

## O 64: New Methods

Time: Wednesday 18:15–21:00

Location: Poster A

O 64.1 Wed 18:15 Poster A

**Transfer chamber from electrochemical cell to UHV** — ●GEORGIJS BAKRADZE<sup>1</sup>, REINER KRAUSE<sup>1</sup>, DIRK VOGEL<sup>2</sup>, BEIBEI PANG<sup>2</sup>, ANDREAS ERBE<sup>2</sup>, MARTIN STRATMANN<sup>2</sup>, MICHAEL ROHWERDER<sup>2</sup>, and KARINA MORGENSTERN<sup>1</sup> — <sup>1</sup>Ruhr-University in Bochum, Faculty of Chemistry and Biochemistry, Bochum — <sup>2</sup>Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

We describe a custom-built transfer chamber dedicated to the transfer of electrodes from the liquid phase into the UHV. The transfer chamber allows to combine several surface analytical techniques, and, thus, to obtain valuable insights into structure and microscopic properties of the electrochemical double layer region on electrodes. The transfer chamber can be coupled to an experimental cluster having facilities for: (i) electrochemical preparation (allowing emersion from electrolyte solution under a constant potential into a controlled humid atmosphere), (ii) in situ electrochemical measurements (Kelvin probe), (iii) surface analysis (ambient-pressure XPS), and (iv) optical characterisation (FTIR spectroscopy). The transfer chamber allows the sample transfer without breaking the UHV conditions directly into a UHV chamber having facilities for microstructural characterisation (low-temperature STM). Efficiency and performance of the setup will be tested on the Au(111) surface, which will be prepared under controlled electrode potentials and relative humidity conditions, revealing the influence of ions on the structure of condensed water layers in realistic electrochemical environments.

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**Space Charge Corrected Electron Momentum Microscope for Time-Resolved Hard X-ray Photoemission at the European XFEL** — ●MARKUS SCHOLZ<sup>1</sup>, GERD SCHÖNHENSE<sup>2</sup>, YVES ACREMANN<sup>3</sup>, KATJA MEDJANIK<sup>2</sup>, NILS GERKEN<sup>1</sup>, and WILFRIED WURTH<sup>1,4</sup> — <sup>1</sup>Physics Department and Center for Free-Electron Laser Science, Universität Hamburg, D-22761 Hamburg, Germany — <sup>2</sup>Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz, Germany — <sup>3</sup>Department Physik, ETH Zürich, CH-8093 Zürich, Switzerland — <sup>4</sup>DESY Photon Science, D-22607 Hamburg, Germany

Photoelectron spectroscopy at synchrotron radiation sources is a well-established technique to study static electronic properties of materials. To overcome limitations in information depth recently hard x-ray photoemission (HAXPES) has been developed as a powerful tool to study electronic structure of the bulk or of buried interfaces. With the new hard x-ray free-electron lasers time-resolved HAXPES will enable dynamic studies of bulk and interface electronic structure down to the femtosecond regime. We will set up a HAXPES endstation for European XFEL, which will be based on a novel electron momentum microscope. To utilize the high-brilliance and ultrashort pulses, we developed new strategies to minimize space-charge induced effects in photoelectron spectroscopy experiments. This project is funded by FSP 302 - FEL, 05K13GU3 and 05K13UM2.

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**Setup for time-resolved STM-induced luminescence** — ●MICHAEL MOHR and RICHARD BERNDT — IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Scanning tunneling microscopy (STM) can be used to induce light emission. The correlation between the arrival times of different STM-induced photons at a detector can be measured with time-correlated single photon counting (TCSPC). These correlation-measurements can provide information about the time scale of rapid processes in the tunnel-junction that influence the STM-induced light emission. These can be, e. g., charge fluctuations on molecules or the fluorescence of molecules themselves. We present a setup for such TCSPC-measurements with a resolution down to the sub-nanosecond range.

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**Surface properties of CeO<sub>2</sub>(111) within kinetic Monte Carlo simulations** — ●STEFANO MATTIELLO<sup>1</sup>, STEFAN KOLLING<sup>1</sup>, MARVIN LEE GUSEN<sup>2</sup>, CHRISTIAN HEILIGER<sup>2</sup>, and HERBERT OVEN<sup>3</sup> — <sup>1</sup>Technische Hochschule Mittelhessen, Gießen, Germany — <sup>2</sup>I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — <sup>3</sup>Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Germany

Recently Kullgren and coworkers claim a incompatibility between density functional theory (DFT) and experimental results of Esch about the density and structure of the vacancies for the surface (111) of CeO<sub>2</sub> under UHV condition and they assume that the claimed oxygen vacancies are in fact fluorine impurities. In order to examine the possibility of a significant fluorine contamination we perform a twice investigation of the ceria surface within kinetic Monte Carlo simulations. Firstly, assuming the formation of vacancies and neglecting fluorine impurities we find that this possibility is not totally incompatible with the relevant DFT results, if microscopic dynamics is considered. Secondly, we investigate the competition between fluorine and oxygen vacancies finding a direct correlation between fluorine and vacancies concentration. This may suggest, that the absence of vacancies and the presence of fluorine only should be unlikely.

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**An approximative method to tackle the modeling of thin film IR spectra** — ●JOCHEN VOGT — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

A vibrational analysis of molecular adlayers based on the calculation of the full Hessian within DFT or other *ab initio* theory is frequently a computationally expensive task. In order to tackle the modeling of IR spectra of thin films with large unit cells, an approximative method is investigated. It is based on the first principles calculation of the Hessians and dipole derivative tensors of individual molecular entities or small clusters using large basis sets. These partial Hessians are used in the second step to reconstruct the full Hessian. The off-diagonal elements representing the intermolecular vibrational coupling are built from the partial dipole derivative tensors assuming that dipole-dipole interaction is the leading coupling term. The inclusion of other types of interaction, however, is possible. First results indicate that calculated Davydov splittings due to dynamic dipole-dipole coupling are larger than observed in experiments and thus require the inclusion of a suitable scheme of electrostatic damping [1].

[1] J. Salas et al., J. Chem. Phys. 133 (2010), 234101

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**Characterizing Measurements at the U55-Beamline at DELTA** — ●ULF BERGES<sup>1,2</sup>, CHRISTOPH KEUTNER<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>DELTA/ZfSy, TU Dortmund, Maria-Goeppert-Mayer Str. 2, 44221 Dortmund — <sup>2</sup>Experimentelle Physik Ib, TU Dortmund, Otto-Hahn-Str.4, 44221 Dortmund

A VUV-Beamline for linearly polarized synchrotron radiation within the energy range between 55 eV and 1500 eV is operated at DELTA, a synchrotron radiation facility at the University of Dortmund, Germany. The beamline is mostly used to perform XPS- and XPD-experiments with an energy resolution of about  $\frac{E}{\Delta E} = 3000$  and a photon flux of about 1e13 photons/s/100mA in the routine mode. New measurements characterizing the present status concerning energy resolution and photon flux of this beamline will be presented. The improved instrumentation of the beamline will be discussed, too.

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**Investigation of glass degradation by X-ray Photoelectron spectroscopy** — ●STEPHANIE REISS<sup>1</sup>, STEFAN KRISCHOK<sup>1</sup>, SABINE URBAN<sup>2</sup>, and EDDA RÄDLEIN<sup>2</sup> — <sup>1</sup>Institut für Physik and Institut für Mikro- und Nanotechnologien, Werk Ilmenau, PF 100565, 98684 Ilmenau, Germany — <sup>2</sup>Institut für Werkstofftechnik, TU Ilmenau, Postfach 100565, 98684, Ilmenau, Germany

Changes in the surface chemical composition during glass degradation were studied by X-ray photoelectron spectroscopy. The samples were manufactured in a float process in which the glass melt is formed on a liquid tin bath leading to a surface with tin enrichment (bath side) and one without (air side). Both sides of fresh and aged glasses were analyzed. The evaluation of the measured O1s core level spectra reveals two components: one at 532eV related to bridging oxygen (BO) linking two silicons and one at 530.3eV related to negatively charged non-bridging oxygen (NBO) where one silicon is substituted by a positive alkali ion. The changes in the ratio of these O1s components give insight in the progress of network dissolution. For the bath side the BO/NBO-ratio decreases from 10.8 to 2.2 after aging. While the fresh sample's air side shows clearly the BO and NBO component with a

ratio of 4.9, the seasoned air side exhibits only one signal. Its FWHM is wider than for each single component of the fresh sample and its binding energy lies with 531.6eV in between them leading to the con-

clusion that both components are almost equal in intensity and hence superimpose to each other. The stronger degradation of the air side hence points to an anticorrosive effect of tin.