O 93: Surface Magnetism (joint session MA/O)

Time: Thursday 9:30–12:00 Location: HSZ 101

Invited Talk O 93.1 Thu 9:30 HSZ 101

Vacuum Resonance States as Atomic-Scale Probes of Noncollinear Surface Magnetism — •Anika Schlenhoff — Department of Physics, University of Hamburg (Germany)

Understanding the spin-dependent scattering of electrons at magnetic surfaces is highly relevant for the control of electron transport in future spintronic applications. However, its atomic-scale variations, e.g. on noncollinear magnetic surfaces, remained inaccessible, due to the laterally averaging nature of the established experimental approaches.

By means of spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy on unoccupied resonance states (RSs) located *in vacuo*, the reflection of electrons at noncollinear magnetic surfaces is investigated [1]. Even for energies up to 20 eV above the Fermi level, the RSs exhibit the same local spin quantization axis as the underlying spin texture. Mapping the spin-dependent electron phase shift upon reflection at the surface on the atomic scale demonstrates the relevance of all magnetic ground state interactions for the scattering of spin-polarized low-energy electrons. Moreover, while conventional SP-STM is restricted to probe at tip-sample distances of a few Å, tunneling into RSs allows for imaging atomic-scale spin textures at technically feasible distances in the nm regime [2]. Experimental results will be discussed in terms of the RS spin-splitting and the magnetic contrast as a function of bias and tip-sample distance, as well as in terms of the atomic-scale nature of the electron reflection at the surface.

[1] A. Schlenhoff, S. Kovaric, S. Krause, and R. Wiesendanger, Phys. Rev. Lett. **123**, 087202 (2019). [2] A. Schlenhoff *et al.*, in preparation.

O 93.2 Thu 10:00 HSZ 101

Dead magnetic layer at the interface - magnetic moment quenching in Mn on W(001) — •Sebastian Meyer[1], Martin Schmitt[2], Matthias Vogt[2], Matthias Bode[2], and Stefan Heinze[1] — [1]Institute for Theoretical Physics and Astrophysics, Christian-Albrechts University of Kiel, 24098 Kiel — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, 97074 Würzburg

The magnetic moment of transition metals can vary strongly due to orbital bonding interactions with ligands, hybridization, or band structure changes induced by reduced coordination, often resulting in high spin–low spin transitions [1]. In contrast, the complete quenching of the magnetic moment, a so-called "dead magnetic layer", has not yet been observed [2]. Using density functional theory in combination with spin-polarized scanning tunneling microscopy, we show that the surface of a Mn double layer on W(001) exhibits a two-dimensional c(2×2) antiferromagnetic ground state. This result can only be confirmed by a complete moment quenching in the interfacial Mn layer caused by the combined action of hybridization and magnetic frustration.

[1] J. L. Fry, *et. al.*, Phys. Rev. B **36**, 868 (1987)
[2] C. A. F. Vaz, *et. al.*, Rep. Prog. Phys. **71**, 056501 (2008)

O 93.3 Thu 10:15 HSZ 101

Tunneling anisotropic magnetoresistance of Pb and Bi adatoms and dimers on Mn/W(110) — •Soumyajyoti Haldar, Mara Gutzeit, and Stefan Heinze — Institute of Theoretical Physics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Noncollinear magnetic structures at transition-metal interfaces are very promising candidates for spintronics applications [1]. A Mn monolayer on W(110) is a prominent example which exhibits a noncollinear cycloidal spin-spiral ground state with an angle of about 173° between neighboring spins. This allows to rotate the spin-quantization axis of an adatom or dimer quasicontinuously and is ideally suited to explore the angular dependence of the tunneling anisotropic magnetoresistance (TAMR) using scanning tunneling microscopy. Here [2], using density functional theory, we explored the TAMR effect of Pb and Bi adatoms and dimers adsorbed on this surface as these elements have a very strong spin-orbit coupling. Pb and Bi adatoms and dimers show a large TAMR up to 60% due to strong spin-orbit coupling (SOC) and the hybridization of 6*p* orbitals with 3*d* states of the magnetic layer. For dimers the TAMR also depends sensitively on the dimer orientation with respect to the crystallographic directions of the surface due to bonds formation with the surface and the symmetry of the SOC induced mixing.

[1] A. Fert et al. Nat. Nanotechnol. **8**, 152 (2013). [2] S. Haldar et al. Phys. Rev. B **100**, 094412 (2019)

O 93.4 Thu 10:30 HSZ 101

Dynamical spin-excitations of transition metal atoms deposited on superconducting surfaces — •Ana Montero, Filipe Souza Mendes Guimarães, Juba Bouaziz, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, the interest in superconductors has been renewed thanks to their application in topological quantum computing — for instance, in the context of qubits, such as Majorana zero modes, which are in-gap states that can arise in nanostructures deposited atop superconductors. Based on ab-initio simulations [1], we systematically scrutinize the electronic and magnetic properties of 3*d* adatoms deposited on various superconducting surfaces above their critical temperature, and investigate their dynamical spin-excitation as probed via inelastic tunneling spectroscopy (IETS). The excitation lifetime, damping and signature in the transport spectra will be presented with a focus on the potential generation of many-body states resulting from the interaction of electrons and spin-excitations.

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] B. Schweflinghaus et al. Phys. Rev. B **89**, 235439 (2014).

O 93.5 Thu 10:45 HSZ 101

Doping graphene with substitutional manganese atoms — •Renan Villarreal[1], Pin-Cheng Lin[1], Harsh Bana[1], Maya N. Nair[2], Ken Verguts[3,4], Steven Brems[4], Stefan De Gendt[3,4], Manuel Auge[5], Hans Hofsäss[5], Chris Van Haesendonck[1], and Lino M. C. Pereira[1] — [1]Quantum Solid-State Physics, KU Leuven, 3001 Leuven, Belgium — [2]CUNY Advanced Science Research Centre, 85 St. Nicholas Terrace, New York, N.Y. 10031, USA — [3]Departement Chemie, KU Leuven, 3001 Leuven, Belgium — [4]Interuniversitair Micro-electronica Centrum (imec), vzw, 3001 Leuven, Belgium — [5]II. Institute of Physics, University of Göttingen, Göttingen 37077, Germany

Several approaches have been explored for the functionalization of 2D materials: the use of different substrates, creation of intrinsic defects, adsorption and intercalation, substitutional doping, among others. For incorporation of substitutional dopants, a major challenge remains: the limited control over the concentration and form of incorporation. An alternative approach is to incorporate the foreign species by ultra-low energy (ULE) ion implantation, precisely tuning the number of implanted ions and their kinetic energy. Here, we demonstrate that it is possible to controllably incorporate manganese (Mn) in graphene as a substitutional dopant using ULE ion implantation. Our approach is based on a wide range of characterization techniques, including STM/STS, synchrotron-based XPS, ARPES, XMCD, transport measurements and Raman spectroscopy. These experimental studies are complemented by DFT and MD calculations.

15 min. break.

O 93.6 Thu 11:15 HSZ 101

Growth and Characterization of Thulium-Cyclooctatetraene-Compounds on Gr/Ir(111) with XANES and XMCD — •Lea Spieker[1], Alexander Herman[1], Benedikt Eggert[1], Tobias Lojewski[1], Nico Rothenbach[1], Stefan Kraus[2], Florin Radu[3], Chen Luo[3,4], Kai Chen[3], Fadi Choueikani[5], Thomas Michely[2], and Heiko Wende[1] — [1]University of Duisburg-Essen — [2]University of Cologne — [3]Helmholz Center Berlin for Materials and Energy — [4]TU Munich — [5]Synchrotron SOLEIL

The magnetic anisotropy and the magnetic coupling of localised 4f elements connected to an organic ligand in a molecular network are a notable point of interest in organic spintronics. We combine the lanthanide thulium (Tm) with the organic molecule cyclooctatetraene (Cot) for the growth of different phases on Gr/Ir(111). Using an undoped substrate Gr/Ir(111) leads the TmCot to self-assemble in a punctiform shape (Dot-phase). On the negatively doped substrate Gr/Eu/Ir(111) TmCot self-assembles in sandwich-molecular wires. As reference, these phases are compared to the metallic sam-

ple Tm/Ir(111) which is known to have an electronic configuration of $4f^{12}$. The electronic and magnetic properties are analysed by X-ray Absorption Spectroscopy using the methods XANES and XMCD, at temperatures down to 1 K. Angular- and field-depended measurements at the thulium $M_{4,5}$-edge revealed magnetic anisotropies. By comparison to multiplet calculations the electronic configuration could be determined as $4f^{12}$ for the three phases. Financial support by DFG (WE 2623/17-1) is acknowledged.

O 93.7 Thu 11:30 HSZ 101

***Ab initio* simulations of hybrid magnetic 2D-materials** — •Nicolae Atodiresei, Vasile Caciuc, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany

We used density functional theory calculations to engineer the electronic and magnetic properties for two classes of two dimensional (2D) materials adsorbed onto Ir(111). In a 1st study, we investigated how to magnetically functionalize a nonmagnetic 2D system as MoS_2 by adsorbing a magnetic cluster made of three Fe atoms. In a 2nd study, we employed non-magnetic molecular systems characterized by different reactivity (e.g. electropositive BH_3 and electronegative NH_3 molecules) to chemically funtionalize a single layer of a magnetic 2D system such as CrI_3. Our *ab initio* simulations can be used as a guide on how the interaction between 2D, atomic clusters and molecules can be used to manipulate the (i) spin-polarization, (ii) magnetic exchange couplings, (iii) magnetic moments and (iv) their orientation of these hybrid 2D materials. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project number 277146847 - CRC 1238 (C01). [1] V. Caciuc *et al.*, Phys. Rev. Mat. **2**, 084001 (2018). [2] V. Caciuc *et al.*, Phys. Rev. Mat. **3**, 094002 (2019).

O 93.8 Thu 11:45 HSZ 101

Emerging 2D-ferromagnetism and strong spin-orbit coupling at the surface of valence-fluctuating $EuIr_2Si_2$ — •Susanne Schulz[1], Ilya A. Nechaev[2], Monika Güttler[1], Georg Poelchen[1], Steffen Danzenbächer[1], Silvia Seiro[3], Kristin Kliemt[4], Evgueni V. Chulkov[5], Clemens Laubschat[1], Eugene E. Krasovskii[5], Christoph Geibel[6], Cornelius Krellner[4], Kurt Kummer[7], and Denis V. Vyalikh[5] — [1]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [2]Centro de Física de Materiales CFM-MPC and Centro Mixto CSIC-UPV/EHU, Donostia/San Sebastián, Spain — [3]IFW Dresden, Germany — [4]Kristall- und Materiallabor, Goethe-Universität Frankfurt, Germany — [5]Donostia International Physics Center, Donostia/San Sebastián, Spain — [6]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [7]European Synchrotron Radiation Facility, Grenoble, France

Here, we present the valence-fluctuating material $EuIr_2Si_2$, where in contrast to its non-magnetic bulk, the Si-terminated surface reveals controllable 2D ferromagnetism. Close to the surface the Eu ions prefer a magnetic divalent configuration and their large $4f$ moments order below 48 K. The emerging exchange interaction modifies the spin polarization of the 2D surface electrons originally induced by the strong Rashba effect. The temperature-dependent intermediate valence of the bulk allows to tune the energy and momentum size of the projected band gaps to which the 2D electrons are confined. This gives an additional degree of freedom to handle spin-polarized electrons at the surface.