O 88: Electronic Structure: Surface Magnetism and Spin Phenomena

Time: Thursday 15:00–18:15 Location: MA 042

O 88.1 Thu 15:00 MA 042

Tuning the zero field splitting of single porphyrin molecules on Pb(111) — •Benjamin W. Heinrich[1], Lukas Braun[1], José I. Pascual[2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE, San Sebastián, and Ikerbasque, Basque Foundation for Science, Bilbao, Spain.

Magnetism in reduced dimensions is governed by the local chemical structure and the interaction with the surrounding on an atomic scale. Here we employ the tip of a low-temperature scanning tunneling microscope to modify reversibly the ligand field of a transition metal atom. Two metal-organic complexes – one high-spin and one intermediate-spin complex – adsorbed on the type I superconductor Pb(111) are studied at 1.2 K. Inelastic electron tunneling spectra reveal changes of the zero field splitting of the spin eigenstates in the order of 10% for both molecules due to the changed potential landscape experienced by the paramagnetic atom.

We explain our results by variations of the ligand field, which modify the *d*-level splitting and thereby the zero field splitting. These experiments highlight the importance of subtle differences in the geometry and surrounding potential, which influence the strength of magnetocrystalline anisotropy in transition metal complexes.

O 88.2 Thu 15:15 MA 042

High out-of-plane spin polarization induced by non-centrosymmetric crystal structure of BiTeI — •Christian Langenkämper[1], Koji Miyamoto[1], Oleg E Tereshchenko[2], Konstantin A Kokh[2], Peter Krüger[3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Novosibirsk State University, Russia — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany

So far, Rashba spin splittings have been discussed mostly for surface states on the basis of the Rashba-Bychkov model. Recently, a new class of Rashba materials has attracted attention: In non-centrosymmetric materials like MoS_2 [1] and BiTeI [2] the bulk Rashba effect is responsible for lifting the spin degeneracy. So far, almost all photoemission studies of BiTeI are focused on Rashba effects in the occupied states around the $\bar{\Gamma}$ point. For future applications, e.g. in opto-spintronics, a substantiated knowledge about the spin-split states above the Fermi level is also needed.

We examined the unoccupied band structure of BiTeI along the $\overline{\Gamma\mathrm{K}}$ direction with spin-resolved inverse photoemission. At the $\bar{\mathrm{K}}$ points at the Brillouin zone boundary, we found a high out-of-plane spin polarization caused by the non-centrosymmetric crystal structure. This case will be discussed on the basis of band calculations.

[1] Suzuki *et al.*, Nat. Nanotechnology **9**, 611 (2014)
[2] Ishizaka *et al.*, Nature Mater. **10**, 521 (2011)

O 88.3 Thu 15:30 MA 042

Barrier free sub-surface incorporation of 3d-transition metals into the Bi(111) surface — •Claudius Klein[1], Nora J. Vollmers[2], Percy Zahl[3], Uwe Gerstmann[2], Wolf Gero Schmidt[2], Peter Sutter[3], and Michael Horn-von Hoegen[1] — [1]Faculty of Physics and Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [3]Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973, USA

For the interesting class of materials with spin-polarized two-dimensional surface states, Bi(111) is a perfect and well understood model system. By combining low temperature scanning tunneling microscopy (LT-STM) measurements and density functional theory, we found the Bi(111) surface to have a well-defined incorporation site for 3d-transition metals within the first bilayer. Atoms like Fe, Co, Ni, Cu become immediately barrier-free embedded and are located within the same specific sub-surface site, as they are not present in STM topography. They only become apparent in STS at tunneling conditions close to the Fermi-energy, as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern. The influence of sample temperature and high coverage regimes for possible surface delta-doping are investigated. Furthermore, this incorporation effect is also observed for some 4d and 5d transition metals.

O 88.4 Thu 15:45 MA 042

Shot noise as a probe of spin polarized transport through single atoms — •Andreas Burtzlaff[1], Alexander Weismann[1], Mads Brandbyge[2], and Richard Berndt[1] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]NanoDTU, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Single Fe and Co adatoms on a Au(111) surface were contacted with a Au coated tip in an STM at 4K. The shot noise of the current through the contacts is strongly suppressed compared to the classical value of 2eI. This is a clear indicator of spin polarization in the electronic transmission. Surprisingly, this effect is observed from single atoms, whose spin moment is expected to fluctuate at 4K. Moreover, Co on Au(111) is a Kondo system and the localized spin is expected to be screened. The results will be discussed on the basis of density functional calculations.

O 88.5 Thu 16:00 MA 042

Spin Chirality in Momentum Space for Surface States on Tl/Si(111) and Tl/Ge(111) — •Sebastian D. Stolwijk[1], Philipp Eickholt[1], Kazuyuki Sakamoto[2], Anke B. Schmidt[1], Peter Krüger[3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Department of Nanomaterials Science, Chiba University, Japan — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The Tl/Si(111)-(1×1) surface is known for its spin-orbit-induced rotating spin pattern in momentum space along $\bar{\Gamma}\bar{\mathrm{K}}$ [1,2]. In this contribution, we focus on the unoccupied surface electronic structure around the $\bar{\mathrm{M}}$ point of Tl/Si(111)-(1×1) and the isoelectronic surface Tl/Ge(111)-(1×1). On both surfaces, our spin- and angle-resolved inverse-photoemission experiments reveal a surface-derived state with giant spin-orbit-induced splitting, in agreement with our theoretical findings. While it lies within a band gap for Tl/Ge(111)-(1×1), it is degenerate with bulk bands on the Si substrate. In both cases, the state is purely in-plane polarized along $\bar{\Gamma}\bar{\mathrm{M}}$, whereas the out-of-plane component is dominant along $\bar{\mathrm{K}}\bar{\mathrm{M}}$. As a consequence, spin chirality is found in momentum space around the $\bar{\mathrm{M}}$ point.

[1] K. Sakamoto et al., Nature Commun. 4, 2073 (2013).
[2] S.D. Stolwijk et al., Phys. Rev. Lett. 111, 176402 (2013).

O 88.6 Thu 16:15 MA 042

Spin-orbit entanglement in the Bi/Ag(111) surface alloy — •Thiago Ribeiro Fonseca Peixoto, Henriette Maass, Christoph Seibel, Hendrik Bentmann, and Friedrich Reinert — Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We investigated the valence band of the Bi/Ag(111) surface alloy by means of spin- and angle-resolved photoelectron spectroscopy (SARPES), with variable photon energy and light polarization. The sample growth and all measurements were performed in ultrahigh vacuum conditions. We obtained ARPES-spectra at room temperature, for photon energies between 20 and 30 eV, with *s*- and *p*-polarized light. The spin-splitted Rashba-type sp_z and p_xp_y surface states [1,2] were observed near Fermi level and exhibit strong intensity variations with the incident light polarization, due to the dipole selection rules. Spin-resolved energy distribution curves were measured at particular points of the surface Brillouin zone, for different photon energies and light polarizations. The surface states are strongly spin-polarized, reaching up to 80% spin-polarization. We show that the spin-polarization has a complex dependence on the parallel momentum, the photon energy and the orbital character of the states. We discuss our results in sight of the peculiar entanglement between the spin and the momentum of the electrons in the Rashba-type surface states [1,2].

[1] H. Bentmann *et al.*, Phys. Rev. Lett. 108, 196801 (2012).
[2] S. N. P. Wissing *et al.*, Phys. Rev. Lett. 113, 116402 (2014)

O 88.7 Thu 16:30 MA 042

Spin-Dependent Size of an Interband Hybridization Gap in the Unoccupied Band Structure of Pb/Cu(111) — •Katharina T. Ritter[1], Sune N. P. Wissing[1], Peter Krüger[2], Anke B. Schmidt[1], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany

Hybridization gaps between states of similar orbital character may become spin dependent in the presence of strong spin-orbit coupling. Using a monolayer of Pb on Cu(111) as a model system, we show that the size of these gaps itself depends on the spin direction of the states.

We use spin- and angle-resolved inverse photoemission in combination with first-principle calculations to investigate the unoccupied electronic structure of Pb/Cu(111). Above the Fermi level we find a spin-dependent hybridization gap where the splitting yields 200 meV for one and even 500 meV for the other spin direction. To gain a greater insight into the hybridization mechanism, an effective two-band tight binding model is developed. Within this model we show that the interaction of substrate and adlayer is crucial to induce a sizeable spin-orbit coupling and hybridization strength to the system.

O 88.8 Thu 16:45 MA 042

Orbital-selective spin characterization of Dirac-cone-like surface state at W(110) — •Koji Miyamoto[1], Henry Wortelen[1], Hossein Mirhosseini[3], Jürgen Henk[4], Taichi Okuda[2], and Markus Donath[1] — [1]WWU Münster, Germany — [2]Hiroshima Univ., Japan — [3]JGU Mainz, Germany — [4]MLU Halle, Germany

Recently, for the topological surface state (TSS) of Bi_2Se_3, several groups have observed an interesting phenomenon by spin- and angle-resolved photoemission (SARPE): the observed spin features of the photoelectrons are strongly dependent on the light polarization [1,2]. This effect is currently highly debated in the field of optospintronics. So far, the observations are limited to surfaces with C_{3v} symmetry.

The surface of W(110) shows a spin-polarized Dirac-cone-like state within a spin-orbit-induced gap, which is reminiscent of a TSS [3]. Here, in contrast to so far studied topological insulators, the surface structure has C_{2v} symmetry.

We studied the orbital dependence of the spin feature of the Dirac-cone-like surface state along $\overline{\Gamma H}$ at W(110) by using SARPE with *s*- and *p*-polarized light. The observed spin textures are found to be reversed between even and odd orbital symmetry. This finding opens a new way to manipulate the spin polarization of photoelectrons in systems with C_{2v} symmetry.

[1] C. Jozwiak *et al.*, Nat., Phys. **9**, 293 (2013).
[2] Z. Xie *et al.*, Nat., Commun. **5**, 3382 (2013).
[3] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012).

O 88.9 Thu 17:00 MA 042

Rashba Splitting of d_{z^2} Surface State on Ta(110) — •Henry Wortelen[1], Koji Miyamoto[1], Hossein Mirhosseini[2], Taichi Okuda[3], Jürgen Henk[4], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz — [3]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan — [4]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

The influence of spin-orbit effects on the surface electronic structure of Ta(110) was investigated by high-resolution spin- and angle-resolved photoemission. We will present photoemission data obtained by excitation with *s*- and *p*-polarized light to reveal the orbital character of the states.

A surface state with d_{z^2} symmetry [1] was detected at a binding energy of 0.45 eV at $\overline{\Gamma}$. It shows a Rashba-type spin splitting, which is large compared with d_{z^2} surface states of other elements of the same period such as Gd(0001) [2] and Tb(0001) [3]. We will discuss our experimental results in the context of electronic-structure calculations concerning spin-dependent spectral densities, spin-dependent photoelectron intensities, and symmetries of the observed states.

[1] E. Kneedler et al., Phys. Rev. Lett. **64**, 3151 (1990)
[2] O. Krupin et al., Phys. Rev. B **71**, 201403 (2005)
[3] O. Krupin et al., New J. Phys. **11**, 013035 (2009)

O 88.10 Thu 17:15 MA 042

State identification and tunable Kondo effect of MnPc — •Andreas Krönlein[1], Jens Kügel[1], Michael Karolak[2], Pin-Jui Hsu[1], Jacob Senkpiel[1], Giorgio Sangiovanni[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Germany — [2]Institut für Theoretische Physik und Astronomie, Theoretische Physik I, Universität Würzburg, Germany

In the past the Kondo effect of transition metal phthalocyanine (Pc) molecules has been intensively studied [1]. Recently, by combined scanning tunneling spectroscopy (STS) and density functional theory we could show that also MnPc/Ag(001) exhibits a Kondo effect [2]. The STS data could, however, not satisfyingly be fit by a single Fano function. Rather they appear to be a superimposition of the Kondo feature and another, yet unknown contribution. In this presentation we will show that the tunneling spectrum can be fitted by either two Fano functions, which would indicate two separate Kondo channels [3], or by a combination of a Fano and a Gauss function, with the latter representing an orbital state. We find that spatially resolved Kondo maps are only consistent with the second scenario. This is corroborated by a systematic investigation that, in addition to MnPc, also includes FePc and CoPc. In either case progressive dehydrogenation leads to a continuous shift of what is identified as the d_{z^2} molecular orbital. The influence on the Kondo temperature of MnPc will be discussed.

[1] A. Mugarza *et al.*, Phys. Rev. B **85**, 155437 (2012).
[2] J. Kügel *et al.*, Nano Lett. **14**, 3895 (2014).
[3] K.J. Franke *et al.*, Science **332**, 6032 (2011).

O 88.11 Thu 17:30 MA 042

Exploring the spectroscopic contrast in spin-polarized scanning tunneling microscopy of the antiferromagnetic e-fct Mn surface: From sub-micrometer to Ångstrom length scales — •Jiaming Song, Chii-Bin Wu, Bin Zhang, and Wolfgang Kuch — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany

We have investigated the antiferromagnetic (AFM) spin structure in AFM/ferromagnetic (FM) exchange-coupled systems in the model system expanded face-centered tetragonal (e-fct) Mn/Co(001) by spin-polarized scanning tunneling microscopy with an in-plane-sensitive Fe ring probe at room temperature. A thickness-dependent study on the surface of Mn films demonstrates that in differential conductance maps on the length scale of 100 nm, Mn exhibits a thickness-dependent layer-wise contrast at +0.2 V sample bias that proves to be mainly of electronic origin and not related to the spin structure. Still, a smaller layer-wise magnetic contribution could coexist. Atomic-scale measurements reveal a non-collinear spin texture of Mn with a (12x2) periodicity and a geometric superstructure with the same unit cell. This spin structure comprises two orthogonal domains, which are ordered on a larger length scale on 6 ML Mn compared to 5 ML. The non-collinear spin texture of Mn could be caused by competing AFM exchange interactions in the reconstructed Mn layer, possibly in combination with the Dzyaloshinsky-Moriya interaction.

O 88.12 Thu 17:45 MA 042

Kondo resonance splitting by a spin current — Deung-Jang Choi[1], Sébastien Guissart[2], Pascal Simon[2], and •Laurent Limot[1] — [1]IPCMS, Université de Strasbourg, UMR CNRS 7504, 67034 Strasbourg, France — [2]Laboratoire de Physique des Solides, Université Paris-Sud 11, UMR CNRS 8502, 91405 Orsay, France

The downscaling of spintronic devices requires developing new strategies for sensing a spin current at the smallest possible length scale. Progress towards this goal has been achieved by experimental advances in probing individual magnetic impurities coupled to non-magnetic electrodes. The spin-flip scattering of an atom is in fact a powerful spin-sensitive spectroscopic probe and information can be gathered on the magnetic interactions, either direct or indirect, between the atom and its environment. Recently, a spin current tunneling into the atom could also be detected in this way provided that the atom ground state is spin-split by a magnetic field (external or effective).

Here we show that the detection of a spin current can be simplified by using the Kondo effect of a single-atom contact. For this purpose, we mimic a multilayered spintronic device by coating a bulk ferromagnetic tip with copper and form a stable single-atom contact with a cobalt atom adsorbed on a copper surface. We find that the strong coupling between the tip and the atom inherent to our contact measurement produces a spin current sufficiently high to promote alone a spin-split Kondo state, the spin polarization of the junction amounting up to 18%.

O 88.13 Thu 18:00 MA 042

Forces during the manipulation of magnetic properties of individual molecules — •Christian Lotze, Olof Peters, Xianwen Chen, Benjamin W. Heinrich, and Katharina J. Franke — Freie Universität Berlin, Inst. f. Experimentalphysik, Arnimallee 14, 14195 Berlin

Molecular magnets are promising candidates for future electronic devices. As such they might be useful, for instance, in memory storage applications. Therefore a requirement is to have control over the molecules magnetic properties. In metal-organic complexes the latter are strongly influenced by the interaction of the metal center with the

substrate and with its ligands.

Here, we characterize the effect of an additional Cl ligand approached to the center of an iron octaethylporphyrin (FeOEP) molecule adsorbed on a Au(111) surface, employing combined scanning tunneling and atomic force microscopy (STM & AFM). The proximity of a Cl-functionalized tip to the Fe center allows to tune the molecule's spin state, magnetic anisotropy and interaction with the surface. This becomes apparent from the evolution of the tunneling spectra when the tip is approached to the molecule. At tip-molecule contact, we finally reach a regime of Kondo screening. We use simultaneous AFM measurements to detect a mechanical distortion of the molecule causing the change of magnetic properties.