

## O 81: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: MA 042

O 81.1 Thu 10:30 MA 042

**Caught in the act! Live observations of catalysts using high-pressure scanning probe microscopy** — ●IRENE M.N. GROOT<sup>1</sup> and JOOST W.M. FRENKEN<sup>2</sup> — <sup>1</sup>Huygens-Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9502, 2300 RA Leiden, the Netherlands — <sup>2</sup>Advanced Research Center for Nanolithography, P.O. Box 41883, 1009 DB Amsterdam, the Netherlands

Recently it has become clear that essential differences can exist between the behavior of catalysts under industrial conditions (high pressure and temperature) and the (ultra) high vacuum (UHV) conditions of traditional laboratory experiments. These observations made it clear that meaningful results can only be obtained at high pressures and temperatures. However, most of the techniques traditionally used to study catalysts were designed to operate under UHV conditions.

This talk focuses on the development of scanning probe microscopy for operando observations of active model catalysts. We have developed set-ups that combine a UHV environment with a high-pressure flow reactor cell, integrated with scanning probe microscopy and mass spectrometry. In this way, we can correlate structural changes of the catalyst with its catalytic performance.

This talk highlights a short overview of the instruments we developed. Some results for CO oxidation will be shown. But additionally, results for a more complex reaction, production of chlorine, will be discussed.

O 81.2 Thu 11:00 MA 042

**High Spatial Resolution Operando IR and X-ray Microspectroscopy Measurements of Multistep Catalytic Reactions in Flow Reactor** — ●ELAD GROSS — Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Molecular-level analysis of catalytic reactions in flow reactors and detection of short lived intermediates are essential for optimization of complex reactions. In this study, multistep catalytic reaction in flow reactor was analyzed by spectral mapping of the catalyst and the organic phase with a spatial resolution of 15  $\mu\text{m}$ , employing micrometer-sized synchrotron-sourced IR and X-ray beams. The catalyst in this reaction was two nanometer sized Au nanoclusters that were encapsulated within a dendrimer matrix and loaded on mesoporous SiO<sub>2</sub> support. The catalyst was packed within a flow microreactor and its reactivity was tested toward the cascade reaction of dihydropyran formation. In-situ synchrotron-sourced IR microspectroscopy detected the reactant-into-product transformation along the flow reactor. By tuning the residence time of the reactants, full kinetic analysis of the catalytic reaction was achieved. X-ray absorption microspectroscopy scan along the flow reactor correlated locally-enhanced catalytic conversion, as detected by IR microspectroscopy, to areas with high concentration of Au(III), the catalytically active species. This study demonstrates the fundamental understanding of mechanism of catalytic reactions that can be gained by detailed in-situ mapping of multistep reactions in flow reactors.

O 81.3 Thu 11:30 MA 042

**Atto-to-Nanosecond Electron Dynamics at Surfaces probed by Time-Resolved Core-Level Photoelectron Spectroscopy** — ●STEFAN NEPPL — Lawrence Berkeley National Laboratory, Berkeley, CA, USA

In the first part of my talk, I will discuss recent experiments that address the ultrafast dynamics inherent to all photoemission processes in condensed phase matter. In these measurements, an XUV attosecond light pulse launches photoelectron wave packets inside a solid. The emission dynamics of the photoelectrons are probed with a few-cycle VIS/NIR laser pulse [1,2]. We demonstrate that this streaking approach is capable of resolving subtle emission delays between electron wave packets that are released from different energy levels of the solid with a precision of only a few attoseconds (1 as = 10<sup>-18</sup> s). For

the simple metal magnesium we show that these time shifts can be interpreted as the real-time observation of photoelectrons propagating through the crystal lattice prior to their escape into vacuum [3]. In the second part, I will describe the implementation of femto- and picosecond time-resolved photoelectron spectroscopy at the Linac Coherent Light Source and at the Advanced Light Source with the goal to follow light-driven electron dynamics at dye-semiconductor interfaces on femto- to nanosecond timescales [4,5].

[1] Cavaliere et al. *Nature* 449, 1029 (2007); [2] Neppel et al. *Phys. Rev. Lett.* 109, 087401 (2012); [3] Neppel et al. *Nature* (2014) accepted; [4] Siefermann et al. *J. Phys. Chem. Lett.* 5, 2753 (2014); [5] Neppel et al. *Faraday Discuss.* 171, 219 (2014).

O 81.4 Thu 12:00 MA 042

**A surface science route towards fully controlled single molecule manipulation** — ●CHRISTIAN WAGNER — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — JARA-Fundamentals of Future Information Technology

Exploring the potential of molecular nanotechnology requires accurate manipulation of large functional molecules. For this purpose, the surface science approach of using a low-temperature scanning probe microscope is currently without alternatives. Still, reliable control requires knowledge of the potential energy surface (PES) experienced by the molecule. In my talk I will outline how the controlled manipulation of organic molecules, in combination with sensitive force-detection, yields new insights into the energetics of adsorption. The freedom to position the tip-attached molecule in any feasible geometry, even far above the surface, allows to reconstruct the entire adsorption potential, from equilibrium height [1] to the asymptotic regime of weak van der Waals interaction [2]. The controlled extraction of a molecule from a monolayer yields complementary information about the intermolecular potential. By comparing differently sized molecules we study the transferability and scalability of experimentally determined molecule-surface potentials. Iteratively improving our knowledge of the PES through more and more precise manipulation, atomic level control over complex molecules might soon become reality.

[1] Wagner, Fournier, Tautz, Temirov, *PRL* 109, 076102 (2012).  
[2] Wagner, Fournier, Ruiz, Li, Müllen, Rohlfing, Tkatchenko, Temirov, Tautz, *Nat. Commun.* 5, 5568 (2014).

O 81.5 Thu 12:30 MA 042

**A phantom force and lateral force microscopy** — ●ALFRED J. WEYMOUTH and FRANZ J. GIESSIBL — University of Regensburg, 93040 Regensburg, Germany

Atomic force microscopy (AFM) allows us to investigate mechanical properties of surfaces and adsorbates at the atomic scale. With a conducting tip, scanning tunnelling microscopy (STM) can be simultaneously performed.

When we measured simultaneous STM and AFM on Si, the unsaturated Si atoms surprisingly appeared repulsive. Our theory is that this is due to a decrease of the electrostatic force [1]. The attractive chemical interaction is still present, but the electrostatic force can be detected at further tip-sample distances. We called this the phantom force, and explained it by an additional resistance within the sample [2]. This resistance can also affect STM measurements, and this effect has recently been observed on Cu surfaces with sub-monolayer oxide layers [3].

Although most AFM measurements are sensitive to vertical forces, we can rotate the AFM sensor and measure lateral forces, a technique we call Lateral Force Microscopy (LFM). We applied LFM to quantify the bending of a CO molecule at the apex of an AFM tip [4]. In this talk, I will compare these findings to new data with a bare metal tip.

- [1] Weymouth et al. *Phys. Rev. Lett.* 106, 226801  
[2] Weymouth and Giessibl, *Appl. Phys. Lett.* 101, 213105  
[3] Matencio et al, submitted  
[4] Weymouth, Hofmann and Giessibl, *Science*, 343, 1120