O 98: Electronic structure: Surface magnetism and spin phenomena I

Time: Thursday 15:00–18:30 Location: MA 042

O 98.1 Thu 15:00 MA 042

Long spin relaxation time in a transition metal atom in contact to a metal substrate — Jan Hermenau[1], Markus Ternes[2], •Manuel Steinbrecher[1], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Department of Physics, Hamburg University, 20355 Hamburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Long spin-energy relaxation times are a prerequisite for the use of spins in data storage or nanospintronics technologies. An atomic-scale solid-state realization of such a system is the spin of a transition metal atom adsorbed on a suitable substrate. For the case of a metallic substrate, which enables a direct contacting of the spin by conduction electrons, the lifetimes reported to date are extremely short and on the order of only hundreds of femtoseconds [1,2]. Here, we show that the spin states of iron atoms adsorbed directly on a conductive platinum substrate have an astonishingly long spin-energy relaxation time in the nanosecond regime, which is comparable to that of a transition metal atom which is decoupled from the substrate electrons by a thin decoupling layer [4]. The combination of long spin-energy relaxation times and strong coupling to conduction electrons implies the possibility to use flexible coupling schemes in order to process the spin-information.

[1] A. A. Khajetoorians *et al.*, PRL **111**, 157204 (2013)
[2] T. Schuh *et al.*, J. Appl. Phys. **107**, 09E156 (2010)
[4] W. Paul *et al.*, Nat. Phys. **13**, 403 (2017)

O 98.2 Thu 15:15 MA 042

Engineering the couplings in atomically crafted spin chains on elemental superconductors — •Anand Kamlapure, Lasse Cornils, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, Germany

Spin chains coupled to s-wave superconductors realized by linear arrays of transition metal atoms on the surface of elemental superconductors may lead to topological superconductivity accompanied by the emergence of Majorana zero modes at the chain ends [1-3]. For realizing braiding of Majonara zero modes, which is ultimately needed for their usage in quantum computation, it is a prerequisite to artificially assemble such chains as well as control the exchange coupling between the chain atoms.

Here, we artificially create chains of different numbers of Fe adatoms [4] and interstitial Fe atoms on an oxygen reconstructed Ta(100) substrate using the tip of a scanning tunneling microscope as a tool. We find that the interaction within the chain can be strengthened by linking the Fe adatoms with interstitial Fe atoms, adding an important step towards the controlled design of quantum circuits employing Majorana end states.

[1] S. Nadj-Perge et al., Phys. Rev. B **88**, 020407(R) (2013).
[2] F. Pientka et al., Phys. Rev. B **88**, 155420 (2013).
[3] J. Klinovaja et al., Phys. Rev. Lett. **111**, 1 (2013).
[4] L. Cornils et al., Phys. Rev. Lett. **119**, 197002 (2017).

O 98.3 Thu 15:30 MA 042

Optically and Electrically Controllable Adatom Spin-orbital Dynamics in Transition Metal Dichalcogenides — Bin Shao[1,2], •Malte Schueler[1,2], Gunnar Schönhoff[1,2], Thomas Frauenheim[2], Gerd Czycholl[1], and Tim Wehling[1,2] — [1]Institute for theoretical Physics, University of Bremen, Bremen, Germany. — [2]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany.

We analyze the interplay of spin-valley coupling, orbital physics, and magnetic anisotropy taking place at single magnetic atoms adsorbed on semiconducting transition metal dichalcogenides, MX_2 (M = Mo, W; X = S, Se). Orbital selection rules turn out to govern the kinetic exchange coupling between the adatom and charge carriers in the MX_2 and lead to highly orbitally dependent spin-flip scattering rates, as we illustrate for the example of transition metal adatoms with d^9 configuration. Our ab initio calculations suggest that d^9 configurations are realizable by single Co, Rh, or Ir adatoms on MoS_2, which additionally exhibit a sizable magnetic anisotropy. We find that the interaction of the adatom with carriers in the MX_2 allows to tune its behavior from a quantum regime with full Kondo screening to a regime of "Ising spintronics" where its spin-orbital moment acts as classical bit, which can be erased and written electronically and optically.

O 98.4 Thu 15:45 MA 042

Probing surface magnetism with a nickelocene tip — •Benjamin Verlhac[1], Nicolas Bachellier[1], Léo Garnier[1], Maider Ormaza[1], Paula Abufager[2], Nicolás Lorente[3], Markus Ternes[4], Marie-Laure Bocquet[5], and Laurent Limot[1] — [1]Université de Strasbourg, CNRS, IPCMS, Strasbourg, France — [2]Instituto de Física de Rosario-CONICET-Universidad Nacional de Rosario,Rosario, Argentina — [3]Donostia International Physics Center (DIPC), San Sebastián, Spain — [4]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [5]ENS-CNRS-UPMC, Paris, France

Inelastic electron tunneling spectroscopy (IETS) within the junction of a scanning tunneling microscope (STM) uses current-driven spin excitations for an all electrical characterization of the spin state of a single object. Here we study the magnetism of a sandwich nickelocene molecule (Nc) adsorbed on Cu(100) by means of X-ray magnetic circular dichroism (XMCD) and density functional theory calculations (DFT), and show with IETS that it exhibits efficient spin excitations. The molecule preserves its magnetic moment and magnetic anisotropy not only on Cu(100), but also in different metallic environments including the tip apex. Taking advantage of this robusteness, we use a functionalized Nc tip to detect the magnetism of a single Fe adatom.

O 98.5 Thu 16:00 MA 042

Controled spin switch in a nickelocene molecular junction — •Benjamin Verlhac[1], Maider Ormaza[1], Nicolas Bachellier[1], Paula Abufager[2], Marie-Laure Bocquet[3], Nicolás Lorente[4], and Laurent Limot[1] — [1]Université de Strasbourg, CNRS, IPCMS, Strasbourg, France — [2]Instituto de Física de Rosario-CONICET-Universidad Nacional de Rosario,Rosario, Argentina — [3]ENS-CNRS-UPMC, Paris, France — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

One of the main challenges in molecular spintronics is to achieve an active control of a molecular spin. This is possible through the modification of the molecular structure either by chemical doping or by external stimuli. Here we investigate the effect of varying the electrode-electrode distance in a controled way in a single nickelocene molecular junction using a low-temperature scanning tunneling microscope. The molecule, when attached to the metallic tip of the microscope, exhibits spin excitations in the tunneling regime, while a Kondo ground state emerges upon contact with a Cu(100) surface, causing then an order of magnitude change in the zero-bias conductance. First principle calculations show that nickelocene reversibly switches from a spin 1 to 1/2 between the two transport regimes.

O 98.6 Thu 16:15 MA 042

Spin-resolved electron transmission through self-assembled layers of PNA — •Paul Möllers[1], Daniel Nürenberg[1], Matthias Kettner[1], Francesco Tassinari[2], Tal Markus[2], Selma Ulku[3], Catalina Achim[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel — [3]Department of Chemistry, Carnegie Mellon University, Pittsburgh, United States

The yield of electrons transmitted through chiral molecules can depend on the electron's spin; chiral molecules can therefore act a spin filters. This effect is referred to as the chirality-induced spin selectivity (CISS) effect. Previous experiments have e.g. been performed with monolayers of double-stranded DNA [1]. In this contribution, we present results of our spin-resolved photoemission experiments performed at room temperature. The samples consist of self-assembled monolayers of helical molecules – various types of double-stranded peptide nucleic acid (PNA) – on polycrystalline gold surfaces. The samples are irradiated by a laser at $\lambda = 213\,\mathrm{nm}$ to generate photoelectrons from the gold substrate which are then transmitted through the adsorbed monolayer. Subsequently, the electrons are analyzed by a Mott polarimeter. We found longitudinal spin polarizations of $-6\,\%$ for PNA and $+25\,\%$ for γ-PNA. The results indicate that the adsorbed molecules act as a spin filter.

[1] B. Göhler et al., Science 331, 894 (2011)

15 min. break

O 98.7 Thu 16:45 MA 042

Inelastic Spin- and Vibrational Excitations on FeTPyP on Au(111) — •Daniela Rolf[1], Friedrich Maass[2], Christian Lotze[1], Benjamin W. Heinrich[1], Constantin Czekelius[3], Petra Tegeder[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin — [2]Universität Heidelberg — [3]Heinrich-Heine Universität Düsseldorf

Porphyrin molecules constitute a class of well-investigated molecules, because of their versatility in terms of self-assembly and electronic and magnetic properties. Numerous studies have been performed with various central metal atoms on different metal surfaces, showing that by a suitable choice of metal center and surface, the molecular properties can be tailored. Interesting phenomena were observed, including the Kondo effect, vibronic coupling and negative-differential resistance. Here, different arrangements of Fe-tetra-pyridil-porphyrin (Fe-TPyP) molecules were investigated on a Au(111) substrate. Employing a low-temperature STM, we show that depending on the molecular geometry, a different number of steps in the dI/dV signal can be observed symmetrically around the Fermi level, with energies up to 115meV. Comparison to HREELS measurements allows for an unambigous identification of vibrational excitations. The lowest energy steps correspond to spin excitations. We correlate the variations in the spectral features to different magnetic ground states and d-level alignments originating from distinct molecular configurations of the self-assembled structures.

O 98.8 Thu 17:00 MA 042

Yu-Shiba-Rusinov states of magnetic adatoms on the quasi 2D superconductor $2H$-$NbSe_2$ — •Eva Liebhaber[1], Rojhat Baba[1], Lisa Rütten[1], Michael Ruby[1], Sebastian Rohlf[2], Kai Rossnagel[2], Benjamin W. Heinrich[1], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

A magnetic impurity adsorbed on a superconducting substrate yields so-called Yu-Shiba-Rusinov (YSR) states. These are low energy bound states inside the superconducting energy gap locally induced by magnetic exchange scattering. $2H$-$NbSe_2$ belongs to the class of transition metal dichalcogenides and is a layered van der Waals material with strong 2D character. In this material, superconductivity coexists with a charge density wave (CDW) at low temperatures.

Here, we investigate YSR states of single transition metal atoms adsorbed on the surface of $2H$-$NbSe_2$ using low temperature scanning tunneling microscopy and spectroscopy. We observe variations in d state resonances as well as in the YSR excitations. We can link these variations to the adsorption in two distinct atomic sites. Furthermore, the energy of the YSR states and their spatial extend appear to be influenced by the CDW.

O 98.9 Thu 17:15 MA 042

Magnetic Vortex Core Pinning at Atomic Scale Surface Perturbations — •Christian Holl[1], Marvin Knol[1], Marco Pratzer[1], Imara L. Fernandes[2], Jonathan Chico[2], Samir Lounis[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52428 Jülich, Germany

Spin polarized scanning tunneling microscopy is used to observe magnetic pinning centers in sub micrometer sized iron platelets. The magnetic ground state of these platelets is a flux closed magnetic vortex whose core can be moved laterally by in-plane magnetic fields[1]. Despite their small volume compared to the vortex core, we show that the core pins to the individual surface adsorbates, presumably oxygen, if the core is squeezed by a perpendicular magnetic field of 1.5 T. Comparison with micro-magnetic simulations reveal a pinning energy of up to 250 meV induced by a single adsorbate. *Ab initio* based calculations show that oxygen adatoms induce anisotropic exchange interactions in the neighbouring substrate atoms[2], which explains the non-concentric pinning position of the core.

[1] A. Wachowiak et al., Science **298**, 577-580 (2002)
[2] Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

O 98.10 Thu 17:30 MA 042

Spin-orbit gaps in ferromagnetic thin films — •Lukasz Plucinski[1], Ewa Mlynczak[1], Stephan Borek[2], Jan Minar[2], Jürgen Braun[2], Mathias Gehlmann[1], Irene Aguilera[3], Gustav Bihlmayer[3], Stefan Blügel[3], Hubert Ebert[2], and Claus M. Schneider[1] — [1]PGI-6, FZ Jülich — [2]LMU, Munich — [3]PGI-1, FZ Jülich

Magnetization direction can control topological phases in ferromagnets by influencing the existence of nodal points and spin-orbit gaps, which control intrinsic magnetotransport properties. Using high resolution angle-resolved photoemission we demonstrate openings of spin-orbit gaps, near the Fermi level [PRX 6, 041048 (2016)]. The gaps and thus the Fermi surface could be manipulated by changing the remanent magnetization direction, and we find qualitative agreement to the one-step model photoemission calculations. For thinner films the quantum confinement leads to quantum wells which also exhibit anisotropy. The analysis of spin-polarized photoemission from these quantum wells allows the unambiguous identification of the initial bands, which has been often challenging due to correlation effects in the band structure, which are beyond the description of popular exchange-correlation potentials. Good agreement is found by comparison to the bulk band structure calculated using the GW method under the assumption of perpendicular momentum broadening due to the finite probing depth of photoemission. This study contributes to better understanding of the role of Berry phase physics in anomalous Hall conductivity and related phenomena in 2D ferromagnetic layers.

O 98.11 Thu 17:45 MA 042

Orbital magnetism of $3d$ adatoms deposited on transition metal surfaces — •Sascha Brinker, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich

The classical definition of the orbital magnetic moment using the ground state charge current is well-defined for finite systems, while for periodic systems the modern theory of orbital magnetization applies. In this work we consider the intermediate case: small magnetic nanostructures deposited on surfaces from first-principles. As an application we consider $3d$ transition metal adatoms deposited on different transition metal surfaces, e.g. Ir(111), Pt(111) and Au(111), and their ground state charge current distributions. We find two contributions to the orbital magnetic moment: a local contribution corresponding to the swirling charge currents around each atom and a non-local contribution related to the net currents flowing between atoms. We show that the non-local contribution, which was neglected in previous works, is an important part of the total orbital magnetic moment, and can even exceed the local contribution. Our findings can be relevant for future experiments with nano-diamonds [1] and ESR-STM [2].

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (ERC Consolidator Grant No. 681405 DYNASORE).
[1] L. Rondin *et al.*, *Rep. Prog. Phys.* **77**, 056503 (2014)
[2] S. Baumann *et al.*, *Science* **350**, 417-420 (2015)

O 98.12 Thu 18:00 MA 042

Fe/Rh(111): a magnetic ground state driven by higher-order spin interactions — Markus Hoffmann, •Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Although for $S > \frac{1}{2}$ systems higher order spin interactions can be expected to get important, the magnetism of transition metals is often studied in the (classical) Heisenberg model. Surprisingly, the two-spin interactions from this model describe many systems rather well, only in some cases biquadratic or cyclic four-spin terms have to be added. Here, we present the system of one monolayer Fe on Rh(111) where an even more exotic term, a 3-site 4-spin interaction, is necessary to explain the ground state that was predicted by density functional theory [1] and recently confirmed experimentally [2]. The Fe layer shows a double–row-wise antiferromagnetic structure, that can be described as double-**Q** state. Another double-**Q** structure, modulating the spins in the orthogonal direction, would be energetically degenerate in the extended Heisenberg model (including biquadratic and cyclic four-spin terms) but is disfavored by the 3-site 4-spin term. Our calculations suggest that the size of this term can be as large (or even exceed) the well known four-spin interactions and that this finding is not limited to the Fe/Rh system.

[1] A. Al-Zubi et al., phys. stat. sol. (b) **248**, 2242 (2011).
[2] A. Krönlein et al., submitted (2017).

O 98.13 Thu 18:15 MA 042

Tuning the spin-related transport properties of FePc on Au(111) through single-molecule chemistry — •Ruoning Li and Yongfeng Wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing, China

Tuning the spin-dependent transport through molecules is of fundamental importance in single-molecule spintronics. Here, the transport properties of iron phthalocyanine (FePc) on Au(111) was investigated by a combination of scanning tunneling microscopy and density functional theory (DFT) calculations. In the high-resolution STS spectrum of FePc measured at 0.5 K, the Kondo resonance was observed. After removing its eight outermost hydrogen atoms, the spectroscopic feature changed to a double-step structure, which reflected a transition of molecular spin states. The DFT calculations revealed that the coupling between Fe and Au(111) got much weaker after cutting the hydrogen atoms. This explained the changing of the spin-related transport FePc on Au(111).