O 52: Focus Session: Spins on Surfaces studied by Atomic Scale Spectroscopies V

Time: Wednesday 15:00–17:15 Location: MA 004

Topical Talk O 52.1 Wed 15:00 MA 004

Locally driven quantum phase transitions in a strongly correlated molecular monolayer — •Markus Ternes — Institute of Physics IIB, RWTH Aachen University, 52074 Aachen, Germany — 2 Peter-Grünberg-Institute (PGI 3), Research Center Jülich, 52425 Jülich, Germany — Jülich Aachen Research Alliance, 52425 Jülich, Germany

The Kondo effect, which appears as a strong zero-bias anomaly, is prototypical for strongly correlated states and therefore cannot be described by single-particle models. Its subtle interplay with magnetically ordered ground states in multi-site Kondo systems continues to attract interest. Here we report on a molecular system of NTCDA molecules on Ag(111) in which individual molecules do not show a Kondo effect even at temperatures of 1K because the π symmetry of their singly occupied orbital hybridizes only weakly with the electrons of the host Ag. In a perfectly ordered lattice, however, newly formed orbital superpositions dramatically increase the hybridization, so that the NTCDA molecules now form a Kondo lattice. Using the electric field exerted by the tip of an STM, we manipulate the orbital superpositions and drive the system through a cascade of quantum phase transitions in which the molecular building blocks change one by one from a Kondo screened to a new paramagnetic ground state, allowing us to reconstruct their complex interactions in detail.

O 52.2 Wed 15:30 MA 004

Evidence for spinarons in Co atoms on noble metal (111) surfaces — •Artem Odobesko, Felix Friedrich, and Matthias Bode — Julius-Maximilians-Universität Würzburg, Physikalisches Institut, Experimentelle Physik II, Am Hubland, 97074 Würzburg, Germany

The first Kondo effect's detection on individual Co atoms on Au(111) surface [1] was associated with a zero-bias anomaly (ZBA) in the differential conductance signal, explained by Fano resonance due to interfering tunneling paths into the Kondo state and atomic orbitals. Recent calculations [2] challenge this interpretation, suggesting that the ZBA is a mix of Co atom spin excitations and the spinaron, a magnetic polaron resulting from the interaction of spin excitations with conduction electrons. Our study used spin-polarised STS on Co atoms on Cu and Au (111) surfaces in magnetic fields up to 12 T. Our comprehensive study of the responses of the ZBA on Co atoms on Cu(111) to an external magnetic field, in conjunction with spin-polarized measurements, allowed us to discriminate between various theoretical models. We observe a field-induced energy shift and experimentally determine the spin character of the spectral features, exhibiting a behavior contrary to Kondo expectations but in line with the spinaron. Consequently, we invalidate the prevailing Kondo-based interpretation of the ZBA in favor of the spinaron and, for the first time experimentally, detect this novel many-body excitation [3].

[1] V. Madhavan *et al.*, Science 280, 567 (1998)
[2] J. Bouazize*t al.*, Nat. Comm. 11, 6112 (2020)
[3] F. Friedrich, *et al.*, Nat. Phys. (2023)

O 52.3 Wed 15:45 MA 004

Spin polarization of the Kondo system in mirror twin boundaries of MoS_2 — •Mahasweta Bagchi[1], Tfyeche Tounsi[1], Afan Safeer[1], Camiel van Efferen[1], Thomas Michely[1], Wouter Jolie[1], Theo A. Costi[2], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

We report spin-polarized scanning tunneling microscopy measurements of the Kondo effect observed in mirror twin boundaries of MoS_2 on graphene, which are consistent with numerical renormalization group calculations. A Kondo resonance appears because the magnetic moment of a singly occupied quantum confined state of the mirror twin boundary is screened by the conduction electrons from the substrate [1]. Using a spin-polarized tip, we measure the Kondo resonance and the singly and doubly occupied confined levels simultaneously, characterizing the full Anderson system. Clear changes in the peak heights of the confined states as well as the magnetic field-split Kondo state provide evidence of their full spin polarization. The magnetization of the confined level as a function of magnetic field and temperature can be described as single quantum spin. This, along with the absence of any higher spin excitations, establishes the mirror twin boundary of MoS_2 as an ideal spin 1/2 system.

[1] van Efferen, et al., Modulated Kondo screening along magnetic mirror twin boundaries in monolayer MoS_2. Nat. Phys. (2023).

O 52.4 Wed 16:00 MA 004

Temperature evolution of the Kondo peak beyond Fermi liquid theory — •David Jacob — University of the Basque Country UPV/EHU, San Sebastian, Spain — IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

The limitation of Fermi liquid theory to very low energies and temperatures poses a fundamental problem for describing the temperature evolution of the Kondo peak. Here Fermi liquid theory for the single impurity Anderson model is extended beyond the low-energy and low-temperature regime by means of an Ansatz for the impurity self-energy based on the accurate description of the Kondo peak by the Frota function and by exploiting Fermi liquid conditions. Analytic expressions for the temperature dependence of the Kondo peak height and width derived from this Ansatz are in excellent agreement with numerical renormalization group data for temperatures up to and beyond the Kondo temperature. The derived expression thus allows to unambiguously determine the intrinsic Kondo peak width and Kondo temperature from finite temperature measurements of the Kondo resonance, as measured by scanning tunneling spectroscopy of magnetic adatoms and molecules on conducting surfaces.

References: D. Jacob, Phys. Rev. B **108**, L161109 (2023); E. Turco *et al.*, arXiv:2310.09326 (2023)

O 52.5 Wed 16:15 MA 004

Accurate Kondo temperature determination of spin-1/2 magnetic impurities — Elia Turco[1], Markus Aapro[2], Somesh C. Ganguli[2], •Nils Krane[1], Robert Drost[2], Nahual Sobrino[3], Annika Bernhardt[4], Michal Jurík̆ek[4], Roman Fasel[1,5], Pascal Ruffieux[1], Peter Liljeroth[2], and David Jacob[3,6] — [1]Empa, Dübendorf, Switzerland — [2]Aalto University, Aalto, Finland — [3]Universidad del País Vasco UPV/EHU, San Sebastián, Spain — [4]University of Zurich, Zurich, Switzerland — [5]University of Bern, Bern, Switzerland — [6]IKERBASQUE, Bilbao, Spain

A localized spin interacting with the electron bath of a metallic surface might give rise to the Kondo effect. The energy scale of this interaction is related to the Kondo temperature T_K and an important quantity when it comes to application of nanoscale magnets. In scanning tunneling spectroscopy (STS) the Kondo effect is observed as a resonance at zero bias. The characteristic temperature evolution of this resonance can be used to prove the Kondo nature of the zero-bias resonance, but only when all other significant broadening methods have been taken properly into account. Using Phenalenyl on Au(111) as an ideal spin-1/2 Kondo system, we demonstrate that the lineshape of a Kondo resonance, measured by STS at finite temperatures, can be described very well by a Hurwitz ζ-function. The extracted intrinsic Kondo linewidth fit very well with a recently derived expression for the temperature evolution of the Kondo resonance. Utilizing the new methodology, we are able to extract the Kondo temperature T_K of a system reliably by a single spectra taken at finite temperature.

O 52.6 Wed 16:30 MA 004

Stable π radical BDPA on Cu(100): adsorption and Kondo signature — •Jacob Teeter[1], Daniel Miller[2], and Stefan Müllegger[1] — [1]Solid State Physics Department, Johannes Kepler University Linz, 4040 Linz, Austria — [2]Hofstra University, New York, USA

Introduction

Stable organic radicals can serve as model systems for investigating metal-free magnetic phenomena. We have investigated one such species, α, γ-bisdiphenylene-β-phenylallyl (BDPA), at the single-molecule level on Cu(100).

Methods

Ultra-high vacuum (UHV) scanning tunneling microscopy (STM) and spectroscopy (STS) were performed using a commercial Omicron Polar STM at 6 K. Spectroscopic measurements were acquired with a W tip using an external lock-in amplifier and a typical modulation voltage of 2.5 mV. The substrate employed was a Cu(100) crystal obtained

from Surface Preparation Laboratory. Density functional theory computations which account for London dispersion forces were performed to elucidate upon the adsorption structure and orientation of BDPA on the Cu(100) surface.

Results and Discussion

Our investigations revealed structural and electronic features of BDPA on Cu(100), including a preferential adsorption orientation and the presence of a Kondo-like feature in differential conductance measurements that suggests survival of the unpaired electron spin.

O 52.7 Wed 16:45 MA 004

Spin excitations and correlations in nanographene-based multi-spin platforms — •Elia Turco[1], Fupeng Wu[2], Nils Krane[1], Ji Ma[2], Roman Fasel[1], Xinliang Feng[2], and Pascal Ruffieux[1] — [1]EMPA, Duebendorf, Switzerland — [2]Faculty of Chemistry, Technical University of Dresden, Dresden, Germany

Chemical design offers the unique opportunity to realize robust molecular spin qubits with tailored magnetic properties, strong qubit interactions, and with practical bottom-up scalability. In this context, much attention has recently been given to open-shell nanographenes (NGs), whose spin interactions can be engineered with atomic precision by on-surface synthesis[1]. In particular, zigzag-edged triangular NGs (triangulenes) are regarded as prototypical magnetic building blocks, with a total spin S scaling with molecular size.

In this contribution, I will discuss multi-spin platforms fabricated via on-surface synthesis from the two smallest S = 1/2 and S = 1 triangulenes[2]. Scanning probe microscopy & spectroscopy of antiferromagnetically coupled hetero-dimers and trimers allow a thorough characterization of these coupled quantum spin systems, with their multiple inelastic spin excitations unambiguously reflecting the underlying spin Hamiltonians. The degenerate spin ground state in asymmetrically coupled spin systems, where each spin unit has a different Kondo exchange with the substrate, also allows to gain novel insights into Kondo correlations. [1] De Oteyza D.G. et al., J. Phys.: Condens. Matter 34 (2022); [2] Turco E. et al., JACS Au, 3, (2023)

O 52.8 Wed 17:00 MA 004

Strong exchange interactions between open-shell nanographenes and a rare earth-gold surface alloy — •Nicolo' Bassi[1], Feifei Xiang[1], Nils Krane[1], Carlo Pignedoli[1], Jan Jan Wilhelm[2], Michal Juríček[3], Roman Fasel[1], and Pascal Ruffieux[1] — [1]Empa, Duebendorf, Switzerland — [2]Institute of Theoretical Physics, Regensburg, Germany — [3]University of Zurich, Zurich, Switzerland

Rare-earth-based intermetallic compounds belong to a family of novel substrates, which is becoming a promising platform to control properties of nanomaterials via specific surface-adsorbates interactions. Different combinations, including GdAu2(1) and TbAu2(2), have been so far studied. They are all characterized by a ordered hexagonal superstructure with similar lattice constants. Here, we investigate various open-shell nanographenes on TbAu2 alloy by means of scanning tunneling techniques. For on-surface synthesized 7 armchair graphene nanoribbons (7-AGNRs), we find that the predicted spin properties of the end states are indeed conserved on TbAu2. Thanks to its lower workfunction, the 7-AGNRs are uncharged and the occupied and unoccupied end states have a spin polarization-induced energy splitting of 1.4eV. In addition, we investigated phenalenyl, the smallest open-shell molecule with spin S = 1/2(4). Low bias spectroscopy reveals a splitting of more than 20mV, which we assign to the exchange interaction between the molecular spin and Tb atoms of the surface layer. These results shows a new substrate for studying different open-shell C structures. 1 Corso, M. et al. ACS Nano 4,(2010). 2 Que, Y. et al. J. Phys. Chem. Lett. 11,(2020). 3 Turco, E. et al. jJACS Au (2023)