O 73: Poster Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules

Time: Wednesday 18:00–20:00 Location: P2

O 73.1 Wed 18:00 P2

In-situ tritium contamination and decontamination of fusion-relevant materials — •Elizabeth Paine[1], Dominic Batzler[2], James Braun[2], Robin Grössle[2], Philipp Haag[2], Marco Röllig[2], Marie-Christine Schäfer[2], Marius Schaufelberger[2], and Kerstin Trost[2] — [1]Eindhoven University of Technology, The Netherlands — [2]Tritium Laboratory Karlsruhe, Karlsruhe Institute of Technology, Germany

Nuclear fusion could offer a solution to the growing global demand for clean, sustainable and abundant energy. The deuterium-tritium fusion reaction offers a high energy yield and feasibility at achievable temperatures. However, the scarcity and radioactive nature of tritium pose significant challenges for its handling in fusion reactors. Tritium adsorption onto surfaces leads to challenges in licensing, process control and maintenance. Ozone is a known decontaminant and may provide a viable solution for the decontamination of these tritiated surfaces. Due to its strong oxidising nature, ozone reacts with the adsorbed tritium, which can then be evacuated. This study aims to investigate tritium accumulation and decontamination on the fusion-relevant materials: beryllium, EUROFER97 and tungsten. These are selected for their critical roles in reactor components and tritium-processing systems. The findings will provide insights into the behaviour of tritium in these materials and assess the potential of ozone-based decontamination techniques compared to established methods. This contributes to the development of effective strategies for tritium handling, decontamination and inventory management in future fusion reactors.

O 73.2 Wed 18:00 P2

Role of the surface for adsorbate motors — •Bensu Günay Ramovic[1], Grant Simpson[1], Mats Persson[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Department of Chemistry, University of Liverpool, Liverpool L69 3BX, United Kingdom

Molecular motors have the ability to perform uni-directional rotation or translation. In addition to such motors in nature, for instance kinesin, artificial molecular motors have seen great developments in the last decades. They have been studied intensely in solutions by averaging methods, but these cannot resolve individual motors. We have studied molecular motors on metal surfaces by scanning tunneling microscopy under ultrahigh vacuum and cryogenic temperatures, allowing us to track the motion of single molecules. Metallic surfaces generally play an important role for physical/chemical processes in molecular adsorbates. Here, we investigate adsorbate motors [1] on different metal surfaces in order to elucidate the role of the substrate for the molecular motion. It turns out that even rather small differences - maintaining the same surface symmetry, but changing the elemental composition - strongly affects the molecular configuration and motion.

[1] Simpson, G. J., Persson, M., & Grill, L. (2023). Adsorbate motors for unidirectional translation and transport. Nature, 621(7977), 82-86.

O 73.3 Wed 18:00 P2

Poisoning resistance of GaPt SCALMS model systems — •Christoph Wichmann[1,2], Michael Moritz[2], Haiko Wittkämper[2], Tzung-En Hsieh[3], Johannes Frisch[3], Macus Bär[2,3,4], Hans-Peter Steinrück[2], and Christian Papp[1] — [1]FU Berlin, Germany — [2]FAU Erlangen, Germany — [3]Helmholtz-Zentrum Berlin, Germany — [4]Helmholtz Institute Erlangen-Nürnberg Germany

Supported catalytically active liquid metal solutions (SCALMS) are a novel concept, where low amounts of a catalytically active transition metal is dissolved in another low melting metal, which acts as a matrix. The highly dynamic surface provides an interesting system offering high activity and remarkable stabilities for dehydrogenation reactions. For industrial applications, different challenges have to be met. One of them is the presence of catalytic poisons in the catalytic feed such as sulfur compounds. Therefore, a model system of a macroscopic GaPt droplet with a low Pt content (1 at.%) and nanoscopic GaPt particles were investigated during the exposure to thiophene as catalyst poison using X-ray photoelectron spectroscopy (XPS) under ultra-high vacuum and near-ambient pressure (0.1-0.2 mbar) conditions. The formation of Ga-sulfides at the surface of the catalyst is observed, leading to an accumulation of Pt in / under this layer. For higher temperatures (>650 K), the dissolution of the formed Ga-sulfides into the liquid metallic Ga-matrix is observed. In all cases, no Pt-sulfide was formed, indicating a resistance of the active Pt sites towards sulfur poisoning of SCALMS.

O 73.4 Wed 18:00 P2

An XPS and molecular beam study of olefin adsorption on ultrathin ionic liquid films on Pt(111) — •Laura Ulm, Cynthia C. Fernández, Leonhard Winter, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Solid catalysts with ionic liquid layer (SCILL) promise improvements for a wide range of applications, e.g. an enhanced selectivity of the 1,3-butadiene hydrogenation to 1-butene by coating a heterogeneous catalyst with thin ionic liquid (IL) films. We studied hydrocarbon adsorption as central step of this reaction by X-ray photoelectron spectroscopy combined with a supersonic molecular beam. Ultrathin films of three different ionic liquids with thicknesses below 1 nm were deposited onto a Pt(111) crystal in UHV by physical vapor deposition and characterized with XPS. These films were exposed to 1,3-butadiene or 1-butene from a supersonic molecular beam at 180 K. The coverage-dependent sticking coefficients of the two olefins were measured using the King-and-Wells method. With increasing IL pre-coverage, the total amounts of adsorbed olefins decreased until further adsorption was completely suppressed by the IL layer. The minimum IL coverage needed for complete suppression of adsorption and the differences between the ionic liquids will be discussed in the context of IL-induced selective 1,3-butadiene hydrogenation.

Supported by the DFG through SFB 1452 (Project ID: 431791331).

O 73.5 Wed 18:00 P2

N heteroatom effects in large aromatic physisorbed adsorbates on metal surfaces: azabenzopyrene on Cu(111) — •Henry Thake[1], Matthew Stoodley[1,2], David A. Duncan[2,3], and Reinhard J. Maurer[1] — [1]University of Warwick, UK — [2]Diamond Light Source, UK — [3]University of Nottingham, UK

Conjugated molecules at metal surfaces are bound by a subtle balance of short- and long-range interactions including charge transfer and dispersion interactions. As such, they represent a challenging opportunity to improve approximations to density functional theory (DFT) where accurate structural and spectroscopic benchmark measurements exist. Accurate structural predictions of the large aromatic molecules naphthalene and pyrene have shown weak adsorption in a flat geometry on Cu(111). Here, we present a combined computational and experimental study of a closely-related molecule featuring a single nitrogen heteroatom - azabenzopyrene on Cu(111). Based on DFT calculations, x-ray standing wave (XSW) structural characterisation, x-ray photoelectron (XPS) and near-edge adsorption fine structure (NEXAFS) spectroscopy simulations, we study the effect of the heteroatom on the adsorption of the conjugated molecule. We develop a structural model consistent with XSW structure determination and simulate XPS and NEXAFS signatures of the sole nitrogen species in the molecule. Nitrogen 1s XPS and K-edge NEXAFS spectra present multiple co-existing chemical environments for the nitrogen species, for which we present a model hypothesis.

O 73.6 Wed 18:00 P2

Surface Charge Modification of Silver Substrates for Enhanced SERS Selectivity — •Georgiana Ion, Stefania Dana Iancu, and Nicolae Leopold — Faculty of Physics, Babes-Bolyai University, 400084, Cluj-Napoca, Romania

Surface-enhanced Raman spectroscopy (SERS) uses the plasmonic properties of metallic nanoparticles for sensitive detection in complex matrices. A key challenge is controlling the detection of specific species. This study developed solid-state SERS substrates with optimized surface properties for selective detection of anionic and cationic analytes.

Citrate-capped silver nanoparticles (cit-AgNPs) were synthesized via the Lee-Meisel method, while hydroxylamine-reduced silver nanoparticles (hya-AgNPs) followed the Leopold-Lendl method. Concentrated nanoparticles were dried into 2 μL droplets on cover glass to create solid substrates. Raman spectra were obtained by immersing the substrates in 2 mL analyte solutions (Nile Blue, Crystal Violet, fumaric acid) using a 532 nm laser.

We found that adding $Ca(NO_3)_2$ only impacts selectivity when added to the colloidal form before drying, making it crucial for developing both substrate types. This optimized cit-AgNPs for anionic detection, while hya-AgNPs, covered with Cl^- ions, selectively detected cationic analytes. Cationic detection can also occur on cit-AgNPs by adding NaCl to the solution. This work highlights how surface modifications enhance SERS substrate selectivity and provide a pathway for tailored systems for specific analyte detection in complex environments.

O 73.7 Wed 18:00 P2

Water adsorption on Bi(111) surfaces calculated from first principles — •Yingjie Xie, Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Deutschland

Bismuth is a semimetal with unique electronic properties, including a strong spin-orbit coupling. Water adsorption on bismuth surfaces is interesting from both a scientific and technological point of view, since the material has numerous electrode applications ranging from analytical chemistry, environmental monitoring, and energy storage to seawater desalination. Surprisingly, relatively little and partially contradiction information is available on the interaction between Bi and water [1,2]. In the present contribution, density-functional theory is used to calculate the adsorption of single water molecules, water clusters and water thin films on Bi(111). We analyze in detail the molecule-molecule and molecule-substrate interaction and provide information on the diffusion characteristics. The calculations are discussed in the context of previous theory and experimental data.

[1] V. Ivanistsev, *et al.*, E. Lust, Surf. Sci. **609**, 91 (2013).
[2] W. Oh *et al.*, J. Phys. Chem. C, **122**, 23084 (2018).

O 73.8 Wed 18:00 P2

Investigation of Na$^+$ ion solvation on the Cu(111) surface by STM — •Anna Shugai and Karina Morgenstern — Physical Chemistry I, Ruhr-Universität Bochum, Bochum, 44801, Germany

Sodium-ion (Na$^+$) batteries offer great potential as an energy storage, making them an attractive alternative to the lithium-ion batteries. However, the practical realization is currently restricted due to the instability of the electrode-electrolyte interface. To reveal the reasons for it, we need to understand the underlying mechanisms that govern the process of Na$^+$ ion on-surface solvation. In this project, we use low-temperature scanning tunneling microscopy (STM) to get the locally resolved structure of D$_2$O-solvated Na$^+$ ions that are supported on the Cu(111) surface. First, the small D$_2$O clusters, containing 10 to 20 molecules, were prepared on the Cu(111) surface. We compare them to the D$_2$O clusters deposited on the Na$^+$-pre-covered Cu(111) surface. The results show that there is strong interaction between the Na$^+$ ion and the D$_2$O solvent molecules. Accordingly, the solvation behaviour of Na$^+$ is more similar to that exhibited by the Li$^+$ ion, than to that of the Cs$^+$ ion.

O 73.9 Wed 18:00 P2

Adsorption of bifunctional methoxy butene on Si(001): the multiplicity of non-selective adsorption — •Jannick Peters, Sophie Göbel, and Michael Dürr — Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

Both, ether group and C=C double bond, adsorb on Si(001) via an intermediate state and with high reactivity. When combining these two functional groups in a bifunctional organic molecule, a variety of different adsorption configurations can be envisioned. However, selective adsorption via the ether group was found for allyl ethers on the Si(001) surface [1]. In the case of methoxy butene (MeBut), the functional groups are separated by an additional CH$_2$ group when compared to allyl ethers. Despite this seemingly small change in the molecules' structure, major differences in the reactivity on Si(001) were observed. At surface temperatures between 90 and 450 K, no selective reaction but a large variety of different adsorption configurations, which are bound either via ether cleavage, the C=C double bond, or both functional groups, was observed when studying intermediates and final products by means of XPS. Depending on the final configuration, the reactivity of the ether group was found to be either enhanced or reduced, which results in an increased temperature window for the reaction from intermediate to final state.

[1] T. Glaser, et al., J. Phys. Chem. Lett. 15, 7168 (2024).

O 73.10 Wed 18:00 P2

Steel Mesh-Supported SNW-1/CsPbBr3 Nanocomposite: Photocatalyst for Sustainable Ammonia Production — •Negin Khosroshahi and Vahid Safarifard — Iran University of Science and Technology, Tehran 16846-13114, Iran

The conversion of solar energy into chemical energy through photocatalysis is an important field of interest in green energy generation and environmental improvement. Nevertheless, its effectiveness currently falls short of expectations, primarily due to the issue of charge recombination. To address this challenge, the photocatalytic effect has become an optimistic approach for enhancing processes. In this research, we have developed a Steel Mesh-Supported SNW-1/CsPbBr3 nanocomposite by combining covalent-organic frameworks with metal halide perovskite. To gauge their effectiveness, the heterostructure was assessed by employing multiple characterization methods including XRD, IR, FESEM, DRS, EDX, VSM, PL, EIS, Zeta, and BET. After the composite's preparation and characterization, we examined its photocatalytic activity in nitrogen reduction. The SNW-1/MHP/Steel mesh nanocomposite exhibited exceptional performance in ammonia generation. These findings suggest that the SNW-1/MHP/Steel mesh nanocomposite holds promise as an environmentally friendly and cost-effective photocatalyst, capable of addressing the challenges of sustainable ammonia production. This study presents a promising method for identifying effective photocatalytic materials using mesh substrates to address environmental concerns.