O 71: Focus Session: Atomic-Scale Studies of Spins on Surfaces with Scanning Tunneling Microscopy 2

Time: Thursday 15:00–18:00 Location: S051

Topical Talk O 71.1 Thu 15:00 S051

Theory for Electron Spin Resonance based on electron transport — •Nicolas Lorente[1], José Reina[2], and Christoph Wolf[2] — [1]Centro de Física de Materiales & DIPC, Donostia, Spain — [2]Center for Quantum Nano Science, Seoul, Korea

Recent progress in electron spin resonance with the scanning tunneling microscope (ESR-STM) [1] is greatly advancing the experimental possibilities of manipulating atomic spins by all-electrical means. Two-qubit operations have been made possible using a pulse-mode in the ESR-STM [2], and addressing remote qubits has been rendered possible by creating a new muti-frequency operational mode [3]. We aim at developing a computational tool that permits us to interpret and predict the outcome of experiments in ESR. The first results of such a simulation tool have addressed one and two spins under an STM current [4,5]. We use a non-equilibrium Green's function approach with Hubbard operators that allows us to write quantum adiabatic Markovian master equations in the presence of an electron current and under the driving of an external electric field. The results are enticing and the modelling is flexible enough to treat many different physical situations. References: [1] S. Baumann et al, Science 350, 417 (2015). [2] K. Yang et al, Science 366, 509 (2019). [3] S.-H. Phark et al, ArXiv:2108.09880. [4] J. Reina et al, Phys. Rev. B 100, 035411 (2019). [5] J. Reina et al, Phys, Rev. B 104, 245435 (2021).

O 71.2 Thu 15:30 S051

Modeling the Electron Spin Resonance Spectrum in Scanning Tunneling Microscopy — •Christian R. Ast[1], Piot Kot[1], Maneesha Ismail[1], and Juan Carlos Cuevas[2] — [1]MPI for Solid State Research, 70569 Stuttgart — [2]Universidad Autónoma de Madrid, 28049 Madrid, Spain

The theory of electron spin resonance (ESR) spectroscopy in scanning tunneling microscopy (STM) has been debated for some time now with a number of different proposals having different origin, but essentially leading to very similar results. While the focus so far has been on the ESR signal itself, the measured DC tunneling spectrum offers more details that allow for a more precise verification of the underlying theory. Here, we discuss the ESR signal from a theory point of view by allowing the tunneling electrons to interact with both the driven spin system and the incident microwave during the tunneling process. We find a more complete description of the whole tunneling current also going beyond the typical approximation of a constant density of states.

O 71.3 Thu 15:45 S051

A new view on the origin of zero-bias anomalies of Co atoms atop noble metal surfaces — Juba Bouaziz[1], Filipe S. M. Guimaraes[1], and •Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich 52425, Germany — [2]Faculty of Physics & CENIDE, University of Duisburg-Essen, 47057, Duisburg, Germany

Many-body phenomena are paramount in physics. In condensed matter, their hallmark is considerable on a wide range of material characteristics spanning electronic, magnetic, thermodynamic and transport properties. In this talk, we address systematically zero-bias anomalies detected by scanning tunneling spectroscopy on Co atoms deposited on Cu, Ag and Au(111) substrates, which remarkably are almost identical to those obtained from first-principles [1]. These features originate from gaped spin-excitations induced by a finite magnetic anisotropy energy, in contrast to the usual widespread interpretation relating them to Kondo resonances. Resting on relativistic time-dependent density functional and many-body perturbation theories, we furthermore unveil a new many-body feature, the spinaron, resulting from the interaction of electrons and spin-excitations localizing electronic states. Besides Co, we will show examples of anomalous spin-excitations characterising adatoms on Nb(110) surface [2,3].
[1] Bouaziz, Guimaraes, Lounis, Nat. Commun. 11, 6112 (2020); [2] Brinker, Küster, Parkin, Sessi, Lounis, Science Adv. 8, eabi7291 (2022); [3] Küster, Montero, Guimaraes, Brinker, Lounis, Parkin, Sessi, Nat. Commun. 12, 1108 (2021).

O 71.4 Thu 16:00 S051

Real-space observation of the Kondo effect in MoS_2 mirror twin boundaries — Camiel van Efferen[1], Jeison Fischer[1], Achim Rosch[2], Thomas Michely[1], and •Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln

Finite mirror twin boundaries in monolayer MoS_2 on graphene confine strongly correlated one-dimensional electronic states [1]. Using scanning tunneling microscopy and spectroscopy, we observe a resonance at the Fermi energy when the highest occupied confined state is filled with one electron. Magnetic field and temperature-dependence of the resonance unambiguously point to the Kondo effect, i.e., screening of the spin-$\frac{1}{2}$ confined state within the mirror twin boundary. Theoretical models for both Kondo resonance and spin-$\frac{1}{2}$ state are used to extract the Kondo coupling strength. Real-space mapping gives access to the correlated beating of both confined state and Kondo resonance along the boundary. Hence, our experiments reveal the behavior of the Kondo effect for a delocalized electronic state on the atomic scale.

[1] Jolie et al., Phys. Rev. X 9, 011055 (2019)

O 71.5 Thu 16:15 S051

Moiré tuning of spin excitations: individual Fe atoms on MoS_2/Au(111) — •Christian Lotze[1], Sergey Trishin[1], Nils Bogdanoff[1], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Magnetic adatoms have been investigated on various surfaces in regard to stabilizing, controlling and manipulating single quantum spins. Here, we study individual iron atoms adsorbed on a single layer of molybdenum disulfide (MoS_2) on a Au(111) crystal. MoS_2 has been recently reported as a well-suited system for decoupling molecules. We show that the Fe atoms are largely decoupled from the Au(111) substrate with the remaining coupling strength varying along the moiré structure. As a consequence, the spectroscopic fingerprints range from pure inelastic excitations to Kondo resonances. Moreover, we see spatial variations of those excitations over one atom, which result from the formation of Fe-S hybrid states and interference effects. In conclusion, our work establishes MoS_2 on Au(111) as a tuning layer for quantum spin properties. This tuning can be realized continuously.

O 71.6 Thu 16:30 S051

Spin excitations on hexagonal zinc oxide — •Lukas Arnhold, Henrik Lichtl, Leon Rullkötter, Nicolaj Betz, Susanne Baumann, and Sebastian Loth — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

Few-layer materials are widely used to tailor different electronic properties, down to the atomic level. We use a double layer of ZnO, a hexagonal wide bandgap semiconductor [1], to mitigate electron scattering between the Ag (111) substrate and Co atoms deposited on the ZnO surface. With low-temperature scanning tunneling microscopy we observe spin excitations and the ability to manipulate transition metal atoms on the surface into hexagonal arrangements. These findings make ZnO a viable candidate for resonant spin spectroscopy methods [2,3] and construction of geometrically frustrated magnetic structures.
[1] A. Shiotari et al., J. Phys. Chem. C 118, 27428 (2014). [2] S. Baumann et al., SCIENCE 350, 417 (2015). [3] M. Hänze et al., SCIENCE ADVANCES 7, eabg2616 (2021).

Topical Talk O 71.7 Thu 16:45 S051

Stochastic resonance as a new tool to investigate spin dynamics — •Susanne Baumann[1], Nicolaj Betz[1], Max Hänze[1], Gregory McMurtrie[1], Susan Coppersmith[2], and Sebastian Loth[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]School of Physics, University of New South Wales, Sydney, Australia

Stochastic resonance is an unusual phenomenon in which noise can be used as a resource to synchronize stochastic dynamics to a control signal [1,2]. In this talk, I will show how stochastic resonance can be induced in the spin switching of magnetic nanostructures on surfaces [3], and, more importantly, how we can use this as a tool to investigate the magnetization dynamics of these spin systems.

With this tool, one can get insight into the interaction of these structures with their environment. This also enables the observation of ultrafast dynamics of excited spin states that are not easily accessible to other scanning probe techniques. The new frequency resolved spectroscopy method allows for the broadband observation of spin dynamics with previously inaccessible bandwidth ranging from milliseconds to picoseconds.

References: [1] R. Benzi, J. Phys. A: Math. Gen 14, L453 (1981). [2] R. Löfstedt, S. N. Coppersmith, Phys Rev. Lett. 72, 1947 (1994). [3] M. Hänze*, G. McMurtrie* et al. Science Adv. 7 eabg2616 (2021).

O 71.8 Thu 17:15 S051

Path-resolved measurement of ultrafast spin dynamics — •Nicolaj Betz[1], Max Hänze[1,2], Gregory McMurtrie[1], Susanne Baumann[1], 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

Transitions between quantum mechanical states are fundamentally random processes. While it is possible to directly observe individual quantum jumps [1] in a time resolved measurement [2], the dynamics of many systems exceed the resolution of real time measurements. This requires the use of time-averaged measurements such as pump probe experiments. These methods typically measure state occupation times and contain little information about the relaxation process itself. Here, we introduce a dynamic response measurement that is sensitive to the switching path between spin states and can be applied in scanning tunneling microscopy. By using stochastic resonance [3], this method resolves spin- switching dynamics of magnetic atoms and nanostructures ranging from milliseconds to picoseconds. Crucially, in more complex spin structures the measurement can distinguish multiple switching paths between higher excited states. This provides deeper insight into ultrafast spin dynamics than possible with relaxometry.

[1] Th. Sauter, et al. Phys. Rev. Lett. 57, 1696 (1986).
[2] M. Hänze, et al. Sci. Adv. 7, 33 (2021).
[3] R. Löfstedt, et al. Phys. Rev. Lett. 72, 1947 (1994).

O 71.9 Thu 17:30 S051

Growth and magnetic characterization of thermally robust cobalt islands on Cu3Au(111) — •Aleš Cahlík, Danyang Liu, Berk Zengin, and Fabian Natterer — Institute of Physics, UZH, Zurich, Switzerland

Due to a larger tunability of the effective lattice parameter, bimetallic alloys can be an appealing choice as an alternative substrate for the growth of thin films and nanostructures. In this respect, we investigate $Cu_3Au(111)$ as a platform for the growth of cobalt nano-islands. Using STM, we demonstrate unique thermal stability of $Co/Cu_3Au(111)$ up to $\sim 340°C$, compared to the fast intermixing of Co/Cu(111) at room temperature. We explore the structural and magnetic properties of the Co islands with spin-polarized and nickelocene functionalized tips. Finally, we find an effective method to produce spin-polarized tips by deliberately lifting off an entire island from the substrate and transferring it to the STM tip.

O 71.10 Thu 17:45 S051

Transport in the Rashba-split surface state of $(\sqrt{3} \times \sqrt{3})$**Bi/Ag(111)**$R30°$ **revealed by MONA** — •Markus Leisegang, Patrick Härtl, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Transport measurements that are sensitive to the band structure of a material require techniques that operate on the length scale of the charge carrier's mean free path. A novel method that fulfills this requirement is the molecular nanoprobe (MONA), which uses a single molecule to detect charge carriers [1].

In this study, we investigate the rotation and tautomerization of phthalocyanine molecules on the $(\sqrt{3} \times \sqrt{3})$Bi/Ag(111)$R30°$ surface and utilize these excitations to investigate transport in the Rashba-split surface state characteristic for this surface [2]. We find that both excitation processes are driven by the N-H stretching mode and can be triggered by a single electron [3]. Our transport measurements proof the sensitivity to hot charge carriers which preferably propagate in the Rashba-split surface state of the $BiAg_2$ alloy. The expected impact of the spin–momentum-locking of this Rashba-split surface state on the surface transport is discussed and first experimental results obtained with spin-polarized tips will be presented.

[1] M. Leisegang *et al.*, Nano Lett. **18**, 2165–2171 (2018)
[2] C. R. Ast *et al.*, Phys. Rev. Lett. **98**, 186807 (2007)
[3] J. Kügel *et al.*, Journ. Phys. Chem. C **121**, 28204–28210 (2017)