# O 112: Electronic structure: Surface magnetism and spin phenomena II

Time: Friday 10:30–13:00 Location: MA 042

O 112.1 Fri 10:30 MA 042

**Composite Kondo impurities created by assembly of entangled spin chains** — •Sebastian Loth[1,2,3], Deung-Jang Choi[2,3,6], Roberto Robles[4], Shichao Yan[2,3], Jacob A. J. Burgess[2,3], Steffen Rolf-Pissarczyk[2,3], Jean-Pierre Gauyacq[5], Nicolas Lorente[6,7], and Markus Ternes[3] — [1]Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Stuttgart — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart — [4]The Barcelona Institute of Science and Technology, ICN2, Barcelona, Spain — [5]Institut des Sciences Moleculaires d'Orsay, CNRS, Univ. Paris-Sud, Orsay Cedex, France — [6]Centro de Fisica de Materiales, CFM/MPC, San Sebastian, Spain — [7]Donostia International Physics Center, San Sebastian, Spain

We create spin chains in which a strongly correlated Kondo state emerges from antiferromagnetic coupling among the atoms of the chain [1]. We used a low-temperature scanning tunneling microscope to construct chains of Fe and Mn atoms on a copper nitride surface on Cu(100). Neither Fe nor Mn are Kondo-screened individually at the temperature of our experiment [2], but composite chains of Fe and Mn can become Kondo-screened. We find that significant inter-atomic entanglement of all magnetic atoms is a requirement for the emergence of the Kondo state. The resulting Kondo resonance is spatially distributed along the chain and can be modified by varying their composition, length and lattice constant. [1] D.J. Choi et al., Nano Lett. 17 6203 (2017). [2] C.F. Hirjibehedin et al., Science 317 1199 (2007).

O 112.2 Fri 10:45 MA 042

**Mechanically-tunable Kondo resonance in a single molecule subjected to the magnetic field reveals pitfalls in determination of the Kondo scale** — •Martin Švec[1], Martin Žonda[2], Oleksandr Stetsovych[1], Richard Korytár[2], Markus Ternes[3], Tomáš Novotný[2], and Pavel Jelínek[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic — [3]Max-Planck-Institut fur Festkorperforschung, Stuttgart, Germany

We study both experimentally and theoretically the mechanically-tunable Kondo resonance using the low-temperature scanning tunneling microscope (STM) to control the coupling of an organic molecule to its underlying metallic substrate. Pulling the molecule with a half-filled orbital and spin 1/2 from the metal surface changes the molecule's magnetic properties from the highly-correlated Kondo-singlet state to the weakly-coupled spin-flip regime, where an externally applied magnetic field can lift the state degeneracy. We employ simulations using the numerical renormalization group (NRG) theory for a reliable quantitative description of the measured low-bias differential conductance spectra and extraction of the characteristic Kondo energy scale spanning about 15 orders of magnitude. We show that the commonly used Fermi-liquid-based (Frota) and perturbative (Appelbaum) fitting procedures can be rather safely used in their corresponding limits of the high correlations and weak coupling, respectively, but they can dramatically fail even without warning signs in the crossover regime.

O 112.3 Fri 11:00 MA 042

**Absorption-site specific Kondo resonance observed in single molecule magnet $TbPc_2$ on Ag(111)** — •Jack Hellerstedt, Ales Cahlik, Martin Svec, Mario Moro, and Pavel Jelinek — Czech Academy of Sciences Institute of Physics

The single molecule magnet bis(phthalocyaninato)terbium(III) ($TbPc_2$) has attracted steady research attention as an exemplar system for realizing molecule based spin electronics. Lattices of these molecules interact through the $\pi$-electrons in their Pc ligands, which manifests itself experimentally as a Kondo resonance in spectroscopy measurements. Understanding these interactions is crucial for their subsequent use in quantum computing schema. We studied $TbPc_2$ molecules evaporated in ultrahigh vacuum onto a single crystal Ag(111) surface, measured at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/ nc-AFM). Submolecular resolution achieved with a CO- functionalized tip offers unprecedented structural information, specifically regarding the two sub-lattices forming tight-packed $TbPc_2$ islands. Kondo resonances are observed on molecules absorbed as a second layer on the larger $TbPc_2$ islands: the presence or absence of the Kondo signature is exactly correlated with the sub-lattice absorption site. Spectroscopies taken with a CO-terminated tip showed the Kondo resonance shifted to the center of the ligand. The latest efforts to understand the structural origin of this site-specific Kondo resonance will be reported.

O 112.4 Fri 11:15 MA 042

**Probing magnetic interactions between Cr adatoms on the $\beta$-$Bi_2Pd$ superconductor** — •Deung-Jang Choi[1,2,3], Carlos García Fernández[3], Edwin Herrera[4], Carmen Rubio-Verdú[3], Miguel M. Ugeda[3], Isabel Guillamón[4], Hermann Suderow[4], Jose Ignacio Pascual[3], and Nicolás Lorente[2,3] — [1]Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [2]Donostia International Physics Center (DIPC), Donostia-San Sebastian, Spain — [3]CIC nanoGUNE, Donostia-San Sebastián, Spain — [4]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain

Recently, the introduction of new impurity states in the superconducting gap has received a lot of attention. Indeed, the search of a new superconducting state dubbed topological superconductivity is strongly based in the combination of doping classical (s-wave) superconductors with magnetic impurities that arrange in a chiral fashion. Magnetic adatoms can be considered as impurities that weaken the binding of superconducting Cooper pairs leading to impurity levels in the gap: so-called Yu-Shiba-Rusinov (YSR) states. By using scanning tunneling microscope (STM), we present the first results of controlled single-atom manipulation to assemble a chain of Cr atoms on a $Bi_2Pd$ superconductor. The interatomic distance between two Cr atoms is thoroughly explored revealing Cr-Cr interactions mediated by the superconductor for the first time[1]. ([1] Choi, D.-J. et al. arXiv:1709.09224)

O 112.5 Fri 11:30 MA 042

**Spin excitations in a 4f–3d heterodimer on MgO** — Aparajita Singha[1], •Fabio Donati[2,1,3], Fabian Donat Natterer[1], Christian Wäckerlin[1,4], Srdjan Stavric[5], Zoran Popovic[5], Zeljko Sljivancanin[5], François Patthey[1], and Harald Brune[1] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, Switzerland — [2]Center for Quantum Nanoscience, Institute for Basic Science, Korea — [3]Department of Physics, Ewha Womans University, Korea — [4]Nanoscale Materials Science, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland — [5]Vinča Institute of Nuclear Sciences, Serbia

Many alloys of transition metals (TM) of the first row and rare earth (RE) elements posses large magnetic anisotropy. Atomic-scale structures made by these elements are intriguing model systems to explore unconventional magnetic phases where structural relaxations and interface effects can play a crucial role. Here we use scanning tunneling microscopy spin-excitation spectroscopy to unravel the magnetic level structure and exchange coupling in the smallest RE-TM cluster, namely HoCo dimers adsorbed on ultrathin layers of MgO on Ag(100). We observe two spin-excitations at $\pm 8$ and $\pm 20$ meV, the former being detectable with spin-polarized tips only. We model their magnetic field dependence with an effective spin Hamiltonian to identify the level splitting and the relative contribution of the two atoms to the spin excitation signal. Combining these results with density functional theory, we infer a ferromagnetic coupling between Ho and Co, which is opposite to what is known for late 4f–3d bulk compounds.

O 112.6 Fri 11:45 MA 042

**Impurity bands and magnetic interactions in the quantum anomalous Hall insulators $(V,Cr):(Bi,Sb)_2Te_3$** — •Thiago R. F. Peixoto[1], Sonja Schatz[1], Can Raphael Crespo-Vidal[1], Hendrik Bentmann[1], Kai Fauth[1], Martin Winnerlein[1], Steffen Schreyeck[1], Charles Gould[1], Karl Brunner[1], Arthur Ernst[2,3], Laurens W. Molenkamp[1], and Friedrich Reinert[1] — [1]Exp. Phys. VII, II and III, Universität Würzburg — [2]Max Planck Institute of Microstructure Physics, Halle (Saale) — [3]Institute for Theoretical Physics, Johannes Kepler Universität Linz, Austria

Recently we have reported on the fingerprint of the 3*d* impurity states in the valence band of the quantum anomalous Hall system

V:$(BiSb)_2Te_3$ by means of resonant photoemission spectroscopy (resPES) [1]. These states lie at the Fermi level and carry a significant magnetic moment, so that they are expected to promote a ferromagnetic superexchange interaction between the magnetic dopants via *pd* hybridization. Here we report x-ray magnetic circular dichroism (XMCD) measurements at the $L_{2,3}$ edges of both V- and Cr-doped $(BiSb)_2Te_3$ thin films. We show the ferromagnetic character of V and Cr 3*d* impurity bands at temperatures below 50 K. We compare our XMCD data with our valence band resPES results, which are supported by *ab initio* calculations of the density of states (DOS), and discuss the implications of V and Cr 3*d*-DOS to the magnetism of magnetically doped topological insulators.

[1] T. R. F. Peixoto *et al.*, Physical Review B **94**, 195140 (2016).

O 112.7 Fri 12:00 MA 042

**Interaction between spin waves and domain walls in ferromagnetic nanostripes** — •Nerea Ontoso[1,2], Luis Lopez-Diaz[1], Luis Torres[1], and Rocio Yanes[1] — [1]University of Salamanca, Salamanca, Spain — [2]CIC nanoGUNE, San Sebastian, Spain

Spin waves are linear low-energy excitations that propagate in ferromagnetic materials. Domain walls, on the other hand, are very stable localized structures that separate regions with uniform magnetization. Both of them are key elements of various spintronic devices, such as racetrack memories or magnon transistors.

By using micromagnetic simulations, we study the interaction between domain walls and spin waves. We analyze two different cases: (i) a head-to-head domain wall in an in-plane magnetized soft ferromagnetic stripe and (ii) a Bloch wall in a nanostripe with high perpendicular anisotropy. We perform a systematic study as a function of the frequency, spin wave amplitude and distance between the spin wave source and the domain wall. We obtain a rather complicated frequency dependence that we try to interpret in terms of spin wave reflection/transmission at the domain wall. However, a general description of this process is complex and requires taking into account dipolar fields, excitation of internal domain wall modes and high order spin wave modes due to the finite stripe width.

O 112.8 Fri 12:15 MA 042

**A first principle-based multiplet description of magnetic adatoms** — •Fernando Delgado[1] and Jhon Wilfred González[2] — [1]Departamento de Física, Universidad de La Laguna, Instituto de estudios avanzados (IUdEA), Avda. Astrofísico Francisco Sánchez, S/N 38203 La Laguna (Tenerife), Spain — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, Manuel de Lardizabal 5, E-20018 Donostia-San Sebastián, Spain

Magnetic atoms absorbed on surfaces has become a particularly attractive system to study the principles of quantum magnetism, in addition to their core interest for digital data storage. From a theoretical perspective, the simulation of these systems is quite challenging. Quite frequently, a density functional theory (DFT) calculation is used to extract the magnetic moments and magnetic anisotropy energy (MAE). Unfortunately, this description fails quite often even at qualitative level in describing the easy axis of the nanomagnet or the MAE. A much better description can be obtained by a dynamical mean field theory calculation, but at a considerably larger computational cost.

Here we have implemented an alternative description in the spirit of the multiplet calculations used in XMCD. A planewave-based spin-unpolarized DFT calculation is carried out to estimate, in combination with a maximally localized Wannier functions calculation, the crystal and ligand fields felt by the adatom electrons. This single electron picture is complemented by a many body exact configuration interaction method to extract the excitation spectra of the correlated system, together with the spin and orbital magnetic moments.

O 112.9 Fri 12:30 MA 042

**Magnetism of thin Cr and Mn films on W(100)** — •Matthias Vogt[1], Martin Schmitt[1], Ryan Cotsakis[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]The University of British Columbia, 2329 West Mall, Vancouver, BC, Canada V6T 1Z4

In this contribution we present spin-polarized scanning tunneling microscopy (SP-STM) data of thin Cr and Mn films on W(001). Due to strong spin-orbit coupling in the W substrate a significant Dzyaloshinskii-Morija interaction (DMI) can be expected, potentially leading to spin structures which are very different from those found in corresponding bulk materials. Quite contrary to this expectation, our results obtained on monolayer and double-layer Cr films on W(001) show an antiferromagnetic order between adjacent terraces, comparable to earlier observations on (001) surfaces of bulk Cr [1,2]. For the Mn double-layer on W(001) our SP-STM data show a checkerboard-like $(\sqrt{2} \times \sqrt{2})$ spin structure with an in-plane easy axis, largely reminiscent of the magnetic state previously found on the Fe monolayer on W(001), but very different from the spin spiral observed for the Mn monolayer on W(001) [3,4].

[1] M. Kleiber *et al.*, Phys. Rev. Lett. **85**, 4606 (2000).
[2] R. Ravlić *et al.*, Phys. Rev. B **67**, 174411 (2003).
[3] A. Kubetzka *et al.*, Phys. Rev. Lett. **194**, 087204 (2005).
[4] P. Ferriani *et al.*, Phys. Rev. Lett. **101**, 027201 (2008).

O 112.10 Fri 12:45 MA 042

**Revealing the interplay between surface reconstruction and magnetic order in Fe bilayers on Ir(111)** — •Nadine Hauptmann[1], Melanie Dupé[2], Tzu-Chao Hung[1], Alexander K. Lemmens[1], Jairo Sinova[2], Stefan Heinze[3], Daniel Wegner[1], Bertrand Dupé[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, Netherlands — [2]Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — [3]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Chiral magnets, e.g. magnetic skyrmions have attracted heavy interest due to their potential application for nano-scale magnetic storage. Their stabilization depends on the interplay between mainly the magnetic exchange and Dzyaloshinskii-Moriya interaction. The latter one strongly depends on the geometric structure. A vast majority of atomic-scale studies have utilized spin-polarized scanning tunneling microscopy (SP-STM). However, with SP-STM it is difficult to distinguish between structural corrugation and electronic and magnetic properties. We use a recently developed combination of SP-STM and magnetic exchange force microscopy (SPEX) to study the spin spirals in the reconstruction line network in a bilayer Fe on Ir(111). We show that with SPEX and DFT calculations we can obtain a detailed understanding of both the structure and the electronic and magnetic properties. Our work is important to understand the origin of magnetic order in atomic-scale magnetic non-collinear systems.