# O 52: Oxide and insulator surfaces: Structure, epitaxy and growth I

Time: Tuesday 14:30–16:00 Location: WILL/A317

**Invited Talk** O 52.1 Tue 14:30 WILL/A317

**Dynamics of catalytically active, atomically precise clusters on reducible oxide supports under the (fast) scanning tunneling microscope** — •Friedrich Esch — TU Munich, Garching, Germany

Reducible oxides are versatile supports for catalytically active particles. Their reducibility offers the possibility to steer fundamental properties such as cluster stability and shape, charge transfer, lattice oxygen reverse spillover, or encapsulation. In this talk, I present our fundamental studies on the dynamics of atomically precise Pt clusters on two complementary supports, $Fe_3O_4(001)$, where reduction leads to interstitial diffusion and hole formation, and $CeO_2(111)$, where it leads instead to the formation of surface-near vacancies. As a local probe, we employ scanning tunneling microscopy (STM) at elevated temperatures and under reactive gas environments, upgraded with sophisticated tools for fast movie acquisition and cluster tracking. We complement this structural characterization with integral pulsed valve molecular beam "sniffer" activity and x-ray photoemission measurements. While on magnetite stabilization of even very small clusters via encapsulation is observed [1,2], on ceria, a dimensionality crossover from 3D to 2D clusters occurs, triggered by the degree of surface reduction [3].

[1] S. Kaiser et al., ACS Catal. 11 (2021) 9519.
[2] S. Kaiser et al., ACS Catal. 13 (2023) 6203.
[3] J. Reich et al., ACS Catal. 15 (2025) 18369.

O 52.2 Tue 15:00 WILL/A317

**Segregation effects in 2D mixed oxide nano-islands: edge structure and composition in V(2-x)FexO3 monolayer islands** — Ying Wang[1], Piotr Igor Wemhoff[1], Ghada Missaoui[1], Niklas Nilius[1], Jacek Goniakowski[2], and •Claudine Noguera[2] — [1]Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne Université, Institut des Nanosciences de Paris, Paris, France

Low-coordinated atoms located at the surface or edges of oxide nanostructures play a crucial role in adsorption and reaction processes in heterogeneous catalysis. Contrary to binary compounds, there is a significant lack of information on their nature and behavior available for ternary materials. In this study, high-resolution scanning tunneling microscopy, DFT calculations and Monte Carlo simulations have been used to decipher the edge structure and composition of mixed V(2-x)FexO3 honeycomb monolayer islands grown on Pt(111).

DFT calculations and MC simulations demonstrate that, in contrast to a clear preference for VO-terminated edges in the pure V2O3 system, Fe segregation to the edges of mixed films tends to produce undercoordinated edge Fe cations, with a ratio of Fe/VO edge species highly sensitive to the oxygen environment. We show that the different oxygen affinity of V and Fe cations, yielding different bonding strengths of terminal vanadyl and ferryl groups are the main cause of the segregation pattern. The sensitivity of edge composition to the oxygen environment thus represents a lever for manipulating the edge configurations and tuning their catalytic response.

O 52.3 Tue 15:15 WILL/A317

**Ultra-high THz-confinement in $LaAlO_3$ twin-walls** — •Jakob Wetzel[1], Javier Taboada-Gutiérrez[2], Susanne C. Kehr[1], Alexey B. Kuzmenko[1,3], Lukas M. Eng[2], and Samuel D. Seddon[1] — [1]TU Dresden, Institute of Applied Physics, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]University of Geneva, Department of Quantum Matter Physics (DQMP), Geneva 1211, Switzerland — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

Recent advancements in polaritonics and nano-photonics have focused on the confinement of optical modes in ultra-thin films, 2D materials, and interfaces in order to uncover pathways toward ultra-compact nanophotonic circuits and sub-diffraction imaging technologies. Such approaches to THz-confinement face fundamental challenges such as inherent strain, defects, and lattice mismatches.

Here we present the experiment- and simulation-based investigations of ferroelastic twin-walls in $LaAlO_3$, which provide a *perfect* strain-free interface to explore optical effects emergent from the coincidence of two equal but directionally rotated optical axes. Scanning near-field optical microscopy (s-SNOM) in combination with the HZDR free electron laser FELBE shows an ultra-high confinement (>250) of THz-fields at these twin-wall. Experimental results are reproduced by COMSOL-simulations and understood with an adapted dipole model.

O 52.4 Tue 15:30 WILL/A317

**Atomic-scale effects of surface modifications on mixed conducting oxides** — •Matthäus Siebenhofer, Claudia Steinbach, and Jürgen Fleig — TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria

Mixed ionic and electronic conducting (MIEC) oxide surfaces play a critical role in various technologies due to their high catalytic activity for processes such as oxygen reduction, oxygen evolution, and (photo)electrochemical water splitting. Recent advances have shown that even minute amounts of surface modifications can dramatically alter the work function and the catalytic performance but the detailed mechanisms behind these effects remain poorly understood.

This contribution discusses our efforts to understand the fundamental processes that occur during modification of MIEC oxide surfaces with ultra-thin oxide layers and acidic contaminants. We employ insitu impedance spectroscopy during pulsed laser deposition (i-PLD) to monitor changes in the oxygen exchange activity of pristine thin film surfaces; X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) provide insights into atomic-scale processes induced by these modifications.

Our results demonstrate that surface modifications introduce charge redistribution between the modification and the MIEC oxide. These effects are governed by the ionic potential and acidity of both the host material and the modifying species. Based on these observations, we provide design strategies to tailor optimized material combinations for targeted catalytic applications.

O 52.5 Tue 15:45 WILL/A317

**Probing electron-transfer between layers of a CrOx/Pt(111) thin film via workfunction and adsorption measurements in the STM** — •Ghada Missaoui[1], Claudine Noguera[2], Jacek Goniakowski[2], and Niklas Nilius[1] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

Low-temperature tunneling spectroscopy has been employed to probe the workfunction of atomically flat Cr-oxide single- and double-stack films grown on Pt(111). The single-stack Cr3O6 trilayer exhibits an exceptionally high workfunction of more than 7.0 eV, decreasing to 5.0 eV for Cr6O11 double-stacks. The charge redistribution behind this workfunction drop was analyzed by density functional theory. The high workfunction of Cr3O6 trilayers originates from a massive electron transfer from the Pt(111) support into empty Cr-states that reduces 2/3 of the oxide cations from their formal 4+ to a 3+ charge state. The negative surface dipole diminishes upon growing a Cr-O honeycomb plane on top of the trilayer, forming a Cr6O11 double-stack. The ad-layer acts as electron donor, allowing the charge transfer from the platinum to decrease substantially. The charge redistribution not only triggers the detected workfunction drop but also leads to a different reactivity of single- versus double-stack CrOx films, as demonstrated with MgPc adsorption experiments performed with the STM.