O 101: Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: TRE Ma

O 101.1 Thu 10:30 TRE Ma

Magnetic resonance imaging of single atoms on a surface — •Philip Willke[1,2,3], Aparajita Singha[1,2], Xue Zhang[1,2], Kai Yang[3], Yujeong Bae[1,2,3], Taner Esat[1,2], Christopher Lutz[3], Andreas Heinrich[1,2], and Taeyoung Choi[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]IBM Almaden Research Center, San Jose, USA

Combining electron spin resonance (ESR) with scanning tunneling microscopy (STM) allowed for spin resonance experiments on individual atoms on surfaces[1], for remote sensing of atomic spins[2] and for accessing the nuclear spin of single atoms in an STM[3]. In this talk, we focus on the interaction of the atomic spin system on the surface with the magnetic STM tip. We show that the tip field allows to tune the spin system into resonance similar to the external magnetic field, and that it can even fully replace the latter[4]. By utilizing this tip magnetic field, we establish magnetic resonance imaging of single atoms[5], exceeding the spatial resolution of other scanning field-gradient techniques by one to two orders of magnitude. We find that MRI scans of different atomic species and with different probe tips lead to unique resonance images revealing the magnetic interaction between tip and atom. [1] Baumann et al., Science, 350, 417-420 (2015). [1] Choi et al., Nat. Nano 12, 420-424(2017). [3] Willke et al., Science 362, 336-339 (2018) [4] Willke, Singha, Zhang et al., Nano Lett. 19, 8201-8206 (2019) [5] Willke et al. Nat. Phys. 15, 1005-1010 (2019).

O 101.2 Thu 11:00 TRE Ma

Probing surface electronic structure and reaction intermediates in situ — •Kelsey Stoerzinger — Oregon State University, Corvallis, Oregon USA — Pacific Northwest National Laboratory, Richland, Washington USA

Catalysts are important constituents in numerous energy conversion and storage processes. Rational design of catalysts with greater activity for higher efficiency devices requires an understanding of the material surface's electronic structure in situ, as well as the reaction intermediates involved.

Many surface science techniques, such as X-ray photoelectron spectroscopy (XPS), collect information from inherently surface-sensitive low-energy processes, requiring operation in ultrahigh vacuum. This constraint is lifted for ambient pressure XPS, which can probe the surface in equilibrium with the gas phase at pressures up to ~a few Torr, or with thin liquid layers using a higher incident photon energy. I will discuss the insights obtained with this technique regarding the electronic structure of well-defined epitaxial oxides in equilibrium with a gaseous atmosphere of small molecules (e.g. O2, H2O, CO2, CH3OH, NO), the adsorption of such species, and their subsequent transformation upon driving a desired reaction by heat, voltage, or additional reactant. Adsorption and reactivity can be manipulated by the oxide composition and electronic structure, crystallographic orientation, strain, and local environment in amorphous materials. This molecular-level understanding of interfacial interactions can guide the rational design of high-surface-area oxide catalysts for technical applications.

O 101.3 Thu 11:30 TRE Ma

Control of molecular spins on surfaces — •Manuel Gruber — IEAP, Christian-Albrechts-Universität zu Kiel, Germany

Controlling the spin of individual molecules is attractive for molecular spintronics, quantum computing, and may turn useful to study many-body physics in yet unexplored regimes. I will report on three approaches pursued in our group. (i) A direct approach is to employ spin-crossover (SCO) complexes, which exhibit an intrinsic spin bistability. Having first demonstrated SCO of Fe^{2+} compounds, we recently extended controlled and reversible switching to single Fe^{3+} complexes on a Cu$_2$N surface. (ii) We integrated a spin switching functionality into robust complexes. It relies on the mechanical movement of an axial ligand strapped to a porphyrin ring. Thus spin and coordination are interlocked and we demonstrate reversible electron-induced switching in this new class of compounds on Ag(111). (iii) Spin is induced in molecules and to some extent controlled through supramolecular manipulation. Spin detection is based on the Yu-Shiba-Rusinov resonances that result from the interaction of the induced spin with Cooper pairs of a superconducting substrate. The induced magnetic moment is fine tuned through the control of the electrostatic potential engendered by neighboring molecules. These experiments notably allow to probe the Yu-Shiba-Rusinov physics caused by fractional charges.

This work has been done in collaboration with the groups of Profs. Berndt, Herges, Rossnagel and Tuczek. Support via SFB 677 and the European Union's Horizon 2020 research and innovation programme (766726) is acknowledged.

O 101.4 Thu 12:00 TRE Ma

Determination and control of charge states of individual molecules — •Shadi Fatayer, Florian Albrecht, Nikolaj Moll, and Leo Gross — IBM Research - Zurich

The physicochemical properties of molecules adsorbed on surfaces are charge-state dependent. Insulating films serve as an ideal platform to study the physics and chemistry of charged molecules, because these films avoid charge leakage. However, investigating individual charged molecules on insulators is experimentally challenging. The atomic force microscope (AFM), operable on insulating substrates and capable of single-electron sensitivity and atomic resolution, is suitable to be used with insulators. Using the AFM, I will first show how the charge state of molecules can be controlled. Then, I will present how different aspects of charged molecules can be accessed with the AFM: (i) How using the AFM as a single-electron current meter allows for tunneling spectroscopy to be performed on insulators and electron-transfer properties probed, (ii) how reversible chemical reactions can be performed via charging molecules and (iii) the insights gained via resolving the atomic structure of individual molecules in different charge states.

O 101.5 Thu 12:30 TRE Ma

Discovery of chiral topological semimetals with multifold fermions and maximal Chern numbers — •Niels Schröter — Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

Chiral topological semimetals (which possess neither mirror nor inversion symmetries) are expected host numerous novel phenomena, such as multifold fermions with large topological charge, long Fermi-arc surface states, unusual magnetotransport and lattice dynamics, and a quantized response to circularly polarized light - the first quantized response in metals. Until recently, all experimentally confirmed topological semimetals crystallized in space groups that contain mirror operations, which means that the aforementioned phenomena cannot appear.

Here I will present the first experimental evidence that AlPt and PdGa are chiral topological semimetals. Using angle-resolved photoelectron spectroscopy and ab-initio calculations, we show that these compounds host multifold fermions that carry the maximal Chern number that can be realized for linear band crossings in any material, which imposes an upper limit to the magnitude of many topological phenomena. Furthermore, by comparing two enantiomers (crystals with mirrored structure that do not coincide), we observe a reversal of their Fermi-arc velocities, which demonstrates that the handedness of chiral crystals can be used as a tuning parameter to manipulate the sign of their Chern numbers. I will furthermore demonstrate how time-reversal symmetry breaking can create novel topological multifold fermions that are elusive in non-magnetic compounds.