O 44: Poster Tuesday: Spins and Magnetism

Time: Tuesday 18:00–20:00 Location: Poster D

O 44.1 Tue 18:00 Poster D

Yu-Shiba-Rusinov States of iron dimers on $2H$-$NbSe_2$ — •Jannik Steinborn[1], Eva Liebhaber[1], Gaël Reecht[1], Sebastian Rohlf[2], Kai Rossnagel[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

A magnetic impurity absorbed on a superconductor leads to bound states (called Yu-Shiba-Rusinov (YSR) states) in the superconducting energy gap. These states are caused by exchange scattering between Cooper pairs and the magnetic impurity. $2H$-$NbSe_2$ is a transition metal dichalcogenide with Van-der-Waals coupled layers. In this material superconductivity and a charge density wave (CDW) coexist at low temperatures.

Here, we investigate the YSR states of iron dimers on the surface of $2H$-$NbSe_2$ with low temperature scanning tunneling microscopy and spectroscopy. We examine the coupling of the YSR states of the two iron atoms and the influence of the CDW.

O 44.2 Tue 18:00 Poster D

Hyperfine fields of magnetic adatoms on MgO/Ag(001) — •Sufyan Shehada, Manuel dos Santos Dias, Filipe Souza Mendes Guimarães, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

The hyperfine interaction couples the atomic nucleus to the surrounding electrons. Nuclear spin states tend to have a very long lifetime, and hold great promise as building blocks for quantum computers. Recently, the hyperfine splitting of the electron spin resonance peak was experimentally detected for Fe and Ti adatoms on MgO/Ag(001) [1]. In this contribution, we report on first-principles calculations of the hyperfine field [2] for a series of magnetic adatoms both on Ag(001) and on MgO/Ag(001) surfaces. We analyze the trends with respect to the type of adatom and its local surface environment, and explore the connection to the stability of the electronic spin states.

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[1] P. Willke *et al.*, Science **362**, 336–339 (2018)
[2] S. Blügel *et al.*, Phys. Rev. B **35**, 3271 (1987)

O 44.3 Tue 18:00 Poster D

Kondo effect of a singly occupied molecular orbital in bis(phthalocyaninato)-dysprosium double decker molecules — •Timo Frauhammer[1], Gabriel Derenbach[1], Svetlana Klyatskaya[2], Eufemio Moreno-Pineda[2], Mario Ruben[2], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany

Double decker bis(phthalocyaninato)-dysprosium single molecule magnets adsorbed on Au(111) have been investigated using low temperature STM. No direct magnetic signal by the 4f electrons could be detected in STS. Interestingly, all molecules adsorbed on step edges show a clear Kondo resonance on the ligands with a Kondo temperature of about 4 K. Some molecules arranged in islands show the same behaviour. This indicates an odd number of electrons residing in the molecular orbitals of the ligands. Assuming there is a strong enough exchange coupling between the unpaired spin on the ligands and the 4-f angular momentum of the Dy central ion, the observed Kondo effect might be used as a means to indirectly address the 4-f magnetic moment.

O 44.4 Tue 18:00 Poster D

Element-Specific Magnetism of Rare-Earth-Cyclooctatetraene Nanowires — •Alexander Herman[1], Stefan Kraus[2], Nico Rothenbach[1], Katharina Ollefs[1], Jan Dreiser[3], Thomas Michely[2], and Heiko Wende[1] — [1]Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47057 Duisburg — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln — [3]Swiss Light Source, Paul Scherrer Institut, Forschungsstrasse 111, CH-5232 Villigen

The analysis of the magnetic coupling and the magnetic anisotropy of localized 4f magnetic moments connected via organic ligands in molecular networks is a highly topical field of research owing to potential applications in organic spintronics. Our on-surface synthesis method allows us to synthesize sandwich-molecular nanowires that consist of alternating ring-like cyclooctatetraene (Cot) molecules and varying rare-earth ions as well as other phases of rare-earth-Cot compounds. The electronic and magnetic properties of these compounds were studied by XAS, XMCD and XLD accompanied by a theoretical approach based on multiplet calculations. The systems show, depending not only on the ligand, but also on the underlying substrate, varying magnetic coupling and magnetic anisotropies. We acknowledge financial support by DFG through the project WE 2623/17-1.

O 44.5 Tue 18:00 Poster D

On-surface chemistry of manganese corroles on Ag(111) — •Hazem Aldahhak[1], Reza Kakavandi[2], Mateusz Paszkiewicz[2], Wolf Gero Schmidt[1], Johannes V. Barth[2], Timur Biktagirov[1], Wolfgang Schöfberger[3], Eva Rauls[4], Florian Klappenberger[2], and Uwe Gerstmann[1] — [1]Department of Physics, Paderborn University, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Physics Department E20, Technical University of Munich, James-Franck-Strasse 1, 85748 Garching, Germany — [3]Institute of Organic Chemistry, Johannes Kepler University, Altenberger Strasse 69, 4040 Linz, Austria — [4]Institutt for Matematikk og Fysikk, University of Stavanger, 4036 Stavanger, Norway.

Corroles are tetrapyrrole macrocycles with promising applications in various fields of science. Here, we present a multi-technique strategy based on density functional theory (DFT) calculations, element-specific X-ray spectroscopy techniques and in situ atomic force microscopy (AFM) to unravel the electronic ground structures and the oxidation states of the prototypical Mn-5,10,15-tris(pentafluorophenyl)corrole complexes as well as of their thermally induced derivatives adsorbed on Ag(111).

Our results, in particular the theory-assisted interpretation of Mn photoemission and absorption fine structure spectra, enable a comprehensive understanding and a deep insight into the on-surface chemistry of such complex molecular systems on the atomic-scale level.

O 44.6 Tue 18:00 Poster D

Changing the Characteristic Critical Current in an STM Josephson Junction by Magnetic Adatoms — •Rika Simon[1], Nils Bogdanoff[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Atomic spins on superconducting surfaces introduce so called Yu-Shiba-Rusinov (YSR) states inside the superconducting gap as a fingerprint of magnetic interaction. Additionally, a renormalization of the local order parameter is predicted by theory, which is not directly reflected in the differential conductance spectra. In contrast, the order parameter can be determined directly in a Josephson junction by measuring its characteristic critical current. The use of a superconducting tip and substrate creates this SIS Josephson junction in a scanning tunneling microscope (STM). The atomic scale spatial resolution of the STM enables the measurement of the critical current on individual magnetic adatoms. A depletion in critical current can be observed on Fe adatoms on a Pb(110) surface [1].
Here, we present further work investigating the seemingly even greater changes in critical current caused by Mn adatoms on Pb(111) in voltage- and current-biased Josephson junctions.
[1] M. T. Randeria, B. E. Feldman, I. K. Drozdov, and A. Yazdani, Scanning Josephson spectroscopy on the atomic scale, Phys. Rev. B 93, 161115(R), 2016

O 44.7 Tue 18:00 Poster D

DFT calculation and experimental study on structural, optical and magnetic properties of Co-doped SrTiO3 — •Pornsawan Sikam[1], Pairot Moontragoon[1,2,3,4], Chayanin Sararat[1], Attaphol Karaphun[1], Ekaphan Swatsitang[1,2,3],

Supree Pinitsoontorn[1,2,3], and Prasit Thongbai[1,2,3] — [1]Department of Physics, Khon Kaen University, Khon Kaen, 40002, Thailand — [2]Integrated Nanotechnology Research Center (INRC), Department of Physics, Khon Kaen University, Khon Kaen, 40002, Thailand — [3]Nanotec-KKU Center of Excellence on Advanced Nanomaterials for Energy Production and Storage, Khon Kaen University, Khon Kaen, 40002, Thailand — [4]Thailand Center of Excellence in Physics, Commission on Higher Education, Bangkok, 10400, Thailand

Outstanding features of SrTiO3 are thermal stability and photocorrosion resistance so the SrTiO3 is widely studied to apply as photocatalyst. However, for further applications, this work would like to study Co doping on the SrTiO3. It is questioned up whether d-orbital of Co could induce magnetism in the non-magnetic SrTiO3 or not because magnetism could improve applications of the SrTiO3. Here, the Co-doped SrTiO3 is studied both experimental and theoretical aspects. In experiment, the Co-doped SrTiO3 is prepared by hydrothermal method. From the experiment, it is seen that Co can improve not only magnetic and optical properties but also surface area of the SrTiO3. These observed results are corresponding to the DFT study. Therefore, it is possible that Co-doped STO might be a potential candidate to be a great photocatalyst and the diluted magnetic semiconductor.