O 33: Spins on Surfaces at the Atomic Scale III

Time: Tuesday 10:30–13:00 Location: REC C 213

Topical Talk O 33.1 Tue 10:30 REC C 213

Fermi liquids, Luttinger integrals, topological invariants ... and magnetic molecules — •Rok Zitko[1,2], German G. Blesio[1,3], Luis O. Manuel[3], and Armando A. Aligia[4] — [1]Jozef Stefan Institute, Ljubljana, Slovenia — [2]Faculty of Mathematics and Physics, University of Ljubljana, Slovenia — [3]Instituto de Fisica Rosario (CONICET) and Universidad Nacional de Rosario, Argentina — [4]INN CNEA-CONICET, Centro Atomico Bariloche and Instituto Balseiro, Bariloche, Argentina

The ground state of a system of interacting fermions is often a Fermi liquid with elementary excitations that are in a one-to-one correspondence with those of a non-interacting Fermi gas. A key idea in Landau's theory is the adiabatic connection between the interacting and the non-interacting system. The adiabatic connection does not, however, always exist and there are several impurity problems where the ground state is known to be a Fermi liquid that is not of the Landau type. I will present the case of the two-channel S=1 Kondo model with single-ion magnetic anisotropy which has a topological quantum phase transition separating two different Fermi-liquid phases. I will discuss how the conservation laws constrain the Luttinger integrals so that their linear combinations become topological invariants, and how the modified Friedel sum rules lead to a peculiar variation of the impurity spectral function. I will then show that the tunneling spectra of iron phthalocyanine molecules on Au(111) surface and of nickelocene molecules on Cu(100) surface can be consistently interpreted in the framework of non-Landau Fermi liquid theory.

O 33.2 Tue 11:00 REC C 213

Locally driven quantum phase transition cascades in a strongly correlated molecular monolayer — Soroush Arabi[1,2,3], Taner Esat[2,5], Aizhan Sabitova[2,5], Yuqi Wang[2,3], Hovan Lee[6], Cedric Weber[6], Kern Klaus[3,4], F. Stefan Tautz[1,2,5], Ruslan Temirov[2,7], and •Markus Ternes[1,2,5] — [1]Institute of Physics IIB, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter-Grünberg-Institute (PGI 3), Research Center Jülich, 52425 Jülich, Germany — [3]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [4]Institut de Physique, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [5]Jülich Aachen Research Alliance, 52425 Jülich, Germany — [6]King's College London, Theory and Simulation of Condensed Matter, London WC2R 2LS, UK — [7]Institute of Physics II, University of Cologne, 50937 Cologne, Germany

The molecular monolayer of 1,4,5,6-naphthalene tetracarboxylic acid dianhydride on Ag(111) creates a perfectly ordered lattice of π-conjugated organic molecules. Using a movable atomically sharp electrostatic gate we drive this lattice of strongly correlated electrons through a cascade of quantum phase transitions. Performing spectroscopic imaging with sub-Angstrom resolution, we show that as the gate field is increased, the molecular building blocks change from a Kondo-screened to a paramagnetic phase one by one, enabling us to reconstruct their complex interactions in detail. We anticipate that the supramolecular nature of the system will, in future, allow engineering quantum correlations in arbitrary patterned structures.

O 33.3 Tue 11:15 REC C 213

Engineering antiferromagnetic spin coupling in carbon based nanostructures — •Elia Turco[1], Nils Krane[1], Fupeng Wu[2], Michal Juricek[3], Xinliang Feng[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa Swiss Federal Laboratories for Materials Science and Technology, Duebendorf, Switzerland — [2]Faculty of Chemistry and Food Chemistry, and Center for Advancing Electronics Dresden, Technical University of Dresden, Germany — [3]Department of Chemistry, University of Zurich, Switzerland

On-surface synthesis offers the possibility to engineer atomically precise nanogaphenes (NGs) with intrinsic magnetic ground states. Unlike atomic magnets, unpaired π-electrons are highly delocalized and prone to hybridize forming entangled quantum states, which are the main requisite for the emerging quantum technologies. Zigzag-edged triangular NGs are regarded as prototypical magnetic building blocks, hosting a total spin S that scales with molecular size [1]. In this contribution, we will present the on-surface synthesis and scanning probe microscopy & spectroscopy of the two smallest S = 1/2 and S = 1 triangulenes on a Au(111) surface, where the Kondo screening of the unpaired spins is a direct evidence of their magnetic ground state. Connecting the two S = 1/2 and S = 1 building blocks into homo- and hetero-dimers an -trimers, we realize multilevel quantum systems with increasing complexity, characterized by multiple inelastic spin excitations. The significant hybridization of the unpaired π-electrons results in strong quantum correlations, which have never been achieved for equivalent atomic systems. [1] J.Su et al. Angew. Chem. 132 (2020)

O 33.4 Tue 11:30 REC C 213

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, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Germany

Magnetic adatoms on properly designed surfaces constitute exquisite systems for addressing, controlling, and manipulating single quantum spins. Here, we show that monolayers of MoS_2 on a Au(111) surface provide a versatile platform for controllably tuning the coupling between adatom spins and substrate electrons. Even for equivalent adsorption sites with respect to the atomic MoS_2 lattice, we observe that Fe adatoms exhibit behaviors ranging from pure spin excitations, characteristic of negligible exchange and dominant single-ion anisotropy, to a fully developed Kondo resonance, indicating strong exchange and negligible single-ion anisotropy. This tunability emerges from a moiré structure of MoS_2 on Au(111) in conjunction with pronounced many-body renormalizations. We also find striking spectral variations in the immediate vicinity of the Fe atoms, which we explain by quantum interference reflecting the formation of Fe-S hybrid states despite the nominally inert nature of the substrate. Our work establishes monolayer MoS_2 as a tuning layer for adjusting the quantum spin properties over an extraordinarily broad parameter range. The considerable variability can be exploited for quantum spin manipulations.

O 33.5 Tue 11:45 REC C 213

Absence of the Kondo effect for Co on Cu(111) — Neda Noei[1], Roberto Mozara[2], Ana M. Montero[3], Sascha Brinker[3], Niklas Ide[1], Filipe S. M. Guimaraes[3], Alexander I. Lichtenstein[2], Richard Berndt[1], Samir Lounis[3], and •Alexander Weismann[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

The zero-bias anomaly in conductance spectra of single Co atoms on Cu(111) observed at $\approx$ 4 K, which has been interpreted as being due to a Kondo resonance, is strongly modified when the Co atoms are attached to monatomic Cu chains. Scanning tunneling spectra measured at 340 mK in magnetic fields exhibit all characteristics of spin-flip excitations. Their dependence on the magnetic field reveals a magnetic anisotropy and suggests a non-collinear spin state indicating that spin-orbit coupling (SOC), which has so far been neglected in theoretical studies of Co/Cu(111), has to be taken into account. According to our density functional theory and multi-orbital quantum Monte Carlo calculations SOC suppresses the Kondo effect for all studied geometries. The interpretation of the zero-bias anomaly in terms of a Kondo resonance is apparently incorrect.

O 33.6 Tue 12:00 REC C 213

Are excitations of the 4f magnetic moment visible to the scanning tunneling spectroscopy? — Daria Kyvala and •Jindrich Kolorenc — Institute of Physics (FZU), Czech Academy of Sciences, Praha, Czech Republic

The inelastic electron tunneling spectroscopy (IETS) has repeatedly proved useful for investigation of spin excitations in transition-metal atoms on surfaces [1,2]. Analogous observations of magnetic excitations in rare-earth atoms remained elusive, the reasoning behind it being that the 4f states that carry the magnetic moment are compact, buried in the atomic core, and the tunneling through a rare-earth atom proceeds via outer, more diffuse orbitals like 5d or 6s. Recently, the

exchange coupling between the spin in these outer orbitals and the 4f magnetic moment was observed in IETS as an excitation in the 50–200 meV range [3]. In the same time, some excitations at lower energies were also seen. Employing a variant of the cotunneling theory [4,5] we demonstrate these excitations to be the elusive crystal-field excitations of the 4f magnetic moment. The selection rules prevent the IETS from detecting enough transitions to fully determine the crystal field by itself, but the visible transitions can be used in conjunction with the x-ray absorption spectra [6] to refine the existing estimates of the crystal field. — [1] A. J. Heinrich *at al.*, Science **306**, 466 (2004); [2] C. F. Hirjibehedin *at al.*, Science **317**, 1199 (2007); [3] M. Pivetta *at al.*, PRX **10**, 031054 (2020); [4] F. Delgado and J. Fernández-Rossier, PRB **84**, 045439 (2011); [5] C. Wäckerlin *et al.*, ACS Nano **16**, 16402 (2022); [6] R. Baltic *et al.*, PRB **98**, 024412 (2018).

O 33.7 Tue 12:15 REC C 213

Tuning the magnetic anisotropy of two coupled spins in a dinuclear Co(II) complex — Chao Li[1], Roberto Robles[2], Nicolas Lorente[3], Alexander Weismann[1], Richard Berndt[1], and •Manuel Gruber[4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastian, Spain — [4]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

The magnetic properties of transition-metal ions are often described using a phenomenological spin Hamiltonian, which suggests that $S = 1/2$ metal ions are isotropic. We investigated a di-nuclear Co(II) complex on Au(111) with low-temperature scanning tunneling microscopy, X-ray magnetic circular dichroism, and density functional theory. The antiferromagnetically coupled Co spins preferentially align along the axis connecting the two Co(II) ions. The magnetic anisotropy is sizable and may be tuned by varying the electronic coupling of the Co(II) ions with the metal electrodes through manipulation of peripheral groups and by approaching the tip toward the complex. These findings may help better describing the magnetic properties of adsorbed molecules, in particular $S = 1/2$ ions, which are viewed as prototypical systems for quantum operations. Funding from the CRC 1242 is acknowledged.

O 33.8 Tue 12:30 REC C 213

Moiré - induced renormalization of singlet-triplet excitations in antiferromagnetically coupled Mn atoms on MoS_2/Au(111) — •Sergey Trishin[1], Christian Lotze[1], Friedemann Lohss[1], Giada Franceschi[1], Leonid I. Glazman[2], Felix von Oppen[3], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [3]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

The properties of single magnetic atoms can change drastically upon adsorption on a surface, for example due to Kondo-like exchange coupling. The magnitude of these interactions can be tuned by a moiré patterned surface [1]. Here, we investigate single Mn atoms and dimers on single-layer molybdenum disulfide grown on a Au(111) substrate. The resulting moiré structure enables variations of the Kondo exchange coupling strength. By additionally varying the spacing between single atoms, we can investigate their properties in the direct and indirect exchange coupling regime. We find that at sufficiently close spacings, the Mn atoms form a non-magnetic singlet ground state. However, the singlet-triplet excitation energies vary strongly depending on the dimer location on the moiré structure. We ascribe these variations to a renormalization of the anti-ferromagentic exchange coupling strength. [1] S. Trishin and C. Lotze and N. Bogdanoff and F. von Oppen and K.J. Franken, Phys. Rev. Lett. **127**, 236801 (2021)

O 33.9 Tue 12:45 REC C 213

Stochastic dynamics of individual and coupled orbital memory on black phosphorus — •Hermann Osterhage, Werner M. J. van Weerdenburg, Niels P. E. van Mullekom, Ruben Christianen, Kira Junghans, Eduardo J. Domínguez Vázquez, Hilbert J. Kappen, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

Recently, the dynamics of Co atoms adsorbed on a black phosphorus (BP) surface were shown to emulate a Boltzmann machine (BM) [1]. The BM relies on a tunable multi-well energy landscape, realized in the stochastic switching of coupled atoms which exhibit orbital memory [2]. Stochastic switching between orbital memory states can be induced using scanning tunneling microscopy (STM). The system response depends on interatomic distances and is adaptable to the position of the STM tip and to the applied DC bias [2].

Here, we present the response of individual and coupled Fe and Co atoms on BP to AC input voltages (i.e. frequency and amplitude response), measured using STM down to millikelvin temperatures. We find a frequency response of the orbital memory of single atoms. The changes in orbital state population with varying AC frequency can be derived from the switching dynamics in the DC case. The interatomic coupling is discussed based on changes in switching rates conditioned on the state of a second atom. Also the AC stochastic response in the multi-well limit will be discussed.

[1] B. Kiraly et al., Nat. Nanotechnol. 16, 414 (2021).
[2] B. Kiraly et al., Nat. Commun. 9, 3904 (2018).