

O 23: Poster: Surface Reactions

Time: Monday 18:00–20:00

Location: P2/EG

O 23.1 Mon 18:00 P2/EG

XPS Studies of 2-Carboethoxy-3-Phenyl-NBD/QC as MOST Energy Storage System — ●FELIX HEMAUER¹, VALENTIN SCHWAAB¹, EVA MARIE FREIBERGER¹, NATALIE J. WALESKA¹, ANDREAS LENG¹, HANS-PETER STEINRÜCK¹, and CHRISTIAN PAPP^{1,2} — ¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ²Freie Universität Berlin, Germany

Molecular solar thermal (MOST) systems are a candidate for storing solar energy in a chemical manner. The energy-lean norbornadiene (NBD) is converted to its energy-rich valence isomer quadricyclane (QC) in a photoconversion reaction, whereby the energy is stored as strain. Molecular design leads to advantageous light-harvesting properties. In a model catalytic approach, we investigated the surface chemistry of the molecule pair 2-carboethoxy-3-phenyl-NBD/QC on Pt(111), Ni(111) and gold by synchrotron radiation-based XPS. Next to in situ observation of the adsorption, temperature-programmed experiments give insights into thermally induced reactions. Hereby, information on the adsorption behavior, the feasibility of the backward reaction of the QC to the NBD derivative, and the respective stability boundaries on the catalyst surfaces is obtained. On Pt(111), the energy release reaction is found to occur between 140 and 230 K. For Ni(111), the back conversion cannot be triggered thermally; instead, individual decomposition routes are monitored. The gold surface shows the highest catalytic activity with an instantaneous reaction upon adsorption at 110 K. The DFG (Project No. 392607742) supported this work. We thank HZB for allocation of synchrotron radiation beamtime.

O 23.2 Mon 18:00 P2/EG

Multiscale modeling and simulation of texture effects on the corrosion of stainless steel in aqueous media — ●VAHID JAMEBOZORGI^{1,2}, KARSTEN RASIM³, and CHRISTIAN SCHRÖDER^{1,2} — ¹Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences, 33619 Bielefeld, Germany — ²Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — ³Miele & Cie. KG, Center for Materials (CFM), Carl-Miele-Straße 29, 33332 Gütersloh

Texture plays a crucial role in physical processes and properties of condensed matter as it is broadly highlighted in the literature. In this work we describe a robust methodology to investigate texture effects which does not suffer from common limitations of quantum based computational approaches in time and space but also can provide the same accuracy as atomistic calculations with orders of magnitude less computational costs. Our methodology is based on the finite element method (FEM) and utilizes 3D digital representations of multi grain microstructures. We demonstrate the efficiency of our approach by studying pitting corrosion in stainless steel. As reflected in literature the irregular geometry of pit expansion through pitting corrosion is mostly caused by texture. We found that the texture significantly affects the pitting corrosion rate and consequently causes various irregular pit growth patterns in granular microstructures. These results are consistent with our DFT and reactive force field molecular dynamics simulations which validate our suggested approach.

O 23.3 Mon 18:00 P2/EG

Model Catalytic Studies on the Thermal Dehydrogenation of 1-Cyclohexylethanol on Pt(111) — ●VALENTIN SCHWAAB¹, FELIX HEMAUER¹, EVA MARIE FREIBERGER¹, NATALIE J. WALESKA¹, HANS-PETER STEINRÜCK¹, and CHRISTIAN PAPP^{1,2} — ¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ²Freie Universität Berlin, Germany

The transition to a sustainable, renewable-based energy system requires novel energy storage technologies. So-called liquid organic hydrogen carriers (LOHCs) enable the safe storage of green hydrogen at high volumetric energy densities through the reversible hydrogenation of organic compounds. Particularly interesting systems are secondary alcohols as they often exhibit exceptionally low dehydrogenation temperatures in their reaction to the respective ketone.

Herein, we investigated the thermal dehydrogenation of the LOHC-pair of 1-cyclohexylethanol and acetophenone on a Pt(111) model catalyst. To gain fundamental insight into the reaction behavior and thermal stability limits of the two compounds, temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) experiments were carried

out. Based on the obtained C 1s and O 1s data, the dehydrogenation of the alcohol and the formation of potential catalyst poisoning decomposition products are discussed.

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O 23.4 Mon 18:00 P2/EG

On-Surface Collision Reactions — MATTHEW JAMES TIMM¹, ●STEFAN HECHT², and LEONHARD GRILL¹ — ¹Institute of Chemistry, University of Graz, Heinrichstraße 28, 8010 Graz, Austria — ²Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

Collisions between atoms and molecules are required to form chemical bonds, and thus lie at the heart of chemistry. Their outcome depends on several parameters: the collision energy, the miss-distance between the centers of the colliding species (the impact parameter), and on the relative alignment of reagents. Studying such reactions on a surface provides a 2D confinement and allows single-molecule imaging by scanning probe microscopy. For surface reactions, it has been demonstrated that the impact parameter can be selected using a 'surface-molecular-beam' of energetic CF₂ 'projectiles' on a Cu(110) surface [1-2]. The inherent corrugation of Cu(110) collimates the projectiles, allowing them to be aimed at nearby molecular 'targets' at chosen impact parameters. However, the relative alignment of reagents could not be varied until now, due to the singular possible adsorption configurations of the studied targets. Here, a singly-debrominated molecular target has been chosen as it can adopt multiple adsorption alignments relative to the incoming CF₂ projectile, thus providing the missing element required for a more general selection of collision geometry. [1] Anggara, K.; Leung, L.; Timm, M. J.; Hu, Z.; Polanyi, J. C.; *Sci Adv.*, 2018, 4, eaau2821. [2] Anggara, K.; Leung, L.; Timm, M. J.; Hu, Z.; Polanyi, J. C.; *Faraday Discuss.*, 2019, 214, 89-103.

O 23.5 Mon 18:00 P2/EG

On-Surface Reaction of Tetraphenylporphyrin with Caesium — ●LEONARD NEUHAUS, FLORIAN MÜNSTER, KASSANDRA ZOLTNER, MARIE IRENE ALBUS, JAN HERRITSCH, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Tetrapyrroles such as porphyrins and their metal complexes play important roles in living organisms and for various modern technologies. While the surface chemistry of their transition metal complexes has been well studied in the last decades, the complexes of alkali metals are almost completely unknown. Here, we have studied the reaction of tetraphenylporphyrin (H₂TPP) with caesium in the multilayer and monolayer on Ag(111). N 1s X-ray photoelectron spectroscopy (XPS) data indicate complete metalation of the porphyrin in both cases. In complementary temperature-programmed reaction (TPR) experiments performed for the multilayer, the desorbing species were clearly identified by mass spectrometry as Cs₂TPP. DFT calculations indicate that this stable complex has a bipyramidal structure with Cs ions on both sides of the molecular plane.

O 23.6 Mon 18:00 P2/EG

Chemicurrent measurements during oxidation of Mg films with varying impact energy — ●TOBIAS PROST and HERMANN NIENHAUS — Fakultät für Physik, Universität Duisburg-Essen, Germany

The chemicurrent originating from the oxidation of super thin magnesium films in correlation with the kinetic energies of the impinging particles is investigated. The magnesium layer thickness is kept well below the mean free path in Magnesium (Mg) to reduce the influence of the carrier recombination in the metal film. The I-V characteristics of such Schottky-Diodes show a homogeneous Schottky barrier of 0.68 eV. The reverse current is below 100 pA. Based on the X-Ray photoelectron spectroscopy (XPS) spectra recorded, it can be demonstrated that the magnesium films are not pre-oxidized. A particular focus lays on the determination of the influence of hyperthermic oxygen on the kinetics of the oxidation process. The kinetic energy of the oxygen molecules could be varied between 25 and 300 meV by adding helium. The chemical current measurements with constant kinetic en-

ergy confirms the nucleation and growth model. Measurements with different oxygen velocities demonstrate that the reaction efficiency in- | creases with kinetic energy of the molecules.