 950 K, the Néel temperature can only be extrapolated from experiments, yielding values in the range of 1300 K to 1600 K [9].

In order to support the validity of our spin model description relying on the assumption of rigid magnetic moments that are stable against magnetic disorder, we also perform calculations using the relativistic Disordered Local Moment (RDLM) theory [20, 21]. This approach assumes a fully spin disordered reference state, and also enables the extraction of spin model parameters by means of the so-called Spin-Cluster Expansion (SCE) [22, 23], which maps the adiabatic magnetic energy surface onto a spin model.

The resulting isotropic Heisenberg couplings are also displayed in Fig. 1. There is a remarkable similarity between the two spin model parameter sets, despite their quantitative differences especially for the first and third neighbor shells. Obviously, the interactions obtained from the SCE-RDLM calculation are also consistent with the layered AFM structure as ground state and we obtain a Néel temperature of 1786(3) K, which is in good agreement with the RTM.

Conceptually, the RTM gives a good approximation near the ground state, whereas the SCE corresponds to a high-temperature phase. The fact that the two sets of parameters agree well despite this fundamental difference between the two methods can be explained by the rigidity of the Mn local spin moments. In order to support this point we compare the density of states (DOS) for the two magnetic states in Fig. 2. As also noted in
FIG. 2. Density of states per atom from the electronic structure calculations in the AFM (top panel) and DLM (bottom panel) states. The DOS for only one Mn sublattice is shown. Positive values correspond to spin up states, negative ones to spin down states.

For our atomistic spin dynamics simulations we combine these anisotropies with the RTM exchange parameters since both are calculated from the same converged potential in contrast to the SCE exchange parameters.
FIG. 3. Calculated induced orbital ($\mu_L$) and spin ($\mu_S$) moments on the two Mn sublattices as a function of the electric field direction for a field of $E = 1 \times 10^7 \text{ V m}^{-1}$ and local magnetic moments oriented along the [110] direction. a) In-plane direction of the induced orbital moments on the two Mn sublattices (black vs. red). The arrows in the center depict the local magnetic moments. b) Cartesian components of the induced orbital moments on the two Mn sublattices (solid vs. dashed) as a function of the in-plane angle of the electric field with respect to the [100] axis. c) and d) same as in a) and b) for the induced spin moments.

the other hand, are not necessarily perpendicular to the electric field direction, but their in-plane components are staggered as well. Additionally, the spin moments display a homogeneous out-of-plane component, i.e., a non-Néel-type contribution.

Interestingly, in all configurations the induced orbital moments are more than one order of magnitude larger than the induced spin moments, yet the former were not included in previous studies [4, 28]. To summarize, there are always quite large staggered orbital moments induced on the Mn sublattices and small induced spin moments with nonstaggered as well as staggered components that can be parallel or antiparallel to the orbital moments depending on the direction of the electric field, see also [12].

IV. ATOMIC SPIN DYNAMICS SIMULATIONS

To include our first-principles calculations in a spin dynamics simulation we extend the semi-classical Heisenberg Hamiltonian [Eq. (1)] by contributions from induced spin and orbital moments,

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} (S_i + s_i) \cdot (S_j + s_j) - \sum_i J_{sd} S_i \cdot s_i + \sum_i \xi S_i \cdot l_i - \sum_i d_z S_{i,z}^2 - \sum_i d_{xy} S_{i,x} S_{i,y},$$

where $S_i = \mu^d_{S,i}/\mu^d_S$ is the local magnetic moment of the d-electrons, $s_i = \mu^s_{S,i}/\mu^s_S$ the induced magnetic moment from the conduction s-electrons and $l_i = \mu^L_{S,i}/\mu^L_S$ the induced orbital magnetic moment. All magnetic moments are normalized with respect to the local magnetic moment. Thus, the Hamiltonian consists of five different contributions: the inter-atomic exchange with exchange constant $J_{ij}$, an additional intra-atomic sd-exchange with exchange constant $J_{sd}$, a spin-orbit coupling (SOC) term with strength $\xi$, as well as second and fourth order anisotropy terms constituting the tetragonal anisotropy.

As our classical spin model employs quantum mechanical and statistical averages of the spin and orbital moments, we also use a classical description of the SOC replacing the spin and orbital momentum operators by their averages. Note that this effective model for the SOC was used by Bruno [29] in order to provide a simple physical interpretation of magnetic anisotropy. In this model only the spin moments couple via the inter-atomic exchange interaction, which is in agreement with the con-
All the contributions from the induced moments can also be represented by a simple Zeeman-like term with a sublattice-specific effective field that represents the staggered field, which was used in previous phenomenological descriptions,

\[
\mu_{\text{d}}^s \mathbf{B}^{\text{ind}}_i = \sum_j J_{ij} \mathbf{s}_j + J^{\text{sd}} \mathbf{s}_i - \xi \mathbf{l}_i .
\]  

For the intra-atomic exchange we estimate from the shift in the up and down s-states \( J^{\text{sd}} = 50 \text{ meV} \). The SOC strength is calculated from the energy difference between the \( d_{3/2} \) and \( d_{5/2} \) resonances yielding \( \xi = 46 \text{ meV} \). Together with the exchange interactions derived in Sec. II and the induced moment calculated for an electrical field of \( 1 \times 10^7 \text{ V m}^{-1} \), this yields staggered fields of about \( 76 \text{ mT} \). Here, the contribution from the induced orbital moments dominates \( \alpha \). It is about a factor of five larger than the contribution from the inter-atomic exchange and more than one order of magnitude larger than that of the intra-atomic exchange. This explains also why the staggered fields calculated here are much larger than those estimated and predicted before \([10, 11, 28]\) as the orbital contribution was previously not taken into account.

The time evolution of the localized Mn moments stemming from the d-electrons is described by the stochastic Landau–Lifshitz–Gilbert (LLG) equation

\[
\dot{\mathbf{S}}_i = -\frac{\gamma}{(1 + \alpha^2)} \mu_{\text{d}}^s \mathbf{S}_i \times [\mathbf{H}_i + \alpha \mathbf{S}_i \times \mathbf{H}_i] ,
\]

where \( \gamma = 1.76 \times 10^{11} \text{ s}^{-1} \) \( T \) is the gyromagnetic ratio and \( \alpha \) a dimensionless damping constant. Temperature is included via Langevin dynamics by adding a random thermal noise \( \mathbf{c}_i \) to the effective field \( \mathbf{H}_i = -\frac{\partial F}{\partial \mathbf{S}} + \mathbf{c}_i \). The field from the induced moments \( \mathbf{B}^{\text{ind}}_i \) is part of this effective field.

The damping constant is a free parameter as there are no experimental values for it in the literature. For comparison with \([10]\) we use a plausible value of \( \alpha = 0.01 \). Similar, for the electrical field a rectangular pulse with pulse length of 20 ps was simulated to compare the results with those from a phenomenological model \([10]\). Since the samples in experiments are mostly of granular type \([11]\), we simulate a system of \( 20.3 \text{ nm} \times 20.3 \text{ nm} \times 20.5 \text{ nm} \) size with open boundary conditions, resembling one grain of a typical sample.

In our simulations we consider electrical fields along \([110]\), i.e. parallel to the local magnetic moments, and along \([100]\), since reversible switching was reported for both directions \([7]\). For both field configurations our model does not switch at \( T = 0 \) for \( E = 1 \times 10^7 \text{ V m}^{-1} \) corresponding to currents of about \( 1 \times 10^{10} \text{ A m}^{-2} \) to \( 1 \times 10^{11} \text{ A m}^{-2} \), which are used in experiments \([2, 31]\). Instead, we need a field strength of at least \( E = 1.9 \times 10^7 \text{ V m}^{-1} \) for the field along the \([110]\) direction, where torques on the local magnetic moments are maximal. For the \([100]\) direction an even larger field of \( 3.1 \times 10^7 \text{ V m}^{-1} \) is required for switching at zero temperature. However, once the system switches, it switches within a few picoseconds, see Fig. 4. This is even faster than predicted in the phenomenological model in Ref. \([10]\), probably because of the inclusion of the orbital induced moments and the exchange interactions beyond the first three nearest neighbors.

As was already pointed out in Ref. \([10]\), the reason for this rapid switching is the so-called exchange enhancement, which is characteristic for antiferromagnetic dynamics \([32]\). The staggered fields do not only rotate the magnetic moments via the damping term in the LLG but also induce a canting between the sublattices via the much stronger precession term. This leads to a very small magnetization resulting in huge torques due to the inter-sublattice exchange field, which tries to realign the sublattices. Here, the damping term is responsible for the realignment. The precession term, on the other hand, rotates the magnetic moments towards the direction of the staggered field. The out-of-plane component of the order parameter remains zero during the process (see Fig. 5). Hence, the inter-sublattice exchange field governs the switching process and, in contrast to the switching in FMs, lower damping allows for faster switching \([33]\).

The electric fields considered so far are much larger than those applied in experiments, but temperature plays an additional major role. A finite temperature does not only lower the energy barrier, here the fourth order in-plane magnetic anisotropy, but thermal fluctuations can also support probabilistic switching. Fig. 6 shows the time evolution of the order parameter at elevated temperatures as well as the switching probability as a function of temperature for electrical fields of \( E = 1 \times 10^7 \text{ V m}^{-1} \). For the \([110]\) direction the system does not switch at temperatures below 250 K, between 250 K and 350 K the process is probabilistic and above 350 K deterministic.

![FIG. 4. Time evolution of the magnetic order parameter during 90° switching at \( T = 0 \text{ K} \). The electric field (applied in the shaded area) is \( 1.9 \times 10^7 \text{ V m}^{-1} \) in \([110]\) direction (top) and \( 3.1 \times 10^7 \text{ V m}^{-1} \) in \([100]\) direction (bottom).](image-url)
FIG. 5. Switching path of the two sublattice magnetization vectors. The antiparallel Mn moments switch over 90° from the initial [110] configuration (semi-transparent) to the final [-110] configuration (opaque). During the switching process the sublattices are canted slightly resulting in huge torques from the inter-sublattice exchange field enhancing the switching process significantly. This exchange enhancement is characteristic for antiferromagnetic dynamics [32]. The out-of-plane component is here scaled by a factor of 100!

In the deterministic regime the energy barrier is so low that the system switches in a few picoseconds, similar to simulations with larger electric fields. In the probabilistic regime, however, it can take several attempts to cross the energy barrier due to thermal agitation. Of course, here the switching probability also depends on the pulse length of the external electric field as longer time scales allow for more stochastic attempts to cross the barrier. For the electric field along the [100] direction the probabilistic regime lies between 400 K and 550 K, above which the switching is deterministic.

Reversible switching for pulse currents along the [100] direction was also observed in experiments [7]. In the same paper, also significant heating resulting in temperatures up to 300 °C was reported and thermal activation was considered to play an important role in the process. A key role of thermal activation was also reported by Meinert et al. [11]. Of course, for thermal switching of nanoparticles the system size is crucial as well, especially for antiferromagnets as their thermal stability is much lower than that of ferromagnets [33]. Here, the system size was chosen such to avoid a purely superparamagnetic switching which would lead to a forth and back switching.

V. CONCLUSIONS

Modeling the current induced switching process in Mn$_2$Au with all its different contributing terms in a quantitative manner is a challenging task. Here, we have presented the first multi-scale model combining first-principles calculations of exchange and anisotropy constants, as well as electrically induced spin and orbital moments in an extended atomistic spin model. We predict much higher effective staggered fields due to the formerly neglected contributions from induced orbital moments. Within the framework of atomistic spin dynamics simulations, we have shown that these fields—combined with inter-sublattice exchange interactions—result in switching processes on the time scale of few picoseconds. However, this switching requires significantly higher electrical fields than in experiments or, alternatively, elevated temperatures. This applies for both considered electrical field directions, [110] and [100], which is in agreement with experimental findings [7]. Hence, in agreement with previous experimental studies [7, 11] we find that thermal activation plays a key role in the current induced switching process and we have consequently distinguished temperature regimes for probabilistic and deterministic switching.

ACKNOWLEDGMENTS

The authors gratefully acknowledge valuable discussions with Karel Carva. L.S. and P.M.O. acknowledge funding from the Swedish Research Council (VR) and the European Union’s Horizon2020 Research and Innovation Programme under FET-OPEN Grant agreement No. 863155 (s-Nebula), and acknowledge computer resources provided by the Swedish National Infrastructure for Computing (SNIC) at the PDC Center for High Performance Computing and the Uppsala Multidisciplinary Center for Advanced Computational Science (UPPMAX). The work of A.D., E.S. and L.Sz. was supported by National Research, Development, and Innovation Office under projects No. PD134579 and No. K131938. The work in Konstanz was supported by the Deutsche Forschungsgemeinschaft via the Sonder-
[1] T. Jungwirth, X. Marti, P. Wadley, and J. Wunderlich, Antiferromagnetic spintronics, Nature Nanotechnology 11, 231 (2016).

[2] J. Zelezný, P. Wadley, K. Olejník, A. Hoffmann, and H. Ohno, Spin transport and spin torque in antiferromagnetic devices, Nature Physics 14, 220 (2018).

[3] V. Baltz, A. Manchon, M. Tsoi, T. Moriyama, T. Ono, and Y. Tserkovnyak, Antiferromagnetic spintronics, Rev. Mod. Phys. 90, 015005 (2018).

[4] J. Zelezný, H. Gao, K. Výborný, J. Zemen, J. Mašek, A. Manchon, J. Wunderlich, J. Sinova, and T. Jungwirth, Relativistic Néel-Order Fields Induced by Electrical Current in Antiferromagnets, Phys. Rev. Lett. 113, 157201 (2014).

[5] P. Wadley, B. Howells, J. Železný, C. Andrews, V. Hills, R. P. Campion, V. Novák, K. Olejník, F. Maccherozzi, S. S. Dhesi, S. Y. Martin, T. Wagner, J. Wunderlich, F. Freimuth, Y. Mokrousov, J. Kuneš, J. S. Chauhan, M. J. Grzybowski, A. W. Rushforth, K. W. Edmonds, B. L. Gallagher, and T. Jungwirth, Electrical switching of an antiferromagnet, Science 351, 587 (2016).

[6] K. Olejník, V. Schuler, X. Marti, V. Novák, Z. Kašpar, P. Wadley, R. P. Campion, K. W. Edmonds, B. L. Gallagher, J. Garces, M. Baumgartner, P. Gambardella, and T. Jungwirth, Antiferromagnetic CuMnAs multilevel memory cell with microelectronic compatibility, Nature Communications 8, 15434 (2017).

[7] S. Y. Bodnar, L. Šmejkal, I. Turek, T. Jungwirth, O. Gomonay, J. Sinova, A. A. Sapozhnik, H.-J. Elmers, M. Kláui, and M. Jourdan, Writing and reading antiferromagnetic Mn$_2$Au by Néel spin-orbit torques and large anisotropic magnetoresistance, Nature Communications 9, 348 (2018).

[8] K. Olejník, T. Seifert, Z. Kašpar, V. Novák, P. Wadley, R. P. Campion, M. Baumgartner, P. Gambardella, P. Němec, J. Wunderlich, J. Sinova, P. Kužel, M. Müller, T. Kamprath, and T. Jungwirth, Terahertz electrical writing speed in an antiferromagnetic memory, Science Advances 4, eaar3566 (2018).

[9] V. M. T. S. Barthem, C. V. Colin, H. Mayaffre, M.-H. Julien, and D. Givord, Revealing the properties of Mn$_2$Au for antiferromagnetic spintronics, Nature Communications 4, 2892 (2013).

[10] P. E. Roy, R. M. Otxoa, and J. Wunderlich, Robust picosecond writing of a layered antiferromagnet by staggered spin-orbit fields, Physical Review B 94, 014439 (2016).

[11] M. Meinert, D. Graulich, and T. Matalla-Wagner, Electrical Switching of Antiferromagnetic Mn$_2$Au and the Role of Thermal Activation, Physical Review Applied 9, 064040 (2018).

[12] L. Salemi, M. Berritta, A. K. Nandy, and P. M. Oppeneer, Orbitally dominated Rashba-Edelstein effect in noncentrosymmetric antiferromagnets, Nature Communications 10, 5381 (2019).

[13] J. Zabloudil, R. Hammerling, L. Szunyogh, and P. Wadley, Electron Scattering in Solid Matter: A Theoretical and Computational Treatise Springer Series in Solid-State Sciences No. 147 (Springer-Verlag, Berlin Heidelberg, 2005).

[14] P. Wells and J. H. Smith, The structure of Mn$_2$Au and Mn$_3$Au, Acta Crystallographica Section A: Crystal Physics, Diffraction, Theoretical and General Crystallography 26, 379 (1970).

[15] A. B. Shick, S. Khmelevskyi, O. N. Myrasov, J. Wunderlich, and T. Jungwirth, Spin-orbit coupling induced anisotropy effects in bimetallic antiferromagnets: A route towards antiferromagnetic spintronics, Physical Review B 81, 212409 (2010).

[16] S. Khmelevskyi and P. Mohn, Layered antiferromagnetism with high Néel temperature in the intermetallic compound Mn$_2$Au, Applied Physics Letters 93, 162503 (2008).

[17] L. Udvardi, L. Szunyogh, K. Palotás, and P. Weinberger, First-principles relativistic study of spin waves in thin magnetic films, Physical Review B 68, 104436 (2003).

[18] P. Weinberger, Magnetic Anisotropies in Nanostructured Matter, Series in Condensed Matter Physics (CRC Press, Boca Raton, 2009).

[19] A. A. Sapozhnik, C. Luo, H. Ryll, F. Radu, M. Jourdan, H. Zabel, and H.-J. Elmers, Experimental determination of exchange constants in antiferromagnetic Mn$_2$Au, Physical Review B 97, 184416 (2018).

[20] B. L. Gyorfy, A. J. Findor, J. Staunton, G. M. Stocks, and H. Winter, A first-principles theory of ferromagnetic phase transitions in metals, Journal of Physics F: Metal Physics 15, 1337 (1985).

[21] J. B. Staunton, L. Szunyogh, A. Buruzu, B. L. Gyorfy, S. Ostanian, and L. Udvardi, Temperature dependence of magnetic anisotropy: An ab initio approach, Physical Review B 74, 144411 (2006).

[22] R. Drautz and M. Fähnle, Spin-cluster expansion: Parametrization of the general adiabatic magnetic energy surface with ab initio accuracy, Physical Review B 69, 104404 (2004).

[23] L. Szunyogh, L. Udvardi, J. Jackson, U. Nowak, and R. Chantrell, Atomic spin model based on a spin-cluster expansion technique: Application to the IrMn$_3$/Co interface, Physical Review B 83, 024401 (2011).

[24] A. A. Sapozhnik, M. Filianina, S. Y. Bodnar, A. Lamirand, M.-A. Mawass, Y. Skourski, H.-J. Elmers, H. Zabel, M. Kláui, and M. Jourdan, Direct imaging of antiferromagnetic domains in Mn$_2$Au manipulated by high magnetic fields, Physical Review B 97, 134429 (2018).

[25] V. M. T. S. Barthem, C. V. Colin, R. Haettel, D. Dufeu, and D. Givord, Easy moment direction and antiferromagnetic domain wall motion in Mn$_2$Au, J. Magn. Magn. Mater. 406, 289 (2016).

[26] L. Salemi, M. Berritta, and P. M. Oppeneer, Quantitative comparison of electrically induced spin and orbital polarizations in heavy-metal/3d-metal bilayers, Phys. Rev. Materials 5, 074407 (2021).

[27] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran, and L. D. Marks, WIEN2k, An Augmented Plane Wave + Local Orbitals
Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria) (2018).

[28] J. Železný, H. Gao, A. Manchon, F. Freimuth, Y. Mokrousov, J. Zemen, J. Mašek, J. Sinova, and T. Jungwirth, Spin-orbit torques in locally and globally noncentrosymmetric crystals: Antiferromagnets and ferromagnets. Physical Review B 95, 014403 (2017).

[29] P. Bruno, Physical Origins and Theoretical Models of Magnetic Anisotropy, in Magnetismus von Festkörpern und Grenzflächen: Vorlesungsmanuskripte des 24. IFF-Ferienkurses, Ferienkurse des Forschungszentrums Jülich, edited by R. Hötzle (Forschungszentrum Jülich, Institut für Festkörperforschung, Jülich, 1993) pp. 24.1–28.

[30] U. Nowak, Classical Spin Models, in Handbook of Magnetism and Advanced Magnetic Materials, edited by H. Kronmüller and S. Parkin (John Wiley & Sons, Ltd, Chichester, UK, 2007).

[31] S. Y. Bodnar, M. Filianina, S. P. Bommanaboyena, T. Forrest, F. Maccherozzi, A. A. Sapozhnik, Y. Skourski, M. Kläui, and M. Jourdan, Imaging of current induced Néel vector switching in antiferromagnetic Mn$_2$Au. Physical Review B 99, 140409 (2019).

[32] T. Dannegger, M. Berritta, K. Carva, S. Selzer, U. Ritzmann, P. M. Oppeneer, and U. Nowak, Ultrafast coherent all-optical switching of an antiferromagnet with the inverse Faraday effect, Phys. Rev. B 104, L060413 (2021).

[33] L. Rózs, S. Selzer, T. Birk, U. Axtitia, and U. Nowak, Reduced thermal stability of antiferromagnetic nanostructures, Physical Review B 100, 064422 (2019), arXiv:1808.07665.