O 81: [MA] Surface magnetism IV

Time: Thursday 15:15–17:15 Location: HSZ 103

O 81.1 Thu 15:15 HSZ 103

SP-STM study on bulk nickel (111) surface — •Liudmila Dzemiantsova, André Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

It has been recently reported that ferromagnetic materials, in particular nickel, can be used as ideal substrates for a high quality graphene formation [1, 2]. Despite the fact that nickel is a good source of spin-polarized electrons, there remains a lack of information about spinpolarized scanning tunneling microscopy (SP-STM) investigations of its surfaces [3, 4].

In our study we used SP-STM to explore the domain structure of a bulk nickel crystal (111) surface on a large scale. We showed that domains can easily be shifted at low magnetic fields or by the stray field of the magnetically coated tip. The strongest magnetic signal was achieved at energies below the Fermi level. This result is in contrast to previous theoretical expectations [3].

[1] A. Varykhalov et al., Phys. Rev. B., 80, 035437 (2009)
[2] Yu.S. Dedkov et al., App. Phys. Lett., 92, 052506 (2008)
[3] K-F. Braun et al., Phys. Rev. B, 77, 245429 (2008)
[4] Y. Nishimura et al., Phys. Rev. B, 79, 245402 (2009)

O 81.2 Thu 15:30 HSZ 103

Orientation-dependent Kondo resonance of the Ni$_2$(hfaa)$_4$(bpm) and Mn$_2$(hfaa)$_4$(bpm) single molecular magnets — •Lei Zhang[1], Michael Schackert[1], Toshio Miyamachi[1], Toyokazu Yamada[1], Frank Schramm[2], Mario Ruben[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruhe Institut of Technology, Germany — [2]Institut of Nanotechnology, Karlsruhe Institut of Technology, Germany

Single molecular magnets (SMM) attract much interest due to their potential applications in spintronics. We investigated metal organic molecules based on (hfaa)$_4$(bpm) containing two $3d$ ions (Ni or Mn) using low temperature scanning tunneling microscopy (STM) at 1 K in ultra-high vacuum. In the bulk, the two metallic ions couple antiferromagnetically leading to an $S = 0$ ground state [1,2].

The Ni$_2$ and Mn$_2$ molecules were sublimed onto atomically clean Cu(100) surfaces resulting in two different absorptions configurations. Scanning tunneling spectroscopy (STS) with a high energy resolution of 0.3 meV showed a strong Kondo resonance on the position of the metal ions inside the molecules indicating that the hybridization of the local spins with the substrate is more efficient than their antiferromagnetic coupling. The Fano resonance showed a pronounced dependence on the adsorption geometry indicating different Kondo temperatures and q-parameters. This is explained by a adsorption dependent hybridization between SMM and the substrate.

[1] G. Brewer *et al.*, Inorg. Chem. **24**, 4580-4584 (1985)
[2] M. Barquín *et al.*, Transition Metal Chemistry **24**, 546-552 (1999)

O 81.3 Thu 15:45 HSZ 103

Search for homochiral magnetic structures along the step edge of Pt(664) — •Benedikt Schweflinghaus, Bernd Zimmermann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Co chains at the step edge of Pt(997) is historically the prime example of a one-dimensional metallic magnet. A series of experimental and theoretical studies uncovered and explained the magnetic properties of this novel magnet. We re-investigate this type of system in the light of the recently discovered Dzyaloshinskii-Moriya interaction (DMI) of ultrathin films causing spin-orbit driven homochiral magnetic structures. The question arises whether the DMI in the Co chain at the Pt edge is strong enough to drive a spin-spiral state of one handedness.

In this contribution we investigate this point applying the material specific density functional theory by means of the Full-Potential Linearized Augmented Plane-Wave (FLAPW) method as implemented in the FLEUR code [1] to a variety of transition-metal (TM) chains on Pt(664). We compare TM chains to the previous analysis of the magnetic anisotropy energy (MAE) for Co chains on Pt(664) [2]. Via a micromagnetic model that includes the MAE, as well as the spin stiffness and the Dzyaloshinskii vector we investigate the possible magnetic phases. While in the Co chain it appears that the ground state is collinear, yet in other TM chains non-collinear states may be possible.

[1] http://www.flapw.de
[2] S. Baud *et al.*, Physical Review B **73**, 104427 (2006)

O 81.4 Thu 16:00 HSZ 103

Magnetism of Cobalt-coordination nodes in 2D supramolecular networks — •Uta Schlickum[1], Willi Auwärter[2], Markus Etzkorn[1], Stefano Rusponi[1], Pardeep Thakur[3], Knud Seufert[2], Svetlana Klyatskaya[4], Mario Ruben[4], Johannes V. Barth[2], and Harald Brune[1] — [1]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Physik Department E20, Technische Universität München, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Germany

Supramocular engineering on crystalline surfaces offers the possibility to fabricate networks with embedded metal centers having specific physicochemical properties. Here we report on the magnetic nature of individual Co atoms in 2D architectures providing different coordination environments probed with X-ray magnetic circular dichroism. Changing the coordination symmetry using related functional organic ligands strongly influences the magnetic characteristics of the metal center. While Co atoms with threefold coordination to carbonitriles show large magnetic moments, these vanish in the case of fourfold coordination to pyrrole ligands in a Co-porphyrin. Further modification of the magnetic properties by site-selective decoration of the individual Co centers by small Fe clusters will be discussed.

O 81.5 Thu 16:15 HSZ 103

Charge-transfer correlation effects on the spin state of magnetic molecules at a metal interface — •Sebastian Stepanow[1], Piter Miedema[2], Aitor Mugarza[1], Gustavo Ceballos[1], Paolo Moras[3], Julio Cezar[4], Carlo Carbone[3], Frank de Groot[2], and Pietro Gambardella[1] — [1]ICN Barcelona — [2]U Utrecht — [3]CNR Trieste — [4]ESRF Grenoble

We investigate the hierarchy of local correlation and hybridization effects in metal-organic molecules adsorbed on metals. Using x-ray magnetic circular dichroism and ligand field multiplet calculations, we demonstrate that the $3d$ electronic ground state of monolayer metal-phthalocyanine (CoPc, FePc) on Au(111) is given by the coherent superposition of two charge states, $d^nE + d^{n+1}$, where E represents a substrate electron bound to the central metal ion and d^n the many-body ionic orbital configuration of the unperturbed molecule. These results differ from previous models of hybrid metal-organic systems, and provide a consistent description of their magnetic properties in terms of spin and orbital multiplicity.

O 81.6 Thu 16:30 HSZ 103

Adsorbate-Dependent Changes in the Surface Magnetization of TiO$_2$ terminated SrTiO$_3$ Surface from *Ab-Initio* Calculations — •Waheed A. Adeagbo, Guntram Fischer, and Wolfram Hergert — University of Halle, Halle, Germany

Motivated by a recent experiment by Khalid *et al.* [1], in which the surface magnetization of STO was increased (weakened) after ultrasonic cleaning in ethanol (acetone), we have studied the magnetic moment formation of the TiO$_2$ terminated STO surface.

For this we have considered the perfect surface as well as one containing an O vacancy or a Ti vacancy. Both of the latter are found to be magnetic, whereas the perfect surface is non-magnetic. Furthermore, we have investigated how the adsorption of the ethanol or acetone influences the results calculated above. We find that the two adsorbates affect the magnetization of the Ti vacancy differently.

Our results are compared to the experimental ones. The calculated observed effects are robust with respect to LDA+U correlation corrections applied to the Ti $3d$ orbitals.

[1] M. Khalid et al., *Phys. Rev. B* **81**, 214414 (2010)

O 81.7 Thu 16:45 HSZ 103

Chiral spin-structure of biatomic Fe chains on Ir(001) — •Yuriy Mokrousov[1], Matthias Menzel[2], Robert Wieser[2], Kirsten von Bergmann[2], Elena Vedmedenko[2], André Kubetzka[2], Roland Wiesendanger[2], Stefan Blügel[1], and Ste-

fan Heinze[3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität zu Kiel, 24098 Kiel, Germany

We investigate from *ab initio* the magnetism of biatomic Fe chains, which form due to self-organization on the (5×1)-reconstructed Ir(001) surface [1]. Using the `FLEUR` code [2], we calculate the magnetic anisotropy and exchange energies with different exchange-correlation functionals, and find very small Heisenberg exchange interactions along the chain of the order of 10 meV/Fe-atom. Upon including spin-orbit coupling we obtain the contribution from the Dzyaloshinskii-Moriya interaction and find that it leads to a 120° spin-spiral ground state of the Fe chains with a unique rotational sense. The results of the Monte-Carlo simulations based on the parameters from *ab initio* are in a very good agreement to STM experiments on the system. We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] L. Hammer *et al.*, Phys. Rev. B **67**, 125422 (2003).
[2] www.flapw.de

O 81.8 Thu 17:00 HSZ 103

Dzyaloshinskii-Moriya interaction in $3d$-$5d$ zig-zag biatomic chains

— V. Kashid[1], •B. Zimmermann[2], T. Schena[2], Ph. Mavropoulos[2], H. G. Salunke[3], V. Shah[4], Y. Mokrousov[2], and S. Blügel[2] — [1]Department of Physics, University of Pune, Pune 411 007, India — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Technical Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India — [4]Interdisciplinary School of Scientific Computing, University of Pune, Pune 411 007, India

We investigate from first principles the influence of the antisymmetric Dzyaloshinskii-Moriya interaction (DMI) on the magnetic properties of free-standing zig-zag biatomic chains consisting of $3d$ (Fe, Co) and $5d$ (Ir, Pt, Au) transition-metal atoms. Using the `FLEUR` code [1], we perform self-consistent spin-spiral calculations while treating the spin-orbit interaction within first-order perturbation theory [2]. In this way we can extract the strength of DMI and analyze it in terms of the electronic structure of the chains. Moreover, within a simple tight-binding model we are able to grasp main features of the DMI in these systems and characterize them in terms of symmetry, band-filling and spin-spiral vector.

We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] www.flapw.de
[2] M. Heide, G. Bihlmayer, S. Blügel, Physica B **404**, 2678 (2009)