O 45: Poster: Solid-Liquid Interfaces - Structure, Spectroscopy, Reactions and Electrochemistry

Time: Tuesday 18:15–20:30 Location: Poster A

O 45.1 Tue 18:15 Poster A

Observation of material movement on KBr surfaces depending on the relative humidity — •Dominik Kirpal, Korbinan Pürckhauer, Alfred J. Waymouth, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

Surfaces exposed to air can change their structure due to external influences like chemical reactions or material exchange and movement. The condensed water layer, present in ambient conditions plays an important role especially on surfaces that dissolve easily in water [1]. Surface atoms can easily diffuse into the thin water layer and, when surface conditions are favourable, they can re-attach to the surface. We collected FM-AFM images of the KBr surface in a climate-controlled glove box at various values of relative humidity. By scratching the surface with the AFM tip, we construct energetically unfavourable hills and scratch sites. We observe the time evolution of these sites. We propose that there is a critical value around 25% relative humidity, under which dissolution and reattachment occurs relatively slowly, in contrast to our observations at 28% relative humidity where these processes occur quickly.

[1] M. Luna, et al., Journal of Physical Chemistry A, 102.34 (1998) 6793-6800.

O 45.2 Tue 18:15 Poster A

Characterization and Chemical Imaging of Aerosols from remote Antarctica — •Johannes Weis[1,2,6], Ricardo H. M. Godoi[1,3], Ana F. L. Godoi[1,3], Simon Mueller[1,2], Sérgio J. Gonçalves Jr.[3], Heitor Evangelista[4], Swarup China[5], Bingbing Wang[5], Alexander Laskin[5], Tristan H. Harder[6], and Mary K. Gilles[1] — [1]Chemical Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [2]Department of Chemistry, University of California, Berkeley, CA 94720, USA — [3]Department of Environmental Engineering, Federal University of Paran UFPR, Curitiba, PR, Brazil — [4]LARAMG, State University of Rio de Janeiro Uerj, Rio de Janeiro, RJ, Brazil — [5]William R. Wiley Environmental and Molecular Science Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99352, USA — [6]Department of Physics, University of Würzburg, Germany

Changes in Antarctica's ice sheets and shelves are of primary concern to the regional and global climate. We hypothesize that the West Antarctic warming can be related to the aerosols transported and formed in this region. Internal composition and characteristics of single aerosol particles were investigated by means of chemical mapping via synchrotron-based scanning transmission X-ray microscopy with near edge X-ray absorption fine structure spectroscopy (STXM/NEXAFS), followed by a rule-based cluster classification. Complementary data obtained from computer-controlled scanning electron microscopy (CC-SEM/EDX) allows us to go a step forward in the understanding of aerosol particles formed in Antarctica's pristine environment.

O 45.3 Tue 18:15 Poster A

A compact and calibratable von Hamos X-Ray Spectrometer based on two full-cylinder HAPG mosaic crystals for high-resolution XES — •Ina Holfelder, Rolf Fliegauf, Yves Kayser, Matthias Müller, Malte Wansleben, Jan Weser, and Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

For high-resolution X-ray Emission Spectroscopy (XES), crystal-based Wavelength-Dispersive Spectrometers (WDS) can be applied for effective speciation characterization of nano- and microscaled materials. A von Hamos geometry provides the highest detection efficiencies combined with high resolving power. This geometry uses a cylindrically bent crystal as dispersive and as a sagittal focusing optic. Highly Annealed Pyrolytic Graphite (HAPG) can be deposited reliably on cylindrical glass substrates and shows highly integrated reflectivity while offering low mosaicity, ensuring high resolving power. A novel calibratable von Hamos X-ray spectrometer based on two full-cylinder optics is being put into operation at the PTB. The spectrometer enables chemical speciation of elements in an energy range from above 10 keV down to 2.3 keV. The first results using synchrotron radiation as the excitation source will be presented. The spectrometer combines high efficiency with high spectral resolution in a compact arrangement also suitable for laboratory arrangements.

O 45.4 Tue 18:15 Poster A

charge accumulation on copper electrode surfaces were studied by means of electrochemical and optical techniques — •Saúl Vázquez-Miranda[1,2], Reza Sharif[1], Kurt Hingerl[1], and Christoph Cobet[1] — [1]Johannes Kepler Universität, Zentrum für Oberflächen und Nanoanalytik, Altenberger Str. 69, 4040 Linz, Austria — [2]Universidad Autónoma de San Luis Potosí ,(IICO) Av, Karakorum 1470, 78216 San Luis Potosí, México

The surface chemistry occurring during electrocatalysis is the key to understand the reaction mechanism.Electrochemical and optical methods were used to investigate the charge accumulation at amorphous and single crystals of Cu surfaces interacting with a supra pure HCl solution.

The investigation of the adsorption/desorption of Cl- ions was carried out using cyclic voltammetry, in which the integrated charge and ion - exchange is measured in a potential window where we prevent damage of the copper surface.

Electrochemical impedance spectroscopy (EIS) measurement on the (111) and (110) faces of copper was used to extract capacitance and resistance parameters. Equivalent circuit modeling was used to suggest the potential of zero charges (PZC).

Spectroscopy Ellipsometry for in operando characterization allows to probe the solid/liquid interface directly while applying an external potential and during chronoamperometry. The correlation of these two techniques allows to shed light on the charge accumulation on the copper surface electrodes.

O 45.5 Tue 18:15 Poster A

The Influence of Li-Imide Salt Additives in Li-Ion Battery Electrolytes on the Solid Electrolyte Interphase Formation on Graphite Electrodes — •Thomas Diemant[1], Varvara Sharova[2,3], Arianna Moretti[2,3], Alberto Varzi[2,3], R. Jürgen Behm[1,2], and Stefano Passerini[2,3] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm — [2]Helmholtz Institute Ulm (HIU) Electrochemic Energy Storage, Helmholtzstr. 11, D-89077 Ulm — [3]Karlsruhe Institute of Technology (KIT), P.O. Box 3640, D-76021 Karlsruhe

The solid electrolyte interphase (SEI), a passivating layer which is formed by electrolyte decomposition during the first electrochemical cycles on the electrodes of Li-ion batteries (LIBs), is one of the main factors influencing the battery performance. In order to ensure the formation of a SEI with well-balanced physico-chemical characteristics, additives are often included into the electrolyte formulation. These additives either decompose prior to the electrolyte main components during the first charge or incorporate into the passive layer, leading to the formation of a more compact, stable and ion conducting SEI.

Herein, we report results of a detailed study on the effect of various Li imide salts (LiTFSI, LiFTFSI, and LiFSI) as electrolyte additives in LIBs, in which the chemical composition and thickness of the SEI layer on graphite anodes is characterized by ex-situ XPS. This is complemented by characterization of the SEI resistance via electrochemical impedance spectroscopy (EIS). Finally, the implications for the cycling performance in half and full cells are discussed.

O 45.6 Tue 18:15 Poster A

Dissolution of noble metals (Au, Ag, Cu) in a trihalide ionic liquid in oxidation state $+1$ as shown by XPS — •Benjamin May[1], Matthias Lexow[1], Hans-Peter Steinrück[1], Florian Maier[1], Nicola Taccardi[2], Juergen Schatz[3], and Harald Maid[4] — [1]Physikalische Chemie II, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Chemische Reaktionstechnik, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]Organische Chemie I, FAU Erlangen-Nürnberg, Erlangen, Germany — [4]Organische Chemie II, FAU Erlangen-Nürnberg, Erlangen, Germany

The corrosion of metals, particularly those generally considered inert, is important to many of the applications of trihalides. In this poster we present the results of X-ray photoelectron spectroscopy analysis of a trihalide ionic liquid, $[C_6C_1Im][Br_2I]$, and its reactions with the group 11 metals copper, silver, and gold. We find that all three of

the metals are susceptible to corrosion by the IL. In addition, we find evidence that all three metals are dissolved in the +1 oxidation state. We propose a reaction of the general form:
$M + [Br_2I]^- \longrightarrow M^+ + 2Br^- + I^\bullet$,

with two iodine radicals recombining to form molecular iodine. Additional testing shows that this reaction occurs in both the presence and absence of water, and that the imidazolium C2 proton is not involved in the corrosion reaction.

O 45.7 Tue 18:15 Poster A

Chemical analysis of solid-liquid interfaces by in-situ Rutherford Backscattering Spectrometry

— •Nasrin B. khojasteh and René Heller — HZDR, Dresden, Germany

Solid-liquid interfaces are important locations for various reactions to occur in biological, chemical and physical processes [1-3]. Recently, an experimental setup for in-situ Rutherford Backscattering Spectrometry (RBS) technique has been installed at the 2 MV Van-de-Graaff accelerator at Ion Beam Center (IBC) of the Helmholtz-Zentrum Dresden-Rossendorf to analyze solid-liquid interfaces as well as to conduct electro-chemistry experiments. The focus of the project is to perform experiments in different fields utilizing this quantitative, non-destructive and standard free ion beam analysis technique for solid-liquid interfaces. A Si3N4 window separates the liquid in the cell from vacuum in the beam line. He+ beam with E = 1.7 MeV is employed to bombard the samples. For feasibility tests, the cell was filled with air, Ne, He, Xe and DIH2O respectively and RBS and Particle Induced X-Ray Emission Spectroscopy (PIXE) spectra were recorded. To examine the efficiency of the technique, ion backscattering studies of the solid-liquid using 0.1M solutions of Cu(NO3) and AgNO3 have been performed and are compared to the literature [4].

[1] Kötz et al., Electrochimica acta. 31 (1986) 169. [2] Morita et al., Radiation Physics and Chemistry. 49 (1997) 603. [3] Hodnik et al., Accounts of chemical research. 49 (2016) 2015. [4] Forster et al., Nuclear Instruments and Methods in Physics Research Section B. 28 (1987) 385.

O 45.8 Tue 18:15 Poster A

Morphology and electronic structure of MnO_2 nanoparticles from first-principles

— •Yonghyuk Lee, Jakob Timmermann, Daniel Opalka, and Karsten Reuter — Technische Universität München, Germany

Manganese oxides are characterized by an outstanding variety of stoichiometries and morphologies. Many structures show high catalytic activity in photo- and electrochemical applications. With Mn as one of the most abundant elements this offers great potential for energy related applications. In the present work we consider MnO_2 which has been identified as an efficient anode material in the electrolysis of water. For a first characterization of polycrystalline MnO_2 we employ ab initio thermodynamics to determine the relative stabilities of hydrated and pristine surfaces as a function of the applied potential. Stable MnO_2 nanoparticle structures are predicted on the basis of the Gibbs-Wulff theorem and the electronic band structure of the particles is analyzed as a function of their size and shape dependence.

O 45.9 Tue 18:15 Poster A

Electrolysis of CO_2 at Platinum/Ionic Liquid Interfaces

— •Andre Kemna and Björn Braunschweig — Institute of Physical Chemistry, WWU Münster, 48149 Münster, Germany

Electrochemical CO_2 reduction reactions (CO2RR) at Pt(poly) and Pt(111)/electrolyte interfaces were studied with cyclic voltammetry (CV). Using different room temperature ionic liquids (RTIL) as electrolytes such as $[BMIM][BF_4]$ and $[EMIM][BF_4]$, we have investigated the influence of both water and the chemical identity of the RTIL as a co-catalyst on the activity for CO2RR. H_2O concentrations between 0.1 and 2 M lead to a substantial rise in activity. In addition, also the surface structure has a significant impact: Compared to polycrystalline Pt, well-ordered Pt(111) electrodes have a substantially lower activity for CO2RR. In order to study the molecular structure of $Pt(poly)/[EMIM][BF_4]$ interfaces in situ and in more detail, we have applied vibrational sum-frequency generation (SFG)[1]. Potentiodynamic SFG spectra reveal a vibrational mode centered at 2355 cm^{-1} which we attribute to a $[CO_2\text{-}EMIM]$ complex at the interface that lifts the inversion symmetry of CO_2 molecules and makes them SFG active. We propose that these interfacial complexes can function as a stable precursor for CO_2 reduction reactions and lead to small overpotentials for CO2RR. Another vibrational band at 2080 cm^{-1} is due to atop CO as the main reduction product of CO_2 electrolysis on Pt surfaces. Strongly adsorbed CO molecules cause a poisoning of the Pt catalyst and lead to a deactivation over many cycles.

[1] B. Braunschweig et. al. J. Electroanal. Chem., 2017, 800, 144-150

O 45.10 Tue 18:15 Poster A

Towards understanding the mechanism of water splitting on TiO2

— Saman Hosseinpour, Simon J. Schlegel, Mischa Bonn, and •Ellen H.G. Backus — Max Planck Institute for Polymer Research, Mainz, Germany

Finding a clean and renewable energy source to replace fossil fuels has attracted much attention, the past few decades, as a requirement for the sustainable development of societies. Direct hydrogen generation on TiO2 by photocatalytic dissociation of water using sunlight was already proposed more than 40 years ago. However, despite extensive work in this area, the fundamentals of the process remain ill-understood, mainly due to the lack of a proper tool to specifically explore the interface between water and TiO2. Sum frequency generation spectroscopy (SFG), is an inherently surface sensitive tool, allowing the study of the water-TiO2 interface. As a first step in understanding the water-splitting reaction, we studied the binding of water to the substrate. From the intensity and frequency of the SFG signal we extract information about the binding of water to the TiO2. Moreover, we show time-resolved SFG data after excitation of the TiO2 with a femtosecond UV pump pulse which mimics the sun light. Preliminary data show that both the surface and the interfacial water molecules undergo changes on ultrafast timescales upon excitation. These UV-pump SFG-probe data illustrate the first steps towards following the photo-induced dissociation of water at the TiO2 interface in real-time.

O 45.11 Tue 18:15 Poster A

DFT study of halogen adsorbate structures on the (100) surfaces of Ag and Au in an electrochemical environment

— •Alexandra Dávila, Lukas Deuchler, Svenja Hövelmann, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

The electrochemical interface between halide containing electrolytes and coinage metal electrodes constitutes an important model system. The chemical potential of the halogen as a function of sample potential, which is crucial for the theoretical description of various processes at the electrode, is in general derived from thermodynamics. Analogously to previous work for halogens/Cu [1] we present a systematic density functional study [2,3] for Cl, Br, and I adsorption on Ag and Au(100). Our DFT calculations include incommensurate adsorbate reconstructions via large unit cells. Differences between the range of stability of equilibrium reconstruction as a function of sample potential as derived from the calculations and the conditions under which the respective structures have been observed experimentally [4] are identified. Furthermore, the atomic structure of the boundary between c(2×2)-Cl adsorption domains on the unreconstructed Au(100) surface have been calculated and are compared to STM images from [5].

[1] I. T. McCrum *et al.*, Electrochim. Acta **173** (2015).
[2] //www.vasp.at. G. Kresse *et al.*, Phys. Rev. B **49**, 14251 (1994).
[3] P. Giannozzi et al., J. Phys. Condens. Matter 21, 395502 (2009).
[4] X. Gao *et al.*, J. Phys. Chem. **98** (1994).
[5] Y.- C. Yang *et al.*, Electrochim. Acta **112** (2013).

O 45.12 Tue 18:15 Poster A

Deposition and reactivity of single Pd clusters at solid-liquid interfaces

— •Clara Rettenmaier, Nicolas Bock, Astrid De Clercq, Ueli Heiz, and Friedrich Esch — Chemistry Department & Catalysis Research Center, Technische Universität München, Garching, 85747, Germany

Electrochemical deposition of Pd monolayers on Au(111) have been studied extensively [1]. Palladium shows high catalytic activities for many chemical reactions and is capable to absorb hydrogen. In particular, submonolayer coverages show significant electrocatalytic enhancement for the hydrogen evolution reaction (HER) [2]. However, size-selected Pd clusters in the non-scalable size regime have barely been studied in aqueous environments, despite their potential for high catalytic activities.

We present the preparation of single size Pd clusters on Au(111) by decomposition of polyoxometalates [3] under controlled electrochemical potential and pH. The clusters are characterized by Electrochemical Scanning Tunneling Microscopy (ECSTM) and Rotating Disc Electrode (RDE) measurements, while the HER activity of single clusters is measured in situ using the STM tip as a microelectrode.

[1] Kibler, L. A., El-Aziz, A. M., Kolb, D. M., Journal of Molecular Catalysis A 2003, 199(1), 57-63.

[2] Pandelov, S., Stimming, U., Electrochimica Acta 2007, 52(18), 5548-5555.

[3] Yang, P., Kortz, U. et al., Angewandte Chemie International Edition 2014, 53, 11974-11978.

O 45.13 Tue 18:15 Poster A

In situ Video-STM Studies of Sulfide Adsorbate Dynamics on Ag(100) in Iodide Solution — •Reihaneh Amirbeigiarab, Bjoern Rahn, and Olaf M. Magnussen — Kiel University

Atomic scale dynamic processes at the interface between electrodes and electrolyte solutions play a pivotal role in electrochemical phase formation reactions. Accordingly, the evaluation of the atomic scale surface dynamic processes on metal electrodes, such as adsorbate diffusion and interaction, is of great importance to understand the reaction mechanisms at solid/liquid interfaces. In situ video-STM allows direct atomic-scale studies of these highly dynamic processes on electrode surfaces. [1-3] We here present results of in situ Video-STM studies on the dynamic behavior of low coverages of sulfide adsorbates on Ag(100) electrode surfaces in iodide-containing solution. We observe clear differences in the potential-dependend diffusion behavior on surfaces covered by a c(2×2)-I coadsorbate layer and by a disordered iodide adlayer, respectively. Futhermore, restructuring of the Ag substrate is found, leading to nanoscale grooves. The results are compared to previous data for sulfide on c(2×2)-Cl and c(2×2)-Br covered Ag(100). [1] T. Tansel, O. M. Magnussen, Phys. Rev. Lett., 96, 026101. (2006) [2] A.Taranovskyy, T. Tansel, O.M. Magnussen, Phys. Rev. Lett., 104, 106101.(2010) [3] Y. C. Yang, A. Taranovskyy, O. M. Magnussen, Angew. Chem. Int. Ed., 51, 1966. (2012)

O 45.14 Tue 18:15 Poster A

Electrochemical Roughening of Pt(111) : Surface Site Reactivity — •Leon Jacobse[1], Yi-Fan Huang[1], Marcel J. Rost[2], and Marc T.M. Koper[1] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Most devices that form the basis of an energy sustainable future, rely on platinum electrocatalysts. To optimize the use of this scarce and expensive metal, it is of the utmost importance to understand the catalyst's degradation on the atomic-scale.

We followed the roughening of Pt(111) upon repeated oxidation and reduction cycles (ORCs), by combining simultaneous cyclic voltammetry and in-situ EC-STM. This approach, together with the long timescale of our experiments, reveals new insights on the roughening process. Within the performed 170 ORCs we observe a continuous increase of the electrode roughness that can be separated into two different growth regimes, each of which exhibits their own correlation with the electrochemically measured number of hydrogen adsorption sites. Comparing the average atomic-scale island structure during the evolution with the disentangled voltammetric signals provides insight into the reactivity of the individual surface sites, like steps, kinks, and corner atoms.

[1] L. Jacobse, Y.-F. Huang, M.T.M. Koper, M.J. Rost, Nature Materials, accepted (2017)

O 45.15 Tue 18:15 Poster A

Chemical Functionalization of Oxide Surfaces: Insights into the Mechanism of Molecular Adsorption at the Solid/Liquid Interface — •Paul Schwarz and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Oxide surfaces are usually functionalized by attaching strongly interacting linker groups, like phosphonic acid or silanol units, employing wet-chemical processes. To obtain a fundamental understanding of the binding and reaction mechanisms at the solid/liquid interface we performed ab initio molecular dynamics (AIMD) simulations to study the anchoring of methylsilanetriol (MST) to aluminum oxide surfaces via condensation reactions in the presence of residual water and liquid isopropanol. Applying Thermodynamic Integration (TI) and Umbrella Sampling (US), we calculated the activation barrier for the surface binding of MST. Depending on whether residual water is present or not, the condensation reaction is found to be spontaneous or activated. Spontaneous condensation can proceed in two different ways, either by an initial protonation of an OH group of the surface or of the MST molecule. In the first case, an intermediate six-membered ring between MST and the desorbing water molecule is formed. In contrast, the protonation of an OH group of MST results in a pentacoordinated Si atom, where the surface OH group at the adsorption site is substituting the leaving OH group of MST.

O 45.16 Tue 18:15 Poster A

Electro-oxidation of CO on Au modified planar and nanostructured Pt(111) electrodes — •Evelyn Artmann, Julian Bösking, Jens Klein, Valeria Chesnyak, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm

The catalytic activity of Platinum (Pt) for the oxidation of CO was shown to increase with increasing amount of low coordinated Pt sites, like Pt step edges, on the surface which may be more active compared to terrace sites.[1] The exact role of step sites in the reaction mechanism is, however, still under debate. A strategy to identify the role of Pt steps in the CO oxidation is to block the steps by decorating them with a narrow Au film and then to compare the activity of the electrode with and without Au decoration. Prior to this it is, however, important to investigate the stability of such Au films on Pt as well as the influence of the Au film on Pt terrace sites for the CO oxidation activity. To this end, we first prepared and structurally characterized, by STM under UHV conditions, Pt(111) single crystals with varying Pt step densities. Subsequently, we decorated the Pt steps with monolayer high Au films and varied the Au coverage from sub-monolayer to full monolayer coverage. Investigating the structural characteristics of the surfaces before and after CO oxidation, as measured in an electrochemical flow cell, provided us information about the electrode stability under reaction conditions and about the influence of the Au film at Pt step and terrace sites on the activity of the electrodes for CO oxidation. [1] G. García et al., *ChemPhysChem.* **12** (2011) 2064.

O 45.17 Tue 18:15 Poster A

Deactivation of Hazardous Chemicals at Oxide Surfaces — •Tobias Klöffel[1], Mariana Kozlowska[2], Bernd Meyer[1], and Pawel Rodziewicz[2] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Institute of Chemistry, University of Bialystok, Poland

After World War II, large quantities of highly toxic chemical warfare agents were disposed in the Baltic Sea, where highly corroded containers, nowadays frequently found in fishing nets or at beaches, constitute a major environmental hazard. A very promising approach for the decomposition of the chemical warfare agents is via hydrolysis reactions using oxide catalysts, in particular, ZnO nanorods. Since it is close to impossible to perform standard surface science experiments for such highly toxic materials, *in silico* research is the only alternative for obtaining insights into the chemical processes at the solid/liquid interface leading to defunctionalization. Here, we will present first results on the adsorption and decomposition of sulfur mustard on ZnO surfaces based on Car-Parrinello Molecular Dynamics (CPMD) simulations. The different types of molecule–surface interactions have been analyzed and the mechanism of the first hydrolysis step has been studied using metadynamics for overcoming reaction barriers. All simulations were done for a full water/ZnO interface, which was created by embedding ZnO in several layers of water.

O 45.18 Tue 18:15 Poster A

Electrochemical Surface Science of Magnetite Fe_3O_4 under Oxygen Evolution Conditions — •Matthias Müllner, Michele Riva, Giada Franceschi, Gareth Parkinson, Ulrike Diebold, and Stijn F.L. Mertens — TU Wien, Institut für Angewandte Physik, Wiedner Hauptstrasse 8-10/134, 1040 Vienna

Earth-abundant oxides such as magnetite Fe_3O_4, with the addition of dopants, are promising candidates for an effective but low-cost catalyst for the oxygen evolution reaction (OER), which is one of the remaining bottlenecks in electrolysis and artificial photosynthesis.

We report electrochemical surface science studies on well-defined magnetite single-crystal surfaces, with the aim of linking reactivity to atomic-level structural information. Preparation and characterisation in UHV (STM, LEED, XPS) are followed by transfer to the electrochemical environment (open-circuit potential measurements, cyclic voltammetry, impedance), using a new sessile-drop cell design. Post-measurement characterisation of the surface in UHV and by ambient AFM indicates stability of $Fe_3O_4(001)$ towards electrolyte exposure (pH 7 up to 14) and during OER. Ongoing work aims to reveal the effects of surface orientation, whether transition-metal-doping of the surface is feasible and how this affects electrocatalytic activity.

O 45.19 Tue 18:15 Poster A

A Novel Electrochemistry Flow Cell for Operando Soft X-Ray Spectroscopy on Catalysts: Demonstrated on a MnOx Film for the Water Oxidation Half Reaction — •Marc F. Tesch[1], Shannon A. Bonke[1], Maryam N. Shaker[1], Travis E. Jones[2], Jie Xiao[1], Rosalie K. Hocking[3], and Alexandr N. Simonov[4] — [1]Helmholtz Zentrum Berlin, Berlin, Germany — [2]Fritz-Haber-Institut, Berlin, Germany — [3]Swinburne University of Technology, Victoria, Australia — [4]Monash University, Victoria, Australia

We present a novel flow cell design for soft X-ray spectroscopy on catalysts optimized for in situ electrodeposition and electrochemistry. Soft X-ray based photon-in - photon-out techniques can probe the electronic structure of a catalyst while it is in contact with an electrolyte and a potential is applied, i.e. operando. Soft X-ray absorption spectroscopy (XAS) allows probing the unoccupied valence states, thereby providing information such as the oxidation state of the catalyst. Resonant inelastic soft X-ray scattering (RIXS) can access valence electronic processes such as charge transfer and dd-transitions. The combination of XAS and RIXS provides a comprehensive picture of electronic changes occurring in a catalyst when tuning the external conditions towards its active state, e.g. by increasing an applied potential across the overpotential. The applicability of the aforementioned experimental techniques is demonstrated on a MnOx catalyst for the water oxidation half reaction measured at different applied potentials. The experimental results are discussed with focus on the potential induced changes in its electronic structure and are compared to theory.

O 45.20 Tue 18:15 Poster A

Wetting properties of CuFeO2 delafossite for photo-catalytic processes — Diego Diaz, Robert Wheatley, Martín Roble, Marcelo Cisternas, Donovan Diaz, •Ulrich G. Volkmann, Alejandro Cabrera, Birger Seifert, and Sascha Wallentowitz — Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile

Metal oxides and ceramics are used universally as catalytic and photocatalytic materials for a very wide range of chemical reaction processes. For water based reactions, hydroxylization, a process dependent upon the wettability of at the surface, can greatly influence catalytic activity of a metal oxide. In this work we present an investigation of the wetting properties CuFeO2 delafossite oxide synthesized using hydrothermal methods. We show how the "as grown" powder produces a strong hydrophobic effect which is described using the Cassie model for suspended droplets upon a rough surface comprised of two materials. Treatment of the powder via milling, pelletization and sintering reveals a hydrophobic surface which is then described by the Wenzel regime. However, in some cases we observe a rapid absorption of the water which we currently attribute to micro-capillaries present in the pellet sample. The material and its surface is characterized via XRD, AFM, FESEM and EDS methods. Acknowledgements: CONICYT Fellowships (MR, MC) and CONICYT-PIA ACT 1409.

O 45.21 Tue 18:15 Poster A

Assets and drawbacks of electrochemical/-catalytic characterization of electrodes prepared under UHV conditions — •Albert K. Engstfeld, Jens Klein, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Our current understanding of the electrochemical/-catalytic properties of complex three dimensional catalyst materials is strongly based on single crystal studies, supported by theoretical studies. In general, the electrochemical properties are characterized on single crystal electrodes prepared under laboratory conditions. These findings are supported by separate UHV studies, in which the electronic and chemical properties of the surfaces are explored by surface sensitive techniques. In order to bridge the gap between UHV and laboratory studies, numerous attempts are presented in the literature over the last decades, where electrochemical techniques are combined with a UHV set-up.[1] In this work, we will first discuss the relevance of the respective approach to prepare single crystals with distinct structural properties under UHV conditions, which can be elucidated with STM measurements and present examples where a clean environment, such as UHV, is indispensable to obtain the respective electrodes. Furthermore, we will present different types of bimetallic structures which can only be formed under laboratory conditions and other types which can only be obtained under UHV conditions. Finally, we will discuss situations where the combination UHV-electrochemistry approach is highly advantageous to in situ electrocatalytic studies. [1] PCCP, 19 (2017) 4141