

## O 99: Spins on surfaces at the atomic scale III

Time: Friday 9:30–12:30

Location: WILL/A317

O 99.1 Fri 9:30 WILL/A317

**Measuring magnetic exchange forces of individual quantum spins** — •NICOLAJ BETZ<sup>1,2</sup>, LUKAS M. VELDMAN<sup>1,2</sup>, MILTON AGULIAR<sup>3</sup>, ERIC LUTZ<sup>3</sup>, SUSANNE BAUMANN<sup>1</sup>, and SEBASTIAN LOTH<sup>1,2</sup> — <sup>1</sup>University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — <sup>2</sup>Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany. — <sup>3</sup>University of Stuttgart, Institute for Theoretical Physics, Stuttgart, Germany

Dynamics of single atomic spins are governed by interactions with the spins immediate, i.e. atomic scale environment. In that, spin-polarized scanning tunnelling microscopy (STM) can give access to some of these interactions, e.g. those between coupled spins, and it can also be used to detect the dynamics in form of individual spin switches. Atomic force microscopy (AFM) on the other hand, gives access to atomic-scale forces, for example the magnetic exchange interaction [1,2]. Here, we show magnetic exchange force detection on a dynamically switching single Fe atom on MgO/Ag(100). We can tune this spin to undergo a ground state reversal as a function of exchange interaction with the tip. We find that the switching spin interacts strongly with the AFM cantilever. Thus, access to these forces provides a new avenue to study dynamically switching single atomic quantum spins revealing information about the interplay between an atom's interactions and the dynamics of the spin.

[1] N. Hauptmann et al., *Nat. Com.* 11, 1197 (2020).

[2] U. Kaiser et al. *Nature* 446, 522-52 (2007).

O 99.2 Fri 9:45 WILL/A317

**Tip induced f-π interaction of YbPc<sub>2</sub> Molecules utilizing STM** — •JONAS ARNOLD<sup>1</sup>, KWAN HO AU-YEUNG<sup>1</sup>, WANTONG HUANG<sup>1</sup>, EUFEMIO MORENO PINEDA<sup>1</sup>, CHRISTOPH SÜRGERS<sup>1</sup>, WOLFGANG WERNSDORFER<sup>1</sup>, MARIO RUBEN<sup>2</sup>, and PHILIP WILLKE<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — <sup>2</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

Individual molecules constitute excellent building blocks for quantum technologies thanks to their small size, reproducibility and the benefit of self assembly. A promising class are rare-earth bis-phthalocyanine complexes (1). In this work, we investigate YbPc<sub>2</sub> molecules using a mK- scanning tunneling microscope (STM) to identify potential indicators of a magnetic signature. In the gas phase, the YbPc<sub>2</sub> molecule is expected to exhibit a radical spin localized at its ligands, an f-shell electron spin S = 1/2 as well as a nuclear spin (I = 1/2 and 5/2) for certain isotopes. Thus, this system is a potential candidate for a spin cascade (1). We perform measurements on self-assembled multi-layer islands of YbPc<sub>2</sub> on Ag(001) and MgO/Ag(001). We find that the proximity of the STM tip changes the spin state of the molecule by tuning states close to the Fermi level (2). We identify the emerging spectral features close to zero bias as inelastic electron tunneling excitations that result from the combined f-π system. This mechanism can be found for the first, second and third molecular layer on Ag(001) as well as MgO/Ag(001). (1) Wernsdorfer, W. et al., *Adv. Mat.*, 2019, 31(26), 1806687. (2) Liao, X. et al., *Nat. Com.*, 2025, 16(1), p.6263.

O 99.3 Fri 10:00 WILL/A317

**Quantifying the interplay between atomic-scale magnetism and Josephson transport atom-by-atom** — •ZHENGYUAN LIU, SEBASTIAN SCHERB, MANUEL STEINBRECHER, NADINE HAUPTMANN, and ALEXANDER KHAJETOORIANS — IMM, Radboud University Nijmegen, the Netherlands

Josephson transport can locally be affected by the presence of magnetic moments in the junction. For example, it was shown that the individual magnetic impurity, and the Yu-Shiba-Rusinov (YSR) excitations they induce in the superconductor can be used to induce a superconducting diode effect [1]. Furthermore, an intrinsic phase shift of  $\pi$  in its ground state can exhibit when a ferromagnetic layer with certain thickness is introduced in the Josephson junction, known as the  $\pi$ -junction [2]. Here, we study the effect of individual and coupled magnetic atoms on the Josephson transport between a superconducting tip and superconducting surface, using scanning tunneling microscopy. We study the evolution of the YSR states going from an individual impurity to a magnetic nanostructure. We correlate this

evolution to changes in the Josephson junction properties locally, by using spatially-dependent I-V spectroscopy. We also review the local diode effect induced in these structures. [1] Trahms, M et al. *Nature* 615, 628\*633 (2023). [2] Ryazanov et al. *Phys. Rev. Lett.* 86, 2427 (2001)

O 99.4 Fri 10:15 WILL/A317

**Exchange-field model for electron spin resonance scanning tunneling microscopy** — •CHRISTOPH WOLF<sup>1,2</sup>, JOSE REINA-GALVEZ<sup>3</sup>, XUE ZHANG<sup>4</sup>, JAN MARTINEK<sup>5</sup>, and NICOLAS LORENTE<sup>6</sup> — <sup>1</sup>Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — <sup>2</sup>Ewha Womans University, Seoul 03760, Republic of Korea — <sup>3</sup>Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — <sup>4</sup>Institute of Molecular Physics, Polish Academy of Science, Smoluchowskiego 17, 60-179 Poznan, Poland — <sup>5</sup>Spin-X Institute, China University of Technology, Guangzhou, China — <sup>6</sup>Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Spain

Since the first experimental demonstration of electron spin resonance in a scanning tunneling microscope the understanding of how spin transitions are driven by oscillating electric fields has gone through several evolutions. In this talk, I will show how an exchange-field model can explain the magnetoelectric coupling between the electric field and a spin impurity. This model is based on an Anderson impurity model and non-equilibrium transport using magnetic electrodes. When the hopping between a magnetic electrode and the impurity is modulated on resonance with the Zeeman splitting one obtains an effective magnetic field that can coherently drive the spin. The sign and magnitude of the exchange field depends on the applied DC bias which gives full control over the position of the resonance and potentially can be used for DC-based quantum-logic operations.

O 99.5 Fri 10:30 WILL/A317

**Revealing spatial inhomogeneities in superconducting 2H-NbS<sub>2</sub> using magnetic sensor atoms** — •WERNER M.J. VAN WEERDENBURG, MARGARETE HUISINGA, CONSTANTIN FLOMMERSFELD, LISA M. RÜTTEN, and KATHARINA J. FRANKE — FachbereichPhysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) are an interesting material class in which multiple quantum phases such as charge-density-wave (CDW) order, superconductivity and pair-density-wave order may co-exist [1]. Within the family of superconducting TMDCs, 2H-NbS<sub>2</sub> stands out as the only material that does not develop a CDW phase, but this interpretation is challenged in the presence of defects, since the material is very close to a lattice instability [2,3].

Here, we present how magnetic adatoms on a superconducting TMDC substrate can be used to investigate spatial inhomogeneities of 2H-NbS<sub>2</sub>. By manipulating an individual Fe atom between binding sites with the tip of a scanning tunneling microscope, we probe the Yu-Shiba-Rusinov (YSR) states and their response to surface variations with high energy resolution. The sensitivity of YSR states to the crystal field, density of states and disorder allows us to analyze the relation between the YSR energies and the properties of the substrate, and to find indications of local charge-density-wave nucleation around intrinsic defects.

[1] Liu et al., *Science* 372, 1447-1452 (2021); [2] Heil et al., *PRL* 119, 087003 (2017); [3] Wen et al., *PRB* 101, 241404 (2020)

O 99.6 Fri 10:45 WILL/A317

**Magnetic quantum corrals on a proximity-superconducting Rashba surface alloy** — •JINKYUNG KIM, HARIM JANG, JENS WIEBE, and ROLAND WIESENDANGER — Department of Physics, University of Hamburg, Hamburg, D-20355, Germany

Quantum corrals can confine and resonate surface-state electrons at discrete eigenenergies. When coupled to superconducting substrates, quantum corrals can be used to sculpt Yu-Shiba-Rusinov (YSR) in-gap states as well as spin-degenerate Andreev bound states, referred to as Machida-Shibata (MS) states, due to proximity-induced Cooper pairing [1,2]. Here, we investigated quantum corrals crafted from Fe atoms on a proximity-superconducting BiAg<sub>2</sub>/Ag/Nb(110) heterostructure. Multiple in-gap states emerge with similar numbers

of antinodes as in the eigenmode closest to the Fermi energy. They show an almost perfect spatial antiphasing between the particle- and hole-like components, reminiscent of long-range YSR states of individual magnetic atoms [3]. By further studying how these in-gap states evolve with corral size and the 3d metal atom species, our work characterizes the interplay between YSR and MS states within the quantum corral. [1] L. Schneider et al., *Nature* 621, 60–65 (2023) [2] K. Ton That et al., *Nat. Phys.* (2025) <https://doi.org/10.1038/s41567-025-03109-y> [3] H. Jang et al., *arXiv:2506.17414* (2025)

O 99.7 Fri 11:00 WILL/A317

**Spin and Charge States of Open-Shell Nanographenes over Functional Substrates** — •FRANCISCO ROMERO-LARA, TRISHA SAI, KATERINA VAXEVANI, DONGFEI WANG, JON ORTUZAR, LEONARD EDENS, STEFANO TRIVINI, FABIAN SCHULZ, and JOSE IGNACIO PASCUAL — CIC nanoGUNE, 20018 San Sebastián, Spain

Atomically precise open-shell nanographenes are platforms hosting spin states, which can be manipulated by local probes and by tuning their local environment. Here, we present the fabrication of aza-triangulenes-based nanostructures over two novel substrates with potential control over their charge and spin state: a rare-earth-gold alloy monolayer and a superconducting surface. The aza-triangulene platforms can host several weakly interacting spin states and a doublet ground state sensitive to Jahn-Teller distortion. We use scanning tunnelling microscopy to resolve their Kondo and spin excitation spectrum. We also resolve the presence of Yu-Shiba-Rusinov (YSR) states inside the proximity gap on the superconducting surface. Owing to an inhomogeneous local contact potential difference, the nanographenes on rare-earth-gold alloy surfaces appear with varying charge states depending on their adsorption site, which is also translated into variations of the spin ground state. Over a superconducting substrate, sub-gap spectral maps reveal with high precision their YSR excitations. They are interpreted based on a model theory as reflecting, in some cases, Jahn-Teller distortions. Overall, our results highlight the potential of unconventional substrates for on-surface nanographene synthesis and for tailoring and probing their intrinsic spin states.

O 99.8 Fri 11:15 WILL/A317

**Extracting mechanical work from quantum spin switching of a single atom** — NICOLAJ BETZ<sup>1,2</sup>, LUKAS M. VELDMAN<sup>1,2</sup>, MILTON AGUILAR<sup>3</sup>, ERIC LUTZ<sup>3</sup>, SUSANNE BAUMANN<sup>1</sup>, and •SEBASTIAN LOTH<sup>1,2</sup> — <sup>1</sup>University of Stuttgart, Institute for Functional Matter and Quantum Technologies — <sup>2</sup>Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart — <sup>3</sup>University of Stuttgart, Institute for Theoretical Physics

Stochastic dynamics are ubiquitous in atomic-scale systems, often arising from dissipative processes through which energy is lost to the environment. Harnessing such dynamics to perform work is at the heart of molecular motors and quantum heat engines. Here, we demonstrate that a single magnetic atom can function as an electric motor that converts spin excitations into mechanical oscillations of a macroscopic cantilever. We couple an Fe atom on MgO/Ag(100) via magnetic exchange interaction to the tip of a combined atomic force (AFM) and scanning tunneling microscope (STM) at milli-Kelvin temperatures. Current-induced inelastic electron tunneling induces cyclic spin switching, creating an alternating exchange force that transfers energy between the quantum spin and the AFM cantilever with a power output sufficient for free-running operation. This single-atom electric motor bridges the quantum-classical divide and provides a platform for studying energy transfer in hybrid quantum-classical systems.

O 99.9 Fri 11:30 WILL/A317

**Tuning the magnetic excitation of a single atom by local gating** — •ANNA M. H. KRIEG, HERMANN OSTERHAGE, JULIAN H. STRIK, NIELS P. E. VAN MULLEKOM, BEN VERLHAC, and ALEXANDER A. KHAJETOORIANS — Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands

The description of single-atom magnetism depends on the interplay of various degrees of freedom and the balance of different interactions. This includes the interplay between the orbital, spin and charge degrees of freedom, as well as the balance between spin-orbit coupling, hybridization, and different exchange interactions, such as Hund's and Kondo exchange. To date, the strategy to change the magnetic behavior of a single atom is to explore different atom/surface combinations. However, in this way, nearly all these parameters are fixed by the material system and when changing the material system, the entire set of parameters changes. Here, we tune the local electrostatic potential

in order to modify the magnetic excitations and tunneling transport of individual Fe atoms. We start with Fe atoms on the surface of InSb(110), and characterize its magnetic excitations as a function of magnetic field. We then harness a newly developed quantum simulator platform, based on patterning Cs atoms on the surface of InSb. We show that by varying the local density of Cs on InSb, we can tune the magnetic excitation of an individual Fe atom. These results serve as a starting point to develop quantum simulation to study magnetic models in which the spin, charge, and orbital degree of freedom can be tuned.

O 99.10 Fri 11:45 WILL/A317

**Spin dynamics of atomic defects in monolayer MoS<sub>2</sub>** — •JOHANNA MATUSCHE<sup>1,2</sup>, KWAN HO AU-YEUNG<sup>1,2</sup>, WANTONG HUANG<sup>1,2</sup>, PAUL GREULE<sup>1,2</sup>, JONAS ARNOLD<sup>1,2</sup>, LOVIS HARDEWEG<sup>1,2</sup>, MÁTÉ STARK<sup>1,2</sup>, LUISE RENZ<sup>1,2</sup>, AFFAN SAFEE<sup>3</sup>, DANIEL JANSEN<sup>3</sup>, JEISON FISCHER<sup>3</sup>, THOMAS MICHELY<sup>3</sup>, WOLFGANG WERNSDORFER<sup>1,2</sup>, CHRISTOPH SÜRGERS<sup>1,2</sup>, JOHANNES SCHWENK<sup>1,2</sup>, WOUTER JOLIE<sup>3</sup>, and PHILIP WILLKE<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — <sup>2</sup>Center for Integrated Quantum Science and Technology (IQST), Karlsruhe Institute of Technology, Karlsruhe, Germany — <sup>3</sup>II. Physikalisches Institut, Universität zu Köln, Köln, Germany

Scanning tunneling microscopy (STM) combined with electron spin resonance (ESR) has enabled coherent control of single ad-atoms and single molecules on surfaces [1]. Additionally, recent studies have revealed that defects in monolayer MoS<sub>2</sub> exhibit well-defined spin signatures [2]. In this talk, we combine these two advances for individual point-like defect spins in monolayer MoS<sub>2</sub> on graphene/Ir(111): First, we focus on stochastic resonance spectroscopy (SRS) [3] to periodically drive rapid transitions between spin states. This allows to identify the main relaxation mechanisms and to determine the T<sub>1</sub> relaxation times. Second, pulsed ESR enables coherent control of the defect spins via Rabi and Ramsey sequences, which provides direct access to their T<sub>2</sub> coherence times. [1] K. Yang et al., *Science*, 366, 509–512 (2019). [2] S. Trishin et al., *Phys. Rev. B*, 108, 165414 (2023) [3] N. Betz et al., *arXiv:2412.12647* (2025).

O 99.11 Fri 12:00 WILL/A317

**Following Spin Interactions into a Chemical Bond Formation** — •DMITRIY BORODIN<sup>1</sup>, MERVE ERCELIK<sup>1</sup>, ANDRES PINAR SOLE<sup>1</sup>, SHADI FATAYER<sup>2</sup>, HARALD BRUNE<sup>3</sup>, CHRISTOPH WOLF<sup>1</sup>, FRANZ J. GIESSEBL<sup>4</sup>, FABIO DONATI<sup>1</sup>, and ANDREAS HEINRICH<sup>1</sup> — <sup>1</sup>IBS Center for Quantum Nanoscience, Seoul, South Korea — <sup>2</sup>KAUST, Thuwal, Saudi Arabia — <sup>3</sup>EPFL, Lausanne, Switzerland — <sup>4</sup>University of Regensburg, Regensburg, Germany

Exchange interactions are essential for the formation of chemical bonds between atoms and dictate the electronic structure of molecules. In a condensed-matter system, a manifold of exchange mechanisms coexist, ultimately defining the local magnetic structure and phase stability. A particularly interesting interaction occurs between transition metal atoms and rare earth elements, where the nature of magnetic coupling in their alloys remains not fully understood. In this work, we use low-temperature scanning probe microscopy to follow the spin interactions between a tip and an adatom on a surface into a chemical bond. By controlling atom-tip separations on the picometer scale, we continuously tune interaction energies and observe spin pairing between the adatom and the magnetic tip, a situation that is reminiscent of covalent bond formation.

O 99.12 Fri 12:15 WILL/A317

**Dark state formation in a zero-field split molecular triplet** — •MARIA STEINER and ANDREA DONARINI — Institute of Theoretical Physics, Regensburg University, Regensburg, Germany

In analogy to atomic physics [1], we propose a protocol to prepare and probe a dark state in a single molecule. To this end, we coherently manipulate with a multifrequency magnetic field a three-level system in the V-configuration. Thus, within a density-matrix formalism for open systems, we extend existing protocols developed to probe Rabi oscillations in ESR-AFM on pentacene [2]. The dissipative dynamics of the reduced density matrix are interpreted in terms of multipole expansion and visualized using three intertwined Bloch spheres. We consider a molecule with a zero-field splitting of the first excited triplet. This splitting typically arises from the spatial anisotropy of the frontier orbitals and the spin dipole-dipole interaction between the unpaired electrons. Pentacene is an archetypal example, which, in addition to these properties, also exhibits anisotropic decay to the ground state

singlet [3] and thus enables experimental readout of the occupied state [2]. We consider both ideal scenarios and realistic parameterization for ESR-AFM on pentacene to model the expected dark state signature.

- [1] Arimondo and Orriols, *Lett. al Nuovo Cim.* **17**, 333 (1976).
- [2] Sellies et al., *Nature* **624**, 64 (2023).
- [3] Peng et al., *Science* **373**, 452 (2021).