

MA 33: Surface Magnetism II (jointly with O)

Time: Wednesday 15:00–17:30

Location: H31

MA 33.1 Wed 15:00 H31

Nanoscale and proximity effects on low-dimensional helical magnetic structures — ●JEISON A. FISCHER, LEONID M. SANDRATSKII, SOO-HYON PHARK, SAFIA OUAZI, DIRK SANDER, and STUART PARKIN — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The finite size of nanoscale magnetic structures with non-collinear spin order influences strongly their magnetic state. Also, the proximity to a ferromagnetic material affects the nanoscale spin-order [1]. We combine symmetry arguments, first-principles calculations and spin-resolved scanning tunneling spectroscopy at 10 K and in magnetic fields to study an 1D helical magnet of some nm extension in proximity to both ferromagnetic Co and vacuum regions. We report a non-uniform distortion of the spin helix in an Fe bilayer on Cu(111)[1], where the spin orientation deviates from that of an ideal helical structure. The proximity to either Co or vacuum leads to distortions of the spin orientation within nm range of the respective interface. The distortions give rise to specific energy and position dependent modifications of the spin-resolved electronic density of states. These effects have not been discussed before. We demonstrate that, in contrast to an ideal helix of infinite length, the lack of symmetry of the nm-long distorted Fe spin helix, induces an energy dependence in STS of the magnetization of the differential tunneling conductance at tip position.

[1] Phark, S. H.; Fischer, J. A.; Corbetta, M.; Sander, D.; Nakamura, K. & Kirschner, J. Reduced-dimensionality-induced helimagnetism in iron nanoislands *Nat. Commun.* 5 (2014) 5183.

MA 33.2 Wed 15:15 H31

Collective magnetism in a hybrid magnetic-superconducting system: Co aggregates on Pb — ●JEISON A. FISCHER, SRIJAN S. SAHA, RÉGIS DECKER, MICHAEL CAMINALE, HIROFUMI OKA, DIRK SANDER, VALERI STEPANIUK, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Combining the quantum phenomena superconductivity and magnetism on the nanoscale opens the path towards the exploitation of new types of electronic excitations, such as Majorana end-states [1]. These phenomena rest on the presence of magnetism in nanoscale hybrid magnetic-superconducting systems. Here, we present a combined experimental low-temperature scanning tunneling spectroscopy (STS) and theoretical first-principles study, which surprisingly finds no evidence for a sizable magnetic moment in Co monomers on a Pb surface. When some ten Co atoms aggregate together, we observe by STS at 1.8 K the appearance of additional peaks in the superconducting gap at ± 1.8 meV. These intragap states are hallmarks of the interaction of magnetic moments with a superconductor. Ab initio calculations reveal that structural relaxation of the Co adatom towards the Pb is the physical origin behind the suppression of the magnetic moment of the adatom. The resulting strong hybridization between Co and Pb leads to a balanced spin-split density of states of Co. In contrast, the Co aggregate binds farther above Pb, and a strong inter-atomic interaction within the Co aggregate leads to a conserved magnetic moment.

[1] R. M. Lutchny et al. *Phys. Rev. Lett.* 105, 077001 (2010); S. Nadj-Perge et al. *Science* 346, 602 (2014).

MA 33.3 Wed 15:30 H31

Magnetic Properties of Hybrid Organic-Ferromagnetic Interfaces — ●NICOLAE ATODIRESEI, VASILE CACIUC, RICO FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Engineering the functionalities in organic spintronic devices requires a reliable description of the electronic properties of the hybrid interface formed by the adsorption of carbon-based materials on magnetic surfaces. The density functional theory provides a framework with predictive power and realistic description of these organic-magnetic hybrid systems. We will present first-principles calculations that demonstrate how the subtle interplay between the chemical, electrostatic and the weak van der Waals adsorption mechanisms determines the geometry, electronic and magnetic structure of such hybrid interfaces. These theoretical studies provide the basic insights required to understand the surface-science experiments and are a key tool to design hybrid interfaces with specific magnetic properties that can be tuned by an

appropriate choice of the organic material and magnetic surface. [1] K. V. Raman *et al.*, *Nature* **493**, 509 (2013); [2] M. Callsen *et al.*, *Phys. Rev. Lett.* **111**, 106805 (2013). [3] N. Atodiresei *et al.*, *MRS Bulletin* 39, 596 (2014). [4] J. Brede *et al.*, *Nat. Nanotech.* 9, 1018 (2014).

MA 33.4 Wed 15:45 H31

Spin-hybridization between molecule and metal at room temperature through interlayer exchange coupling — ●MANUEL GRUBER^{1,2,3}, FATIMA IBRAHIM¹, SAMY BOUKARI¹, LOIČ JOLY¹, WULF WULFHEKEL², FABRICE SCHEURER¹, ERIC BEAUREPAIRE¹, MEBAREK ALOUANI¹, WOLFGANG WEBER¹, and MARTIN BOWEN¹ — ¹IPCMS, CNRS-UdS, Strasbourg, France — ²Karlsruher Institut für Technologie, Germany — ³IEAP, CAU Kiel, Germany

Strong coupling may exist between paramagnetic molecules and a ferromagnetic substrate. However, the study of such hybrid interfaces was so far limited to sublimable molecules deposited in ultra-high vacuum conditions in order to prevent the oxidation of the FM substrate. Here we investigated the possibility to use interlayer exchange coupling as the mediator of the molecule/FM magnetic coupling. Using X-ray magnetic circular dichroism (XMCD), we studied the magnetic coupling between manganese phthalocyanine (MnPc) molecules and a Cu(001)/Co FM substrate separated by a wedge-shaped Cu spacer. The XMCD data show that the Mn ion within MnPc molecules can be magnetically coupled to the Co substrate at room temperature when separated by up to 4 ML of Cu. The XMCD intensity evolves in an oscillatory manner with increasing Cu thickness. By decreasing the temperature, we could observe stronger oscillations in the magnetic coupling and this over a much larger Cu thickness range (up to 12 ML). The phase and the periods of the oscillatory coupling is found to be in agreement with interlayer-exchange-coupling theory [1].

[1] Gruber *et al.*, *Nano letters*, DOI:10.1021/acs.nanolett.5b02961

MA 33.5 Wed 16:00 H31

Exchange bias and room temperature magnetic order in molecular layers — ●MANUEL GRUBER^{1,2,3}, FATIMA IBRAHIM¹, SAMY BOUKARI¹, HIRONARI ISSHIKI², LOIČ JOLY¹, WULF WULFHEKEL², FABRICE SCHEURER¹, WOLFGANG WEBER¹, MEBAREK ALOUANI¹, ERIC BEAUREPAIRE¹, and MARTIN BOWEN¹ — ¹IPCMS, CNRS-UdS, Strasbourg, France — ²PI, Karlsruhe Institut für Technologie, Germany — ³IEAP, CAU Kiel, Germany

Considerable attention was focused at the interface between a ferromagnet and an organic molecular layer, where promising spintronic properties appear. Separately, molecular semiconductor may exhibit antiferromagnetic (AF) correlations well below RT. Yet, surprisingly, while magnetic pinning of a FM layer through exchange bias with an AF layer constitutes a cornerstone of spintronics, this ingredient remains missing in molecular spintronics. We performed X-ray magnetic circular dichroism measurements on paramagnetic manganese-phthalocyanine (MnPc) molecules deposited onto a FM Co(001) surface. The measurements, in combination with ab initio calculations, show that the Co/MnPc spinterface stabilizes an AF ordering at room temperature within subsequent MnPc monolayers away from the interface. In turn, we studied the impact of the AF MnPc layer on the Co substrate using the magneto-optic Kerr effect: the molecular AF layer magnetically pins the underlying Co film at temperatures below 100 K [1].

[1] Gruber *et al.*, *Nat. Mater.* 14, 981 (2015)

15 min. break

MA 33.6 Wed 16:30 H31

New approach to determine the microscopic interatomic Dzyaloshinskii-Moriya parameters from DFT calculations — ●MARKUS HOFFMANN, BERND ZIMMERMANN, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The Dzyaloshinskii-Moriya interaction (DMI) is the key ingredient for the formation of so-called chiral magnetic skyrmions – topological magnetization solitons – in materials with broken structure inversion symmetry. Realistic extended Heisenberg Hamiltonians obtained from a mapping of density functional theory (DFT) calculations provide theoretical insight into the DMI and are the starting point for the in-

vestigation of the thermodynamics and spin-dynamics of skyrmions in real chiral magnets. So far most DFT calculations provided either micromagnetic DM-vectors or microscopic DM-vectors but of limited interaction range between the magnetic atoms. This prohibits for example the analysis of frustration in the DMI or the consequence of Fermi surface nesting on the DMI. Here, we present a generalization of the derivation of interatomic exchange interactions in ferromagnets [1] to the interatomic DMI in chiral magnets. Applying the magnetic force theorem in a spin-spiral state and calculating $\vec{D}(\vec{q})$ in the full Brillouin zone, the DMI vectors \vec{D}_{ij} can be found via Fourier transformation. We present the analytical expressions relating \vec{D}_{ij} to the single-particle energies and apply our new approach to 2Fe/W(110), a commonly studied system in the field of surface magnetism.

[1] M. Ležaić *et al.*, Phys. Rev. B **88**, 134403 (2013).

MA 33.7 Wed 16:45 H31

Spin Excitation Spectroscopy on Fe4 Molecular Magnets Compressed in the Junction of a Scanning Tunneling Microscopy —

•JACOB BURGESS^{1,2}, LUIGI MALAVOLTI^{1,2,3}, VALERIA LANZILOTTO³, MATTEO MANNINI³, SHICHAO YAN^{1,2}, SILVIYA NINOVA³, FEDERICO TOTTI³, STEFFEN ROLF-PISSARCZYK^{1,2}, ANDREA CORNIA⁴, ROBERTA SESSOLI³, and SEBASTIAN LOTH^{1,2} — ¹Max-Planck Institut für Struktur und Dynamik der Materie — ²Max-Planck Institut für Festkörperforschung — ³Department of Chemistry Ugo Schiff, University of Florence & INSTM RU of Florence — ⁴Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia & INSTM RU of Modena and Reggio Emilia

Here we present inelastic tunneling spectroscopy measurements on individual Fe4 single magnetic molecules. Magnetic excitations at meV energies can be detected. Strong tip interactions are inherent in the measurement and present an experimental challenge. This necessitates the use of a correlation between excitation energy and general topography to identify intact molecules. The spectra of intact molecules indicate that the intramolecular exchange interaction is boosted significantly when compared to bulk molecular crystals. Ab initio calculations show that this can be explained by a minimal tip induced compression of the molecular core[1]. Fe4 remains suitable for spintronics applications when incorporated into prototype device and may have its magnetic properties tuned by mechanical interactions.

[1] J.A.J. Burgess *et al.*, Nature Communications 6, 8216 (2015).

MA 33.8 Wed 17:00 H31

Orienting the magnetic easy axes of molecular single-ion magnets by a graphene interlayer —

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gen PSI — ²Laboratory of Nanostructures on Surfaces, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne — ³CNRS, CRPP, UPR 8641, F-33600 Pessac and CNRS, ICMCB, UPR 9014, F-33600 Pessac — ⁴Department of Chemistry, Copenhagen University, DK-2100 Copenhagen — ⁵Condensed Matter Theory, Paul Scherrer Institut, CH-5232 Villigen

Molecular single-ion magnets (SIMs) [1] are attractive for spintronics applications because of the quantum nature of their spin and the long magnetization lifetimes. We have studied Er(trensals) SIMs [2] adsorbed on graphene/Ru(0001), graphene/Ir(111) and on bare Ru(0001) by scanning tunneling microscopy and x-ray magnetic circular dichroism. On graphene the molecules self-assemble into a densely packed layer with their magnetic easy axes oriented perpendicular to the surface. In contrast, on bare Ru(0001) the molecules are disordered and exhibit different orientations of the easy axes. The graphene-substrate moiré pattern which exhibits a stronger periodic corrugation on Ru(0001) than on Ir(111) does not influence the adsorption and magnetic properties of the molecules. [1] J. Dreiser, J. Phys.: Condens. Matter 27, 183203 (2015). [2] K. S. Pedersen *et al.*, Chem. Sci. 5, 1650 (2014).

MA 33.9 Wed 17:15 H31

Monte Carlo study of chiral magnetic structures in transition-metal multilayers —

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Due to their unique topological and dynamical properties and hence the possible application in data storage devices [1], chiral magnetic structures, such as skyrmions, have recently received a lot of interest. One of the main challenges is the stabilization of skyrmions at room temperature. To study the temperature dependence, we performed parallel tempering Monte Carlo (MC) [2] simulations. The advantage of this method is the possibility to overcome local energy minima via temperature and sample large volumes of the phase space. In order to increase the critical temperature of skyrmion systems, we explore transition-metal multilayers built from a repetition of atomic and biatomic layers of Pd, Fe and Ir [3]. We show that the critical temperature in these systems can be significantly enhanced by the interlayer exchange coupling between adjacent Fe bilayers in the multilayer structure. An increase of the exchange coupling in multilayers which may be achieved, e.g. by varying the number or species of $4d$ or $5d$ layers within the multilayer, may even yield critical values close to room temperature.

[1] A. Fert *et al.*, Nature Nanotechnology 8 (2013). [2] K. Hukushima and K. Nemoto, J. Phys. Soc. Japan **65** (1996). [3] B. Dupé *et al.*, arXiv:1503.08098 (2015).