

O 57: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Wednesday 10:30–12:45

Location: MA 042

Invited Talk

O 57.1 Wed 10:30 MA 042

Hydrogen Atom Adsorption on Surfaces Studied in Inelastic Scattering Experiments — •OLIVER BUENERMANN — Georg-August Universität Göttingen, Germany

The first step in most reactions at surfaces is the adsorption of the reactants. For this to happen their translational and binding energy have to be dissipated to the solid. In inelastic scattering experiments, adsorption can be studied on model systems in great detail. Based on such experiments new theoretical models can be developed that accurately describe the delicate interplay between electronic and nuclear motion in prototypical chemical reactions. Hydrogen adsorption is of special interest, as the small mass of the atoms leads to an inefficient phonon coupling, but sticking probabilities on surfaces can still be high.

Recently, we could show that in case of H-atom scattering from Au(111) a large amount of the translational energy can be transferred to electronic excitation of the metal [1]. We expanded our studies to various surfaces including a set of metals, insulators, and graphene. Furthermore, the influence of the projectile mass was investigated by replacing hydrogen by its heavier isotope deuterium. The experimentally observed dependencies are presented and their implication for the underlying energy transfer processes are discussed.

[1] Bünermann, O. et al., *Science* 350, 1346-1349 (2015).

O 57.2 Wed 11:00 MA 042

Work function measurements on heterogeneous surfaces: The role of electrostatic potentials for ultraviolet photoelectron spectroscopy (UPS) — •THORSTEN SCHULTZ¹, THOMAS LENZ², NARESH KOTADIYA², GEORG HEIMEL¹, GUNNAR GLASSER², RÜDIGER BERGER², PAUL W. M. BLOM², PATRICK AMSALEM¹, DAGO M. DE LEEUW², and NORBERT KOCH¹ — ¹Humboldt Universität zu Berlin, 12489 Berlin — ²Max Planck Institute for Polymer Research, 55128 Mainz

UPS is a primary technique to determine the work function of surfaces. According to literature, heterogeneous surfaces are expected to exhibit one secondary electron cut-off (SECO) representing an area-averaged work function. However, several reports show that more than one cut-off can be observed for heterogeneous surfaces. To clarify this discrepancy, heterogeneous model surfaces consisting of bilinear arrays, providing a work function contrast of more than 1 eV, were investigated. With UPS we measure two SECOS, one reflecting the high work function surface fraction and the other an averaged work function. The electrostatic potential away from the surface was measured by Kelvin-probe force microscopy and compared to electrostatic modeling. With this we can quantitatively explain that the high work function areas lead to an additional energy barrier for electrons emitted from the low work function areas.[1] We detail the role of experimental parameters on the appearance of SECOS and how this influences the determination of ionization energy of molecules deposited on heterogeneous surfaces.

[1] T. Schultz et. al, *Adv. Mat. Interf.* 4, 1700324 (2017)

O 57.3 Wed 11:15 MA 042

1,3-Di(methoxy)imidazolium ionic liquid mixtures investigated by angle-resolved X-ray photoelectron spectroscopy — •BETTINA HELLER¹, CLAUDIA KOLBECK¹, INGA NIEDERMAIER¹, SABINE DOMMER², JÜRGEN SCHATZ², HANS-PETER STEINRÜCK², and FLORIAN MAIER² — ¹Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — ²Lehrstuhl für Organische Chemie I, FAU Erlangen-Nürnberg, Germany

Ionic liquids (ILs) - salts with melting points typically well below 100 °C and an extremely low vapour pressure - allow for applying surface science methods under UHV condition such as X-ray photoelectron spectroscopy (XPS). In this work, the functionalised IL 1,3-di(methoxy)imidazolium hexafluorophosphate ([([MeO]2Im)[PF₆]])[1] and its mixtures with two non-functionalised 1,3-dialkylimidazolium ILs, namely 1-methyl-3-octylimidazolium bis[(trifluoromethyl)sulfonyl]imide ([C₈C₁Im][Tf₂N]) and 1,3-diethylimidazolium hexafluorophosphate ([C₂C₂Im][PF₆]), were investigated. We were using our Dual Analyser System for Surface Analysis (DASSA)[2] for simultaneous measurements in 0° (bulk sensitive) and 80° (surface sensitive) emission relative to the surface normal of the sample. Changes in the angle-resolved XP spectra directly reveal differences in surface and

bulk composition of the mixtures, whereas pronounced differences in the electronic structure due to functionalisation are reflected in large chemical shifts.

[1] G. Laus et al., *Z. Naturforschung* 2007, 62b, 295-308.

[2] I. Niedermaier et al., *Rev. Sci. Instrum.* 2016, 87, 045105.

O 57.4 Wed 11:30 MA 042

A three electrodes electrochemical setup for XPS studies in ionic liquids — •FRANCESCO GRECO, RADHA GOBINDA BHUIN, HANS-PETER STEINRÜCK, and FLORIAN MAIER — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) are widely used in electrochemical studies due to their large electrochemical window, good ionic conductivity and thermal stability. These properties together with their extremely low vapor pressure make them unique candidates to perform electrochemistry in liquid media in combination with ultra-high-vacuum-based surface science techniques. In this work, a three electrodes electrochemical cell for X-ray-Photoelectron-Spectroscopy (XPS) studies has been developed, which allows in-situ cyclic voltammetry and chronoamperometry using the molybdenum sample holder as counter electrode, a platinum wire as quasi-reference electrode and a wire of chosen material as working electrode. The experiments are performed in a "Dual Analyzer System for Surface Analysis (DASSA)"[1] which enables angle-resolved X-ray Photoelectron Spectroscopy (ARXPS) using two electron analyzers mounted for simultaneous measurements in 0° (bulk-sensitive) and 80° (surface-sensitive) emission relative to the surface normal.

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[1] I. Niedermaier, C. Kolbeck, H.-P. Steinrück, F. Maier, *Rev. Sci. Instrum.* 87 (2016) 045105

O 57.5 Wed 11:45 MA 042

Correction and Suppression of the Space-Charge Effect in Cathode-Lens Microscopes — •BENEDIKT SCHÖNHENSE¹, KATERINA MEDJANIK², DMITRY VASILYEV², SERGEY BABENKOV², MARTIN ELLGUTH², HANS-JOACHIM ELMERS², and GERD SCHÖNHENSE² — ¹Imperial College London, UK — ²56

Previous pump-and-probe photoemission experiments have revealed that the Coulomb interaction in the pulsed beam (commonly referred to as "space-charge problem") is a serious obstacle, in particular due to background electrons released by the pump pulse [1]. Theoretical work [2] has uncovered the reason for the dramatic deterioration of the imaging performance in conventional cathode lenses (PEEMs, k-microscopes): All slow electrons are efficiently focused into the lens column where they travel along the optical axis and exert strong forces on the primary photoelectrons. Shifts up to 10 eV have been measured at the conditions of beamline P04 of PETRA III. We present strategies of an a-posteriori correction of the Lorentzian deformation of the momentum distributions [2] and of an a-priori suppression of the deterministic part of Coulomb interaction by "extraction-field tailoring".

[1] L.-P. Oloff et al., *J. of Appl. Phys.* 119, 225106 (2016)

[2] B. Schönhense et al., *New J. Phys.*, under review

O 57.6 Wed 12:00 MA 042

On multi-electron emission from surfaces — IURI S. BRANDT, ZHENG WEI, JÜRGEN KIRSCHNER, and •FRANK O. SCHUMANN — Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

We have studied the electron pair emission process from surfaces due to the impact of a primary positron. The existence of this process implies a two-step scattering event. In the first step the primary positron scatters with a valence band electron. Each particle of the positron-electron pair can collide with another valence electron. We find that the electron pair intensity is on the same scale as the positron-electron pair intensity. This suggests that a significant contribution of the pair intensity is actually due to the emission of three particles. Our instrument is only able to detect two particles in coincidence. We also observe a strong material dependence of the coincidence intensity. In previous studies with primary electron excitation or photon absorption we observed that NiO displays the highest coincidence rate.[1,2] The same observation we have made in this work. We find that NiO has a factor of 3 higher coincidence intensity compared to the Ag(100)

substrate. We also note that the pair intensity scales with the single electron rate. The higher the singles rate the higher the coincidence rate. We discuss the fact that very different excitation processes leading to pair emission give similar results.

[1] I.S. Brandt et al., Phys. Rev. B 92, 155106 (2015).

[2] F.O. Schumann et al., Phys. Rev. B 93, 235128 (2016).

O 57.7 Wed 12:15 MA 042

Spin-resolved ARPES measurements on Sn/Si(111) —
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In systems with spin-orbit coupling (SOC) and electronic correlations of comparable strength, like Pb/Si(557), a Spin-Orbit-Density-Wave is formed at low temperatures resulting in an insulating state below 78K [1]. It is characterized by Rashba-type spin-split bands with nesting between opposite helical states at the Fermi surface.

For Si(111) covered by 0.3 ML Sn, a $\sqrt{3} \times \sqrt{3}$ reconstruction is formed which shows a Mott-type Metal-insulator transition upon cooling below 70 K [2]. Recently, this system was investigated by ARPES and DFT suggesting a collinear antiferromagnetic order with a $2\sqrt{3} \times \sqrt{3}$ spin cell at low temperatures [3].

Spin-resolved ARPES measurements reveal the existence of a spin-ordered surface unit cell larger than $\sqrt{3} \times \sqrt{3}$. However, the SOC induced effects are small, thus the insulating state is mainly governed by electronic correlation effects.

[1] C. Brand et al., Nat. Comm. **6**, 8118 (2015).

[2] S. Modesti et al., PRL **98**, 126401 (2007).

[3] G. Li et al., Nat. Comm. **4**, 1620 (2013).

O 57.8 Wed 12:30 MA 042

Fermi Surface, Fermi-Velocity and Circular Dichroism of Rhenium Measured with Soft X-Rays — •KATERINA MEDJANIK¹, DMITRY VASILYEV¹, SERGEY BABENKOV¹, MARTIN ELLGUTH¹, BENEDIKT SCHÖNHENSE², JENS VIEFHAUS³, HANS-JOACHIM ELMERS¹, and GERD SCHÖNHENSE¹ — ¹JGU, Inst. für Physik, Mainz — ²Imperial College London, UK — ³DESY Photon Science, Hamburg

Parallel-imaging k -space microscopy with time-of-flight energy recording has substantially advanced photoemission data recording. In combination with the circularly-polarized high-brilliance soft X-rays at beamline P04 at PETRA III (Hamburg), we acquired 4D photoemission data arrays $I(E_B, k_x, k_y, k_z)$ for both photon helicities in the full bulk Brillouin zone and energy range of the d-band complex. Here, we present the experimental Fermi surface map for rhenium (hcp), revealing unprecedented detail quality. The full data set, including Fermi-velocity distribution $v_F(\mathbf{k})$ and circular dichroism texture have been obtained in a few hours of acquisition time. Maximum k_z -resolution has been achieved by variation of the photon energy in small steps. Data are compared with our previous results for tungsten (bcc) [1] and iridium (fcc) [2].

[1] K. Medjanik et al., *Nat. Materials* **16**, 615 (2017); [2] G. Schönhense et al., *Ultramicrosc.* **183**, 19 (2017).