

## O 81: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: H24

**Invited Talk**

O 81.1 Thu 10:30 H24

**Zooming in on the electronic properties of van der Waals Heterostructures** — ●SØREN ULSTRUP<sup>1</sup>, JYOTI KATOCH<sup>2</sup>, ROLAND J. KOCH<sup>3</sup>, SIMON MOSER<sup>3</sup>, KATHLEEN M. MCCREARY<sup>4</sup>, SIMRANJEET SINGH<sup>2</sup>, JINSONG XU<sup>2</sup>, BEREND T. JONKER<sup>3</sup>, ROLAND K. KAWAKAMI<sup>2</sup>, AARON BOSTWICK<sup>3</sup>, ELI ROTENBERG<sup>3</sup>, and CHRIS JOZWIAK<sup>3</sup> — <sup>1</sup>Department of Physics and Astronomy, Aarhus University, DK — <sup>2</sup>Department of Physics, Ohio State University, USA — <sup>3</sup>Advanced Light Source, Berkeley Lab, USA — <sup>4</sup>Navel Research Lab, USA

Two-dimensional (2D) semiconducting transition metal dichalcogenides (TMDs) exhibit a diverse collection of intriguing electronic phenomena. These include single-particle effects related to new spin and valley physics, as well as exotic many-body interactions. The latter are exemplified by the presence of tunable band gaps and tightly bound excitons and trions. Here, I will show how the electronic properties of complex heterostructures composed of tungsten disulfide and boron nitride (WS<sub>2</sub>/hBN) can be accessed using angle-resolved photoemission spectroscopy with nano-scale spatial resolution (nanoARPES). I will present three major discoveries in such stacks: (i) The direct observation of the energy- and momentum-dependent electronic structure of one-dimensional TMD nanoscrolls, (ii) a substrate-induced lateral band bending, demonstrating ultimate control of band offsets at the nanoscale, and (iii) a doping dependent three-particle excitation in the measured spectral function which is consistent with the formation of a trion.

**Invited Talk**

O 81.2 Thu 11:00 H24

**Directly measuring the anisotropic magnetic exchange force field of a spin spiral** — ●NADINE HAUPTMANN<sup>1</sup>, TZU-CHAO HUNG<sup>1</sup>, WOUTER JOLIE<sup>1</sup>, SOUMYAJYOTI HALDAR<sup>2</sup>, DANIEL WEGNER<sup>1</sup>, STEFAN HEINZE<sup>2</sup>, and ALEXANDER A. KHAJETOORIANS<sup>1</sup> — <sup>1</sup>Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, Netherlands — <sup>2</sup>Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Chiral magnets, e.g. magnetic skyrmions and spin spirals, are hot candidates for nano-scale magnetic storage. These magnetic structures are stabilized by an interplay between competing exchange interactions at the atomic-scale. Spin-polarized scanning tunneling microscopy (SP-STM) has achieved great success in investigating the magnetization of such structures, but faces a number of limitations in being able to directly detect the underlying exchange forces, as well delineate between structural and electronic contributions to the spin-polarized density of states. To go beyond these limitations, we have developed a new method, which combines SP-STM and magnetic exchange force microscopy (SPEX) based on nc-AFM utilizing a tuning fork design. The method has been successfully applied to independently determine the structural corrugation from the electronic and magnetic contributions for single and bi-layers of Fe/Ir(111). Here, we investigate a new regime for SPEX, namely characterizing the distance-dependent spectroscopy of the noncollinear magnetic exchange force derived from the antiferromagnetic spin spiral in a monolayer Mn/W(110).

**Invited Talk**

O 81.3 Thu 11:30 H24

**Scanning Probe Microscopy at Ambient Pressures** — ●BARAN EREN — Department of Chemical and Biological Physics, Weizmann Institute of Science, 234 Herzl Street, Rehovot, Israel

We perform surface science studies in the presence of gases, while avoiding significant sacrifices in terms of measurement resolution and accuracy. This involves microscopy and spectroscopy techniques that have been specially adapted to be performed at ambient pressures. Atomic structure and chemical properties of low Miller-index Cu surfaces exposed to CO, CH<sub>3</sub>OH, and CO<sub>2</sub> will be presented. Cu surfaces break up into nanoclusters at RT in the presence of CO in the Torr pressure range. This finding has implications in heterogeneous cataly-

sis as it shows how the surface evolves, affecting its electronic structure and chemical properties. The reason behind clustering is the high difference in adsorption energy of CO on low-coordinated Cu atoms as compared to high-coordinated Cu atoms. In addition, adsorbed CO weakens the binding of the Cu atom to its neighbors, which facilitates the detachment of the edge Cu atoms and their diffusion. Unlike CO, CH<sub>3</sub>OH does not cause the break-up of Cu into clusters because methoxy adsorbs strongly both on step and terrace atoms.

STM is limited to electrically conducting surfaces but many real catalysts are supported on insulating oxides. We built an AFM system to operate under reactant gases, and we are developing a new methodology to use Hamaker constants to obtain chemical fingerprints at the lower nanometer scale.

**Invited Talk**

O 81.4 Thu 12:00 H24

**High energy surface x-ray diffraction from surfaces and particles in operando catalysis** — ●UTA HEJRAL<sup>1</sup>, STEFANO ALBERTIN<sup>1</sup>, MIKHAIL SHIPILIN<sup>2,3</sup>, JIANFENG ZHOU<sup>1</sup>, SEBASTIAN PEAFF<sup>1</sup>, SARA BLOMBERG<sup>1</sup>, JOHAN ZETTERBERG<sup>1</sup>, JOHAN GUSTAFSON<sup>1</sup>, ANDREAS STIERLE<sup>2</sup>, and EDVIN LUNDGREN<sup>1</sup> — <sup>1</sup>Lund University, Lund, Sweden — <sup>2</sup>DESY, Hamburg, Germany — <sup>3</sup>Stockholm University, Stockholm, Sweden

Catalysts are widely employed in chemical industry, in fuel cells and car exhaust control systems, where they accelerate desired chemical reactions. To improve catalyst performance, a time-resolved atomic-scale understanding of the interplay between the catalyst surface structures, the catalytic activity/selectivity, and the gas phase surrounding the catalyst surface is inevitable.

High energy surface x-ray diffraction (HESXRD) provides a fast data acquisition for the structural characterization of model catalyst samples under operando conditions. We demonstrate how we used HESXRD to study the shape-dependent sintering of supported Pt-Rh alloy nanoparticles during CO oxidation. Flat-shaped Pt-rich particles underwent strong vertical sintering, while Rh-rich compact-shaped particles proved to be sinter-resistant. In another experiment we combined HESXRD with gas phase diagnostics to investigate the structure-gas phase correlation during self-sustained reaction oscillations over Pd(100) during CO oxidation. We found that the surface features epitaxial PdO(101) bulk oxide decorated by metallic Pd islands on top, which play a crucial role for the self-sustained oscillations.

**Invited Talk**

O 81.5 Thu 12:30 H24

**Batteries at Work: Towards Operando Photoelectron Spectroscopy on Lithium Ion Batteries** — ●JULIA MAIBACH<sup>1,2</sup>, IDA KÄLLQUIST<sup>3</sup>, KRISTINA EDSTRÖM<sup>2</sup>, HÅKAN RENSMO<sup>3</sup>, HANS SIEGBAHN<sup>3</sup>, and MARIA HAHLIN<sup>3</sup> — <sup>1</sup>Karlsruhe Institute of Technology, Institute for Applied Materials, Germany — <sup>2</sup>Uppsala University, Department of Chemistry - Ångström Laboratory, Sweden — <sup>3</sup>Uppsala University, Department of Physics and Astronomy, Sweden

Almost 40 years after the first commercially available lithium ion battery, the solid electrolyte interphase (SEI) is still considered one of the least understood parts in a lithium ion battery. While it is known that the SEI forms from decomposition products of the liquid battery electrolyte on the negative electrode, the exact formation mechanism and this results in the functionality of an electrode protection layer with Li ion conductivity are not yet fully understood. In this presentation, we will first discuss the challenges of SEI characterization and then present our approach to operando ambient pressure x-ray photoelectron spectroscopy (AP-XPS) on lithium ion battery systems. This technique can provide the key tool that has been missing so far to probe the functionality of the electrode/electrolyte interface in more realistic battery environments. We will show our results of AP-XPS characterizations of liquid carbonate-based battery electrolytes, battery electrodes with the liquid electrolyte present, and how the electrochemical reactions of a battery can be driven and followed under the measurement conditions pertaining to photoelectron spectroscopy.