O 89: Spins on surfaces at the atomic scale II

Time: Thursday 15:00–18:00 Location: WILL/A317

O 89.1 Thu 15:00 WILL/A317

Magnetization Curves of Antiferromagnetic Spin Chains: Probing the Quantum to Classical Crossover — •Henrik Lichtl[1,2], Lukas Veldman[1,2], Nicolaj Betz[1,2], Johannes Schust[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart. — [3]Carl-Zeiss- Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm. — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna.

As the size of a magnetic structure increases it undergoes a transition from a quantum system to a classical magnet, yet the evolution of the magnetization behavior at this crossover is largely unexplored. Here we introduce an approach to record high-speed magnetization curves in a scanning tunneling microscope (STM), reaching magnetic field sweep rates of up to 40kT/s. We analyze the statistics of the transitions between the two antiferromagnetic ground states of antiferromagnetic Fe spin chains on a Cu2N surface, which allows us to distinguish between quantum and classical regimes in their magnetization curves. Quantum signatures diminish rapidly with size of the chain, where chains longer than five atoms already show characteristics of classical nanoscale magnets. Accessing such high-speed magnetization curves at the atomic scale brings concepts originally developed for bulk materials into the STM, offering insight into how quantum spins interact with their environment during the quantum-to-classical transition.

O 89.2 Thu 15:15 WILL/A317

Optimizing On-Surface Quantum Spins for Quantum Information Processing — •Denis Jankovic[1,2], Hoang-Anh Le[1,2], Saba Taherpour[1,3], and Christoph Wolf[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Departement of Physics, Ewha Womans University, Seoul, Republic of Korea

The bottom-up engineering of quantum-coherent spins on surfaces with STM enables atomically precise quantum logic in on-surface qubits, and atomic-scale multi-qubit devices.

We use optimal control on an open-system model of exchange-coupled surface spins to counter decoherence, static coupling, and imperfect initialization, identifying high-fidelity gates compatible with current ESR-STM constraints.

Finally, building on advances in electrically driven nuclear spins, we will outline ongoing experiments using lanthanides on surfaces, where ESR-STM manipulates hyperfine-coupled nuclear-spin manifolds as on-surface qudits.

O 89.3 Thu 15:30 WILL/A317

Spin Lifetime Engineering using Superconducting Surfaces — •Máté Stark, Luise Renz, Jonas Arnold, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Extending the spin lifetime (T_1) and decoherence time (T_2) of atomic and molecular spins is central to realizing quantum-coherent spin systems on surfaces studied by scanning tunneling microscopy (STM). For instance, previous studies have demonstrated that T_1 can be extended to nanoseconds for Fe-OEP-Cl on superconducting Pb(111) to milliseconds for Fe on MgO/Ag(001) by exploiting superconducting protection or electronic decoupling, respectively [1,2].
Building on these concepts, we aim here to combine protection by a superconducting gap and insulating decoupling layers to explore and control spin lifetimes of single FePc spins. By switching from the normal-conducting into the superconducting state we discuss how superconductivity as well as decoupling from the substrate and tip govern the lifetime and dynamics of molecular spin excitations. We show first results using all electric pump-probe spectroscopy, which are performed in a home-built dilution refrigerator scanning tunneling microscope operating at 50 mK. [1] Nat. Phys. 9, 765 (2013) [2] Nat. Phys. 13, 403 (2017)

O 89.4 Thu 15:45 WILL/A317

Bottom-up realization of band structure using arrays of individual Cs atoms on InSb(110) — •Niek M.M. Aarts, Kira Junghans, Roel Burgwal, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud Universiteit, Nijmegen, Netherlands

The combination of atomic manipulation and scanning tunneling spectroscopy has become a powerful platform for quantum simulation of electronic structure. The approach is based on the atomically precise placement of atoms and the flexibility to realize structures with a variety of shapes and symmetry. Inherent to this approach is role of finite size effects in the tailored electronic structure. This plays an integral role in understanding the influence of various interactions, like spin-orbit interactions, or electron-electron interactions, on any potential quantum phase of matter to be simulated.

Here, we study the evolution of the electronic structure as a function of lattice size, using the recently discovered quantum simulator platform of Cs on InSb(110). Using STM, we start by studying structures that exhibit atomic like states and expand these structures into the molecular limit. We study the changes in the localized states and the symmetry of the responsible wavefunctions. We then quantify the increase of states as the number of sites in the system increases, and band structure emerges. We also discuss the role of the size of the artificial atomic sites. This extension of the Cs/InSb(110) quantum simulator to larger systems enables the study of artificial band structure in the presence of strong SOC.

O 89.5 Thu 16:00 WILL/A317

Crystal field manipulation of magnetic atoms on an insulating surface — •Julian Zeitler[1], Johannes Schust[1], Nicolaj Betz[1,2], Lara Mezger[1], Lukas Veldman[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Philip Willke[5], Sebastian Loth[1,2], and Susanne Baumann[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart. — [3]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm. — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna. — [5]Karlsruhe Institute of Technology, Physikalisches Institut.

The magnetic behavior of ions in solid-state materials is predominantly driven by their immediate atomic-scale environment. The specific arrangement of surrounding charges creates a crystal field (CF), which alters and mixes the electronic states. For magnetic atoms on insulating thin films, this CF is strongly influenced by the atom's adsorption site on the underlying lattice. Using combined scanning tunneling microscopy (STM) and atomic force microscopy (AFM), we investigate the CF influence on magnetic atoms on thin-film MgO and use tip-atom forces to precisely reposition the atoms within their binding sites, thereby tuning the CF. We quantify changes of the local binding geometry by combining our measurements with multiplet calculations. Our measurements pave the way for harnessing magneto-elastic effects in individual atoms either by manipulating their magnetic properties via electric fields or local forces, such as mechanical strain.

O 89.6 Thu 16:15 WILL/A317

Topological End States of Chiral Graphene Nanoribbons on Proximitized Superconducting Au (111) — •Trisha Sai[1], Frederik Bauer[1], Stefano Trivini[1], and Jose Ignacio Pascual[1,2] — [1]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Graphene nano-structures may host localized magnetic moments characterized by their geometry, heteroatom substitution, topological frustration, or bulk-boundary correspondence. However, observation of their open-shell configuration via on-surface synthesis can be inhibited due to charge transfer. This is in the case of (3, 2, 8) chiral graphene nanoribbons (chGNRs) synthesized on Au(111), whose symmetry-protected topological end states (SPTES) are quenched due to electron depopulation. In this work, we synthesize (3, 2, 8) chGNRs on thin films of Au (111) grown on a superconducting Nb (110) single crystal. Through controlled deposition of monolayers of Au, we observe a modulation in the surface state of Au (111), thereby a reduction in the work function of the resulting platform. Moreover, the substrate

is also complemented with proximity induced superconductivity. Low-Temperature scanning tunneling spectroscopic (STS) measurements reveal that the SPTES of (3, 2, 8) chGNRs are retained in a mixed-valence regime where their spectral weight is distributed between an in gap Yu-Shiba-Rusinov (YSR) state and an orbital state close to Fermi energy. In case of a depopulated terminus, the YSR states are weak and suppressed while the orbital state is more pronounced.

O 89.7 Thu 16:30 WILL/A317

Confinement-modulated spin-orbit coupling tuned with atomic-scale gating fields — •Hermann Osterhage, Julian H. Strik, Anna M. H. Krieg, Ivan Ado, Mikhail Titov, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

In 2D, inversion symmetry breaking combined with a sizeable potential gradient leads to the well-known Rashba spin-orbit coupling (SOC), locking the spin and momentum. Using potential gradients to induce SOC is not limited to the Rashba case, but may be extended to lower dimensional structures, such as quantum dots. However, tuning SOC in these limits is challenging: it requires potential gradients that are comparable to the size of the confined structure itself.

Here, we demonstrate a new type of SOC, akin to the Rashba effect, where large potential gradients are formed within an atomically patterned quantum dot. Using low-temperature scanning tunnelling microscopy and spectroscopy we create quantum dots of various shapes and sizes by patterning individual Cs ions on the surface of InSb(110). We find that we can tune the confinement potential, as shown by the presence of multiple localized states. In addition, by probing the resultant multiplet structure, we identify zero-field splittings within a given quantum dot that are induced by the geometry of the potential. We also discuss the magnetic field dependence of this level structure and explain the findings based on the 8-band Kane model.
[1] E. Sierda et al, Science 380, 1048 (2023).

O 89.8 Thu 16:45 WILL/A317

Tuning the Kondo temperature of MoS_2 mirror twin boundaries on graphene — •Tfyeche Y. Tounsi[1], Kuber Vyas[1], Camiel van Efferen[1], Affan Safeer[1], Achim Rosch[2], Jeison Fischer[1], Thomas Michely[1], Theo A. Costi[3], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

In scanning tunneling spectroscopy, the dI/dV signatures of the Kondo effect in MoS_2 mirror twin boundaries (MTBs) are the zero-bias resonance peak, in addition to the impurity levels [1]. The experimental data give access to the Anderson model parameters; The splitting U of the non-degenerate states, the impurity orbital's position ϵ with respect to E_F, and the impurity level's bare width γ_0.

In this work, we compare the Kondo temperature T_K measured in MTBs of MoS_2 grown on three different substrates. In the case of MoS_2 / Graphene (Gr) / Ir (111), T_K was in the range [10^{-4} K, 10^{-10} K] [1]. By intercalating with a single layer of Eu under Gr, we have noticed a decrease of γ_0, leading to a drop in T_K. The third system, MoS_2 / Gr / Ir (110), T_K increased significantly to the range [1 K, 10 K]. This enabled us to study the Kondo effect at the boundary between the weakly screened magnetic state above T_K and the Kondo singlet state below T_K.

References: [1] C. van Efferen et al, Nat. Phys. 20, 82-87 (2024).

O 89.9 Thu 17:00 WILL/A317

Statistical analysis of electron-induced switching of a spin-crossover complex — •Jonas Fussangel[1], Björn Sothmann[1], Sven Johannsen[2], Sascha Ossinger[3], Felix Tuczek[3], Richard Berndt[3], Jürgen König[1], and Manuel Gruber[1] — [1]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [3]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spin-crossover complexes switch between two spin states, but the microscopic pathway remains unclear. Using low-temperature STM, electron-induced switching of $[Fe(H_2B(pz)(pypz))_2]$ on Ag(111) has opened new perspectives for understanding the switching mechanisms. Current time traces show two levels matching the spin states. An analysis of waiting-time distribution yields switching rates whose voltage dependence is explained by a simple model where transient molecular charging triggers switching. Comparing experiment and theory provides previously inaccessible estimates of LUMO energies [1]. The approach offers new insights into the switching mechanism and predicts higher switching rates when the molecule is electronically decoupled from the substrate, e.g., by introducing an ultrathin insulating layer.
[1] J. Fußangel et al., *arXiv*: 2506.13373 (2025)

O 89.10 Thu 17:15 WILL/A317

Decoupling strategies for YPc_2 molecular spin qubit platforms on metal surfaces — Franklin H. Cho[1,2], Soyoung Oh[1,2,3], Dan Chi Nguyen[1,2], Jinjoo Lee[1,2], We-hyo Soe[1,2], Luciano Colazzo[1,2], Jisoo Yu[1,2], Pierre Josse[1,2], Caroline Hommel[1,2], Lukas Spree[1,2], Christoph Wolf[1,2], and •Fabio Donati[1,2] — [1]IBS Center for Quantum Nanoscience, South Korea — [2]Ewha Womans University, South Korea — [3]The Clarendon Laboratory, University of Oxford, The United Kingdom

Yttrium phthalocyanine double-decker (YPc_2) is an appealing building block for surface spin-qubit architectures due to its delocalized $S = 1/2$ radical and planar structure [1]. Here, we investigated the morphology, electronic structure, and spin properties of single- and multi-layer YPc_2 on Cu(111) single crystals and on zinc phthalocyanine (ZnPc) grown on Cu(111). Low temperature scanning tunneling microscopy reveals the molecular layer structure and the variation of its electronic configuration when directly adsorbed on Cu(111) versus on a ZnPc decoupling layer [2]. X-band electron spin resonance using our custom-built surface-sensitive spectrometer [3] shows that the YPc_2 radical is preserved on ZnPc but quenched upon direct contact with Cu(111). Density functional theory attributes this quenching to the hybridization of molecular orbitals with the substrate electrons. Our study highlights the necessity of suitable decoupling layers to preserve radical spins near metallic surfaces. [1] F. Branzoli et al., Phys. Rev. B 83, 174419 (2011). [2] S. Oh et al., Nanoscale 17, 22163 (2025). [3] F. H. Cho et al., Rev. Sci. Instrum. 95, 063904 (2024).

O 89.11 Thu 17:30 WILL/A317

Inelastic Zoo: Spin, Vibrational, and Orbital Excitations in Conductance Spectra — •Arnab Banerjee, Richard Berndt, and Alexander Weismann — Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany

First-principle predictions of excitation energies and cross sections in inelastic tunneling spectroscopy are challenging, making it difficult to assign experimental features to specific excitations. There is a need for a reliable identification of conductance features. We investigated the spin-1/2 molecule cobaltocene on superconducting Pb(110) and use Yu-Shiba-Rusinov states combined with a superconducting tip to detect a large number of sharp spectral features. From a peak shape analysis, we find the coexistence of spin, vibrational, and orbital excitations within a single conductance spectrum.

O 89.12 Thu 17:45 WILL/A317

Current-induced Electron Spin Polarization in Magnetic Molecules — •Paul Greule, Wantong Huang, Máté Stark, Kwan Ho Au-Yeung, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron spins of single molecules offer a promising platform for quantum information processing. To harness such spins as functional qubits, efficient initialization is essential. Electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) has emerged as a powerful technique to probe molecular spins at the atomic scale. Using this technique, it has been shown that a spin-polarized tunnelling current can polarize the nuclear spin of a single Cu atom [1]. In this talk, we show that this concept can be transferred to the electron spin of molecules: Using Fe-FePc complexes with an electron spin of S=1/2 [2], we build molecular dimers. Here, the first complex serves as a readout and pumping system, while the energy-level occupation of the second complex is probed and manipulated. The exchange interaction between them enables remote spin-pumping, where angular momentum is transferred. Controlling the spin-polarized tunnel current via the bias voltage allows us to tune the spin polarization of the second complex remotely. Our findings establish an all-electrical technique to initialize molecular spin qubits and provide insights for enhanced control schemes. [1] K. Yang et al., Nat Nano 2018, 13, 1120-1125 [2] W. Huang et al., Nat Commun 2025, 16, 5208