

O 67: Competition for the Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00

Location: H45

O 67.1 Thu 10:30 H45

Magnon Rashba effect at ferromagnetic surfaces — ●KHALIL ZAKERI LORI — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Rashba effect refers to as a spin–splitting phenomenon of the electronic band structure in the absence of any external magnetic field. It originates from a fundamental effect known as spin–orbit coupling. Basically, the relativistic motion of electrons produces a magnetic field, which couples to their spins and causes a splitting in the energy levels of electrons with different spins. It offers a way to control and manipulate the electrons spin and thus lies in the central idea of spintronics. We report a similar effect on the spin integer quasi-particles i.e. magnons at a ferromagnetic surface. We provide the first direct experimental evidence, which demonstrates that the dispersion relation of surface magnons in the presence of spin–orbit coupling and in the absence of time-reversal symmetry shows a splitting for different magnetization directions, similar to the electron dispersion relation at metal surfaces [1]. Moreover, we will show that the lifetime, amplitude, group and phase velocity of surface magnons propagating along two opposite (but equivalent) directions perpendicular to the magnetization are different [2]. Our findings can inspire ideas for designing new spintronic devices based on this new effect. [1] Zakeri *et al.*, Phys. Rev. Lett. **104**, 137203 (2010). [2] Zakeri *et al.*, Phys. Rev. Lett. **108**, 197205 (2012).

O 67.2 Thu 11:00 H45

Emergent quantum size effects at surfaces of correlated and topological solids — ●PHIL KING — Kavli Institute for Nanoscale Science, Cornell University, USA

We use angle-resolved photoemission (ARPES) to probe quantum-confined electron systems created, at the surfaces of correlated oxides and topological insulators, by control of surface charge. In transition-metal oxides, we write this directly by forming surface oxygen vacancies through UV light irradiation. We use ARPES to image the *d*-electron subband ladder of the resulting oxide two-dimensional electron liquids, revealing a delicate interplay between quantum-confinement, orbital ordering, spin-orbit interactions and electronic correlations.^{1,2} In topological insulators, we show that creation of similar surface quantum wells leads to a hierarchy of electronic states with simultaneous confinement of electron- and hole-like subbands,^{3–5} the former showing giant tuneable Rashba spin splittings.^{4,5} We uncover a complex band and binding energy dependence of the coupled spin-orbital texture of this surface electronic system through circular dichroism in ARPES. We show how this results from a novel connectivity between quantum well and topological surface states, enforced by the topologically non-trivial nature of the host system.⁵ Together, these studies reveal the drastic reconstruction of electronic structure that occurs from electric field-induced confinement across a variety of emerging quantum materials. ¹ Nature Mat. **10** (2011) 114; ² Phys. Rev. Lett. **108** (2012) 117602; ³ Nature Commun. **1** (2010) 128; ⁴ Phys. Rev. Lett. **107** (2011) 096802; ⁵ Nature Commun. **3** (2012) 1159.

O 67.3 Thu 11:30 H45

Comparative Density Functional Theory Study of Acetaldehyde Hydrodeoxygenation Mechanisms on Ru and RuO₂ Catalysts — ●LARS GRABOW — Chemical and Biomolecular Engineering, University of Houston, 4800 Calhoun Rd., S222, Houston, TX 77204-4004

The hydrodeoxygenation (HDO) mechanism of acetaldehyde, a surrogate molecule for the over 400 different oxygenated species in biomass-derived pyrolysis oil, is presented for the Ru(0001) and RuO₂(110) surfaces based on Density Functional Theory results. Under typical HDO reaction conditions, the thermodynamic phase diagram indicates that the RuO₂(110) surface is partially reduced and terminated by OH-groups on the bridging O-sites. Further reduction and creation of a surface O-vacancy site are necessary to create an active site for ac-

etaldehyde adsorption through its terminal O-atom and selective conversion to ethylene. In contrast, acetaldehyde is more easily activated on Ru(0001), but metallic Ru favors C-C bond over C-O bond scission which leads to the unwanted formation of CO and CH₄. Given the higher C-O bond scission selectivity on the metal-oxide, a rapid prediction method for surface phase diagrams and equilibrium O-vacancy concentrations of other rutile(110) surfaces is developed. In combination with a more detailed understanding of the HDO mechanism on metal and metal-oxide catalysts this model can be used for the development of new and efficient catalysts that can lead to an increased utilization of biofuels.

O 67.4 Thu 12:00 H45

Controlling the Conformation of Peptides and Proteins on Solid Surfaces in Ultrahigh Vacuum — ●STEPHAN RAUSCHENBACH — Max-Planck-Institute for Solid State Reseach, Stuttgart

The hierarchical self-assembly of functional proteins through folding is a versatile and robust approach to generate functional nanoscale structures. It can, however, not be mimicked outside of biological systems.

We developed an electrospray ion beam deposition (ES-IBD) system capable of depositing nonvolatile molecules including proteins and polypeptides on surfaces in ultrahigh vacuum (UHV). In this environment we study their structure and electronic properties with resolution at the atomic level using scanning tunneling microscopy (STM).

We show that the structure of polypeptides adsorbed on a surface can be controlled on several length scales, using features unique to ES-IBD. Bradykinin, a short peptide of 9 amino acids (AA) folds into an equilibrium structure, influenced by the molecule-substrate interaction. Long polypeptide chains (unfolded cytochrome-c, 104 AA) do not reach an thermal equilibrium, but instated fold randomly, perfectly following polymer statistics in two dimensions (2d). In this case, ES-IBD allows us to select the mechanical properties of the gas phase ion before deposition and steer the structure on the surface between extended chains for high charge states and refolded 2d-random coils for low charge states.

This result shows that ES-IBD combined with high resolution UHV STM, opens the door to conformational control of 2d polypeptides and its application to rationally fold functional nanostructures at surfaces.

O 67.5 Thu 12:30 H45

Surface-aligned femtochemistry: Uni- and bimolecular reaction dynamics on oxide surfaces — ●MIHAI E. VAIDA¹, THORSTEN M. BERNHARDT², and STEPHEN R. LEONE¹ — ¹Departments of Chemistry and Physics, University of California and Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States — ²Institute of Surface Chemistry and Catalysis, University of Ulm, 89069 Ulm, Germany

The breaking and making of chemical bonds in molecules attached to a substrate constitute the elementary steps of surface chemical reactions and occur on the ultrafast time scale of nuclear motion. Their understanding is fundamental to the molecular level conception of chemical reaction mechanisms on surfaces, especially, for example, in catalytic materials. In this contribution a combination of an optical pump-probe configuration with time-of-flight mass spectrometry is employed to monitor in real time the mass and the relative velocity of intermediates and products of photoinduced surface reactions. Results are presented for the application of this technique to the photodissociation dynamics of methyl iodide and methyl bromide as well as to the formation dynamics of iodine, bromine and iodine monobromide molecules on magnesia ultrathin films on a Mo(100) single crystal surface. A new perspective and a further improvement of the experimental procedure will also be presented regarding the study of surface chemical reactions with femtosecond high order harmonic vacuum ultraviolet and extreme ultraviolet laser pulses by core level photoemission spectroscopy and mass spectrometry.