O 35: Poster: Surface Reactions

Time: Tuesday 18:00–20:00 Location: Poster C

O 35.1 Tue 18:00 Poster C

Surface Science Investigations of Oxanorbornadiene/ Oxaquadricyclane Ester Derivatives as MOST Systems on Pt(111) — •Felix Hemauer[1], Valentin Schwaab[1], Eva Marie Freiberger[1], Natalie J. Waleska-Wellnhofer[1], Daniel Krappmann[1], Hans-Peter Steinrück[1], and Christian Papp[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Freie Universität Berlin, Germany

The harvesting and storage of solar power is feasible in a chemical manner with so-called molecular solar thermal (MOST) systems. In one-photon one-molecule processes, the conversion of the energy-lean norbornadiene (NBD) into its strained quadricyclane (QC) isomer takes place upon irradiation. On demand, the energy-releasing back reaction is triggered. For a sustainable storage and release cycle, the catalytic release needs to occur without loss of the MOST molecules. Since the methylene bridgehead group was found to be the weakest link, the surface chemistry of derivatized hetero-NBD/QC pairs was assessed on Pt(111). Specifically, synchrotron radiation-based XPS experiments were performed on 2,3 bis(methylester)-oxa-NBD/QC derivatives and its extended 2,3-bis(benzylester) substitution. Next to qualitative information on adsorption motifs, respective reaction pathways were deduced by means of temperature-programmed measurements. That is, the energy release in the cycloreversion reaction from the energy-rich isomers was studied, as well as competing desorption and decomposition steps determined. The DFG (392607742) supported this work. We thank HZB for allocation of synchrotron radiation beamtime.

O 35.2 Tue 18:00 Poster C

Non-thermal plasma modification of unsized carbon fibers — •Torben Noah Gärtig, Viktor Udachin, and Wolfgang Maus-Friedrichs — Clausthal Center of Material Technology, Clausthal University of Technology, Clausthal-Zellerfeld, Germany

Bonding of carbon fibers to the resin matrix for carbon-fiber-reinforced polymers is mostly achieved with sizing materials. An alternative treatment by oxidizing fibers with a non-thermal dielectric barrier discharge (DBD) plasma in air or oxygen atmospheres may provide a more environmentally friendly approach, which can simplify recycling of fibers and exclude the usage of sizing substances. In the present study, unsized carbon fibers were plasma treated in air and oxygen atmospheres at 1000 hPa and 25 °C with treatment times up to 10 minutes. The fiber surface before and after treatment was analyzed with X-Ray Photoelectron spectroscopy as well as microscopic methods like atomic force microscopy (AFM) and confocal laser scanning microscopy (CLSM). The plasma was characterized with optical emission spectroscopy (OES). It was found that air DBD plasma under ideal power parameters can oxidize fibers better than oxygen DBD plasma due to nitrogen reactive species aiding ozone generation. The observed oxidation does not result in significant morphology changes.

O 35.3 Tue 18:00 Poster C

Model Catalytic Studies on the Thermal Dehydrogenation of Alcohol-Based Liquid Organic Hydrogen Carrier Systems — •Valentin Schwaab[1], Felix Hemauer[1], Natalie J. Waleska-Wellnhofer[1], Eva Marie Freiberger[1], Hans-Peter Steinrück[1], and Christian Papp[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Freie Universität Berlin

The transition to a sustainable, renewable-based energy system requires novel energy storage technologies. Hydrogen production through electrolysis is a promising approach, however, under standard conditions the gas has a low volumetric energy density and is difficult to handle. So-called liquid organic hydrogen carriers (LOHCs) enable safe storage of hydrogen at high volumetric energy densities through the reversible hydrogenation of organic compounds. Alcohols are particularly interesting systems, as they often exhibit exceptionally low dehydrogenation temperatures in their reaction to the respective hydrogen-lean carbonyl compounds.

We investigated the dehydrogenation reactions of two alcohol-based LOHC pairs, namely, benzaldehyde/cyclohexylmethanol and acetophenone/1-cyclohexylethanol, on a Pt(111) model catalyst. The adsorption and the thermal evolution of the compounds was monitored in situ in synchrotron radiation photoelectron spectroscopy (SRPES) experiments at BESSY II, Helmholtz-Zentrum Berlin (HZB).

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O 35.4 Tue 18:00 Poster C

Grazing incident extended X-ray absorption fine structure on liquids at Beamline P64 at Petra III — •Lukas Voss, Dirk Lützenkirchen-Hecht, Frederic Braun, Franz Eckelt, and Carlo Schneider — Bergische Universität Wuppertal, NRW

The existing setup for grazing incidence X-ray absorption spectroscopy at Beamline P64, PETRA III, has been expanded to accommodate liquid samples. This enhancement involved the integration of a mirror device in front of the reflectometer, redirecting the X-ray beam downward onto the liquid sample surface. The adjustable mirror facilitates variations in both height and angle, enabling diverse incident angles on the surface. Leveraging this improved configuration, our investigation focused on the formation of germanium nanoparticles on the surface of deionized water. The high-speed scanning monochromator at P64 allowed for the rapid acquisition of complete EXAFS spectra within fractions of a second. Consequently, we successfully captured the exceedingly swift reaction between germanium(IV)-isopropoxide and water in situ. To further advance our capabilities, a specialized liquid sample chamber is currently under construction. This chamber aims to facilitate the study of surface reactions in liquids at controlled gas interfaces and temperatures. Its versatile design enables the detection of the reflected X-ray beam for Refl-EXAFS, while also facilitating fluorescence detection using a PIPS detector. This integrated approach enhances our ability to comprehensively investigate and analyze diverse liquid systems, such as e.g. Langmuir-Blodgett-films, providing valuable insights into surface interactions.

O 35.5 Tue 18:00 Poster C

Oxide reduction mechanisms on Cu and Fe surfaces under non-thermal plasma — •Viktor Udachin, Fabien Krebs, Oliver Höfft, Lienhard Wegewitz, and Wolfgang Maus-Friedrichs — Clausthal University of Technology, Clausthal-Zellerfeld, Germany

Oxide layers on metal surfaces usually limit the performance of materials in different industrial applications like coating or bonding. Therefore, the ability of rapid reduction of such oxides is of a big interest. Whereas methods as chemical reduction usually require complex procedures to obtain metallic surfaces, non-thermal plasmas have been shown as a quick and environmental-friendly method for surface deoxidation without notable morphological changes. Nevertheless, no detailed information on mechanisms of reduction on different metal systems is accessible. In the current work, the mechanisms of surface oxide reduction under non-thermal dielectric barrier discharge (DBD) Ar/H2 plasma were investigated. We performed depth profile characterization of oxidized Cu and Fe surfaces before and after treatment via angle resolved X-ray photoelectron spectroscopy (AR-XPS). Surface topography of Cu was studied in vacuum with atomic force microscopy (AFM), scanning tunneling microscopy (STM) as well as spectroscopy (STS) directly after oxide reduction, showing individual steps of surface deoxidation. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 394563137 - SFB 1368

O 35.6 Tue 18:00 Poster C

CO_2 reduction by trapped electrons at the NH_3/Cu(111) interface. — •Maya Heine, Lukas Gierster, and Julia Stähler — Humboldt Universität zu Berlin

When electrons are photoinjected from a metal substrate into D_2O or NH_3 adlayers they can become trapped and exhibit lifetimes up to minutes. The energetics and dynamics of such trapped electrons have been studied across picoseconds to minute timescales using time-resolved two-photon photoelectron spectroscopy and are well understood [1]. An exciting next step is to investigate the interactions of such electrons with molecules. For example, trapped electrons have already been shown to participate in the water splitting reaction at the amorphous solid water interface [2]. We investigate the interaction of CO_2 with the crystalline NH_3/Cu(111) interface, as much remains to be understood regarding the timescales and energetics of possible reactions of this important molecule. We show first results where we observe quenching of the trapped electron signal and work function modifications upon CO_2 addition, suggesting activation of CO_2 by the trapped electrons.

[1] Stähler et al. *Chemical Science 2, no. 5, 907-16* (2011)

[2] King et al. *The Journal of Physical Chemistry C 121, no. 13, 7379-86* (2017)

O 35.7 Tue 18:00 Poster C

Experimental investigation of GaInP(100) surfaces exposed to H2O — •David Ostheimer[1], Christian Dressler[2], Mohammad Amin Zare Pour[1], Sahar Shekarabi[1], Max Grossmann[3], Agnieszka Paszuk[1], and Thomas Hannappel[1] — [1]TU Ilmenau, Grundlagen von Energiematerialien, Ilmenau, Deutschland — [2]TU Ilmenau, Theoretische Festkörperphysik, Ilmenau, Deutschland — [3]TU Ilmenau, Theoretische Physik I, Ilmenau, Deutschland

Despite GaInP being employed in photoelectrochemical devices with world-record efficiencies, stability remains a significant challenge. A detailed understanding of the reactions at the semiconductor/electrolyte heterointerface is crucial to tailor the semiconductor surface appropriately to avoid losses of the photogenerated charge carriers and to reduce corrosion. As a first step, we investigate the interaction of phosphorous-rich (P-rich) and group-III-rich-GaInP(100) surfaces, with water vapor. Our analysis reveals that the initial surface reconstruction of GaInP(100) has a significant effect on the interaction with water. The P-rich GaInP(100) surface showed minimal alteration following exposure to 300 kL of water vapor. In contrast, the group-III-rich surface exhibits no RAS anisotropy after exposure. XPS measurements indicate a reduction of In-In- bonds, and that the initial pathway toward oxidation mainly involves the hydroxylation of these dimers, which subsequently leads to a formation of InOx species. Both findings could be further confirmed by ab-initio Born-Oppenheimer molecular dynamic simulations with 0.5 fs timesteps and 30 ps total simulation time for each system.