

## CPP 11: Thin Oxides and Organic Thin Films (joint session DS/CPP)

Time: Thursday 15:15–16:15

Location: H5

CPP 11.1 Thu 15:15 H5

**Hybrid electronic states in epitaxially layered perovskite oxide electrocatalysts for water electrolysis** — ●LISA HEYMAN<sup>1</sup>, MORITZ WEBER<sup>1</sup>, MARCUS WOHLGEMUTH<sup>1</sup>, FELIX GUNKEL<sup>1</sup>, and CHRISTOPH BAEUMER<sup>1,2</sup> — <sup>1</sup>Peter Gruenberg Institute and JARA-FIT, Forschungszentrum Juelich GmbH, Germany — <sup>2</sup>MESA+ Institute for Nanotechnology, University of Twente, Netherlands

In electrochemical water splitting catalyzed by perovskite oxides (ABO<sub>3</sub>), the B-O hybridization degree has a major impact on the electrocatalytic activity. Additionally, space charge layers at the interface to the electrolyte may hamper the electron transfer into the electrode, complicating the analysis of hybridization phenomena. The goal in this work was to explore whether A site doping in cobaltites (ACoO<sub>3</sub>) has a major impact on the oxygen evolution reaction (OER) through a different degree of hybridization or the extend of a surface space charge layer. We investigated La<sub>0.6</sub>Sr<sub>0.4</sub>CoO<sub>3</sub> and LaCoO<sub>3</sub> bilayer structures in epitaxial thin films that enabled us to create a near surface depth profile of both, the hybridization degree and the doping concentration confirmed by x-ray photoelectron spectroscopy (XPS). In a Mott Schottky (MS) analysis, we showed that in the OER potential regime the catalytic activity is not limited by a space charge layer. Therefore, we can correlate the observed OER activity trend to the degree of hybridization in cobaltites. The combined XPS and MS analysis enables to differentiate between the influence of the hybridization degree and intrinsic space charge layers, which are indistinguishable in a sole physical or electrochemical characterization.

CPP 11.2 Thu 15:30 H5

**tailored electrical characteristics in TiOx/HfOx-based memristive device for targeting neuromorphic computing** — ●SEONGAE PARK<sup>1,2</sup>, STEFAN KLETT<sup>1</sup>, TZVETAN IVANOV<sup>1,2</sup>, ANDREA KNAUER<sup>2</sup>, JOACHIM DOELL<sup>2</sup>, and MARTIN ZIEGLER<sup>1,2</sup> — <sup>1</sup>Department of Electrical Engineering and Information Technology, TU Ilmenau, Ilmenau, Germany — <sup>2</sup>Institute of Micro and Nanotechnologies MacroNano, TU Ilmenau, Ilmenau, Germany

Over the last few years, memristive devices have shown their high potential for neuromorphic computing. In particular, redox-based memristive devices have become the focus of research interest, since they enable precise emulation of synaptic functionality through local ionic processes. However, for targeted device functionality, a detailed understanding of ionic processes at the atomic level is required, which is often severely hampered by coupled electronic and ionic processes. In this talk, the bi-layer oxide system TiOx/HfOx is presented. In a combined approach using a 4-inch wafer process technology and a physical device model, we show the contribution of physical device parameters such as device area size, the thickness of HfOx, interface modification, as well as the stoichiometry of HfOx to the electrical characteristics. Furthermore, we present how those parameters can be tuned for customized device functionalities. In that respect, memristive devices with tailored I-V characteristics and analog resistive switching are obtained that own an intrinsic self-compliance and do not need electroforming-free cycles.

CPP 11.3 Thu 15:45 H5

**Arrangement and electronic properties of cobalt phthalocyanine molecules on Si(111) ( $\sqrt{3} \times \sqrt{3}$ ) R30°-B** — ●MILAN KUBICKI, MARTIN FRANZ, SUSI LINDNER, HOLGER EISELE, and MARIO DÄHNE — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The formation of self-assembled monolayers of organic molecular materials on solid surfaces is an important subject because of their possible application in advanced optical and electronic devices. Here, the molecular arrangement and the interfacial electronic properties of cobalt phthalocyanine (CoPc) on the deactivated Si(111) ( $\sqrt{3} \times \sqrt{3}$ ) R30°-B surface are studied by scanning tunneling microscopy and spectroscopy [1,2]. It is found that for submonolayer coverages the CoPc molecules lie flat on the Si surface with the Co  $d_{z^2}$  orbital of the molecule forming a hybrid state with the  $p_z$  orbital of the Si adatom at the surface. For multilayer coverages in contrast, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films, and the electronic properties resemble those of pure CoPc.

[1] S. Lindner, M. Franz, M. Kubicki, S. Appelfeller, M. Dähne, and H. Eisele, *Phys. Rev. B* **100**, 245301 (2019).

[2] M. Kubicki, S. Lindner, M. Franz, H. Eisele, and M. Dähne, *J. Vac. Sci. Technol. B* **38**, 042803 (2020).

CPP 11.4 Thu 16:00 H5

**Experimental Quantification of Interaction Energies in Organic Monolayers** — ●PIERRE-MARTIN DOMBROWSKI, STEFAN RENATO KACHEL, LEONARD NEUHAUS, TOBIAS BREUER, J. MICHAEL GOTTFRIED, and GREGOR WITTE — Philipps-Universität Marburg, Germany

The formation of molecular nanostructures is determined by the interplay of intermolecular and molecule-substrate interactions. However, these interactions are experimentally hardly accessible. Temperature-programmed desorption (TPD) is a fairly well-established experimental technique capable of quantifying both types of interaction, but its quantitative analysis is by no means trivial. In the present study, we analyse the desorption kinetics of the two organic semiconductors pentacene (PEN) and perfluoropentacene (PFP) from Au(111) and MoS<sub>2</sub> surfaces to show the potential of TPD, but also highlight challenges for large adsorbates. Combining TPD with scanning tunnelling microscopy, work function measurements and theoretical modelling, we show that intermolecular interactions are dominated by the intramolecular charge distribution, resulting in net intermolecular repulsion in unitary and attractive interactions in mixed PEN:PFP monolayers. We determine the coverage-dependent prefactor of desorption with unprecedented precision and correlate its evolution with the activation of specific degrees of freedom of motion of adsorbed molecules. Lastly, we compare differences in molecule-substrate interactions on Au(111) and MoS<sub>2</sub>, revealing that (sub-)monolayers on MoS<sub>2</sub> are stabilized only by entropy.