O 84: Focus Session: Spins on Surfaces II (joint session O/MA)

Time: Thursday 15:00–18:00 Location: H15

Invited Talk O 84.1 Thu 15:00 H15

Long-lived magnetic states in atomic-scale magnets — •Sebastian Stepanow — ETH Zürich, Switzerland

Magnetic atoms on surfaces are emerging as a new class of systems with exceptionally long spin relaxation times, which allows for reading and writing magnetic bits on the atomic scale. The magnetic properties of the single-ion magnets depend crucially on their atomic environment and enhancing their spin dynamics may lead to the development of single-atom qubits. Recent observations of magnetic remanence in individual Ho atoms adsorbed on ultrathin MgO(100) layers on Ag(100) provided the first evidence of a single atom magnet on a surface. The opening of the hysteresis loop indicates that the lifetime of Ho atoms is on the order of hours at cryogenic temperatures. Meanwhile more rare-earth adatom systems have been identified having exceptionally long spin relaxation time T_1. Despite the raising interest in these systems, it is still not clear which factors determine their very long relaxation time and if a long coherence time can be expected. The talk highlights our recent efforts in the understanding of the different contributing factors, i.e., the strong uniaxial magnetic anisotropy, the symmetry protection of the ground state from quantum tunneling and other first order scattering processes, and the peculiarities of the spin-phonon coupling with the supporting substrate.

O 84.2 Thu 15:30 H15

Mechanism of spin-dependent electron transfer on ferromagnetic interfaces: an ab initio study — •Simiam Ghan, Karsten Reuter, and Harald Oberhofer — Chair of Theoretical Chemistry, Technical University of Munich, Garching, Germany.

Self-assembled monolayers of organic molecules (SAMs) on surfaces show great promise in the emerging field of molecular electronics due to tunable charge transport properties, long-range 2-dimensional order and ease of manufacture. Growth of SAMs on ferromagnetic surfaces offers the additional possibility of spin-dependent transport for molecular spintronics in e.g. spin-valves and magnetic tunneling junctions. To establish design principles for such applications, a thorough understanding of (spin)charge transport mechanisms over SAM-metal interfaces is of great importance.

As an initial benchmark, we report calculations of spin-dependent electron transfer in model systems of Argon monolayers on ferromagnetic Fe(110), Co(0001) and Ni(111) substrates. Spin-polarized charge transfer rates are calculated from the Fermi Golden Rule using a Hamiltonian derived from first-principles density functional theory. A faster transfer of minority spins from Argon to substrate is predicted, in excellent agreement with experiment. The scheme allows us to compare the roles of orbital geometries (i.e. their spatial character) and couplings, versus densities of acceptor states in determining a final preferential spin transfer. The benchmarked protocol is applied to thiol-based model SAMs with an aim towards predicting tunable spin-transport behavior.

O 84.3 Thu 15:45 H15

Unraveling the Oxidation and Spin State of Mn-Corrole — •Reza Kakavandi[1], Mateusz Paszkiewicz[1], Hazem Aldahhak[2], Uwe Gerstmann[2], Wolfgang Schofberger[3], Wolf Gero Schmidt[2], Johannes V. Barth[1], and Florian Klappenberger[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Department of Physics, Paderborn University, Germany — [3]Institute of Organic Chemistry, Johannes Kepler University, Austria

The ability of engineering oxidation states and spin configurations in metal-corroles have fueled the vision of metal complexes-based platform for faster catalysis and more efficient fuel cells. One of the challenges in the functionality of corroles is to devise ways to unveil and ultimately control the electronic structure of the metal centers. However, despite the importance in implementation this class of molecules in novel devices, their electronic structure is hardly accessible with traditional techniques and thus is still under debate, especially at the interfaces. Here, via X-ray spectroscopic investigations and density functional theory calculations we explore the electronic ground state of the prototypical Mn-5,10,15-tris(pentafluorophenyl) corrole complex within a highly pure multilayer. The theory-based interpretation of Mn photoemission and absorption fine-structure spectra (3s and 2p and L2,3-edge, respectively) evidence a Mn(III) oxidation state with an S = 2 high-spin configuration. Furthermore, we shine light on the influence of being in contact to a Ag(111) surface and discuss mechanism such as charge transfer and annealing induced chemical conversions and their impact on the spin properties.

O 84.4 Thu 16:00 H15

Magnetic excitation spectra of single atoms on magnetic and non-magnetic substrates — •Juba Bouaziz, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

At low temperatures, inelastic scanning tunneling spectroscopy is a tool of predilection for the inspection of magnetic excitation spectra of single atoms deposited on surfaces. We employ a first-principles approach for the computation of the inelastic tunneling spectra relying on the Korringa-Kohn-Rostoker Green function method in combination with time-dependent density functional theory and many-body perturbation theory [1]. We extend the method to account for non-collinear magnetism and spin-orbit driven phenomena. The central quantity of our work is the electron's self-energy which encodes the coupling of the electron to the spin-excitation and renormalizes the electronic structure. We investigate 3*d* transition metal adatoms deposited on non-magnetic substrates such as Re(0001) and on magnetic surfaces such as PdFeIr(111) capable of hosting magnetic skyrmions [2,3].

[1] B. Schweflinghaus *et al.* Physical Review B **89**, 235439 (2014).
[2] N. Romming *et al.* Science **341**, 636-639 (2013).
[3] D. M. Crum *et al.* Nature Communications **6**, 8541 (2015).

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC consolidator Grant No. 681405 DYNASORE).

O 84.5 Thu 16:15 H15

Anisotropic spin-split surface states in momentum space from molecular adsorption — •Rico Friedrich[1,2], Vasile Caciuc[1], Bernd Zimmermann[1], Gustav Bihlmayer[1], Nicolae Atodiresei[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Present address: Center for Materials Genomics, Duke University, Durham, NC 27708, USA

Achieving control over the surface state spin texture can open new prospects in spintronics. We have recently demonstrated from first principles that the spin texture of a surface Rashba system can be controlled by the adsorption of molecules [1].

The molecular adsorption can also be employed to modulate the surface electronic structure in different momentum space directions, creating anisotropic spin splittings in **k**-space [2]. This effect is caused by an asymmetric adsorption of the molecules. Physisorbed NH_3 gives rise to variations of the surface state Rashba parameters up to a factor of 1.4 over the surface Brillouin zone. In contrast, chemisorption of BH_3 leads to variations by more than a factor of 2.5. Consequently, the anisotropy carries over to a modulation of the surface state spin texture: the spin direction can be changed from in-plane to predominantly out-of-plane by modifying the electronic momentum by 90°.

[1] R. Friedrich, *et al.*, New J. Phys. **19**, 043017 (2017).
[2] R. Friedrich, *et al.*, Phys. Rev. B **96**, 085403 (2017).

This work was supported by the Volkswagen-Stiftung (Optically Controlled Spin Logic project) and DFG SFB 1238 (Project C01).

O 84.6 Thu 16:30 H15

Tuning the coupling of an individual magnetic impurity to a superconductor: quantum phase transition and transport — •Laëtitia Farinacci[1], Gelavizh Ahmadi[1], Gaël Reecht[1], Michael Ruby[1], Nils Bogdanoff[1], Olof Peters[1], Benjamin W. Heinrich[1], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Germany — [2]Dahlem Center for Complex Systems, Berlin, Germany

Magnetic impurities on superconductors induce via exchange scattering local bound states, so called Yu-Shiba-Rusinov states, in their vicinity. Depending on the coupling strength between the impurity and the substrate, the system can be in a free- or screened-spin ground state.

Here, we use the flexibility of a Fe-porphin molecule on a Pb(111)

surface to tune continuously and reversibly between these ground states. By approaching the STM tip toward the molecule we modify on the one hand the bound state energy and on the other hand the junction transport properties so that we can resolve the YSR excitations by single-electron as well as by (multiple) Andreev reflections. [1]

[1] Farinacci et al., PRL 121, 196803 (2018)

O 84.7 Thu 16:45 H15

Investigation of the effect of Mn adatoms on the critical current in a STM Josephson junction — •Nils Bogdanoff[1], Rika Simon[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Inistitut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Atomic spins on superconducting surfaces introduce so called Yu-Shiba-Rusinov (YSR) states inside the superconducting gap as fingerprint of a magnetic interaction. Furthermore, theory predicts a renormalization of the local order parameter. Differential conductance spectroscopy reveals the YSR states but not the intrinsic order of the superconducting groundstate. Using a Josephson junction the order parameter can be determined directly by measuring its characteristic critical current. We use a Pb tip in a scanning tunneling microscope (STM) and a Pb substrate as a SIS junction. The precise control over the STM tip enables high real-space resolution to study for example defects on atomic length scales. As was shown before [1], a reduction of the critical current can be observed on iron adatoms on a Pb(110) surface.

Here, we measure the critical current caused by Mn adatoms on Pb(111) in voltage- and current-biased Josephson junctions. We show that these more strongly reduce the critical current than the Fe adatoms.

[1] M. T. Randeria et al., Scanning Josephson spectroscopy on the atomic scale, Phys. Rev. B 93, 161115(R), 2016

O 84.8 Thu 17:00 H15

Broadband noise spectroscopy of antiferromagnetic iron dimers — •Gregory McMurtrie[1,2,3], Max Hänze[1,2,3], Luigi Malavolti[1,2,3], and Sebastian Loth[1,2,3] — [1]Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

Spin and charge dynamics are particularly pronounced in nanoscale materials, where they give rise to exciting effects such as quantum interference or quantum critical behavior. Accessing these dynamics on their intrinsic length and time scales is an important step towards a microscopic understanding of quantum physics on the atomic scale. Applying pulses [1] or continuous wave signals [2] to individual atoms has proven a powerful technique for the characterization of fast magnetic surface dynamics using scanning tunneling microscopy. We show that the dynamics of individual atoms can be observed in the frequency domain using broadband noise detection, thereby non-invasively revealing picosecond-scale fluctuations. This method is a powerful tool for characterizing both state lifetimes and measuring surface scattering effects, giving deeper insight into the fundamental dynamic behavior of spins coupled to dissipative environments. [1] S. Loth, M. Etzkorn, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 329 1628 (2010) [2] S. Baumann, W. Paul, T. Choi, C. P. Lutz, A. Ardavan, A. J. Heinrich, Science 350 6259 (2015)

O 84.9 Thu 17:15 H15

Ab-initio study of the electron-phonon interaction of a single Fe adatom on the MgO/Ag(100) surface — •haritz garaimarin[1,2], julen ibañez-azpiroz[3], peio g. goiricelaya[1,2], idoia g. gurtubay[1,2], and asier eiguren[1,2] — [1]Materia Kondentsatuaren Fisika saila, Euskal Herriko Unibertsitatea UPV/EHU, Bilbo, Spain — [2]Donostia International Physics Center, Donostia, Spain — [3]Centro de Física de Materiales CSIC-UPV/EHU, Donostia, Spain

Breakthrough experimental studies have recently shown that it is possible to create stable magnetic quantum states in individual adatoms [1,2]. While the role of electronic interactions on the magnetic stability has been thoroughly investigated theoretically [3], the coupling with phonons has attracted much less attention. The aim of this work is to study, via ab-initio calculations, the effect of the electron-phonon interaction (EPI) in Fe adatoms deposited on MgO/Ag(100), a benchmark system where the EPI is believed to determine to large extent its magnetic stability [2]. Here we present the calculated electronic structure and vibrational dynamics of this system, including the local vibrations of the adatom. Furthermore, we analyze the effect of the EPI on the magnetic stability via the renormalization of the electronic properties of the adatom.

[1] F. Donati *et. al.*, Science **352**, 318 (2016). F. D. Natterer *et. al.*, PRL **121**, 27201 (2018). [2] W. Paul *et. al.*, Nat. Phys. **13**, 403 (2017). [3] N. Lorente and J.-P. Gauyacq, PRL **103**, 176601 (2009). J. Fernández-Rossier, PRL **102**, 256802 (2009). J. Ibañez-Azpiroz *et. al.*, Nano Lett. **16**, 4305 (2016).

O 84.10 Thu 17:30 H15

Spin excitations in non-collinear magnetic clusters deposited on Pt(111) from TD-DFT — •Sascha Brinker, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich

Small magnetic clusters hold great promise for future information technology. The smallest stable magnetic nanostructure on a metallic surface is a Fe trimer on Pt(111) [1]. The spin stability is strongly influenced by the excitation spectrum and by relativistic effects, like e.g. the Dzyaloshinskii-Moriya-interaction [2], which is among others responsible for non-collinear magnetic ground states. In this contribution, we generalize our time-dependent density functional theory calculations already including the spin-orbit interaction [3, 4] to non-collinear magnetic structures, focusing on magnetic clusters on Pt(111). We interpret our results with a generalized Landau-Lifshitz-Gilbert equation. We pay special attention to the anisotropic and non-local contributions to the spin pumping and damping, and to their dependence on the magnetic structure.

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] J. Hermenau *et al.*, Nat. Comm. **8**, 642 (2017)
[2] J. Hermenau, S. Brinker *et al.*, arXiv:1811.02807 (2018)
[3] M. dos Santos Dias *et al.*, Phys. Rev. B **91**, 075405 (2015)
[4] F. S. M. Guimarães *et al.*, Phys. Rev. B **96**, 144401 (2017)

O 84.11 Thu 17:45 H15

Hyperfine interaction of individual atoms on a surface — •Philip Willke[1,2,3], Yujeong Bae[1,2,3], Kai Yang[3], Jose Lado[4,5], Alejandro Ferrón[6], Taeyoung Choi[1,2], Arzhang Ardavan[7], Joaquín Fernández-Rossier[4], Andreas Heinrich[1,2], and Christopher Lutz[3] — [1]Center for Quantum Nanoscience, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]IBM Almaden Research Center, San Jose, USA — [4]International Iberian Nanotechnology Laboratory, Braga, Portugal — [5]ETHZ, Zurich, Switzerland — [6]Universidad Nacional del Nordeste, Corrientes, Argentina — [7]University of Oxford, Oxford, UK

The combination of electron spin resonance (ESR) with scanning tunneling microscopy (STM) enabled spin resonance on individual atoms on surfaces [1]. Making use of the increased energy resolution of ESR-STM we can resolve and control the hyperfine interaction of single atoms [2]. Using atom manipulation we find that the hyperfine interaction strongly depends on the binding configuration of the atom as well as the proximity to other magnetic atoms. This allows us to extract atom- and position-dependent information about the electronic ground state as well as properties of the nuclear spin. Moreover, we show that the populations of the nuclear spin states can be controlled by utilizing the spin-polarized tunnel current [3].

[1] S. Baumann *et al.*, Science **350** (2015). [2] P. Willke *et al.*, Science **362** (2018). [3] K. Yang, PW, *et al.*, Nature Nano (2018).