

## O 64: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: S051

O 64.1 Thu 10:30 S051

**Gold-colored metallic water solution** — ●TILLMANN BUTTERSACK<sup>1</sup>, PHILIP MASON<sup>2</sup>, CHRISTIAN SCHEWE<sup>2</sup>, RYAN McMULLEN<sup>3</sup>, FLORIAN TRINTER<sup>1,4</sup>, DANIEL NEUMARK<sup>5</sup>, STEPHAN THÜRMER<sup>6</sup>, ROBERT SEIDEL<sup>7</sup>, BERND WINTER<sup>1</sup>, STEPHEN BRADFORTH<sup>3</sup>, and PAVEL JUNGWIRTH<sup>2</sup> — <sup>1</sup>Fritz-Haber-Institute, Berlin, GER — <sup>2</sup>Czech Academy of Sciences, Prague, CZ — <sup>3</sup>US Southern California, Los Angeles, USA — <sup>4</sup>DESY, Hamburg, GER — <sup>5</sup>UC Berkeley, USA — <sup>6</sup>Kyoto U, JP — <sup>7</sup>BESSY, Berlin, GER

Whereas tap water and common aqueous solutions conduct some electricity, pure water is an almost perfect insulator. The required pressures to transform water into a metallic state will not be achievable on Earth. Liquid Ammonia undergoes a gradual phase transition from a blue electrolyte solution to a bronze-colored metallic solution if the concentration of solvated alkali metal is enhanced. Water and alkali metals react vigorously, as the valence electrons of the alkali metal are transferred to the aqueous solution almost instantly, leading to a Coulomb explosion. Here, we demonstrate, that water from the gas phase adsorbs onto the surface of sodium-potassium alloy droplet leading to the formation of a thin shiny and golden layer. Characterization of the liquid with photoelectron and UV/Vis spectroscopy revealed a plasmon energy of 2.7 eV and signatures of liquid water. These observations are spectroscopic evidence for an aqueous solution with metallic properties. Its plasmon frequency is in the visible region of the spectrum and thus is the reason for the fascinating golden color.

O 64.2 Thu 11:00 S051

**Standing molecules for quantum sensing** — ●TANER ESAT — Peter Grünberg Institute (PGI 3), Forschungszentrum Jülich, 52425 Jülich, Germany — Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany

Artificial nanostructures, fabricated by placing building blocks like atoms and molecules in well-defined positions, are an almost universal playground where quantum effects can be studied and exploited on the atomic scale. In my talk, I will show that the manipulation capabilities of a scanning tunneling microscope (STM) allow the fabrication of metastable structures which do not form spontaneously in nature and that these structures offer attractive functionalities for quantum information and sensing. Specifically, I will demonstrate that a large planar aromatic molecule can be lifted into an upright standing geometry on a pedestal of two metal adatoms using the STM tip. This atypical and surprisingly stable upright orientation of the single molecule enables the system to function as a quantum dot and a coherent single-electron field emitter. Utilizing a novel homebuilt STM that uses adiabatic demagnetization refrigeration (ADR) to reach millikelvin temperatures, I will show that the standing molecule is weakly coupled to the surface and that it exhibits spin-flip excitations corresponding to a spin-1/2 system. If the standing molecule is fabricated on the tip, it can be used for the measurement of surface potentials and magnetic fields on the atomic scale at the same time - possibly even as an electron spin resonance sensor on the tip.

O 64.3 Thu 11:30 S051

**On-surface synthesis and characterization of cyclo[18]carbon** — ●KATHARINA KAISER<sup>1</sup>, LOREL SCRIVEN<sup>2</sup>, FABIAN SCHULZ<sup>1</sup>, PRZEMYSŁAW GAWEL<sup>2</sup>, LEO GROSS<sup>1</sup>, and HARRY ANDERSON<sup>2</sup> — <sup>1</sup>IBM Research - Zurich, Säumerstrasse 4, 8803 Rüschlikon, CH — <sup>2</sup>Department of Chemistry, Oxford University, Chemistry Research Laboratory, Oxford, OX13TA, UK

Cyclo[*n*]carbons, purely *sp*-hybridized carbon allotropes with unique structural and electronic properties, have been predicted for decades to exist. Although a synthetic route was already elaborated in the 1980's, and glimpses of cyclocarbons were detected in gas phase, they could never be stabilized long enough for characterization. A distinctive feature of cyclo[*n*]carbons is their two conjugated  $\pi$ -systems that can

lead to the formation of two orthogonal ring currents and so-called double-aromatic stabilization. However, distortions in the geometry can lead to a lowering in ground state energy, and theoretically predicted ground state structures were found to depend on the level of theory. Consequently, cyclo[*n*]carbon's structures remained unknown.

AFM and STM at low temperatures allow triggering certain on-surface chemical reactions by atom manipulation and can thus facilitate the controlled formation of highly reactive molecules on inert surfaces from more stable precursors. Using this approach, we formed cyclo[18]carbon on a thin layer of NaCl. By comparing high-resolution AFM images with a functionalized tip and AFM simulations of different predicted resonance structures, we identified two possible ground state structures of cyclo[18]carbon adsorbed on bilayer NaCl.

O 64.4 Thu 12:00 S051

**Correlative in situ microscopy of hydrogen oxidation on rhodium: from the meso- to the nanoscale** — ●JOHANNES ZEININGER — Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria

Catalytic surface reactions, such as CO oxidation, may produce a variety of spatio-temporal effects on the catalyst surface. To reveal the mechanisms behind such spatio-temporal effects, it is advantageous to apply multiple techniques to the same samples, particularly at different length scales. In other research areas than catalysis this idea has led to the correlative microscopy approach. In catalysis, this approach is, if at all, used for sample characterization, often in two separate setups. In the present contribution, the correlative microscopy approach has been applied in situ to the catalytic hydrogen oxidation on rhodium to reveal the mechanism of multifrequential kinetic oscillations, a novel effect recently detected in this reaction. Such oscillations were first observed on a polycrystalline Rh foil, where the reaction oscillated in a self-sustained way between the states of high and low activity (a known behavior), but with different frequencies on adjacent domains (a new and unexpected behavior). Later on, such an effect was also observed on the nanofacets of a Rh tip modeling a single catalytic particle. Such behavior contradicts previous observations and expectations based on the known spatial coupling mechanisms and was never observed before, for any surface reaction.

O 64.5 Thu 12:30 S051

**Efficient electronic passivation schemes for surface calculations of semiconductors exhibiting spontaneous polarization: Thermodynamic and electronic properties of GaN surfaces** — ●SU-HYUN YOO<sup>1</sup>, MIRA TODOROVA<sup>1</sup>, LIVERIOS LYMPERAKIS<sup>1</sup>, CHRIS VAN DE WALLE<sup>2</sup>, and JÖRG NEUGEBAUER<sup>1</sup> — <sup>1</sup>Department of Computational Materials Design, MPI für Eisenforschung, Germany — <sup>2</sup>Computational Materials Group, Materials Department, UCSB, USA

Semiconductor surfaces play a central role in modern technology related to catalysis, electronics, and energy applications. The most widespread approach to study surfaces with density-functional theory calculations is to use slab geometries with periodic boundary conditions. A common strategy employed to avoid artificial charge transfer from one side of the slab to another, is to passivate the dangling bonds at its backside. Using the examples of wurtzite polar and semipolar surfaces, we demonstrate that the conventional passivation scheme using pseudo-H atoms fails to describe the electronic structure of low-symmetry semiconductors. We therefore developed an improved passivation method [npj Comp. Mater. 7, 58, 2021/PR Mater. 5, 044605, 2021] that takes the polarization effect and the concept of surface reconstructions into account. It accurately describes surface electronic properties and enables computationally efficient surface energy calculations. Using this novel approach we have studied the orientation-dependent thermodynamic stability and electronic properties of GaN surfaces. The resulting Wulff shape provides insight of how to avoid facet-related defects such as V-pits hampering GaN-based electronics.