MA 19: Surface Magnetism

Time: Tuesday 9:30–12:30 Location: EB 407

MA 19.1 Tue 9:30 EB 407

Magnetism and electronic structure of a Dy adatom on a MgO(001) substrate — •Alexander B. Shick[1,2], Eduard Belsch[1,3], and Alexander I. Lichtenstein[3,4] — [1]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, Prague, CZ — [2]Weizmann Institute of Science, Rehovoth, IL — [3]Institute of Theoretical Physics, University of Hamburg, Hamburg, DE — [4]European X-Ray Free-Electron Laser Facility, Holzkoppel 4, Schenefeld, DE

The electronic structure and magnetism of individual Dy atom adsorbed on the MgO(001) substrate is investigated using the combination of DFT with the Hubbard-I approximation to the Anderson impurity model (DFT+U(HIA)). The divalent Dy^{2+} adatom in f^{10} configuration is found. The calculated XAS and XMCD spectra are compared to the experimental data. Quantum tunneling between degenerate $|J = 8.0, J_z = \pm 4.0\rangle$ states leads to formation of $|J = 8.0, J_z = 0.0\rangle$ ground state with an in-plane orientation of the magnetic moment. It explains absence of remanent magnetization in Dy adatom on the top of MgO(001) substrate. Our studies can provide a viable route for further investigation and prediction of the rare-earth single atom magnets.

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MA 19.2 Tue 9:45 EB 407

The magnetic domain structure of Tb(0001)/W(110) — •Patrick Härtl, Markus Leisegang, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Rare earth metal films are known to exhibit an extremely rich magnetic behavior. In the first instance it depends on the element-specific sign and wavelength of the RKKY interaction, but details of the film preparation procedure have also been shown to influence the domain structure [1]. Here we report on an investigation of epitaxial Terbium (Tb) films on W(110) by means of spin-polarized scanning tunneling microscopy (SP-STM). Tb is a ferromagnetic metal with a Curie temperature of 221 K [2]. It exhibits a large magnetic anisotropy [3] attributed to its non-spherical $4f$ charge distribution arising from a large atomic orbital momentum ($L = 3$). The easy magnetization axis is within the basal plane along $\langle 10\bar{1}0\rangle$. Our investigation on Tb(0001) films grown on W(110) indeed shows a sixfold magnetic contrast, consistent with the expected in-plane orientation of magnetic domains and comparable to earlier studies of Dy(0001)/W(110) [4]. Thickness-dependent studies reveal that the magnetic domain sizes increases with increasing film thicknesses. Domain walls are identified as Néel walls with a width of $1.4 - 3.6$ nm.

[1] P. Härtl *et al.*, Phys. Rev. B **105**, 174431 (2022).
[2] J. E. Prieto *et al.*, Phys. Rev. B **94**, 174445 (2016).
[3] J. J. Rhyne *et al.*, J. Appl. Phys. **38**, 1379 (1967).
[4] L. Berbil-Bautista *et al.*, Phys. Rev. B **76**, 064411 (2007).

MA 19.3 Tue 10:00 EB 407

Exploring the complex magnetism of hexagonal Mn mono- and double-layers on Ir(111) — •Mara Gutzeit, Tim Drevelow, Soumyajyoti Haldar, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstraße 15, 24098 Kiel, Germany

Ultrathin transition-metal films can host complex magnetic states with intriguing properties due to competing magnetic interactions. Prominent examples are antiferromagnetic (AFM) hexagonal Mn monolayers (MLs) on Re(0001) exhibiting depending on the Mn stacking either the RW-AFM or the 3Q state as the magnetic ground state [1], a double layer (DL) of Mn on the W(110) surface which holds a conical spin spiral state [2] or a Mn DL on W(001) for which the moments of the interface Mn atoms even vanish [3]. Here, employing density functional theory calculations we calculate the energy dispersion of spin spirals of both an AFM hexagonal Mn ML and a DL on Ir(111) in order to investigate their magnetic phase space. While for the ML the Néel state turns out to be energetically lowest, the situation becomes more involved for the Mn DL due to the possibility of spin spirals propagating in two interacting magnetic layers. We show that this system is characterized by a strong AFM interlayer exchange coupling giving rise to a variety of complex magnetic states that govern the low-energy regime.

[1] Spethmann *et al.* PRL **124**, 227203 (2020)
[2] Yoshida *et al.* PRL **108**, 087205 (2012)
[3] Meyer *et al.* PRR **2**, 012075(R) (2020)

MA 19.4 Tue 10:15 EB 407

Exchange engineering of a two-dimensional half-metal — •Xin Liang Tan[1,2], Arthur Ernst[3], Kenta Hagiwara[1], Ying-Jiun Chen[1,2], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut, Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]Institut für Theoretische Physik, Johannes Kepler Universität, A 4040 Linz, Austria

Ideal half-metals, showing conductivity only in one spin channel, would open the way to efficient spin-injection devices for spintronics. Prototypical examples of half-metals, such as Heusler alloys and complex oxides, lose their high spin polarization at the surface or when reduced to sub-nm thickness, complicating the realization of nanoscale spintronics. Here we present a bottom-up optimization pathway for the realization of a two-dimensional(2D) itinerant half-metallic iron-palladium film via direct band structure engineering. Spin-resolved momentum microscopy enables 2D spin-resolved mapping of the full Brillouin zone. A fully polarized Fermi surface, the hallmark of a half metal, was engineered via direct control of the film-film composition and alloying. The balancing acts between the exchange interaction and the spin-orbit coupling in the 2D film allow the direct tuning of electronic states. We highlight the local critical regions in momentum space contributing to the opening up of a spin gap. Layer- and spin-resolved Korringa-Kohn-Rostoker calculations with coherent potential approximation corroborate our experimental findings and reveal the interplay between the exchange and spin-orbit interactions.

MA 19.5 Tue 10:30 EB 407

Ab-initio exploration of complex magnetism of frustrated Mn films on Ag(111) surface — •Selcuk Sözeri[1,2], Nihad AbuAwwad[2,1], Amal Aldarawsheh[2,1], and Samir Lounis[1,2] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulations, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

Utilizing ab-initio simulations we explore the complex magnetism emerging in antiferromagnetic Mn films deposited on Ag(111) surface. While the associated triangular lattice is prone to magnetic frustration, contradictory behaviors were reported theoretically [1,2,3] and experimentally [4]. We use the full-potential relativistic Korringa-Kohn-Rostoker Green function method to extract the magnetic exchange interaction tensors for one and two Mn monolayers grown on Ag(111). Notably, we find the free-standing Mn layer to host a spin spiraling state as the ground state, while the hybridization with the electronic states of Ag promotes the Néel state to be the lowest in energy in agreement with [4]. We extract the magnetic phase diagrams and highlight the impact of both long-range Heisenberg exchange and Dzyaloshinskii-Moriya interactions.

– Project funded by DFG (SPP 2137: LO 1659/8-1).
– [1] P. Kurz, PhD-Thesis @ RWTH-Aachen University (2000); [2] Heinze et al., Appl. Phys. A 75, 25 (2002); [2] B.R. Malonda-Boungou, et al., Comp. Cond. Mat. 16. e00368 (2019); [3] C.L. Gao, et al., PRL 101, 267205 (2008).

MA 19.6 Tue 10:45 EB 407

The Impact of Lattice Distortions on the Magnetic Stability of Single Atoms: Dy and Ho on BaO(100) — Boris V. Sorokin[1], Marina Pivetta[1], Valerio Bellini[2], Darius Merk[1], Sébastien Reynaud[1], •Alessandro Barla[3], Harald Brune[1], and Stefano Rusponi[1] — [1]Institute of Physics, EPFL, CH-1015 Lausanne, Switzerland — [2]S3-Istituto di Nanoscienze-CNR, I-41125 Modena, Italy — [3]Istituto di Struttura della Materia, CNR, Trieste, Italy

With a view to the operation as qubits and memories of surface-adsorbed single-atom magnets, there is currently a strong focus on un-

derstanding the factors determining their spin dynamics. We present our investigations of the magnetic properties of Dy and Ho atoms adsorbed on BaO(100) thin films on Pt(100) [1] and a comparison with previous results for the same two elements on MgO/Ag(100). On BaO(100), Dy shows hysteresis in magnetic fields up to ≈ 3.5 T and long spin lifetime, exceeding 300 s at 2.5 K and 0.5 T. Surprisingly, Ho shows paramagnetism, as opposed to its long spin lifetime on MgO. Our combined experimental and theoretical approach shows that the critical differences bewteen BaO(100) and MgO(100) originate from the local surface distortions induced by the adatoms: while on MgO minimal distortions involve only the closest O atoms, on BaO they affect both the closest anions and cations.

[1] B. V. Sorokin, M. Pivetta, V. Bellini, D. Merk, S. Reynaud, A. Barla, H. Brune, and S. Rusponi, Adv. Funct. Mater. 33, 2213951 (2023).

15 min. break

MA 19.7 Tue 11:15 EB 407

The quest for Single Atom Magnets: the case of Dy adatoms on $SrTiO_3$ surfaces — •Valerio Bellini[1], Stefano Rusponi[2], Marina Pivetta[2], Pietro Gambardella[3], Harald Brune[2], Carlo Carbone[4], and Alessandro Barla[4] — [1]S3-Istituto di Nanoscienze-CNR, Modena, Italy — [2]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland — [3]Department of Materials, ETH Zurich, Zurich, Switzerland — [4]Istituto di Struttura della Materia-CNR, Trieste, Italy

We present a case study of rare-earth Dy and Ho single atoms deposited on the surface of $SrTiO_3$ using a combined theoretical and experimental approach [1]. X-ray magnetic circular dichroism reveals slow relaxation of the Dy magnetization on a time scale of about 800 s at 2.5 K, unusually associated with an easy-plane magnetic anisotropy. With the help of first-principles calculations and atomic multiplet simulations we rationalise this observation in terms of the magnetic properties of the Dy atoms as a function of the occupation sites on the coexisting TiO_2 and SrO-terminated surface. Interestingly, the adsorption of Dy on the insulating $SrTiO_3$ crystal leads to the formation of a spin-polarized two-dimensional electron gas, that couples antiferromagnetically to the Dy spin moments.

[1] V. Bellini, S. Rusponi, J. Kolorenč, S. K. Mahatha, M.A. Valbuena, L. Persichetti, M. Pivetta, B. V. Sorokin, D. Merk, S. Reynaud, D. Sblendorio, S. Stepanow, C. Nistor, P. Gargiani, D. Betto, A. Mugarza, P. Gambardella, H. Brune, C. Carbone, and A. Barla. ACS Nano 16, 11182 (2022).

MA 19.8 Tue 11:30 EB 407

Bismuthene on a three-dimensional spin-structure realized in Mn/Ag(111) — •Gustav Bihlmayer[1], Chia-Ju Chen[2], Yen-Hui Lin[2], Stefan Blügel[1], and Pin-Jui Hsu[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, National Tsing Hua University, Hsinchu, 30013, Taiwan

Depositing Mn on a $BiAg_2$/Ag(111) surface alloy leads to the formation of a honeycomb (HC) lattice on the surface, that can be observed with scanning tunneling microscopy (STM). The HC lattice is commensurate with a p(2×2) Ag(111) unit cell and can be assigned to Bi atoms, as can be derived from comparison to density functional theory (DFT) calculations. Furthermore, in spin-polarized STM no spin-signal is visible from the HC, but islands with different spin-polarization patterns with p(2×2) periodicity are found. These patterns can be manipulated via an external magnetic field, substantiating their magnetic origin. They show similarities with a 3**Q** structure, predicted for Mn/Cu(111) [1] and observed in Mn/Re(0001) [2]. The DFT calculations confirm the stability of the 3**Q** state compared to other ground states found theoretically [3] and experimentally [4] for Mn/Ag(111). This system realizes a quantum-spin-Hall system in contact with a non-collinear three-dimensionally modulated spin structure.

[1] Ph. Kurz et al., Phys. Rev. Lett. **86**, 1106 (2001). [2] J. Spethmann et al., Phys. Rev. Lett. **124** 227203 (2020). [3] M. dos Santos Dias et al., Phys. Rev. B **83**, 054435 (2011). [4] C. L. Gao et al., Phys. Rev. Lett. **101**, 267205 (2008).

MA 19.9 Tue 11:45 EB 407

Prospecting gigantic magnetic anisotropy energies with 3d-O molecules on MgO films — •Sufyan Shehada[1,2], Manuel dos Santos Dias[3], Muayad Abusaa[2], and Samir Lounis[1,4] — [1]Peter Grünberg Institute & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Arab American University, Jenin, Palestine — [3]Scientific Computing Department, STFC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom — [4]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Realizing stable atomic magnetic bits hinges on large out-of-plane magnetic anisotropy energy (MAE). Rau et al. detected the maximum MAE for a 3d element by inserting a Co atom on MgO(100) [1], which, however, did not show magnetic bi-stability. While simulations based on standard density functional theory (DFT) fails to capture the detected large MAE, our approach, incorporating a Hubbard U correction and spin-orbit coupling, reproduces the large MAE for a Co adatom on MgO(001). We identify the underlying mechanisms and take one step further by exploring the case of 3d-O molecules as a potential scenario to enhance the MAE while reducing the hybridization of the electronic states of the adatoms with those of the substrate in order to increase the chances for magnetic bi-stability. We investigate different structural geometries of 3d-O molecules on MgO and focus in particular on the case of molecules perpendicular to the surface.

–Work funded by (BMBF–01DH16027).

[1] Rau *et al.*, Science **344**, 988 (2014).

MA 19.10 Tue 12:00 EB 407

Complex non-collinear spin structure of a Mn double layer on Ag(111) — •Tim Drevelow and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstraße 15, 24098 Kiel, Germany

Non-collinear spin structures in ultrathin transition-metal films are interesting for spintronic applications and can be stabilized by competing magnetic interactions. Higher-order exchange interactions have been shown to stabilize nontrivial spin structures such as a distorted 3Q state in a Mn monolayer on Re(0001) [1] and a conical spin spiral in a Mn double layer on W(110) [2]. The Ag(111) surface is a different type of substrate since it exhibits only a weak hybridization with magnetic overlayers and a small spin-orbit interaction such that exchange interactions should play a dominant role. Here, we present first-principles calculations for a Mn double layer on the Ag(111) surface using density functional theory. We reveal a complex three-dimensional magnetic ground state which is stabilized by higher-order exchange interactions.

[1] Haldar *et al.* Phys. Rev. B. **104**, L180404 (2021).
[2] Yoshida *et al.* Phys. Rev. Lett. **108**, 087205 (2012)

MA 19.11 Tue 12:15 EB 407

Magnetic state of rare earth atoms on NaCl films — •María Blanco-Rey[1,2,3], Fernando Delgado[4], Andrés Arnau[1,2,3], Marina Pivetta[5], Stefano Rusponi[5], and Harald Brune[5] — [1]Universidad del País Vasco UPV/EHU, Spain — [2]Donostia International Physics Center DIPC, Spain — [3]Centro de Física de Materiales MPC-CSIC-UPV/EHU, Spain — [4]Universidad de La Laguna, Spain — [5]École Polytechnique Fédérale de Lausanne EPFL, Switzerland

A combination of STM and XAS experiments shows that rare earth atoms on NaCl/Ag have $4f^n$ and $4f^{n-1}$ electronic configurations depending on the adsorption site. The NaCl film thickness determines the preferred adsorption site, which in turn defines the occupation of the $5d$ shell. In this contribution we show that DFT calculations for Gd and Eu ad-atoms can mimic the energetics and electronic occupation of the $6s5d$ shells, predicting a $4f^{n-1}$ configuration for the rare earth as a Na substitutional, an adsorption geometry that is favorable for 2ML of NaCl only. For thicker films, defect formation is hindered and only $4f^n$ species are allowed. As the rare earth atom becomes decoupled from the Ag substrate, there is a preference for adsorption sites with reduced coordination.