

## O 99: Gerhard Ertl Young Investigator Award: Finalists session

Time: Thursday 13:30–15:30

Location: R1

O 99.1 Thu 13:30 R1

**Magnetic resonance imaging in a scanning tunneling microscope** — ●PHILIP WILLKE<sup>1,2,3,4</sup>, APARAJITA SINGHA<sup>2,3</sup>, XUE ZHANG<sup>2,3</sup>, KAI YANG<sup>4</sup>, YUJEONG BAE<sup>2,3,4</sup>, TANER ESAT<sup>2,3</sup>, CHRISTOPHER LUTZ<sup>4</sup>, ANDREAS HEINRICH<sup>2,3</sup>, and TAEYOUNG CHOI<sup>2,3</sup> — <sup>1</sup>Karlsruhe Institute of Technology, Physikalisches Institute, Karlsruhe, Germany — <sup>2</sup>IBS Center for Quantum Nanoscience, Seoul, Republic of Korea — <sup>3</sup>Ewha Womans University, Seoul, Republic of Korea — <sup>4</sup>IBM Almaden Research Center, San Jose, USA

Combining electron spin resonance (ESR) with scanning tunneling microscopy (STM) allowed for spin resonance experiments on individual atoms on surfaces[1], for remote sensing of atomic spins[2] and for accessing the nuclear spin of single atoms in an STM[3]. In this talk, we focus on the interaction of the atomic spin system on the surface with the magnetic STM tip. We show that the tip field allows to tune the system into resonance similar to the external magnetic field, and can even fully replace the latter[4]. By utilizing this tip magnetic field, we establish magnetic resonance imaging of single atoms[5], exceeding the spatial resolution of other scanning field-gradient techniques by one to two orders of magnitude. We find that MRI scans of different atomic species and with different probe tips lead to unique resonance images revealing the magnetic interaction between tip and atom. [1] Baumann et al., *Science*, 350, 417-420 (2015). [2] Choi et al., *Nat. Nano* 12, 420-424(2017). [3] Willke et al., *Science* 362, 336-339 (2018) [4] Willke, Singha, Zhang et al., *Nano Lett.* 19, 8201-8206 (2019) [5] Willke et al. *Nat. Phys.* 15, 1005-1010 (2019).

O 99.2 Thu 14:00 R1

**Ab-initio studies of exciton  $g$  factors: Monolayer transition metal dichalcogenides in magnetic fields** — ●THORSTEN DEILMANN, PETER KRÜGER, and MICHAEL ROHLFING — Institute of Solid State Theory, University of Münster, Germany

The effect of a magnetic field on the optical absorption in semiconductors has been measured experimentally and modeled theoretically for various systems in previous decades. We present a new first-principles approach [1] to systematically determine the response of excitons to magnetic fields, i.e. exciton  $g$  factors. By utilizing the *GW*-Bethe-Salpeter equation methodology we show that  $g$  factors extracted from the Zeeman shift of electronic bands are strongly renormalized by many-body effects which we trace back to the extent of the excitons in reciprocal space. We apply our approach to monolayers of transition metal dichalcogenides (MoS<sub>2</sub>, MoSe<sub>2</sub>, MoTe<sub>2</sub>, WS<sub>2</sub>, and WSe<sub>2</sub>) with strongly bound excitons for which  $g$  factors are weakened by about 30%.

[1] *Phys. Rev. Lett.* 124, 226402 (2020)

O 99.3 Thu 14:30 R1

**Manipulating charge states of individual molecules on insulators** — ●SHADI FATAYER, FLORIAN ALBRECHT, NIKOLAJ MOLL, and LEO GROSS — IBM Research - Zurich

The physicochemical properties of molecules adsorbed on surfaces are charge-state dependent. Insulating films serve as an ideal platform to study the physics and chemistry of charged molecules, because these films avoid charge leakage. However, investigating individual charged molecules on insulators is experimentally challenging. The atomic force microscope (AFM), operable on insulating substrates and capable of single-electron sensitivity and atomic resolution, is suitable to be used with insulators. Here, I will present how different aspects of charged molecules can be accessed with the AFM: (i) How using the AFM as a single-electron current meter allows for tunneling spectroscopy to be performed on insulators and electron-transfer properties probed, (ii) how molecules in excited states can be prepared, (iii) how reversible chemical reactions can be performed via charging molecules and (iv) the insights gained via resolving the atomic structure of individual molecules in different charge states.

O 99.4 Thu 15:00 R1

**Probing surface electronic structure and reaction intermediates in situ** — ●KELSEY STOERZINGER — Oregon State University, Corvallis, Oregon USA — Pacific Northwest National Laboratory, Richland, Washington USA

Catalysts are important constituents in numerous energy conversion and storage processes. Rational design of catalysts with greater activity for higher efficiency devices requires an understanding of the material surface's electronic structure in situ, as well as the reaction intermediates involved.

Many surface science techniques, such as X-ray photoelectron spectroscopy (XPS), collect information from inherently surface-sensitive low-energy processes, requiring operation in ultrahigh vacuum. This constraint is lifted for ambient pressure XPS, which can probe the surface in equilibrium with the gas phase at pressures up to ~a few Torr, or with thin liquid layers using a higher incident photon energy. I will discuss the insights obtained with this technique regarding the electronic structure of well-defined epitaxial oxides in equilibrium with a gaseous atmosphere of small molecules (e.g. O<sub>2</sub>, H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>3</sub>OH, NO), the adsorption of such species, and their subsequent transformation upon driving a desired reaction by heat, voltage, or additional reactant. Adsorption and reactivity can be manipulated by the oxide composition and electronic structure, crystallographic orientation, strain, and local environment in amorphous materials. This molecular-level understanding of interfacial interactions can guide the rational design of high-surface-area oxide catalysts for technical applications.