

O 42: Metal substrates 2

Time: Wednesday 10:30–11:45

Location: S053

O 42.1 Wed 10:30 S053

Atomic structure determination of epitaxially grown tin perovskite CsSnBr₃ on gold surfaces — ●MADAD ABBASLI¹, JENNY SCHRAGE¹, JIAQI CAI¹, JEREMY HIEULLE², ALEX REDINGER², CARSTEN BUSSE¹, and ROBIN OHMANN¹ — ¹University of Siegen, Department of Physics, Germany — ²University of Luxembourg, Department of Physics and Materials Science, Luxembourg

Tin perovskites can be efficient and environmentally friendly substitutions to lead perovskites, but they have a drawback due to oxidation from Sn²⁺ to Sn⁴⁺. Here, we present an in-situ study of epitaxially grown CsSnBr₃ on Au(111) and Au(100) in ultrahigh vacuum (UHV) using scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and x-ray photoelectron spectroscopy (XPS). By co-evaporation of the precursor molecules CsBr and SnBr₂ submonolayers up to a few monolayers are obtained. On Au(111), CsSnBr₃ grows in three differently oriented domains due to the hexagonal symmetry of the substrate. On Au(100), which has square symmetry, identical to CsSnBr₃, but with about half of the lattice constant of the perovskite, we observe a (2x2) superstructure. Chemical analysis shows no indication of tin oxidation, which demonstrates the importance of preparation of tin perovskites in vacuum using evaporation.

O 42.2 Wed 10:45 S053

Peculiar growth of Mn on Ir (111) investigated by SP-STM — ●ARTURO RODRIGUEZ SOTA, VISHESH SAXENA, ANDRÉ KUBETZKA, JONAS SPETHMANN, ROLAND WIESENDANGER, and KIRSTEN VON BERGMANN — Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg

The growth of metallic layers has been studied for many years, from single atom coverages via clusters and islands to extended films. The experimental parameters used during the growth, such as deposition temperature or amount of material, determine the resulting phase. Usually, only one phase is present for a given preparation, but for europium on graphene the coexistence of clusters and islands of has been documented. This was attributed to several effects including charge transfer from the metal clusters to the substrate in a precise window of coverage and temperature [1].

Here we study the growth of Mn on Ir(111) using spin polarized scanning tunneling microscopy (SP-STM). In this metallic system we have found the coexistence of clusters and islands for any Mn submonolayer coverage. We have characterized the clusters in detail at low temperature and found several different configurations made out of three atoms. The Mn islands exhibit a reconstruction that disappears when the layer is completely closed. The monolayer presents the Néel state as its magnetic ground state.

[1] D. F. Förster et al., *New J. Phys.* 14, 023022 (2012).

O 42.3 Wed 11:00 S053

Breaking down of Stoner band ferromagnetism induced by interface formation — ●DAVID JANAS¹, ANDREA DROGHETTI², IULIA COJOCARIU³, VITALIY FEYER³, STEFANO PONZONI¹, MILOS RADONJIĆ⁴, IVAN RUNGGER⁵, LIVIU CHIONCEL⁶, GIOVANNI ZAMBORLINI¹, and MIRKO CINCHETTI¹ — ¹TU Dortmund University, Dortmund, Germany — ²Trinity College, Dublin, Ireland — ³Forschungszentrum Jülich, Jülich, Germany — ⁴University of Belgrade, Belgrade, Serbia — ⁵National Physics Laboratory, Teddington, United Kingdom — ⁶University of Augsburg, Augsburg, Germany

Interfaces between ferromagnetic transition metals and molecules or atoms display intriguing spin properties that have been invoked to explain the peculiar behavior of a variety of molecular spintronic and spin-optoelectronic devices [1]. Despite its relevance, a satisfying

model for the hybridization occurring at such interfaces has not yet been presented. Experimentally, this is due to the lack of information on the interface band structure in the whole Brillouin zone, while, theoretically, the role of electron correlation has up to now mostly been neglected. Here, we overcome these limitations using state-of-the-art experimental and theoretical methods to explore the model interface between iron and an ordered oxygen layer. We use spin-resolved momentum microscopy to provide access to the complete spin-resolved interface band structure and explain our findings using DFT+ Σ_2 calculations that go beyond the one-electron approximation [2].

[1] Cinchetti, M. et al. *Nature Mater* **16**, 507-515 (2017).

[2] Droghetti, A. et al. *Phys. Rev. B* **105**, 115129 (2022).

O 42.4 Wed 11:15 S053

Computational screening of self-intercalated transition metal dichalcogenides for enhanced electrocatalytic activity — ●STEFANO AMERICO and KRISTIAN S. THYGESEN — Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark

Self-intercalation of metal atoms in bilayer transition metal dichalcogenides (TMD) has been recently realized experimentally through chemical vapor deposition (CVD) and molecular beam epitaxy (MBE), giving rise to completely new phases of the materials with controlled stoichiometry. However, little is known yet about the possible applications for this novel class of compounds. In this work, we use density functional theory to evaluate the catalytic activity towards electrochemical water splitting for 22 self-intercalated TMDs, including both metallic and semiconducting ones. We assess the thermodynamic and chemical stability of the compounds at different pH values and perform a systematic study of the hydrogen and oxygen adsorption energies at 33%, 66% and 100% intercalation degrees, identifying potential anode and cathode materials. Temperature-pressure phase diagrams are also calculated in order to guide the synthesis of compounds with the desired intercalation degree through CVD.

O 42.5 Wed 11:30 S053

A μ -Photoreactor for Investigating Planar Hydrogen Evolution Catalysts at Ambient Condition — ●CLARA ALETSEE, MARTIN TSCHURL, and UELI HEIZ — Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technical University of Munich

Photocatalytic water splitting and alcohol reforming offer promising alternatives for clean H₂ production, in contrast to the industrially applied steam reforming of fossil fuels. However, the understanding of the reaction mechanisms, which is indispensable for tailored performance improvement, is complicated by the structural complexity of powdered catalyst. In contrast, well-defined planar catalysts are already used for fundamental studies in ultra-high vacuum, but a simple extrapolation of the results to applied conditions is impractical due to a significant pressure difference.

Herein, we present a μ -photoreactor for the evaluation of planar model catalysts like single crystals or epitaxially grown semiconductors at ambient conditions in a continuous gas flow. In this system, the catalyst serves as the bottom of the reactor, while a 200 μ m O-ring on top defines the reactor volume of 12 μ L. It is sealed by a UV-vis transparent lid with lithographically implemented channels for the gas flow toward the quadrupole mass spectrometer for product analysis. The functionality is demonstrated by ethanol photoreforming over a Pt loaded TiO₂ catalyst. This concept will not only enable the evaluation of planar photocatalysts, but also the investigation of the transferability of UHV results to applied systems.