TT 6: Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)

The electron spin, a fundamental quantum mechanical property, plays a crucial role in determining the electronic and magnetic properties as well as the dynamics of matter. Its role becomes even more important at surfaces, 2D materials and nanomagnets as the low-dimensionality increases electron correlation. A fundamental understanding of spin excitations is significant for both fundamental science and modern applications. For decades, the interpretation of experimental signatures of spin excitations were focused on the Kondo effect paradigm, with Co atoms on the (111) surface of noble metals as the prototypical example. However, recent first-principles predictions and spin-polarized scanning tunnelling spectroscopy in high magnetic fields have demonstrated the existence of many-body states, called spinarons. These states arise from the binding of electronic states to spin excitations in the presence of spin-orbit coupling. Such findings, along with other studies, challenge the Kondo interpretation. Furthermore, related non-trivial many-body states may emerge in thin-film geometries, as shown by photoemission spectroscopy and first-principles manybody investigations or in quantum spin liquids. These examples testify that many-body phenomena are not only critically important for the fundamental understanding of spin excitations, they also impact a wide range of material characteristics, including electronic, magnetic, thermodynamic, and transport properties. This focus session will provide a forum to discuss intriguing many-body states driven by spin excitations, and serve as a forum to discuss the current knowledge on their origins, unique properties, and implications.

Organized by
Matthias Bode (Würzburg University), Yujeong Bae (Swiss EMPA), and Stefan Blügel (FZ-Jülich).

Time: Monday 15:00–18:15 Location: H24

Invited Talk TT 6.1 Mon 15:00 H24
Kondo and Yu-Shiba-Rusinov resonances: transport and coupling — •Laëtitia Farinacci[1,2,3], Gelavizh Ahmadi[3], Gaël Reecht[3], Benjamin W. Heinrich[3], Contanstin Czekelius[3], Felix von Oppen[3], and Katharina J. Franke[3] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Germany — [3]Fachbereich Physik, Freie Universität Berlin, Germany

The exchange coupling between a magnetic impurity and a superconducting substrate leads to the formation of magnetic bound states, known as Yu-Shiba-Rusinov (YSR) states, inside the superconducting gap, as well as a Kondo resonance outside the gap. Studying these two many-body phenomena in parallel provides valuable insights into their characteristic properties.

We observed striking correlations between the asymmetries of the YSR state and the Kondo effect induced by FeTPyP molecules on Pb(111) in a scanning tunneling microscope (STM) [1]. We show that both asymmetries originate from interfering tunneling paths via a spin-carrying orbital and the highest occupied molecular orbital.

Additionally, we studied the formation of YSR bands in a self-assembled kagome lattice of magnetic molecules on Pb(111) and track YSR hybridization from kagome precursors to larger islands [2]. This work will motivate further studies to resolve possible spin-liquid or Kondo-lattice-type behavior.

[1] PRL 125, 256805 (2020). [2] Nat. Comm. 15, 6474 (2024).

Invited Talk TT 6.2 Mon 15:30 H24
Electron delocalization in a 2D Mott insulator — •Amadeo L. Vazquez de Parga[1,2,4,5], Cosme G. Ayani[1,2], Michele Pisarra[3], Iván M. Ibarburu[1], Clara Rebanal[1], Manuela Garnica[2,4], Fabián Calleja[2], and Fernando Martín[1,2] — [1]Universidad Autónoma de Madrid, Madrid, Spain — [2]IMDEA Nanociencia, Madrid, Spain — [3]Universitá della Calabria, Rende, Italy — [4]Instituto Nicolás Cabrera, Madrid, Spain — [5]Condensed Matter Physics Center (IFIMAC), Madrid, Spain

We follow by means of low temperature Scanning Tunneling Microscopy and Spectroscopy, the buildup of a 2D Kondo lattice in a system composed by a 2D Mott insulator, a single 1T-TaS2 layer, stacked on the surface of a metallic crystal, 2H-TaS2. When the sample temperature is lower than 27K, the magnetic moments present in the Mott insulator experience the Kondo screening by the conduction electrons of the metal, leading to the appearance of a Kondo resonance at the Fermi level. Below 11 K, a gap opens within the Kondo resonance, which is the signature of the formation of a coherent quantum state that extends all over the sample, i.e., a Kondo lattice [1]. Quasi particles interference maps reveal the emergence of a Fermi contour in the 2D Mott insulator when the temperature drops below 11K, indicating the delocalization of the highly correlated Mott electrons [2]. The observed modifications in the LDOS are well explained by state-of-the-art Density Functional Theory calculations.

[1] Small 20, 2303275 (2024) [2] Nat. Commun. 15, 10272 (2024)

Invited Talk TT 6.3 Mon 16:00 H24
Kondo or no Kondo, that is the question — •Alexander Weismann, Neda Noei, Niklas Ide, and Richard Berndt — Institut für experimentelle und angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

The spin properties of individual atoms and molecules can produce distinctive spectral features in tunneling spectra near zero bias. Among these features, Kondo resonances and inelastic spin-flip excitations are often challenging to distinguish, despite their markedly different spectral line shapes. A Kondo resonance indicates a non-magnetic ground state, where the atomic spin is screened by conduction band electrons. In contrast, spin-flip excitations observed in zero-field tunneling spectra require magnetic anisotropy, which arises from spin-orbit coupling (SOC), to play a significant role. In this study, we demonstrate that the well-known Co/Cu(111) system, long believed to exhibit a Kondo resonance, instead adopts a magnetic ground state that is protected from Kondo screening by substantial magnetic anisotropy. The zero-bias anomaly in scanning tunneling spectra undergoes significant modification when Co atoms are attached to monoatomic Cu chains. Measurements conducted at 340 mK in a magnetic vector field reveal clear signatures of inelastic spin-flip excitations, with the anisotropy axis tilted away from the surface normal. The magnitude and orientation of this anisotropy are consistent with density functional theory (DFT) calculations. Moreover, quantum Monte Carlo many-body simulations confirm that the Kondo effect is suppressed when SOC is properly accounted for.

Invited Talk TT 6.4 Mon 16:30 H24
Evidence for spinarons in Co atoms on noble metal (111) surfaces — •Artem Odobesko — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg

The zero-bias anomaly in the tunnelling differential conductance of Co atoms on Au(111) [1], long attributed to the Kondo effect, has recently been reinterpreted [2] as evidence of the spinaron – a novel many-body excitation arising from the interplay between spin excitations and conduction electrons. In our study, we used spin-polarized scanning tunneling spectroscopy (STS) on Co atoms on Cu(111) and Au(111) under high magnetic fields, revealing field-induced energy shifts and spin-resolved spectral features that challenge the conventional Kondo interpretation. Instead, our findings provide the first experimental confirmation of the spinaron [3].

We also investigated the role of hybridization with the substrate in spinaron formation, focusing on the reconstructed Au(111) surface. The unique local electronic environments created by the herringbone reconstruction strongly influence the hybridization strength and spectral features of Co adatoms, revealing a clear link between adsorption site, hybridization, and spinaronic excitations. Our results shed light on the fundamental mechanisms driving spinaron formation.

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

Invited Talk TT 6.5 Mon 17:00 H24

Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures — •Samir Lounis — Peter Grünberg Institut, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

Many-body phenomena are crucial in physics, particularly in condensed matter, influencing electronic, magnetic, thermodynamic, and transport properties. They leave distinct spectroscopic signatures, such as Kondo, excitonic, and polaronic features, arising from specific degrees of freedom. Since more than two decades Cobalt atoms on the (111) surfaces of noble metals have been a paradigm for the Kondo effect in scanning tunnelling spectroscopy experiments [1]. However, our recent first-principles predictions [2] followed by STS experiments in high magnetic fields [3,4] challenge this notion. Our findings reveal that the observed transport anomalies stem from spin excitations of Co atoms, forming a new many-body state – the spinaron – distinct from the Kondo resonance. I will delve into the spinaron origins, their unique properties, and implications explored through the recent atomic manipulation experiments. This work opens pathways to investigate and engineer these hybrid states in nanostructures, offering new insights into fundamental many-body states.

[1] V. Madhavan et al., Science 280, 567 (1998); [2] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [3] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [4] N. Noei et al., Nanoletters 23, 8988 (2023)

TT 6.6 Mon 17:30 H24

Emergence of spinaronic states in Fe adatoms — Ilias Klepetsanis[1,2], Juba Bouaziz[4], •Philipp Rüssman[1,3], and Samir Lounis[1,2] — [1]Forschungszentrum Jülich & JARA, Germany — [2]University of Duisburg-Essen and CENIDE, Germany — [3]University of Würzburg, Germany — [4]Research Center for Advanced Science and Technology, University of Tokyo, Japan

In recent years, spinarons, predicted from first-principles calculations [1], have been observed in Co adatoms on the Cu(111) surface, using spin-polarized scanning tunnelling spectroscopy (STS) in high magnetic fields [2]. Spinarons leave a non-trivial spectroscopic signature, for long interpreted to originate from the Kondo effect [3]. Here, we employ relativistic time-dependent density functional and many-body perturbation theory, to investigate the case of Fe adatoms on the Cu(111) surface, which carry a large magnetic moment of $3.25\mu_B$ preferring an out-of-plane orientation as dictated by a magnetic anisotropy energy of 2meV. In contrast to the Co adatom, the spinarons in Fe do not overlap with trivial spin-excitations. We discuss the spinaronic response to an out-of-plane magnetic field, the orbital character and the impact of spin-orbit coupling. [1] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [2] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [3] V. Madhavan et al., Science 280, 567 (1998)

TT 6.7 Mon 17:45 H24

Revising the Superconductivity in Iron Based Superconductors from the Perspective of Electron Phonon Coupling — •Lanlin Du[1,2] and Sheng Meng[1,2,3] — [1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong, China

There are currently two mainstream superconducting pairing mechanisms, namely electron phonon coupling and spin fluctuation, which are believed to play a dominant role in conventional superconductors like simple metal superconductors and unconventional superconductors like Copper oxides, respectively. Iron based superconductors are believed to connect these two aspects, that is, both mechanisms are important in it. In fact, some studies have shown that electron phonon coupling is also important in cuprates, and even provide evidence for s-wave pairing symmetry in them. Therefore, it is important to consider the role of electron phonon coupling in unconventional superconductors. Here, we revise the superconductivity in Iron based superconductors using Migdal-Eliashberg formalism and electron phonon coupling strength corrected by many body method from the two perspectives of doping and pressurization. Our results are in good agreement with the experiments. Based on this, we predict a new two-dimensional high-Tc Iron based superconductor.

TT 6.8 Mon 18:00 H24

Theoretical model for multiorbital Kondo screening in strongly correlated molecules with several unpaired electrons — •Manish Kumar[1], Aitor Calvo-Fernandez[2], Diego Solar-Polo[1], Asier Eiguren[2], Maria Blanco-Rey[3], and Pavel Jelinek[1] — [1]Institute of Physics, Academy of Sciences of the Czech Republic , Cukrovarnicka 10, Prague 6, CZ 16200, Czech Republic — [2]Department of Physics, University of the Basque Country UPV-EHU, 48080 Leioa, Spain — [3]Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, University of the Basque Country UPV-EHU, 20018 Donostia-San Sebastián, Spain

The mechanism of Kondo screening in strongly correlated molecules with several unpaired electrons on a metal surface is still under debate. Here, we provide a theoretical framework that rationalizes the emergence of Kondo screening involving several extended molecular orbitals with unpaired electrons. We introduce a perturbative model, which provides simple rules to identify the presence of antiferromagnetic spin-flip channels involving charged molecular multiplets responsible for Kondo screening. The Kondo regime is confirmed by numerical renormalization group calculations. In addition, we introduce the concept of Kondo orbitals as molecular orbitals associated with the Kondo screening process, which provide a direct interpretation of experimental dI/dV maps of Kondo resonances. We demonstrate that this theoretical framework can be applied to different strongly correlated open-shell molecules on metal surfaces, obtaining good agreement with previously published experimental data.