O 67: Poster: Oxide, Insulator and Semiconductor Surfaces

Time: Wednesday 18:00–20:00 Location: Poster C

O 67.1 Wed 18:00 Poster C

DFT study of the adsorption of small molecules on a vicinal ZnO surface — •Marlene Sell and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Understanding the adsorption of reactants on the surface of a catalyst is not only of interest for exploring reaction mechanisms, but the adsorption itself can also alter the structure of the catalyst surface.

In this study, the adsorption of carbon dioxide, formaldehyde, and formic acid, three important intermediates in the synthesis of methanol from syngas, on the vicinal ZnO(10$\bar{1}$4) surface was investigated using density-functional theory (DFT). Four different structures of the surface were considered: two previously proposed truncated bulk terminations, both include 2-fold coordinated surface atoms, and two new structural model, which are found to be lower in energy due to the elimination of the 2-fold coordinated atoms by a shift of atomic rows. For each of the three molecules and four surface models, the energetically most favorable structure was determined and characterized by calculation of the XPS core level shifts.

In addition, the stabilization of the different surface models by a successively increasing number of water molecules was compared. The resulting adsorption energies show that once water molecules adsorb on the undercoordinated Zn surface atoms, the bulk-truncated surface structure becomes energetically more favorable than the structure with shifted atomic rows.

O 67.2 Wed 18:00 Poster C

A structural study of CO ligation to Cu adsorbed on Fe3O4 (001) — •Fulden Eratam[1], Benedikt Klein[1,2], Lena Puntscher[3], Matthew Stoodley[1,2], Alexander Generalov[4], Alexei Preobrajenski[4], Tien-Lin Lee[1], Gareth Parkinson[3], and David A. Duncan[1] — [1]Diamond Light Source, Didcot, UK — [2]University of Warwick, Coventry, UK — [3]TU Wien, Vienna, Austria — [4]MAX IV, Lund, Sweden

Single atom catalysis (SAC) utilizes atomically dispersed single species of metals to serve as isolated active sites on a support and offers a promising tool for maximizing catalytic activity, selectivity and stability. Iron oxides are a popular support for such catalysts (e.g. [Angew. Int. Ed. 132 (2020), 12968]), where X-ray absorption near edge spectroscopy (XANES) is typically used to identify the coordination state of the SAC. The (001) surface of single crystal magnetite (Fe3O4) has been shown to coordinate a high density of single metal atoms [Science 346 (2014), 1215]. We have previously demonstrated that CO coordination pulls these atoms out of the surface by 0.2 Å [J. Chem. Phys. 152 (2020), 051102]. The current work highlights the effect of one such CO distortion on the XANES data and presents Cu L-edge XANES of Cu single metal adatoms adsorbed on Fe3O4(001) before and after CO coordination. In the absence of CO, it is found that Cu adatoms produce a XANE spectrum very similar to that of Cu2O. Meanwhile, CO coordination is found to produce a significant enhancement in the intensity of a pre-edge feature, resolved at an energy range typical of CuO.

O 67.3 Wed 18:00 Poster C

Enhanced Infrared Reflectance-Absorbance Spectroscopy on Magnetite Surfaces via Platinum Nanoparticle Encapsulation — Eric Sauter[1], •Lachlan Caulfield[1], Christof Wöll[1], Johanna Reich[2], Sebastian Kaiser[2], and Barbara A.J. Lechner[2] — [1]Karlsruhe Institute for Technology — [2]Technical University Munich

This study delves into the surface science of magnetite (Fe3O4) using ultra-high vacuum (UHV) techniques, concentrating on platinum nanoparticles' (Pt NPs) encapsulation and its impact on Infrared Reflectance-Absorbance Spectroscopy (IRRAS) bands. Magnetite, widely explored for diverse applications, possesses unique surface properties that can be tailored for enhanced functionality. Pt NPs, known for catalytic prowess, were precisely deposited on the magnetite surface in UHV conditions, ensuring a uniform distribution. Advanced surface science techniques characterized resulting morphology and composition. Surface ligand infrared spectroscopy (SLIR) revealed significant enhancements in CO-specific infrared bands' intensity after Pt NP encapsulation, signifying a notable influence. The study elucidates mechanisms driving this enhancement, emphasizing Pt NPs' role in influencing vibrational modes on the magnetite surface. This research advances understanding of magnetite surface modification and systematically explores enhancement effects on infrared bands from Pt NP encapsulation. Implications extend to designing and optimizing catalytic and sensing applications, where surface reactivity and spectroscopic sensitivity are critical.

O 67.4 Wed 18:00 Poster C

AAO template-guided preparation of ordered ZnO nanopore arrays — •Yu Duan[1,2], Jiajia Qiu[1], Mo Sha[1], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Center for Advanced Thin Films and Devices, School of Materials and Energy, Southwest University, Chongqing, 400715, China

The nanostructural design of zinc oxide (ZnO) has been of great interest as it can effectively affect its photoelectric conversion efficiency, photocatalytic activity, electrochemical activity, and other properties. In this work, we employed an anodic aluminum oxide (AAO) template-guided approach. The structural design and replication of the AAO template enabled the controlled growth of ZnO nanostructures with precise porous morphology. As a result, highly ordered ZnO nanopore arrays were prepared with tunable pore size and height. This unique array of ZnO nanopores may have potential applications in the fields of photovoltaic conversion, gas sensing, and water decomposition. In addition, the present synthesis strategy also has the potential for precise structural design of other metal and oxide materials.

O 67.5 Wed 18:00 Poster C

Initial stages of epitaxial growth of Fe$_3$O$_4$ films on SrTiO$_3$(111) — •Luis Witte, Tobias Pollenske, and Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastrasse 7, 49076 Osnabrück, Germany

Magnetite films hold promising perspectives in spintronics as, e.g., MRAM (Magnetic Random Access Memory) devices. MRAMs, based on magnetic tunnel junctions, promise non-volatile storage with improved energy efficiency and extended battery life for electronic devices. The ferromagnetism-controlled spin polarization of electrons in magnetite enables precise switching operations. Specific adjustments to the layer properties can be achieved by selectively varying the deposition temperature.

In this study, ultrathin Fe$_3$O$_4$ layers were deposited on SrTiO$_3$ (111) using reactive molecular beam epitaxy evaporating in $5 \cdot 10^{-6}$mbar O$_2$ with deposition temperatures from 200°C to 600°C. The focus of this work is on the temperature-dependent growth modes of magnetite during the initial stages of growth. LEED and XPS measurements were conducted after each step to gain insights into the structural and chemical compositions of the magnetite layers within the first monolayers. Upon completion of the growth process, additional XRR and (HE)XRD measurements were performed to obtain information about the structure and final thickness of the film.

O 67.6 Wed 18:00 Poster C

Polaron formation on BaTiO$_3$ surfaces induced by oxygen vacancies — •Andreas Ziegler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

BaTiO$_3$ is widely used as substrate and recently found interest in catalysis for oxidative coupling reactions. For these applications it is important to understand its surface properties in an oxygen-deficient state. While the localization of electrons due to oxygen vacancies has been studied intensely for bulk BaTiO$_3$, excess electrons on the surfaces of BaTiO$_3$ have not been elucidated yet.

We applied spin-polarized density functional theory (DFT) with an on-site Hubbard+U correction to determine the behavior of defect electrons created by oxygen vacancies on the Ba- and Ti-terminated BaTiO$_3$(001) surface. By applying atomic distortions before geometry optimization we achieved different localization/delocalization pattern of the two defect electrons. We find that localization of both electrons is energetically always more favorable than solutions with delocalized electrons. On the Ba-terminated surface, in the lowest-energy configuration, one electron is localized within the oxygen vacancy on the surface and the other on a Ti ion in the subsurface layer. This is in contrast to the bulk, where both defect electrons preferentially localize on neighboring Ti sites. On the Ti-terminated surface, strong surface relaxations occur, hindering an electron to localize in the vacancy and allowing localization only on two specific Ti sites.

O 67.7 Wed 18:00 Poster C

In situ X-ray photoelectron spectroscopy study of atomic layer deposited ceria on SiO$_2$: substrate influence on the reaction mechanism during the early stages of growth — •Max Gertig, Carlos Morales, Karsten Henkel, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Straße 1, 03046 Cottbus, Germany

Atomic layer deposition (ALD) is known to produce amorphous and defect-rich films in a layer-by-layer fashion, which can potentially give rise to unexpected material properties. In particular, ultrathin films (few monolayers) will show the highest complexity, as the substrate-material interaction will play a major role during deposition. Therefore, it is crucial to understand the early stages of growth of the ALD process to control and potentially tailor this interfacial interaction. Applying a surface science approach combined with complementary ex-situ characterization, we have studied by in-situ X-ray photoelectron spectroscopy (XPS) the early stages of ceria (CeO$_x$) growth on SiO$_2$ substrates deposited by thermal-ALD using Ce(thd)$_4$/O$_3$. Interestingly, an initial mixture of Ce^{3+} and Ce^{4+} was observed, although only Ce^{4+} may be expected considering the used precursor and oxidant. This fact, together with a deviation from the ideal layer-by-layer growth and a higher growth rate during the first cycles, indicates a significant influence of the substrate of the ALD reaction mechanism as well as a correlation between morphology and ceria oxidation state.

O 67.8 Wed 18:00 Poster C

Adsorption of methanol on Si(001) revisited: alternative reaction pathways at increased surface temperature — •Sophie Göbel[1], Timo Glaser[1], Gustav Nolte[1], Denys Jockel[1], Christian Länger[1], Julian Heep[1], Hendrik Weiske[2], Jan-Niklas Luy[2], Ralf Tonner-Zech[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialwissenschaften, Justus-Liebig-Universität Giessen, Germany — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany

Molecular electronics is seen as a possibility to advance semiconductor technology beyond Moore's law. With silicon as the technologically most important substrate, understanding the interaction between organic molecules and silicon surfaces is crucial for tailoring the properties of the required organic/inorganic interfaces. While low energy pathways have been extensively studied in the past, our research focuses on the question if channels with higher barriers can be addressed at higher surface temperatures. In this context, we studied the binding of methanol, the simplest alcohol, on Si(001) using X-ray photoelectron spectroscopy, scanning tunneling microscopy, and DFT calculations. Exploring this in principle simple system reveals a multitude of possible reaction channels spanning a wide range of energy barriers. However, experimentally we find the initial methanol adsorption always to proceed via O-H dissociation and further reaction channels to be operative only in the further course of the reaction.

O 67.9 Wed 18:00 Poster C

Preparation and characterization of P- and In-rich AlInP(100) by XPS and in-situ RAS — •Mohammad Amin Zare Pour, Sahar Shekarabi, Agnieszka Paszuk, and Thomas Hannappel — Grundlagen von Energiematerialien, Institut für Physik, Technische Universität Ilmenau

n-AlInP(100) is commonly used for a selective transport of electrons in so-called window layers in high-efficiency III-V multijunction solar or photoelectrochemical (PEC) cells. A fundamental understanding of water interaction with the window layer is crucial for PEC applications as well as for atomic layer deposition of passivation layers such as TiO2. In this study we focus on the preparation of different surface reconstructions of AlInP(100) by metalorganic chemical vapour deposition (MOCVD) utilizing in-situ reflection anisotropy spectroscopy (RAS) and benchmarking of the in-situ signals by X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). Our findings show that annealing the AlInP(100) surface at 310 °C leads to a P-rich surface reconstruction displayed by a (2x1)-like LEED pattern, while annealing it at 440 °C forms an In-rich surface reconstruction with a diffuse (2x4) LEED pattern. XPS results show the presence of P-P dimers on the surface of P-rich AlInP, while In-In bonds were resolved on In-rich surfaces. We determine a band bending of 1.0 eV and 1.7 eV toward the surface in the band alignment of P- and In-rich AlInP surfaces, respectively, indicating that In-rich surface has more surface states.

O 67.10 Wed 18:00 Poster C

Structure and Stability of Al-alloyed β-Ga$_2$O$_3$(100) surfaces — •Ming-Chao Kao[1,4], Lukas Paul Schewe[2], Arub Akhtar[3], Jana Rehm[3], Saud Bin Anooz[3], Zbigniew Galazka[3], Andreas Popp[3], Jan Ingo Flege[2], Vedran Vonk[1], and Andreas Stierle[1,4] — [1]Centre for X-ray and Nanoscience, Deutsches Elektronen-Synchrotron, Hamburg, Germany — [2]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus, Germany — [3]Leibniz-Institut für Kristallzüchtung , Berlin, Germany — [4]Department of Physics, University of Hamburg

β-Ga$_2$O$_3$ (GaO) holds great promise in high-power applications. GaO is predicted to outperform the leading technologies based on SiC and GaN due to a three times higher calculated critical field strength. It has been identified that alloying with Al results in an almost linear increase in the bandgap between Ga$_2$O$_3$ (4.85eV) and Al$_2$O$_3$ (7eV). A critical issue in the bandgap engineering of GaO is maintaining reasonable electron mobility, which is low for the pure material ($150cm^2/V/S$). This project aims to explore GaO by Al alloying, which allows tunable wide bandgaps for engineering material properties and at the same time maintains excellent crystal quality. PXRD and their Rietveld refinement on several AlGaO crystals indicate a preferential ordering of Al and Ga over octahedral and tetrahedral sites. The results of an SXRD study using synchrotron radiation addressing the surface structure of β-Al$_x$Ga$_{2-x}$O$_3$(100) substrates with $x = 0 - 0.25$. Our results indicate that the GaO(100) surface is nearly bulk terminated and remains smooth up to 800°C and 10^{-5}mbar of molecular oxygen.