O 7: Spins on Surfaces at the Atomic Scale I

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

Topical Talk O 7.1 Mon 10:30 REC C 213

Superconductivity in atom-by-atom crafted quantum corrals — •Lucas Schneider[1], Khai That Ton[1], Ioannis Ioannidis[2,3], Jannis Neuhaus-Steinmetz[1], Thore Posske[2,3], Roland Wiesendanger[1], and Jens Wiebe[1] — [1]Department of Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]I. Institute for Theoretical Physics, University of Hamburg, D-20355 Hamburg, Germany — [3]Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany

Gapless materials in electronic contact with superconductors acquire proximity-induced superconductivity in a region near the interface. Here, we investigate the most miniature example of this so-called proximity effect on only a single quantum level of a surface state confined in a quantum corral on a superconducting substrate, built atom-by-atom using a scanning tunneling microscope. Whenever an eigenmode of the corral is pitched close to the Fermi energy by adjusting the corral's size, a pair of particle-hole symmetric states is found to enter the superconductor's gap. By comparison to a resonant level model of a spin-degenerate localized state coupled to a superconducting bath, we identify the in-gap states as scattering resonances theoretically predicted 50 years ago by K. Machida and F. Shibata, which had so far eluded detection. We further show that the observed anticrossings of the in-gap states indicate proximity-induced pairing in the quantum corral's eigenmodes. In a final step, we study how individual magnetic adatoms interact with the corral's eigenmodes.

O 7.2 Mon 11:00 REC C 213

Tailoring Yu-Shiba-Rusinov bands in a Kagome lattice by molecular self-assembly — •Laetitia Farinacci, Gael Reecht, Nils Bogdanoff, Benjamin W. Heinrich, Felix von Oppen, and Katharina J. Franke — Freie Universitaet Berlin, Germany

Coupling of magnetic bound states in superconductors (so-called Yu-Shiba-Rusinov or YSR states) leads to fascinating phenomena; such as the formation of topological states. Bottom up approaches allow for a precise characterization of the coupling parameters, shedding light onto the formation of YSR bands and their properties. Most studies so far rely on atom manipulation, which is time demanding and typically limits the size of the systems to below a hundred sites.

Here, we show that self-assembly of Fe-porphine-chloride (FePCl) molecules on Pb(111) can be controlled by varying the sample temperature during and after molecular deposition. In particular, we show that we can obtain islands in which the FeP molecules arrange in a Kagome lattice or in its precursors. This way, we can, on the one hand, characterize the YSR hybridization with molecular precision and, on the other hand, study the long-range band formation across 2D islands.

O 7.3 Mon 11:15 REC C 213

Atom-by-Atom Study of Spin Lattices on a Superconducting Rashba Material — •Khai That Ton, Lucas Schneider, Jens Wiebe, and Roland Wiesendanger — Department of Physics - University of Hamburg, Hamburg, Germany

In the research field of topological superconductivity, Rashba-spin-orbit-coupling is believed to be a stabilizing parameter for topological phases, increasing the size of the topological gap.

One well-known category of materials with large spin-orbit coupling are Bismuth-based surface alloys, which have been extensively studied by surface-sensitive methods like angle-resolved photoemission and scanning tunneling spectrosopy [1,2,3,4]. However, studies of such materials proximitized by superconducting substrates are lacking so far. In this work, we grew Bismuth-based surface alloys on thin films proximitized by elementary superconducting substrates, adsorbed transition metal atoms, and then built dimers, chains and small two-dimensional lattices of these atoms via STM-tip based atom manipulation. We will present a scanning tunneling spectroscopy investigation of the low-energy electronic structure of these different spin lattices.

[1] C. R. Ast et al. Phys. Rev. Lett. 98, 186807 (2007).
[2] C. R. Ast et al., Phys. Rev. B 75, 201401(R) (2007).
[3] M. Steinbrecher et al., Phys. Rev. B 87, 245436 (2013).
[4] W. Jolie et al., ACS Nano 16, 4876*4883 (2022).

O 7.4 Mon 11:30 REC C 213

Symmetry-dependent coupling in Yu-Shiba-Rusinov dimers — •Lisa Rütten[1], Eva Liebhaber[1], Harald Schmid[1], Gaël Reecht[1], Kai Rossnagel[2,3], Felix von Oppen[1], and Katharina Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany — [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Unpaired adatom spins on superconductors interact with the Cooper pairs of the substrate and cause Yu-Shiba-Rusinov (YSR) states inside the superconducting gap. These can be probed by scanning tunneling spectroscopy at the single-atom scale. On superconducting van der Waals materials, the YSR wave functions of magnetic impurities can extend over several nanometers. This provides a wide range of adatom spacings over which their interaction is sufficiently strong to be potentially observed as a splitting in the tunneling spectra. Additionally, the YSR wave functions inherit their symmetry from the substrate. Depending on the symmetry and spacing in YSR dimers, the spins may interact differently via RKKY and Dzyaloshinskii-Moriya interactions. This manifests in splittings and/or shifts of the YSR states.

Here, we manipulate Fe atoms on superconducting $2H$-$NbSe_2$ using the tip of a scanning tunneling microscope and build dimers with different symmetries. Depending on the orientation of the dimers with respect to the crystal symmetry of the substrate we find YSR hybridization but also more complex effects caused by spin interactions.

O 7.5 Mon 11:45 REC C 213

Magnetic impurity states proposed as 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 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 current is sensitive to quasiparticles above the gap. We show, based on a simple rate equation model, how the control of the magnetic field, as well as the voltage bias, allows the operation of the junction as a thermometer for the effective temperature of quasiparticles.

[1] W.-V. van Gerven Oei, *et al.*, "Magnetic impurities in spin-split superconductors", Phys. Rev. B **95**, 085115 (2017).

O 7.6 Mon 12:00 REC C 213

Magnetic phase diagram of a YSR-molecule — •Niels P.E. van Mullekom[1], Benjamin Verlhac[1], Werner M.J. van Weerdenburg[1], Hermann Osterhage[1], Manuel Steinbrecher[1], Katharina J. Franke[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — [2]Fachbereich Physik, Freie Universität Berlin, Germany.

Yu-Shiba-Rusinov (YSR) states arise from the exchange coupling between a local spin and a superconductor, and are strongly linked to Kondo screening. Understanding the interplay of this exchange interaction with other energy scales, as well as the role of higher spin degrees of freedom, requires magnetic field dependent characterization. To date, most studies of YSR states have been limited to bulk superconductors, which easily quench in the presence of modest magnetic fields.

Here, using high resolution milliKelvin scanning tunneling microscopy and spectroscopy, we characterize the magnetic phase diagram of a molecule on the surface of a thin film superconductor. We see nontrivial changes in the YSR excitations, that go beyond the trends that are expected in a spin 1/2 picture. We relate these changes to the various properties of the molecule, including the role of multiple channels and magnetic anisotropy. We additionally propose a model to understand the various changes in the excitation. These results provide an in-depth and detailed approach to understand the role of high spin systems in the presence of Kondo and YSR states.

O 7.7 Mon 12:15 REC C 213

Spin currents in helical molecular wires — •Richard Korytár[1], Jan van Ruitenbeek[2], and Ferdinand Evers[3] — [1]Univerzita Karlova, Prague, Czech Republic — [2]Leiden University — [3]University of Regensburg

Various spin-selective phenomena have been recently reported for helical molecular wires. The explanation of these phenomena is still lacking [1]. I will present a theoretical analysis of spin currents in non-magnetic molecular junctions. First, constraints based on time-reversal invariance will be summarized. Second, I will present results based on Landauer formalism and a simple model Hamiltonian. Possible experimental detection setups will be discussed.

[1] Evers et al., Adv. Mater. 2022, 34, 2106629

O 7.8 Mon 12:30 REC C 213

Controlling the Spin States of iron porphyrin on Au(111) — •Xiangzhi Meng[1], Jenny Möller[2], Masoud Mansouri[3,4], Daniel Sánchez-Portal[3,4], Aran Garcia-Lekue[3,5], Alexander Weismann[1], Chao Li[1], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, 24098 Kiel, Germany — [3]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain — [4]Centro de Física de Materiales CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain; — [5]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Spin-flip excitations of FeTBrPP molecules on Au(111) are investigated with a low-temperature scanning tunnelling microscope under ultrahigh vacuum condition. The molecules show two distinct adsorption configurations that exhibit different magnetic anisotropy energies. Density functional theory calculations show that the different structures and excitation energies reflect unlike occupations of the Fe 3d levels. We demonstrate that the magnetic anisotropy energy can be well controlled by adjusting the adsorption site, the orientation, or the tip-molecule distance.

O 7.9 Mon 12:45 REC C 213

Mapping magnetism with a molecule — •Alex Fétida[1], Michelangelo Romeo[1], Olivier Bengone[1], Marie-Laure Bocquet[2], Nicolas Lorente[3], and Laurent Limot[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR 7504, 67000 Strasbourg, France — [2]PASTEUR, Ecole Normale Supérieure, PSL University, Sorbonnes Université, CNRS, 24 Rue Lhomond, 75005 Paris, France — [3]Centro de Fisica de Materiales (CFM MPC) CSIC-EHU, 20018 San Sebastián, Spain

The decoration of metal probe-tips by a molecule intentionally picked up from a surface has proven to be a powerful method to improve the measurement capabilities of a scanning tunneling microscope (STM). The success of this approach opens the prospect of introducing spin sensitivity through the tip functionalization by a magnetic molecule. We show here that a metallocene-terminated tip can probe surface magnetism through the inelastic component of the tunneling current, which provides an electrical access to the metallocene spin states. When the tip is 100 picometers away from point contact, the exchange interaction between the tip and a magnetic sample changes the metallocene spin states. This detection scheme can then be used to independently measure the sample exchange field and spin polarization with atomic-scale resolution with knowledge of spin orientation as we show on ultra-thin cobalt layers.