O 13: Poster Session I: Surface magnetism I

Time: Monday 10:30–12:30 Location: P

O 13.1 Mon 10:30 P

Scaling Information Technology to the Atomic Limits — •Brian Kiraly, Elze J. Knol, Werner M.J. van Weerdenburg, Daniel Wegner, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The end of the scaling era in microelectronics and the expanding demand for computational resources will require new fundamental approaches to energy-efficient computing. The successes of software-based artificial intelligence are promising in this direction, yet the big payoffs promised from hardware implementations are much rarer, as they require the development of dynamic physical systems with tunable, memory-bearing coupling. In this talk, I will discuss our efforts to connect these computational requirements to the physics of single atoms on the surface of the semiconductor black phosphorus. I will show how the screening characteristics of the surface play an important role in stabilizing multiple orbital configurations, or valencies, and how these valencies realize robust non-volatile memory. I will then discuss the valency dynamics in coupled cobalt ensembles on black phosphorus. After revealing how the anisotropic surface- mediated interactions enable tunable atomic coupling, I will demonstrate that a fully functional atomic scale neural network, or so-called Boltzmann machine, can be derived from just seven cobalt atoms on black phosphorus. With two naturally separated time scales, one for computation and one for learning, this atomic Boltzmann machine further presents the possibility for autonomous learning based on the response of the system to external stimuli.

O 13.2 Mon 10:30 P

Chiral spin coupling arising from step edges in ultrathin magnetic films — Anika Schlenhoff, •Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Germany

Step edges represent a local break of lateral symmetry in ultrathin magnetic films. In our experiments, we investigate the spin coupling across atomic step edges on Fe/W(110) by means of spin-polarized scanning tunneling microscopy and spectroscopy.

As we show in our experiments, atomic step edges induce a chiral spin coupling, with outreaching consequences on the local spin texture in the film [1]. Local modifications of the spin texture toward step edges separating double from single layer areas of Fe on W(110) are observed, and selection rules indicate a chiral spin coupling that significantly changes with the propagation along different crystallographic directions. The experimental results will be presented, and the findings are explained in terms of anisotropic Dzyaloshinskii-Moriya interaction arising from the broken lateral symmetry at atomic step edges.

Our experiments strongly indicate that surface roughness and interface quality on the atomic scale is of high relevance for spin manipulation and transmission in terms of tailored magnetic coupling for future spintronic applications.

[1] A. Schlenhoff, S. Krause, and R. Wiesendanger, Phys. Rev. Lett. **123**, 037201 (2019).

O 13.3 Mon 10:30 P

Trends of higher-order exchange interactions in transition metal trilayers — •Mara Gutzeit, Soumyajyoti Haldar, Sebastian Meyer, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Higher-order exchange interactions (HOI) beyond the pair-wise Heisenberg exchange can play a crucial role in the formation of the magnetic ground state of a system. Prominent examples are both Rh/Fe atomic bilayers on Ir(111) [1] and a monolayer Fe on Rh(111) [2] which are shown to exhibit a double-row-wise antiferromagnetic (↑↑↓↓) ground state stabilized by HOI. Here, employing density functional theory as implemented in the FLEUR and VASP code, we investigate the behaviour of HOI in magnetic trilayer systems. Choosing the above-mentioned Rh/Fe/Ir system as a starting point, we systematically study how the HOI change not only with the band filling as Rh (Ir) is replaced by other elements of the 4*d* (5*d*) series but also how they are affected by different stackings of the involved transition metals. Additionally, trends for HOI parameters are presented for the case that the central 3*d* element Fe is replaced by Co. Finally, the values obtained for the biquadratic exchange, the four-site-four-spin term and the three-site-four-spin interaction of the trilayers are compared with values calculated for respective ultrathin film systems.

[1] Romming *et al.* PRL 120, 207201 (2018)
[2] Krönlein *et al.* PRL 120, 207202 (2018)

O 13.4 Mon 10:30 P

Evidence of topological Shiba bands in artificial spin chains on superconductors — •Lucas Schneider[1], Philip Beck[1], Thore Posske[2,3], Daniel Crawford[4], Eric Mascot[5], Stephan Rachel[4], Roland Wiesendanger[1], and Jens Wiebe[1] — [1]Department of Physics, Hamburg University — [2]I. Institute for Theoretical Physics, Hamburg University — [3]Centre for Ultrafast Imaging Hamburg — [4]School of Physics, University of Melbourne — [5]Department of Physics, University of Illinois at Chicago

Magnetic chains on superconducting substrates are a promising system to realize topological superconductivity and Majorana states [1-3]. In this study, we use the tip of a scanning tunneling microscope to assemble magnetic chains atom-by-atom on the surface of an elemental superconductor. We analyze Bogoliubov quasiparticle interference, reveal the formation of multiple in-gap bands and access momentum information about the band dispersions. Using this information, we find evidence that one of the bands is topologically non-trivial and gapped by effective *p*-wave correlations. This work features an important step towards the distinct experimental determination of topological phases from bulk properties only. We acknowledge funding by the ERC via the Advanced Grant ADMIRE (No. 786020), by the Cluster of Excellence 'Advanced Imaging of Matter' (EXC 2056 - project ID 390715994) and by the DFG (SFB-925 - project 170620586). [1] J. Li *et al.* PRB **90**, 235433 (2014). [2] S. Nadj-Perge *et al.*, Science **346**, 6209 (2014). [3] H. Kim *et al.*, Science Advances **4**, eaar5251 (2018).

O 13.5 Mon 10:30 P

Epitaxial growth of Fe on Be(0001) studied by STM — •Karoline Oetker, Hermann Osterhage, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Structural and magnetic properties of Fe thin films can be tuned by the choice of substrate material and lattice structure [1]. Under high pressure, bulk Fe is known to undergo a phase transition to the hexagonal close-packed (hcp) structure [2]. Despite experimental and theoretical efforts, the magnetism of hcp Fe remains unclear [3]. Utilizing substrates with hcp structure as hosts for pseudomorphic growth potentially forces Fe films into the hcp phase, which may then be investigated by spin-polarized scanning tunneling microscopy (SP-STM) [1].

In preparation for such studies, Fe growth on clean Be(0001) surfaces has been investigated in dependence of coverage and substrate temperature during deposition. High resolution STM images and Auger electron spectroscopy will be presented and discussed in terms of growth behavior and chemical composition of the films at room temperature and at elevated temperatures.

[1] R. Wiesendanger, Rev. Mod. Phys. **81**, 1495 (2009).
[2] I. Leonov *et al.*, Phys. Rev. Lett. **106**, 106405 (2011).
[3] R. Lizárraga *et al.*, Phys. Rev. B **78**, 064410 (2008).

O 13.6 Mon 10:30 P

Temperature and magnetic field dependent behavior of atomic-scale skyrmions in Pd/Fe/Ir(111) nanoislands — •Philipp Lindner, Lennart Bargsten, Stepan Kovaric, Johannes Friedlein, Jonas Harm, Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Jungiusstraße 11A, 20355 Hamburg, Germany

The thermal stability of atomic-scale skyrmions is of high relevance for potential spintronics applications and validation of theoretical models, but atomic-scale skyrmion observation was hitherto limited to very low temperatures.

In our recent study [1], we employed our unique experimental setup [2] to systematically explore the thermomagnetic phase space of Pd/Fe nanoislands on an Ir(111) substrate in an external magnetic field up to 3 T within the temperature range between 1 K and 100 K via scanning

tunneling microscopy and spectroscopy.
Evidence is found for the spin spiral, field-polarized and fluctuating disordered magnetic phases. Irrespective of considerable thermally driven magnetization dynamics, evidence for skyrmions is found at up to approximately 80 K. This critical temperature is almost tripled compared to the Fe/Ir(111) system without Pd capping [3], thereby demonstrating the stabilization of atomic-scale skyrmions against thermal agitation by highly polarizable adlayers.
[1] P. Lindner *et al.*, Phys. Rev. B **101**, 214445 (2020).
[2] J. Friedlein *et al.*, Rev. Sci. Instrum. **90**, 123705 (2019).
[3] A. Sonntag *et al.*, Phys. Rev. Lett. **113**, 077202 (2014).

O 13.7 Mon 10:30 P

Bloch-type spin helix in bilayer Fe islands on Ir(110) measured by spin-polarized STM — •Jeison A. Fischer[1], Timo Knispel[1], Vasily Tseplyaev[2], Markus Hoffmann[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Most work on interfacial chiral spin textures focused on films exhibiting C_{3v} symmetry and isotropic Dzyaloshinskii-Moriya interaction (DMI), known to only support Néel-type spin helices and skyrmions [1]. In contrast, C_{2v} symmetry systems such as the (110) surface of an fcc crystal are predicted to show anisotropic DMI, leading to various scenarios of topological pattern formation [2]. Fully unexpectedly, our spin-polarized STM/STS study reveals a magnetic stripe phase, due to a spin helix with a period of 1.2 nm along the $[\bar{1}10]$ direction in bilayer Fe islands on unreconstructed Ir(110). Based on detailed field dependent measurements with a vector magnet, we conclude that the chirality of the spin helix is of Bloch-type, where the rotation is perpendicular with the propagation direction. This contradicts the assumption of the spin helix being induced by an interface in-plane DMI vector. Combined with theoretical insights, we discuss our findings in terms of the formation energy in systems with C_{2v} symmetry.
[1] S. Heinze et al. Nat. Phys. Vol.7, p.713 (2011).
[2] M. Hoffmann et al. Nat. Commun. Vol.8, p.308 (2017).

O 13.8 Mon 10:30 P

Efficient Ab-initio Multiplet Calculations for Magnetic Adatoms on MgO — •Christoph Wolf[1], Fernando Delgado[2], Jose Reina[3], and Nicolas Lorente[3] — [1]Center for Quantum Nanoscience, Seoul, Korea — [2]Universidad de La Laguna, Spain — [3]Centro de Fisica de Materiales CFM/MPC, Spain

Scanning probe microscopy and spectroscopy, and more recently in combination with electron spin resonance, have allowed the direct observation of electron dynamics on the single-atom limit. The interpretation of data is strongly depending on model Hamiltonians. However, fitting effective spin Hamiltonians to experimental data lacks the ability to explore a vast number of potential systems of interest. By using plane-wave density functional theory (DFT) as starting point, we build a multiplet Hamiltonian making use of maximallylocalized Wannier functions. The Hamiltonian contains spinorbit and electron-electron interactions needed to obtain the relevant spin dynamics. The resulting reduced Hamiltonian is solved by exact diagonalization. We compare three prototypical cases of 3d transition metals Mn (total spin S=5/2), Fe (S=2) and Co (S=3/2) on MgO with experimental data and find that our calculations can accurately predict the spin orientation and anisotropy of the magnetic adatom. Our method does not rely on experimental input and permits us to explore and predict the fundamental magnetic properties of adatoms on surfaces.