O 22: Poster Surface Reactions

Time: Monday 18:00–20:00 Location: P2

O 22.1 Mon 18:00 P2

TRACE/TRIADE: A setup to investigate tritium accumulation of solids — •Marie-Christine Schäfer, Dominic Batzler, James Braun, Robin Grössle, Philipp Haag, Elizabeth Paine, Marco Röllig, Marius Schaufelberger, and Kerstin Trost — Tritium Laboratory Karlsruhe, Eggenstein-Leopoldshafen, Germany

In the context of the KArlsruhe TRItium Neutrino experiment (KATRIN), sufficient knowledge of the accumulation of tritium on surfaces is crucial for minimising systematic effects, thus optimising the experiment. On a bigger scale, the understanding of these specific tritium gas-surface interactions is relevant when it comes to fusion reactors and their fuel cycles. In search of materials with small tritium memory effects, the Tritium Activity Chamber Experiment (TRACE) at Tritium Laboratory Karlsruhe (TLK) provides the possibility of exposing solid samples to high purity tritium gas while monitoring the near-surface activity via beta-induced X-ray-spectrometry (BIXS). Similarly, the TRItium Adsorption Desorption Experiment (TRIADE) also measures the tritium accumulation via the BIXS method but is being upgraded to additionally provide the option of studying adsorption and desorption processes at temperatures down to 100 K. For this, a newly designed sample holder is currently being tested. Besides investigating the tritium accumulating properties of different materials, the compatibility with UV/ozone in the context of decontaminating the surfaces is also of relevance. For this, experiments with an additional setup are set to be conducted in the near future. This contribution will present the TRACE/TRIADE setups as well as their planned modifications.

O 22.2 Mon 18:00 P2

Exploring TiO_2-water-interfaces with AIMD and Machine Learning Force Fields — •Johannes Laurenz Wolf, Christian Dressler, and Malte Grunert — Technische Universität Ilmenau, Department of Physics, 98693 Ilmenau, Germany

Titanium dioxide (TiO_2) is a pivotal material in photocatalysis, particularly for water splitting applications in artificial leaves. In this study, we employ ab initio molecular dynamics (AIMD) and machine learning force fields (MLFF) within the MACE framework to investigate systems comprising, TiO_2 layers in different crystalline phases on indium phosphide (InP) and water. A central focus is placed on the structural and dynamic properties of the TiO_2-water interface.

To enhance our understanding of interfacial interactions, we introduce nanoscale pinholes into the TiO_2 layer, exploring their impact on water adsorption and hydrogen bonding dynamics. AIMD simulations provide atomic-scale insights, while MLFF extends these analyses to longer time scales, enabling a comprehensive investigation of adsorption mechanisms, titanium coordination, and local surface distortions.

O 22.3 Mon 18:00 P2

Investigation of the water-GaN(10$\bar{1}$0) and water-GaN(0001) interface by ab initio molecular dynamics simulations — •Marius Otto, Christian Dressler, Fabian Ullmann, and Stefan Krischok — Technische Universität Ilmenau

We have performed ab initio molecular dynamics simulations to investigate the dissociative adsorption of water at the water-GaN(10$\bar{1}$0) and water-GaN(0001) interfaces. Our results confirm that water undergoes dissociative adsorption on both surfaces, with notable differences in the protonation states of the adsorbed oxygen species. On the non-polar GaN(10$\bar{1}$0) surface, Ga atoms are exclusively coordinated by hydroxyl (OH) groups, whereas the polar GaN(0001) surface shows a mixed coverage of hydroxyl (OH) and water (H_2O) species. The dissociation of water is significantly more pronounced on the GaN(10$\bar{1}$0) surface due to the availability of distinct adsorption sites for both hydrogen and hydroxyl groups. In contrast, on the GaN(0001) surface, steric shielding of the adsorption sites inhibits water dissociation, resulting in reduced reactivity. In addition, we have also compared our simulations to XPS and UPS measurements.

O 22.4 Mon 18:00 P2

kinetics and thermodynamics of dehalogenation on metal surfaces — •Yu He[1], Hao Jiang[1], Zhiwen Zhu[1], Juan Xiang[1], Jinyang Xu[2,3,4], Zhaofeng Liang[2], Lei Xie[2], Fei Song[2], and Qiang Sun[1] — [1]Materials Genome Institute of Shanghai University,Shanghai,China — [2]Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai,China — [3]Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai,China — [4]University of Chinese Academy of Sciences, Beijing,China

In the field of on-surface synthesis, dehalogenative aryl-aryl coupling has become the key strategy for the fabrication of covalently bonded carbon-based nanomaterials. However, studies on the kinetics and thermodynamics of these reactions are still scarce. Also, most of the works focus on debromination while overlooking the dechlorination reaction which is a fundamental reaction with significant implications for environmental protection and sustainable chemistry. Here, we combined synchrotron-based x-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM) to study the dehalogenative polymerization reactions of chlorinated and brominated aromatic hydrocarbons on the Au(111) surface. We resort to high-resolution surface-sensitive techniques to identify the reactants and products as well as the important reaction intermediates. Using the fast XPS, we are able to extract the kinetic curves of the reactions and obtain detailed insight into the reaction process. Our research deepens the understanding of the reaction mechanism.

O 22.5 Mon 18:00 P2

Self-assembly and reactions of benzonitriles on metal surfaces — •Anran Bao[1] and Wenshao Yang[2] — [1]Physikalische Chemie I, Ruhr-Universität Bochum, Bochum, Germany — [2]Hangzhou Institution of Advanced Studies, Hangzhou,China

Surface synthesis enables innovative material design, with the self-assembly of organic molecules on metal surfaces. Among on-surface reactions, the Ullmann coupling is significant. Notably, despite the considerable differences in the chemical structures of cyanides and halogen atoms, they exhibit similarities in organic reactions. This provides a new perspective on surface synthesis and possibilities for synthesizing novel nanomaterials. This study focuses on the unique self-assembly and chain formation of benzonitrile derivatives, particularly iso-phthalonitrile (IPN), tere-phthalonitrile (TPN) and ortho-phthalonitrile (OPN), on the Co(0001) surface. We observed that IPN and TPN molecules adsorb randomly at room temperature using Scanning Tunneling Microscopy. However, these molecules undergo significant transformations upon annealing, forming chain-like structures. OPN forms disordered chains at room temperature, which become more linear and ordered upon heating. Compared to Au(111) and Ag(111), where simpler self-assemblies or dimers form, Co(0001) uniquely enables complex, ordered chain formation. This work provides critical insight into the catalytic properties of cobalt, enhancing understanding of molecular assembly on metal surfaces and offering new directions for designing nanostructured materials with precise molecular ordering.

O 22.6 Mon 18:00 P2

Characterization of an unexpected mu3 adsorption of molecular oxygen on Ag(100) with LT-STM — •Merve Ercelik[1], Andrés Pinar Solé[1], Liang Zhang[2], Hua Guo[2], Andreas J. Heinrich[1], Yujeong Bae[1], and Dmitriy Borodin[1] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul 03760, South Korea — [2]Department of Chemistry and Chemical Biology, Center for Computational Chemistry, University of New Mexico, Albuquerque, New Mexico 87131, USA

The interaction between molecular oxygen and metal surfaces is a key topic in quantum chemistry and surface science, with significant implications for electrochemistry and heterogenous catalysis. Using low-temperature scanning tunneling microscopy (STM), we investigate a previously unknown adsorption state of molecular oxygen on Ag(100), where the molecule binds to three silver atoms simultaneously (mu3-O2). We characterize vibrational excitations through inelastic electron tunneling spectroscopy (IETS): out-of-plane hindered rotation, in-plane hindered rotation, and in-plane hindered translation. Tunneling electron induced rotations reveal a rotational isomerization barrier of 69.3 meV. Interestingly, GGA-level DFT calculations fail to identify mu3-O2 as a stable adsorption state, likely due to self-interaction errors affecting the description of localized charges. We speculate that the mu3-O2 configuration corresponds to a formal molecular oxygen anion, with the 11 meV excitation observed in IETS attributed to a transition between spin-orbit states of the surface-bound molecular anion.