O 11: Focus Session: Spins on Surfaces studied by Atomic Scale Spectroscopies II

Time: Monday 15:00–17:45 Location: MA 004

Topical Talk O 11.1 Mon 15:00 MA 004

Unusual magnetism of closed-shell molecules on metal substrates — •Alexander Weismann[1], Arnab Banerjee[1], Manuel Gruber[2], Jan Homberg[1], Niklas Ide[1], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

Molecular magnetism is studied using low temperature scanning tunneling spectroscopy by resolving spectroscopic fingerprints close to the Fermi energy like Kondo resonances, inelastic spin excitations and Yu-Shiba-Rusinov (YSR) states. We find a variety of closed-shell molecules that can become paramagnetic in suitable environments or by molecular switching. Furthermore, an unexpectedly large orbital moment related to molecular ring currents is observed. Using YSR states we sensitively detect a large number of molecular vibrations via inelastic tunneling. Magnetic and vibrational excitations are spatially mapped and energy shifts caused by intermolecular interactions are resolved on a 100 μeV scale. Taken together our results highlight the importance of electrostatic stray fields due to polar bonds in molecules.

O 11.2 Mon 15:30 MA 004

Theory of a Single Magnetic Impurity on a Thin Metal Film in Proximity to a Superconductor — •Jon Ortuzar Andres[1], Stefano Trivini[1], Katerina Vaxevani[1], Jingchen Li[2], F. Sebastian Bergeret[3,4], Miguel A. Cazalilla[4,5], and Jose Ignacio Pascual[1,5] — [1]CIC nanoGUNE, Donostia-San Sebastián, Spain — [2]School of Physics, Sun Yat-sen University, Guangzhou 510275, China — [3]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, Donostia-San Sebastián, Spain — [4]Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Magnetic impurities on proximitized thin films can host Yu-Shiba-Rusinov states, entangled excitation between the spin of the impurity and the electrons of the substrate. We argue that the formation of YSR excitations in proximitized thin films is largely mediated by a type of Andreev-bound state named after de Gennes and Saint-James. This is shown by studying an experimentally motivated model and computing the overlap of the wave functions of these two sub-gap states. We find the overlap stays close to unity even as the system moves away from weak coupling across the parity-changing quantum phase transition. Based on this observation, we introduce a single-site model of the bound state coupled to a quantum spin. This model can qualitatively explain the complex behaviour of magnetic impurities interacting with the proximitized metal. The adequacy of this description is assessed by reintroducing the coupling to the continuum as a weak perturbation within the framework of Anderson's poor-man's scaling.

O 11.3 Mon 15:45 MA 004

Microwave excitation of atomic scale superconducting bound states — Janis Siebrecht[1], Haonan Huang[1], Piotr Kot[1], Robert Drost[1], Ciprian Padurariu[2], Björn Kubala[2], Jochim Ankerhold[2], Juan Carlos Cuevas[3], and •Christian R. Ast[1] — [1]MPI für Festkörperforschung, Stuttgart — [2]Institut für Komplexe Quantensysteme, Universität Ulm, Ulm — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

Magnetic impurities on superconductors lead to bound states within the superconducting gap, so called Yu-Shiba-Rusinov (YSR) states. They are parity protected, which enhances their lifetime, but makes it more difficult to excite them. Here, we realize the excitation of YSR states by microwaves facilitated by the tunnel coupling to another superconducting electrode in a scanning tunneling microscope (STM). We identify the excitation process through a family of anomalous microwave-assisted tunneling peaks originating from a second order resonant Andreev process, in which the microwave excites the YSR state triggering a tunneling event transferring a total of two charges. We vary the amplitude and the frequency of the microwave to identify the energy threshold and the evolution of this excitation process. Our work sets an experimental basis and proof-of-principle for the manipulation of YSR states using microwaves with an outlook towards YSR qubits.

O 11.4 Mon 16:00 MA 004

YSR-STM thermometer for superconducting quasiparticle temperatures — •Ciprian Padurariu[1], Sujoy Karan[2], Haonan Huang[2], Björn Kubala[1,3], Christian R. Ast[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

The occupation of the quasiparticle continuum in a superconductor is of critical importance for the functionality of Josephson junction-based quantum devices. While significant progress has been made recently, the detection and removal (trapping) of quasiparticles remains a significant challenge. This talk will describe the design of a thermometer that detects the presence and effective temperature of superconducting quasiparticles. The device consists of a mK-STM functionalized with a single Yu-Shiba-Rusinov (YSR) state inside the gap. Transport between the tip and a clean superconducting substrate shows Zeeman-split peaks in the differential conductance associated to the YSR state [1]. The width of the peaks is sensitive to the effective temperature of quasiparticles above the gap. We show that this width manifests not only in the voltage-dependence, but also in the magnetic field- and exchange coupling-dependence of the current. This allows determining the effective temperature below the limit of the STM energy resolution. [1] W.-V. van Gerven Oei, *et al.*, "Magnetic impurities in spin-split superconductors", Phys. Rev. B **95**, 085115 (2017).

O 11.5 Mon 16:15 MA 004

Non-local detection of Yu-Shiba-Rusinov states in quantum corrals — Khai Ton That[1], Chang Xu[2], Ioannis Ioannidis[3], Lucas Schneider[1], Thore Posske[3], Dirk K. Morr[2], Roland Wiesendanger[1], and •Jens Wiebe[1] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]University of Illinois at Chicago, Chicago, USA — [3]Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany

Quantum mirages are non-local projections of local quantum states induced by an atomic-scale defect in a bath of conduction electrons that can be tailored by cages of nonmagnetic atoms, so-called quantum corrals [1,2]. Here, we observe, by scanning tunnel spectroscopy, the mirage of the Yu-Shiba-Rusinov (YSR) state induced by a magnetic atom in the gap of a superconductor and a characteristic corral-eigenenergy dependent oscillation in its particle-hole asymmetry. Our modelling shows that the mirage is dominated by an indirect coupling of the YSR state induced in the bulk superconductor with the corral eigenmodes. [1] H. Manoharan et al., Nature 403, 512 (2000); [2] L. Schneider et al., Nature 621, 60 (2023).

O 11.6 Mon 16:30 MA 004

Yu-Shiba-Rusinov bands in a self-assembled kagome lattice of magnetic molecules — •Laëtitia Farinacci[1], Gaël Reecht[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

The kagome lattice features both a flat-band and a Dirac cone, which makes it of particular interest for electronic correlations and relativistic effects. Moreover, if anti-ferromagnetic nearest-neighbour coupling takes place, its geometry ensures magnetic frustration. This further broadens the range of physical phenomena that a kagome lattice can host.

However, it is challenging to realize an ideal two-dimensional lattice as interlayer coupling or interactions with a solid-state support may suppress the correlations. Here, we initiate a study a kagome lattice hosting unpaired electron spins on a superconductor. Using molecular self-assembly we show that the deposition of Fe-porphine-chloride molecules on a Pb(111) surface can lead to the formation of a kagome lattice in 2D molecular islands, and also of smaller units that correspond to kagome precursors. Each FeP molecule induces a magnetic bound state, called Yu-Shiba-Rusinov (YSR) state and we show that these hybridize in the kagome precursors and lead to YSR bands in large islands.

O 11.7 Mon 16:45 MA 004

Spin-flip excitations in organometallic chains — •Jung-Ching Liu[1], Chao Li[1], Outhmane Chahib[1], Xing Wang[2], Ping Zhou[2], Robert Häner[2], Silvio Decurtins[2], Ulrich Aschauer[3], Shi-Xia Liu[2], Ernst Meyer[1], and Rémy Pawlak[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern — [3]Department of Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Strasse 2A, A-5020 Salzburg

Controlling the spin of metal adatoms in well-ordered organometallic (OM) frameworks is a key step towards the realization of molecular electronics and spintronics. Here, we present the study of magnetic signatures at metal centers in the complex structure coordinated by PTO and Fe adatoms[1]. STM and AFM with CO-terminated tips[2] reveal the structure of the OM chains. STS at 1K indicates three spin-flip excitations and collective spin-state excitations of Fe on Ag(111). On Pb(111), PTO-Fe chains only show two spin-flip excitations outside the superconducting gap. By comparing these two systems, we conclude that the spin characteristics of the PTO-Fe chain do not change drastically between these substrates, while spin-state excitation is expected to have a longer lifetime on superconductors[3,4]. We believe our study provides a route for fundamental studies in spin-spin and spin-substrate interactions with different lattice structures.[1]Chem. Eur. J., 2016, 22, 8105-8112. [2]PRL, 2011, 107, 086101. [3]Nat. Phys., 2013, 9, 765-768. [4]Nano Lett. 2022, 22, 6075-6082.

O 11.8 Mon 17:00 MA 004

Tunable ferromagnetic order in 2D layers of transition metal dichlorides — •Andrea Aguirre[1,2], Andrés Pinar[3], Jon Ortuzar[2], Oleksandr Stesovych[3], Nacho Pascual[2], Celia Rogero[1], Pavel Jelínek[3], Maxim Ilyn[1], and Martina Corso[1] — [1]Materials Physics Center (CSIC-UPV/EHU), San Sebastian, Spain — [2]CIC nanoGUNE-BRTA, San Sebastian, Spain — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

Metal dihalides TMX2, where TM is a transition metal and X a halogen, are a class of 2D layered materials bonded through van der Waals interactions. These binary compounds exhibit magnetic texture with semiconducting electronic properties. Since single layers can grow epitaxially on metal substrates, there is a strong interest in determining whether these properties persist at the 2D limit.

Here we study the epitaxial growth of FeCl2 and NiCl2 on Au (111). Their chemical and electronic properties were explored high-resolution X-ray photoelectron spectroscopy (XPS) and low-temperature scanning tunneling microscopy and spectroscopy (STM). These 2D materials grow in large and flat monolayers electronically decoupled from the substrate. Our studies on the magnetic properties by X-ray absorption spectroscopy (XAS) revealed a ferromagnetic order related to the 3d electrons of the metal in the compound. The magnetic alignment depends on the TM used, so that it can be switched from out-of-plane to in-plane by substituting the metal ion from iron to nickel. Additionally, we probed the same magnetic behavior at the atomic scale by using nickelocene functionalized STM tips.

O 11.9 Mon 17:15 MA 004

Distinct Quantum States in Topological Insulator Surfaces of Nanowires and Nanoribbons of Bismuth Selenide — •Christian Nweze[1], Tomke Eva Glier[1], Mika Rerrer[1], Malte van Heek[1], Sarah Scheitz[1], Lewis Akinsinde[1], Niklas Kohlmann[2], Lorenz Kienle[2], Yalan Huang[1], Wolfgang Parak[1], Nils Huse[1], and Michael Rübhausen[1] — [1]Institute of Nanostructure and Solid-State Physics, University of Hamburg, Hamburg, 22761, Germany. — [2]Institute for Materials Science, Faculty of Engineering, Kiel University, Kaiserstrasse 2, 24143, Kiel, Germany

Topological insulators (TIs) exhibit unconventional quantum phases that can be manipulated with external quantum confinements. The geometry of the surface of 3D TIs plays a crucial role in tuning the quantum confinement in TIs. For instance, morphing a 3D TI into a 1D cylinder results into a curved surface in which the electron spin is locked perpendicular to the momentum and, as well as, tangential to the perimeter of the TI nanowire. This leads to a new state with a Spin-Berry Phase (SBP). We utilized Surface-Enhanced Raman Scattering (SERS) as sensor to study the confinement of quasi-relativistic electrons in TI nanowires. Our result shows diameter-dependent SERS in nanowires which is attributed to the self-interference effect of the electronic wavefunction along the curved surface of the nanowires. Rectangular shaped Nanoribbons do not show this effect. Plasmonic gold nanoparticles attached at the distinct topological surface states enables us to discriminate different subband splitting between nanowires and nanoribbons.

O 11.10 Mon 17:30 MA 004

Quantum simulator to emulate lower-dimensional molecular structure — •Emil Sierda, Xiaochun Huang, Danis Badrtdinov, Brian Kiraly, Elze Knol, Anna M.H. Krieg, Gerrit C. Groenenboom, Mikhail I. Katsnelson, Malte Rösner, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Bottom-up quantum simulators have been developed to quantify the role of various interactions, dimensionality, and structure in creating electronic states of matter. Here, we demonstrated a solid-state quantum simulator emulating molecular orbitals, based solely on positioning individual cesium atoms on an indium antimonide surface. Using scanning tunneling microscopy and spectroscopy, combined with ab initio calculations, we showed that artificial atoms could be made from localized states created from patterned cesium rings. These artificial atoms served as building blocks to realize artificial molecular structures with different orbital symmetries. These corresponding molecular orbitals allowed us to simulate two-dimensional structures reminiscent of well-known organic molecules. The platform could further be used to monitor the interplay between atomic structures and the resulting molecular orbital landscape with submolecular precision.