O 92: Gerhard Ertl Young Investigator Award

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

O 92.1   Thu 10:30   TRE Ma

Controlling the magnetic state of individual single atom magnets — •Fabian D. Natterer[1,2], Kai Yang[1,3], William Paul[1], Philip Wilke[1,4], Taeyoung Choi[1], Thomas Greber[1,5], Andreas J. Heinrich[1,6], and Christopher P. Lutz[1] — [1]IBM Almaden Research Center, San Jose, USA — [2]EPFL, Lausanne, Switzerland — [3]University of Chinese Academy of Sciences, Beijing, China — [4]University of Göttingen, Germany — [5]University of Zürich, Switzerland — [6]Ewha Womans University, Seoul, Republic of Korea

The possibility of data storage in single atom magnets represents the natural limits of a thought experiment for miniaturization in magnetic storage media. Up to now, the magnetic bit size was reduced to clusters containing few atoms, but a recent investigation showing magnetic remanence in ensembles of single holmium atoms on magnesium oxide (MgO) presented the prospect of data storage at the atomic limit. However, it was unclear how the magnetic state of a selected rare earth magnet could be controlled. We demonstrate here the reading and writing of individual Ho atoms on MgO. The Ho atoms independently retain their magnetic state over several hours. A selected Ho bit is read by tunnel magnetoresistance and written by current pulses using a scanning tunneling microscope. Using STM enabled electron spin resonance, we unambiguously prove the magnetic origin of the Ho states and reveal a large Ho magnetic moment of $(10.1 \pm 0.1)\,\mu_\mathrm{B}$. The long lifetime of the magnetic state, combined with electrical reading and writing shows that the programming of single atom magnets is possible.

O 92.2   Thu 11:00   TRE Ma

Fascinating two-dimensional oxide quasicrystals — •Stefan Förster[1], Sebastian Schenk[1], Klaus Meinel[1], Eva Maria Zollner[1], Rene Hammer[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

When approaching the two-dimensional limit, oxides are known to exhibit strong variations in their structures and properties as compared to the respective bulk materials[1]. One of the best examples are the two-dimensional oxide quasicrystals (OQCs), which have been discovered for reduced $BaTiO_3$ on Pt(111) [2]. We report here on a second OQC derived from $SrTiO_3$ on Pt(111) as well as on approximant structures for both OQC systems, in which selected motifs of the OQC are periodically repeated. Those approximants differ drastically in their complexity. For $BaTiO_3$ a simple approximant structure is observed, which contains six of the building blocks (tiles) of the OQC in the unit cell and which has been structurally fully resolved recently [3]. For $SrTiO_3$ the more complex approximant contains a patch of 36 tiles in the unit cell. This approximant very closely resembles the ideal OQC. Our studies unravel OQCs as best-controlled QC model systems for addressing the fundamental questions related to the driving forces for aperiodic structure formation.

[1] F. Netzer, S. Fortunelli (Eds.), Oxide Materials at the two-dimensional limit, Springer (2016) [2] S. Förster K. Meinel, R. Hammer, M. Trautmann, W. Widdra, Nature 502, 215 (2013) [3] S. Förster et al., Phys. Rev. Lett. 117, 095501 (2016)

O 92.3   Thu 11:30   TRE Ma

Tuning the electrocatalytically active site: atomic ensemble effects and surface strain — •Maria Escudero-Escribano — Technical University of Denmark, Department of Physics, Fysikvej, 2800 Kgs. Lyngby (Denmark)

In order to improve the kinetics of the oxygen reduction reaction (ORR), we can modify the geometric structure (1) and/or alter the electronic properties of the surface atoms (2,3) of the catalyst.

We used a self-ordered molecular pattern, cyanide-modified Pt(111), to study the ORR (1) and to decorate surfaces at the atomic scale (4,5). My electrochemical scanning tunneling microscopy images provided an atomically resolved visualization of the honeycomb structure in the presence of cations (4). Interestingly, CN groups block the adsorption of spectator anions in the electrolyte, while allowing the adsorption of oxygen. As a consequence, CN-Pt(111) presents a 25-fold enhancement over Pt(111) (1).

In addition, we have studied novel Pt-lanthanide alloys for ORR. A Pt overlayer is formed onto the bulk alloys by acid leaching. Our surface-sensitive X-ray diffraction measurements on Gd/Pt(111) show the formation of a crystalline Pt overlayer under compressive strain (6). The ORR activity versus the lattice parameter follows a volcano relation (2). We use the lanthanide contraction to control surface strain effects and tailor the activity, stability and reactivity of Pt.

(1) Nature Chem. 2010, 2, 880; (2) Science 2016, 352, 73; (3) J. Am. Chem. Soc. 2012, 130, 16476; (4) ChemPhysChem 2011, 12, 2230; (5) J. Phys. Chem. C 2009, 113, 12340; (6) Nano Energy 2016.

O 92.4   Thu 12:00   TRE Ma

Towards Accurate Electronic Structure Predictions for Hybrid Interfaces — •David A. Egger — Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

A highly relevant physical quantity for nanostructured molecule-metal interfaces is the energy level alignment of the molecular electronic states with respect to the Fermi level of the metal. Typical density functional theory (DFT) calculations, especially those using local and semi-local functionals, often underestimate level alignment and lead to inaccurate descriptions of electronic structure and charge transport properties of interfaces. Here, we introduce an efficient theoretical method that is based on DFT, but in contrast to common approximations fulfills physically motivated criteria for exchange-correlation interactions relevant for surfaces and interfaces. To this end, we combine the optimally-tuned range-separated hybrid (OT-RSH) functional with a DFT-derived image-charge model to accurately determine level alignment at molecule-metal interfaces in a non-empirical but system-dependent manner.[1,2] We apply our fully self-consistent approach to several physisorbed and chemisorbed molecule-metal interface systems. For both the level alignment and work-function changes, we find that our calculated results are in very good agreement with reference data from photoemission spectroscopy. Our findings indicate new ways of accurate and efficient electronic structure predictions for hybrid interfaces. [1] Egger, D. A.; Liu, Z.-F.; Neaton, J. B.; Kronik, L.: Nano. Lett. 15, 2448 (2015). [2] Liu, Z.-F.; Egger, D. A.; Refaely-Abramson, S.; Kronik, L.; Neaton, J. B.: under review.

O 92.5   Thu 12:30   TRE Ma

Structural Lubricity under Ambient Conditions — •Mehmet Z. Baykara — Department of Mechanical Engineering, Bilkent University, Ankara, Turkey — UNAM - Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey

Despite its fundamental importance, physical mechanisms that govern friction are poorly understood. While a state of ultra-low friction, termed structural lubricity, is expected for any clean, atomically flat interface consisting of two different materials with incommensurate structures, associated predictions could only be quantitatively confirmed under ultra-high vacuum (UHV) conditions so far. In this contribution, we report structurally lubric sliding under ambient conditions at mesoscopic (4,000-130,000 nm^2) interfaces formed by gold islands on graphite, in excellent agreement with theory [1]. Ab initio calculations reveal that the gold-graphite interface is expected to remain largely free from contaminant molecules, leading to structurally lubric sliding. The experiments reported here demonstrate the potential for practical lubrication schemes for micro- and nano-electromechanical systems that would mainly rely on an atomic-scale structural mismatch between the slider and substrate components.

[1]: E. Cihan, S. Ipek, E. Durgun, M.Z. Baykara, Nature Communications 7, 12055 (2016).