O 118: Surface Magnetism II (joint session O/MA)

Time: Friday 10:30–13:45 Location: GER 38

O 118.1 Fri 10:30 GER 38

Observation of tunable single-atom Yu-Shiba-Rusinov states — •Artem B. Odobesko[1], Domenico DiSante[2], Alexander Kowalski[2], Felix Friedrich[1], Ronny Thomale[2], Giorgio Sangiovanni[2], and Matthias Bode[1] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, Würzburg, Germany

Through scanning tunneling spectroscopy, we analyze the interdependence of Kondo screening and superconductivity. Our data obtained on single Fe adatoms on Nb(110) show that the coupling and the resulting Yu-Shiba-Rusinov (YSR) bound states are strongly adsorption site-dependent and exhibit a quantum phase transition, where two YSR resonances cross at zero bias. By sweeping the external magnetic field to turn off and on superconductivity in the Nb substrate, we were able to study the interaction of individual magnetic adatoms with the normal-metallic or superconducting substrate in two consecutive experiments. The data show that the in-gap position of YSR states scales with the Kondo temperature and exhibits a cross-over at 0.7Δ, in good agreement with theoretically predicted value. The observed experimental signatures are rationalized by combined density functional theory and continuous-time quantum Monte-Carlo calculations. This treatment shows that the size of the magnetic moment and the hybridization of the impurity orbitals with the substrate are key parameters for understanding the interaction between magnetic adatoms and superconductors.

O 118.2 Fri 10:45 GER 38

YSR states in manually assembled clusters of molecules on a superconducting surface — •Jan Homberg, Manuel Gruber, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24118 Kiel, Germany

The interaction between magnetic adsorbates and Cooper pairs of a superconducting substrate leads to Yu-Shiba-Rusinov (YSR) resonances. This effect has so far been investigated with low-temperature scanning tunneling microscopy (STM) on adsorbates containing a metal atom, which provides the magnetic moment. We show that non-magnetic molecules without any metal ion can acquire a net magnetic moment upon assembly into clusters as evidenced by YSR resonances. The magnetic moment is due to a partial filling of the lowest unoccupied molecular orbital of the adsorbed molecules. We show that the filling and the corresponding magnetic moment depend on the number of neighboring molecules, on their relative orientations, and on the positions of hydrogen atoms in neighboring molecules. The YSR resonances are due to fractional charges that we analyze using an Anderson-like model.

Support via the European Union's Horizon 2020 research and innovation programme (766726) is acknowledged.

O 118.3 Fri 11:00 GER 38

Tunneling of Cooper pairs through a molecular junction — Cristina Mier[1], Rose Reina[1], Leonard Garnier[2], Benjamin Verlhac[2], Laurent Limot[2], Nicolas Lorente[1], and •Deung-Jang Choi[1] — [1]Centro de Física de Materiales (MPC) CSIC-EHU San Sebastián, Spain — [2]Université de Strasbourg, CNRS, IPCMS, UMR 7504 Strasbourg, France

The tunneling of Cooper pairs between two superconductors connected through a weak link is called Josephson effect. Cooper pairs tunnel through Andreev bound states (ABS) which is localized to the weak link. The dependence of the ABS on the phase difference between the two superconductors fixes the way the Cooper pairs tunnel. ABS are a characteristic of the junction and they cannot be probed by varying the bias between the two superconductors since they take place at zero bias. This is very different from Yu-Shiba-Rusinov (YSR) in-gap state that can take place already for one superconductor and are due to the weakening of Cooper pairs produced by a magnetic impurity [1]. We will present experimental data and theoretical analysis characterizing the ABS of a reproducible Scanning Tunneling Microscope molecular junction giving us access to the elusive phase difference in an STM setup.

[1] Choi, D.-J. et al. Mapping the orbital structure of impurity bound states in a superconductor. Nat. Commun. 8, 15175 (2017).

O 118.4 Fri 11:15 GER 38

Charge transport between discrete superconducting bound states at the atomic scale — •Haonan Huang[1], Ciprian Padurariu[2], Jacob Senkpiel[1], Robert Drost[1], Björn Kubala[2], Juan Carlos Cuevas[3], Alfredo Levy Yeyati[3], Joachim Ankerhold[2], Klaus Kern[1,4], and Christian R. Ast[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]Institut für komplexe Quantensysteme, Universität Ulm, Ulm, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [4]EPFL, Switzerland

A Yu-Shiba-Rusinov (YSR) state is a pair of in-gap states resulting from the interaction of magnetic atoms with a superconductor. While YSR states have received intensifying attention especially in the field of scanning tunneling microscopy (STM) due to its capability to resolve and measure the transport through single atom, the tunneling processes between YSR states still remain elusive. We are now able to controllably introduce YSR state of desired properties to the apex of the STM tip and measure the tunneling between the tip YSR state and a sample YSR state, which we call *Shiba-Shiba tunneling*. This results in a current peak at the sum of the two YSR energies. We observe a blockade in Shiba-Shiba peak when increasing conductance, which renders YSR tip a general probe of the single level lifetime at the atomic scale.

O 118.5 Fri 11:30 GER 38

Theory of Shiba-Shiba tunneling at the edge of a Majorana chain — •Ciprian Padurariu[1], Haonan Huang[2], Björn Kubala[1], Christian R. Ast[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The realization of the Majorana chain [1], a 1D-chain of Yu-Shiba-Rusinov (YSR) states created by magnetic impurities on the surface of a superconductor, suggests that Majorana states emerging at the edges can be probed by the STM.

Recently, we have developed an ideal tool to probe and manipulate the edge states of a Majorana chain. It consists of a superconducting STM tip with its own in-gap YSR state created by a magnetic impurity on the tip. With this device we have studied the sharp resonant transport between the YSR state on the tip and another one on the superconducting sample, and have developed its theory.

This talk will expand on the theory of Shiba-Shiba tunneling and present the possible opportunities to manipulate edge states of the Majorana chain. We discuss the effects of spin-orbit coupling on tunneling, that may be relevant to the experimental realization. In certain parameter regimes theory predicts that the edge state will transfer from the chain to the tip. This may provide a first step towards realizing braiding of edge states using the STM.

[1] S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A.H. MacDonald, B.A. Bernevig, A. Yazdani, Science **346**, 602 (2014).

O 118.6 Fri 11:45 GER 38

Bloch-type spin helix in bilayer Fe islands on Ir(110) by spin polarized STM — Jeison A. Fischer[1], •Timo Knispel[1], Mahasweta Bagchi[1], Jens Brede[1], Vasily Tseplyaev[2], Markus Hoffmann[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, 50937 Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Most work on interfacial chiral spin textures focused on films exhibiting C3v symmetry and isotropic Dzyaloshinskii-Moriya interaction (DMI), known to only support Néel-type spin helices and skyrmions [1]. In contrast, C2v symmetry systems such as the (110) surface of an fcc crystal, are predicted to show anisotropic DMI leading to various scenarios of topological pattern formation [2]. Fully unexpectedly, our spin-polarized STM/STS study reveals a magnetic stripe phase, due to a spin helix with a period of 1.2 nm along the [-1 1 0] direction in bilayer Fe islands on unreconstructed Ir(110). Based on detailed field dependent measurements with a vector magnet, we conclude that the chirality of the spin helix is of Bloch-type, where the rotation is perpendicular with the propagation direction. This contradicts the assumption of the spin helix being induced by an interface in-plane DMI vector. Combined with theoretical insights, we discuss our findings in terms of the formation energy in systems with C2v symmetry. Funding: CRC1238 and the Jülich Supercomputing Center project CJIAS1F

[1] S. Heinze et al. Nat. Phys. Vol.7, p.713 (2011).
[2] M. Hoffmann et al. Nat. Commun. Vol.8, p.308 (2017).

O 118.7 Fri 12:00 GER 38

Study of the skyrmion formation on Co monolayers deposited on superconducting Ru(0001) substrate — •Loic Mougel[1], Julian Skolaut[1], Marie Hervé[1,2], Timofey Balashov[1], Jasmin Jandke[1], Bertrand Dupé[3], and Wulf Wulfhekel[1] — [1]Physikalisches Institut ,KIT, Karlsruhe, Germany — [2]Institut des Nanosciences de Paris, CNRS, Sorbonne université, Paris, France — [3]Institute of Physics, Johannes Gutenberg-Universität (JGU), Mainz, Allemagne

It has been theoretically proposed in the last years that magnetic skyrmions, when positioned in proximity to a superconductor might host Majorana bound states. These states are predicted to appear in pair of entangled states, as a zero-energy excitation in a superconducting gap. Such states are of great interest for the realization of Topological Quantum Computation.

Recently we demonstrated that it was possible to stabilize skyrmions using low magnetic field, on monolayers of Co deposited on a Ru(0001) surface. By submitting the system to a magnetic field one can create skyrmions that will remain meta-stable in the remanent state. In this communication we report on the preliminary experiments realized on the Co monolayers deposited on the superconducting Ru(0001) surface. We will present the measurements of Ruthenium superconducting gap, as well as the study of the proximity effect that arise at the Ferromagnetic/Superconductor interface, and how the superconducting state can influence the spin-spiral structure.

O 118.8 Fri 12:15 GER 38

Theoretical description of single-Co Kondo effect in atomic Cu wires on Cu(111) — Nicolas Néel[1], Markus Bohn[1], Jörg Kröger[1], •Malte Schüler[2,3], Bin Shao[2,3], Tim Wehling[2,3], Alexander Kowalski[4], and Giorgio Sangiovanni[4] — [1]Institute for Physics, Technical University of Ilmenau — [2]Bremen Center for Computational Materials Science, University Bremen, — [3]Institute for Theoretical Physics, University Bremen — [4]Institute for Theoretical Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg

Linear atomic chains containing a single Kondo atom, Co, and several nonmagnetic atoms, Cu, assembled atom by atom on Cu(111) with the tip of a scanning tunneling microscope show a peculiar evolution of the Kondo resonance. The evolution of this resonance can be inferred from changes in the line shape of the Abrikosov-Suhl-Kondo resonance. Strikingly, for two geometries no Kondo resonance at all is observed. We perform state-of-the-art first-principles calculations to describe the resonance and unravel possible microscopic origins of the remarkable experimental observations. We focus on the fact that the theoretical results are in line with experimental findings for all but two geometries which show no resonance and draw conclusions on the current state of theoretical description of many-body phenomena in real materials.

O 118.9 Fri 12:30 GER 38

Ensembles of Orbital Memories on Black Phosphorus — •Elze Knol[1], Brian Kiraly[1], Hilbert Kappen[2], and Alexander Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Donders Institute for Neuroscience, Radboud University, Nijmegen, The Netherlands

Cobalt atoms at the surface of black phosphorus (BP) have demonstrated bistable valencies [1], which can be utilized to store digital information. According to density functional theory calculations, each valency hosts a unique magnetic moment. The calculations further reveal that the bistable valencies arise due to a vertical atom displacement which modifies the screening from the underlying BP. In order to study the role of this screening, we take advantage of the tip-induced band bending occurring at the tip-sample junction of a scanning tunneling microscope to probe the energy landscape governing the valency stability. We find, both in single atom memories and ensembles of atomic memories, that the effects of local band bending are depending on the black phosphorus surface. We visualize this dependency directly with a scanning tunneling microscope by carefully studying the position dependence of the stochastic current noise. The inherent properties of this system [2] provide a unique opportunity for atomic ensembles in solids.

[1] Kiraly, et. al., Nature Commun. 9, 3904, (2018). [2] Kiraly, et. al., Phys. Rev. Lett. 123, 216403, (2019).

O 118.10 Fri 12:45 GER 38

Efficient Ab-initio Multiplet Calculations for Magnetic Adatoms on MgO — •Christoph Wolf[1], Fernando Delgado[2], Jose Reina[3], and Nicolas Lorente[3] — [1]Center for Quantum Nanoscience, Seoul, Korea — [2]Universidad de La Laguna, Spain — [3]Centro de Fisica de Materiales CFM/MPC, Spain

Scanning probe microscopy and spectroscopy, and more recently in combination with electron spin resonance, have allowed the direct observation of electron dynamics on the single-atom limit. The interpretation of data is strongly depending on model Hamiltonians. However, fitting effective spin Hamiltonians to experimental data lacks the ability to explore a vast number of potential systems of interest.

By using plane-wave density functional theory (DFT) as starting point, we build a multiplet Hamiltonian making use of maximally-localized Wannier functions. The Hamiltonian contains spinorbit and electron-electron interactions needed to obtain the relevant spin dynamics. The resulting reduced Hamiltonian is solved by exact diagonalization. We compare three prototypical cases of 3d transition metals Mn (total spin S=5/2), Fe (S=2) and Co (S=3/2) on MgO with experimental data and find that our calculations can accurately predict the spin orientation and anisotropy of the magnetic adatom. Our method does not rely on experimental input and permits us to explore and predict the fundamental magnetic properties of adatoms on surfaces.

O 118.11 Fri 13:00 GER 38

Probing the magnetism of single atoms with orbital sensitivity — Aparajita Singha[1,2], Daria Sostina[1,2], Christoph Wolf[1,2], Safa Ahmed[1,2], Denis Krylov[1,2], Luciano Colazzo[1,2], Alessandro Barla[3], Pierluigi Gargiani[4], Stefano Agrestini[4], Woo-suk Noh[5], Marina Pivetta[6], Stefano Rusponi[6], Harald Brune[6], Andreas J. Heinrich[1,2], and •Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [3]Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Trieste, Italy — [4]ALBA Synchrotron Light Source, Cerdanyola del Vallès, Catalonia, Spain — [5]Pohang University of Science and Technology, Pohang, Republic of Korea — [6]Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Individual Ho atoms adsorbed on MgO/Ag(100) show large magnetic anisotropy and long magnetic lifetime up to 40 K [Science 352, 318 (2016)]. Investigating the distribution of the electron spins among the valence orbitals is crucial to understand the quantum level structure and the origin of magnetic stability in these atoms. Here, we use the orbital sensitivity of x-ray absorption spectroscopy to investigate the valence magnetism of rare earth atoms and clusters on MgO/Ag(100). We find both Gd and Ho atoms in a monovalent state, with one electron transferred to the underneath substrate. Combining our findings with density functional theory, we clarify the controversy on the ground state of Ho single atom magnets [Phys. Rev. Lett. 121, 027201 (2018)].

O 118.12 Fri 13:15 GER 38

Quantum stochastic resonance of single Fe atoms — •Max Hänze[1,2], Gregory McMurtrie[1], Luigi Malavolti[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Stochastic resonance [1] can be observed in a variety of different systems, ranging from the periodicity of glacial periods in paleontology [2] to the time-dependent behavior of individual neurons [3] in the field of neuroscience. All such systems exhibit stochastic behavior which, because of a strong nonlinear response, can be synchronized to a small harmonic excitation. We observe quantum stochastic resonance in a single Fe atom deposited on the copper nitride surface [4] using scanning tunneling microscopy. Unlike in standard stochastic resonance, the atomic-scale process is dominated by quantum fluctuations where the magnetic state of the Fe atom is driven resonantly between two states in a classically forbidden regime. This phenomenon enables the direct observation of spin dynamics in open quantum system.

[1] R. Benzi, J. Phys. A: Math. Gen 14, L453 (1981) [2] P. N. Pearson et al. Paleontological Society Papers 18, 1-38 (2012) [3] A. J.

Bulsara et al. Theor. Biol. 152, 531-555 (1991) [4] C. F. Hirjibehedin et al. Science 317, 1199-1203 (2007)

O 118.13 Fri 13:30 GER 38

Electronic transport properties in bidimensional ferromagnet GdAu2 with atomic scale resolution — •Alberto Moya[1,2,3], David Serrate[1,2], M. Ricardo Ibarra[1,2], and Matthias Bode[3] — [1]Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, E-50009 Zaragoza, Spain — [2]Instituto de Nanociencia de Aragón, Universidad de Zaragoza, E-50018 Zaragoza, Spain — [3]Physikalisches Institut, Lehrstuhl für Experimentelle Physik 2, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Electronic properties of atomic scale motifs are difficult to measure because of complexity associated to patterning such small electrical probe contacts. In this work, we measure the electrical resistance of an antiphase boundary of a GdAu2 surface alloy. The GdAu2 monolayer is prepared on a Au(111) substrate and is known to be in-plane ferromagnetically ordered at low temperatures. It exhibits occasional antiphase boundaries which separate structurally identical but phase shifted domains by an atomically sharp 1D lattice defect. Here we measure the magnetotransport response across the boundary.

The measurements were performed by means of the recently developed Molecular Nanoprobe (MONA) technique. In this technique charge carriers (electrons or holes) are injected from the tip of a scanning tunneling microscope (STM) and detected by conformational switching processes excited inelastically by hot electrons reaching dehydrogenated phthalocyanine molecules. By statistically analyzing thousands of injection sequences the charge transport between two surface spots can be evaluated.