

O 77: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: S051

Invited Talk

O 77.1 Thu 10:30 S051

The first single atom magnet — ●FABIO DONATI¹, STEFANO RUSPONI¹, SEBASTIAN STEPANOW², CHRISTIAN WÄCKERLIN¹, APARAJITA SINGHA¹, LUCA PERSICHETTI², ROMANA BALTIC¹, KATHARINA DILLER¹, EDGAR FERNANDES¹, FRANÇOIS PATTHEY¹, JAN DREISER^{1,3}, ŽELJKO ŠLJIVANČANIN^{4,5}, KURT KUMMER⁶, CORNELIU NISTOR², PIETRO GAMBARELLA², and HARALD BRUNE¹ — ¹Ecole Polytechnique Fédérale de Lausanne — ²ETH Zurich — ³Paul Scherrer Institute — ⁴Vinča Institute of Nuclear Sciences — ⁵Texas A&M University at Qatar — ⁶European Synchrotron Radiation Facility

Realizing magnetic remanence in a single atom is the key to store and process information in the smallest unit of matter. To achieve this goal, one needs to protect the magnetic states of the single atom from quantum tunneling of the magnetization and from scattering with the electrons of the supporting substrate. Here we demonstrate that individual rare-earth atoms adsorbed on ultra-thin insulating layers grown on non-magnetic metal substrates exhibit magnetic remanence up to a temperature of 30 K and a relaxation time of 1500 s at 10 K. This first example of a single atom magnet shows bistability at a temperature which is significantly higher than the best single molecule magnets reported so far. Its extraordinary performances are achieved by a suitable combination of magnetic ground state and adsorption site symmetry, as well as by suppressing spin-electron scattering with conduction electrons by ultra-thin insulating layers.

Invited Talk

O 77.2 Thu 11:00 S051

When Electron Acceptors Donate Charge: Molecular Orbitals vs Hybrid Bands at Inorganic/Organic Interfaces — ●OLIVER T. HOFMANN¹, PATRICK RINKE², MATTHIAS SCHEFFLER³, and GEORG HEIMEL⁴ — ¹TU Graz, Graz, Austria — ²Aalto University, Helsinki, Finland — ³Fritz-Haber-Institut der MPG, Berlin, Germany — ⁴Humboldt University of Berlin, Germany

At inorganic/organic interfaces, the concept of electrons moving in extended bands collides with the notion of localized molecular orbitals. For the adsorption of most electron accepting molecules, theory and experiment concordantly report an average charge-transfer smaller than one electron per molecule, raising the question how such an (indivisible) object can be divided between the subsystems. Using hybrid density functional theory (DFT) we prepare and contrast both situations for TCNE molecules on clean and NaCl-passivated Cu substrates. Hybrid DFT functionals localize electrons on a subset of individual molecules, who become charged and whose signatures and associated observables differ markedly from the delocalized band states of fractionally charged molecules obtained with semi-local DFT. We then apply our computational framework to F4TCNQ on ZnO(10 $\bar{1}$ 0), which exhibits two different charge transfer types. Charge donation again leads to integer charging of individual molecules, whereas charge back-donation proceeds via covalent bonds and thus delocalized hybrid bands. Since back-donation also occurs for the uncharged F4TCNQ molecules in the organic film, we end up with the counterintuitive situation of positively charged electron acceptors on the ZnO surface.

Invited Talk

O 77.3 Thu 11:30 S051

Direct observation of H-bond dynamics using scanning tunneling microscopy — ●TAKASHI KUMAGAI — Fritz-Haber Institute

H-bond dynamics is involved in many important processes in chemistry and biology. However, it is still poorly understood at the microscopic level because the dynamics, H-bond rearrangement and H-atom (proton) transfer, remains difficult to directly probe at the single-molecule level. Additionally, quantum nuclear effects, like tunneling and zero-point energy, play a crucial role due to the small mass of the H atom, which could cause difficulty in accurately describing the H-bond dynamics. We have used low-temperature STM to directly observe the H-bond dynamics, which were examined with a variety of models as-

sembled from single atoms/molecules by STM manipulation [1-8].

I will discuss the direct observation of several different types of H-bond dynamics; 1) the H-bond exchange reaction governed by tunneling in a water dimer [1], 2) vibrationally-induced H-atom relay reactions in one-dimensional H-bonded water-hydroxyl complexes [4], and 3) the intramolecular H-atom transfer (tautomerization) in a porphycene molecule [6,7]. These results provide a novel insight into H-bond dynamics at the single-molecule level and unveiled the impact of the local environments on the process that is hidden in studies of molecular ensembles probed by spatially-averaging spectroscopies [8].

References; [1] PRL 100, 166101. [2] PRB 79, 035423. [3] PRB 81, 045402. [4] Nat. Mater. 11, 167. [5] Visualization of hydrogen-bond dynamics, Springer (2012). [6] PRL 111, 246101. [7] Nat. Chem. 6, 41. [8] Prog. Surf. Sci. 90, 239.

Invited Talk

O 77.4 Thu 12:00 S051

Visualizing topological states of matter and their interaction with perturbations using local probes — ●PAOLO SESSI — Universität Würzburg

Topological insulators (TIs) are a new class of materials insulating in the bulk but conductive on their surface where they host linearly dispersing gapless Dirac states. The strong spin-orbit coupling perpendicularly locks the spin to the momentum, leads to a chiral spin texture that restricts scattering channels, and results in spin currents intrinsically tied to charge currents. Since all these properties manifest at surfaces, scanning probe techniques are ideal tools to visualize them with both high spatial and energy resolution. In my talk, I will present a series of experiments that allow not only to visualize the presence of Dirac boundary modes, but also to directly prove some of their most remarkable properties. In particular, I will discuss recent efforts focused onto the controlled manipulation of topological states, which is achieved by coupling TIs to well-defined perturbations. First, I will demonstrate that surface magnetic doped TIs can establish magnetic order at very dilute concentrations. Then, I will report on the realization of spin networks of different symmetries conveniently created at TI surfaces by self-assembly processes. Finally, I will illustrate how the introduction of strain can be successfully used to engineer TI transport properties.

Invited Talk

O 77.5 Thu 12:30 S051

Surface Chemistry of Oxygen and Water on Anatase TiO₂ (101) — ●MARTIN SETVIN¹, ULRICH ASCHAUER², JAN HULVA¹, MICHAEL SCHMID¹, ANNABELLA SELLONI³, and ULRIKE DIEBOLD¹ — ¹TU Wien — ²ETH Zurich — ³Princeton University

TiO₂ is a prototypical material used in photocatalysis, e.g. in water remediation or photocatalytic water splitting. Two polymorphs of TiO₂, rutile and anatase, are used industrially with anatase typically preferred in applications. The surface chemistry of water and oxygen is the basis for majority of (photo)catalytic processes on TiO₂; most prominently in the photocatalytic water splitting and the oxygen reduction reaction. We report adsorption of water and oxygen studied by a combination of experimental and theoretical techniques (STM, nc-AFM, TPD, XPS, DFT). Special attention is paid to the activation of adsorbed O₂ molecules, i.e. electron transfer from the reduced anatase sample to the adsorbate. We show that this can occur in regions with a surplus of excess electrons, e.g., in the vicinity of subsurface donors and at step edges. In other regions the adsorbed O₂ molecules remain neutral. With nc-AFM we show they can be charged by an electron injected from the tip. We find a small energy barrier of 0.3 eV for this process. Interaction between co-adsorbed H₂O and O₂ is used to illustrate the reactivity of thus activated O₂. When the two species react they both dissociate, with terminal (OH)⁻ groups as the final product of the reaction, stable at room temperature. This species as well as the reaction intermediates, OOH and HOOH, are identified with atomically-resolved SPM measurements.