

O 18: Poster Session II: Metal substrates II

Time: Monday 13:30–15:30

Location: P

O 18.1 Mon 13:30 P

Atom exchange and registry shift upon formation of surface tellurides on Ag(111) and Cu(111) — ●ANDREAS RAABGRUND, MAXIMILIAN AMMON, TILMAN KISSLINGER, LUTZ HAMMER, and M. ALEXANDER SCHNEIDER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

The formation of (surface) metal alloys using Te achieved a lot attention lately, e.g. for photovoltaics or thermoelectrics [1]. In this work, we study the initial stages of Te surface alloy formation on Ag(111) and Cu(111) by STM, STS, LEED, and DFT. For coverages below 0.14 ML tellurium is readily incorporated into the topmost substrate layer via local atomic exchange. The process occurs already at or below room temperature and eventually leads to a $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ short-range order. Increasing the Te coverage leads to coexisting islands of a $(\sqrt{3} \times \sqrt{3})R30^\circ$ superstructure on Ag(111) [2] and a $(2\sqrt{3} \times \sqrt{3})R30^\circ$ superstructure on Cu(111) [3], which are well-ordered and fully developed at $\Theta = 1/3$ ML Te. In these two phases, the top layer has 1 : 1 stoichiometry in hcp registry to the substrate and only 2/3 of the surface sites are occupied. The Te atoms are only threefold coordinated in-plane. STS data shows that the substitutional Te phases have a distinctly different electronic structure from that of the well-ordered phases at $\Theta = 1/3$ ML. Notably, the unoccupied dispersing states with sp_z character are not found anymore in the range E_F to $E_F + 2.5$ eV. [1] Ibers J., Nat. Chem. 1, 508 (2009) [2] Ünzelmann et al, Phys. Rev. Lett. 124, 176401 (2020) [3] Kisslinger T., Phys. Rev. B. 102, 155422 (2020)

O 18.2 Mon 13:30 P

Growth of samarium thin films and subsequent oxidation on polycrystalline copper — ●EMILIA POZAROWSKA, CARLOS MORALES, and JAN INGO FLEGE — BTU Cottbus-Senftenberg, Konrad-Zuse-Str. 1, 03046 Cottbus, Germany

The growth of samaria thin films on copper sheets has been chemically studied by in situ X-ray photoelectron spectroscopy (XPS). The early stages of growth (0.1-14 ML) were studied by consecutive evaporations of Sm by chemical vapor deposition followed by XPS measurements. Subsequently, samaria films of different thicknesses, namely 0.1, 1, and 14 ML, were oxidized at room temperature (RT). The evolution of the sample morphology was determined through inelastic peak shape analysis (IPSA) using the QUASES software as an indirect method to study the relationship between Sm oxidation state and its surface arrangement. Our results show that samarium grows as 2D islands up to 2ML, which is followed by 3D growth. Chemical analysis indicates that at low coverages (<0.5 ML) Sm is already oxidized, leading to the appearance of Sm³⁺ as the only oxidation state. The increase in the intensity of the O1s peak with time and the absence of spectral changes in the Cu2p and LMM Auger (substrate) indicate that the transformation is mainly due to adventitious oxidation of the layer. With further deposition at RT the metallic state Sm⁰ appears at higher coverages, which is readily postoxidized by subsequent exposure to molecular oxygen, leading to complete oxidation. No intermediate oxidation states (Sm²⁺) were observed, in contrast to the reported prevalence of Sm²⁺ on single crystal surfaces during the early stages of growth.

O 18.3 Mon 13:30 P

The influence of charge transfer on molecular structure and conformation at surfaces: TCNQ on metals — ●LUKE ROCHFORD¹, DAVID DUNCAN¹, PHIL WOODRUFF², and REINHARD MAURER² — ¹Diamond Light Source, UK — ²Warwick University, UK

Electron acceptors such as TCNQ are believed, based on previous studies, to adopt bent conformations when adsorbed on metal surfaces due to electron transfer. Our recent, quantitative, structural experiments show definitively that this is not the case on a variety of metal surfaces.

Our experimental work has combined powerful complimentary surface science techniques in the home lab with synchrotron light-based techniques, mainly synchrotron x-ray photoelectron spectroscopy (SXPS) and x-ray standing waves (XSW). XSW has been central here, as it allows quantitative measurement out-of-plane structure of molecules with chemical specificity and sub-bond-length precision.

These data are supported by DFT calculations which show that dispersion force corrections are vital to properly reproduce our observed

structures. The explicit inclusion of metal adatoms in structural models is also of key importance to explain our experimental observations.

This fundamental understanding has allowed us to understand the lateral charge transfer at work between native metal adatoms and electron acceptor molecules. We have applied this knowledge to design and create two-dimensional charge transfer salts using low concentrations of alkali metal atoms.

O 18.4 Mon 13:30 P

Heat of Adsorption on Single Crystals: Microcalorimetry — ●ANN-KATRIN BAUMANN and SWETLANA SCHAUERMANN — Max-Eyth-Str.2, 24118 Kiel

Rational design of new heterogeneous catalysts requires detailed understanding of the bonding interactions between the gaseous species and the catalytic surface. One of the crucial parameters in this interaction is the adsorption enthalpy of the involved surface species.

Adsorption enthalpies can be determined with high level of accuracy by a direct method of single crystal adsorption calorimetry (SCAC), which has a number of advantages over the commonly used indirect method of temperature programmed desorption. In contrast to indirect methods, SCAC provides heats of adsorption without relying on assumptions on the details of the desorption kinetics or reversibility of the desorption processes.

In this work, an improved experimental setup of SCAC is presented. In ultra high vacuum, a pulsed molecular beam is employed to dose a known amount of molecules on a well-defined thin metal single crystal (1-2 μ m) or nanostructured model surfaces containing supported metallic nanoparticles. The arising heat of adsorption is detected by a pyroelectric material (β -PVDF) pressed against the back of the thin metal crystal. Simultaneously, the sticking coefficient of the molecules is recorded in order to determine the amount of molecules contributing to the signal (short-term sticking) and the total amount of molecules remaining permanently adsorbed on the surface (long-term sticking).

O 18.5 Mon 13:30 P

Dynamics of Adsorption and Desorption on Chiral Surfaces — ●SABINE CHARLOTTE MATYSIK and STEPHEN JOHN JENKINS — Department of Chemistry, University of Cambridge, Cambridge, United Kingdom

The relationship between structural chirality and chiral motion is not well understood and often involves different length scales for both phenomena. In this dispersion-corrected density functional theory study, we focus on the dissociative adsorption of small achiral molecules on both chiral and achiral surfaces. The interplay between chirality and surface dynamics is explored by using the transition state of the dissociation reaction as a starting point for ab initio molecular dynamics simulations. Special focus in the analysis of these reactive trajectories lies on the time evolution of rotational momenta.

O 18.6 Mon 13:30 P

Study of tritium uptake in thin palladium-titanium-gold films by Beta-Induced X-ray Spectrometry — ●MAX AKER¹, SONJA SCHNEIDEWIND², SEBASTIAN VETTER¹, CHRISTIAN GOFFING¹, and MAGNUS SCHLÖSSER¹ — ¹Institute for Astroparticle Physics, Karlsruhe Institute of Technology — ²Institute of Nuclear Physics, University of Münster

Metallic multilayer-systems are promising materials for tritium storage utilizable for passive tritium pumps, dedicated radioisotope heat sources, or calibration standards for the analysis of tritium in solids. Beta-Induced X-ray Spectrometry (BIXS) is a technique for tritium activity measurements and depth profiling in solids.

BIXS was used for activity measurements on Pd/Ti/Au multilayers in air which were tritiated at T_2 pressures up to 0.7 mbar. The measurements were complemented by activity quantifications using liquid scintillation counting. Combined with GEANT4 simulations the activity determination in samples consisting of three different metals with total thicknesses up to 300 nm and activities of 10^4 Bq to 10^8 Bq was accomplished. Pd/Ti/Au systems are interesting for tritium capture studies since Ti allows a quasi-irreversible tritium capture at room temperature, Pd prevents the formation of an oxide barrier on the Ti, and Au has low permeation to tritium, but increases the BIXS detection efficiency due to high stopping power. The findings on the influence of

T₂ pressure, Pd layer thickness and bake-out on the final activity and its stability in the sample are reported in this poster.

O 18.7 Mon 13:30 P

Tritium adsorption on a gold surface from a gaseous tritium source — MAX AKER and •FRANK HERMANN — Institute for Astroparticle Physics and Institute of Experimental Particle Physics, Karlsruhe Institute of Technology

The KATRIN collaboration aims to determine the neutrino mass with a sensitivity of 0.2 eV/c² (90% CL). This will be achieved by measuring the endpoint region of the β -electron spectrum of gaseous tritium. A gold-coated stainless steel disk defines the physical limit of the tritium source. This so-called rear wall and any potential adlayer on it are exposed to impinging β -electrons, tritium cluster ions and neutral tritium molecules which allows ad- and absorbing tritium.

The beta-spectrum from tritium decays on or below the rear wall surface differs from that of the gaseous tritium source. This leads to a spectral distortion which needs to be considered in the neutrino mass determination. Investigations with regard to spectral shape, radial distribution and temporal evolution will be presented in this poster. Also first models predicting its future increase and hypotheses for the state of the surface-near bound tritium will be discussed.

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O 18.8 Mon 13:30 P

Adsorption and reactivity of monodispersed silver clusters stabilized by an organic network — •VISHKAYA JAYALATHARACHCHI¹, ELIZABETH GRAHAM^{1,2}, JENNIFER MACLEOD¹, and JOSH LIPTON-DUFFIN^{1,2} — ¹Queensland University of Technology, Brisbane, Australia — ²Central Analytical Research Facility (CARF)

In this study, we investigate the chemical and electronic structures of Ag metal clusters coordinated by deprotonated 1,3,5-benzenetricarboxylic acid (TMA) molecules on Ag(111) using soft x-ray spectroscopy techniques. Deprotonation was examined by X-ray photoemission spectroscopy (XPS) and scanning tunnelling microscopy (STM). We used Near edge X-ray absorption fine structure spectroscopy (NEXAFS) in these experiments to study the molecular geometry after deprotonation of the carboxylic/ carboxylate groups via C-K edge/ O-K edge measurements. Evolution of HOMO-LUMO levels has been studied using combination of Valence band spectra and Resonant photoemission spectroscopy (RESPES) and compared with the calculated density of states with corresponding charge distribution of intact TMA and deprotonated TMA molecules.

Careful study of the chemical and electronic structure of these clusters will allow us to better understand how to use organic molecules to engineer arrays of single-atom catalysts on surfaces, with the goal of tailoring these 2D materials systems for reactivity and selectivity in targeted catalysed reaction.