O 28: Oxide and insulator surfaces: Structure, epitaxy and growth – Poster

Time: Monday 18:00–20:00 Location: P2

O 28.1 Mon 18:00 P2

Probing Reactions at the Plasma-Catalyst Interface — •Maarten van Dorp and Roland Bliem — ARCNL, Amsterdam, The Netherlands

Efficient conversion of CO2 into value-added chemicals is a major step towards tackling climate change. However, chemical activation of CO2 by conventional catalysis requires exceedingly high reaction temperatures, straining energy efficiency and consequently industrial viability. Plasma-assisted catalytic conversion (PLAC) circumvents this by activating CO2 dissociation through the repeated impact of *hot* electrons from a non-thermal plasma, lowering the reaction barrier while selectively heating chemically activated CO2 species. However, to rationally design new PLAC catalysts, and therefore unlock the full potential of PLAC, crucial information about the short-lived intermediates is still unknown.

Here, a NiAl(110) substrate with an epitaxially grown alumina layer (Al10O13) was selected as well-defined support for carrying Cunanoparticles as a model system for the hydrogenation of CO2 with PLACIn this model system, a complete characterization of transient intermediates * both within the ECR microwave plasma and on the catalyst surface * requires a combination of complementary spectroscopic techniques, such as XPS, in-situ IRAS, LEED, and OES. . We establish the model system for plasma applications by synthesizing different alumina thicknesses, characterizing them with LEED, and testing their stability during exposure to plasma-activated species using in situ XPS.

O 28.2 Mon 18:00 P2

Influence of sample temperature on electron-beam-induced modifications in ultrathin CaF_2 films on Si(111) — •Luis Witte, Chris Schröder und Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

The development of modern transistor technologies based on 2D materials requires gate dielectrics with low defect densities and high chemical stability. CaF_2 layers on Si(111) are well suited for this purpose due to their low lattice mismatch and large band gap. However, a crucial aspect is their stability under electron irradiation, e.g. during LEED analysis of the layers, which can lead to structural and chemical changes.

In this study, ultrathin CaF_2 layers were deposited on Si(111) using molecular beam epitaxy. First, a growth temperature study was carried out at substrate temperatures between 400 °C and 700 °C. In a second step, the influence of the sample temperature during LEED measurements on the structural stability of the layers was studied. The electron beam of the LEED served both as a source of excitation for structural changes and as a probe for detecting these modifications. The measurements were conducted at sample temperatures from −150 °C to 600 °C in order to systematically investigate temperature-related effects. The results show that modifications induced by the electron beam exhibit a pronounced temperature dependence. In addition, ex-situ XPS measurements were performed to analyse chemical changes.

O 28.3 Mon 18:00 P2

Growth of MgO on Ag(100) for promoting charge transfer of organic molecules — •Christian Haberland, Felix Otto, Maximilian Schaal, Jonas Brandhoff, Leon Bojunga, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Integer charge transfer between metal substrates and adsorbed organic molecules is a central mechanism governing interfacial electronic structure and thus the functionality of molecular devices. To control this process, ultrathin insulating films offer a powerful strategy by decoupling molecular orbitals from metallic states while still enabling quantized charge exchange. In this work, we report the successful preparation of MgO monolayer films on Ag(100) using controlled deposition of Mg and annealing procedures in an oxygen atmosphere. The resulting MgO/Ag(100) system provides a reliable platform for studying charge-transfer phenomena at oxide-supported interfaces. Comprehensive characterization was performed using photoelectron spectroscopy (UPS, XPS, XPD), revealing the electronic structure and stoichiometry, while scanning tunneling microscopy confirmed atomic-scale order and film continuity. The established growth of MgO serves as a robust model system for investigating integer charge transfer in metal/organic hybrid interfaces.

O 28.4 Mon 18:00 P2

Epitaxy of ultrathin α-Fe_2O_3(0001) and Fe_3O_4(111) on α-Al_2O_3(0001) — •Hanna Laguta, Tobias Pollenske, Chris Schröder, Luis Witte, Felix Johannsmann, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Iron oxides have a lot of technological applications and occur in magnetic, catalytic or electronic devices. Fe_3O_4 (magetite) and α-Fe_2O_3 (hematite) belong to the most stable iron oxides which can be found in nature.

Hematite is antiferromagnetic and has a lot of potential to be used for magnetic data storage. Thus it is of interest to study ultrathin hematite films. In this work, on the one hand α-Fe_2O_3 was grown directly onto the α-Al_2O_3(0001)-substrate using MBE. On the other hand Fe_3O_4 was deposited first to be oxidised to hematite in a second step. The magnetite films underwent exposures of oxygen between $6 \cdot 10^{-3}$ mbar·s and $180 \cdot 10^{-3}$ mbar·s, one sample was oxidised step-by-step.

The samples were respectively investigated using Soft and Hard X-ray Photoelectron Spectroscopy to determine the stoichiometries of near-surface and subsurface regions. Low Energy Electron Diffraction is used to determine the surface structure of the ultrathin oxide films and to distinguish hematite (α-Fe_2O_3) from maghemite (γ-Fe_2O_3) films. Additional measurements using SQUID provide insight into the magnetic properties of the samples.

O 28.5 Mon 18:00 P2

STM and LEED studies on the stabilization of two-dimensional scandium oxides on Pt(111) by Ba and Ti incorporation — •Selina Schmechel, Muriel Wegner, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The formation of two-dimensional oxides on metal support crucially depends on a charge transfer between the film and the substrate. For the particular case of M_2O_3 transition metal oxide honeycomb (HC) structures, it was found that potentially di- and quadrivalent metal cations form HC structures by charge exchange with the support [1]. This is not possible for trivalent metals and, therefore, they do not form 2D oxides.

Here we study the growth of submonolayer scandium oxide films. We confirm the 3D growth for the binary Sc_2O_3 compound with the bulk lattice parameter of 3.2Å. However, when incorporating Ti an immediate transition into a 2D layer is observed. For different compositions, these mixed Sc-Ti-O films develop long-range ordered 2D wagonwheel structures. By incorporating Ba into Sc_2O_3 we succeed in the formation of a HC structure. In this case, all HC pores are filled with Ba ions, which donate their valence electrons to the substrate. This HC posses a lattice parameter of 6.1Å as determined from LEED. This points to an increased Sc-Sc distance as compared to bulk conditions. This host atom-assisted HC stabilization will be applied to the preparation of lanthanide HC oxides in the future.

[1] J. Goniakowski et al., J. Phys. Chem. C **123**, 9272 (2019)

O 28.6 Mon 18:00 P2

Oxidation behaviour of nickel on magnesium oxide (001): An in situ study of structural development. — •Tobias Pollenske, Laurenz Hüffmeier, Hannah Hilmer, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Precise control of nickel oxidation on magnesium oxide (MgO)(001) surfaces under ultra-high vacuum (UHV) conditions is of fundamental importance for understanding metal/oxide interfaces and developing novel materials with tailored magnetic, electronic or catalytic properties. In this study, an approximately 15 nm thick Ni layer was deposited on MgO(001) using molecular beam epitaxy (MBE) and oxidised in situ at 250°C, 300°C and 400°C under 1×10^{-5} mbar O_2. The structural changes during oxidation were monitored by X-ray diffraction (XRD) near the MgO(002) Bragg reflection. In addition, GIXRD,

XRR and soft XPS measurements were performed between the oxidation steps. The results show that structured NiO formation only occurs at 400°C, while lower temperatures only lead to surface-limited oxidation. The soft XPS data confirm that the Ni surface oxidises almost immediately once a sufficient temperature is reached, with longer exposure to oxygen having little additional effect. Furthermore, the diffraction data show that annealing above 250°C improves the crystalline order of the Ni film. These combined in situ measurements provide a detailed picture of the oxidation kinetics and temperature-dependent structure development at the Ni/MgO(001) interface.

O 28.7 Mon 18:00 P2

Initial stages of gold nanoparticle growth on sapphire — •Hannah Hilmer[1], Chris Schröder[1], Tobias Pollenske[1], Timo Kuschel[2,4], Arno Jeromin[3], and Joachim Wollschläger[1] — [1]Institute of Physics, Univ. Osnabrück, 49076 Osnabrück, Germany — [2]Faculty of Physics, Univ. Bielefeld, 33615 Bielefeld, Germany — [3]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Sychrotron DESY, 22607 Hamburg, Germany — [4]Institute of Physics, Johannes Gutenberg Univ. Mainz, 55128 Mainz, Germany

Gold nanoparticles are of great interest for applications in catalysis, sensor technology, and electronics due to their shape- and size-dependent optical, electrical, and chemical properties. Their morphological and electronic properties depend heavily on the growth conditions. $Al_2O_3(0001)$ is particularly well suited as a substrate due to its chemical stability and well-defined surface structure.

For this purpose, gold was deposited in ultra-high vacuum using thermal molecular beam evaporation at different deposition durations and varying substrate temperatures. In addition, thermal post annealing was carried out at different temperatures.

The growth processes of Au on $Al_2O_3(0001)$ substrates were characterized using XRR, XPS and LEED. The results show that gold grows on sapphire in the initial stage according to Volmer-Weber growth as discontinuous islands. SEM and EDX analyses show clearly defined gold particles whose size and distribution depend strongly on the substrate temperature, the evaporation time per interval, and annealing temperature.

O 28.8 Mon 18:00 P2

Local Characterization of Structural and Electronic Properties of the ZnO(0001) Surface — •Yuyang Zhang and Martin Wenderoth — IV Physical Institute, University of Göttingen

Zinc oxide (ZnO) serves as a key model system for understanding Proton-Coupled Electron Transfer (PCET) at interfaces.[1] To unravel electron dynamics on hydrated and doped surfaces, a profound understanding of the pristine surface is the indispensable baseline. Here, high-quality single-crystalline ZnO (0001) surface were prepared under ultra-high vacuum (UHV) conditions. The desired reconstruction was achieved by optimizing cycles of Ar+ sputtering and annealing. The structural properties were characterized by Low-Energy Electron Diffraction (LEED), confirming the long-range order and the intrinsic hexagonal surface symmetry. Similar to [2], Scanning Tunneling Microscopy (STM) revealed an ordered morphology dominated by atomically flat terraces with a high concentration of defects characteristic of polar face. Complementary atomic force microscopy (AFM) measurements provided additional information on the mesoscale morphology. Tunneling current measurements were utilized to probe the local electronic properties, providing insight into the surface band structure. This work was financially supported by the DFG through the CRC1633. [1] Hammes-Schiffer et al, ACS Nano 2017, 11, 10295-10302 [2] Diebold et al, Surf. Sci. 2002, 519, 201-217