HL 12: Heterostructures, Interfaces and Surfaces: Photonics

Time: Monday 16:45–18:30 Location: POT/0051

HL 12.1 Mon 16:45 POT/0051

Surface patterning for high index contrast AlOx/GaAs distributed Bragg reflectors — •Frederike Jaeschke[1,2], Yurii Kutovyi[1,2], Nils von den Driesch[1,2], Serhii Darahan[3], Christoph Krause[1], Benjamin Bennemann[1], Frank Vewinger[3], and Alexander Pawlis[1,2] — [1]Peter Gruenberg Institute, Forschungszentrum Juelich GmbH, Juelich, Germany — [2]JARA-Fundamentals of Future Information Technology, Juelich-Aachen Research Alliance, Aachen, Germany — [3]Institut für Angewandte Physik, Universitaet Bonn, Bonn, Germany

Enhancing the refractive index contrast between the constituent materials in a distributed Bragg reflector (DBR) leads to stopband broadening and an increase in the attainable reflectivity for a given number of layer pairs, thereby mitigating the impact of growth-induced thickness variations on optical properties. One promising approach involves the post-growth wet-oxidation of AlAs to amorphous AlOx, which substantially increases the index contrast relative to conventional AlAs/GaAs stacks. In this talk, we present optimization of the AlAs/GaAs DBR growth parameters alongside different substrate patterning approaches which facilitate controlled lateral oxidation for micrometer-scale AlOx/GaAs pillar structures. We compare the optical properties of wet-oxidized AlOx/GaAs and as-grown AlAs/GaAs DBRs to explore the potentials and limitations of such pre-structuring concepts for realizing high index contrast DBRs with decreased growth times and improved layer thickness accuracy.

HL 12.2 Mon 17:00 POT/0051

Improving Photoelectrochemical Nitrate Reduction on Copper (I) Oxide Electrodes — •Maximilian Christis[1,2], Jasmin Zitzmann[1,2], Saswati Santra[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The photoelectrochemical (PEC) nitrate reduction reaction (NO_3RR) offers a green approach for simultaneous production of ammonia (NH_3) and removal of the wastewater pollutant nitrate (NO_3*) in ambient conditions. Copper (I) oxide (Cu_2O) was recently reported to be active for both electrochemical (EC) and PEC NO_3RR, but its practical application is limited by stability issues. Thus, optimal reaction conditions that balance NH_3 selectivity and catalyst stability remain to be established. In the current investigation, we find that alkaline electrolytes enhance Cu_2O-catalyzed PEC NO_3RR compared to neutral conditions, and higher NH_3 selectivity is achieved at lower applied potentials. However, under illumination and at potentials < 0.3 V vs. RHE, the catalyst rapidly reduces to metallic Cu, favoring EC rather than PEC NO_3RR. To address this challenge, we are exploring possible strategies to reduce in-situ decomposition of Cu_2O photocathodes, aiming to enable their long-term use for solar NH_3 synthesis.

HL 12.3 Mon 17:15 POT/0051

InGaN/GaN nanowire arrays for photoelectrochemical biosensors — •Hannah Nell, Genrietta Steingelb, Rudolfo Hötzel, Ruben Neelissen, Stephan Figge, Tim Grieb, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

Group III-nitride materials are known for their stability under physiological conditions, making them promising candidates for use as electrochemical biosensors [1]. In this work, we analyse the simultaneous detection by photoluminescence (PL) and photocurrent measurements of InGaN/GaN nanowire (NW) arrays, enabling sensitive and selective sensing of redox-active biomolecules. However, the performance of the NW photoelectrode is constrained by non-radiative surface recombination of photogenerated carriers at the semiconductor-electrolyte interface, leading to irreversible photooxidation of the NW surface, mainly driven by non-passivated surface states. The deposition of ultra-thin metal oxide films is a possibility to suppress such effects. The influence of TiO2 as a surface coating on the sensor properties was analysed by photoelectrochemical characterisation, demonstrating how surface modifications can affect the sensor performance in biochemical environments. [1] G. Steinhoff, et al., Appl. Phys. Lett. 83, 177 (2003)

HL 12.4 Mon 17:30 POT/0051

Metal-oxide passivation for high-efficiency photoelectrochemical devices — •Negin Mogharehabed[1], Mohammad Amin Zare Pour[1,2], Christian Höhn[3], Roel van de Krol[3], Thomas Hannappel[2], and Agnieszka Paszuk[1] — [1]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Thin metal-oxide protection layers are crucial in highly efficient III-V photoelectrochemical (PEC) devices to suppress interfacial recombination and ensure long-term stability. Here, we study TiO_2 layers deposited on AlInP/GaInP(100) photoabsorbers, examining how surface preparation prior to atomic layer deposition and the Ti-precursor chemistry affect the chemical composition and band alignment at the TiO_2/III-V heterointerface, as well as the TiO_2 bulk and surface properties. Before TiO_2 deposition, the native oxide on AlInP(100) was removed by wet-chemical etching. TiO_2 films were grown using either TTIP or $TiCl_4$ with H_2O at various substrate temperatures. X-ray photoelectron spectroscopy was used to characterize the interface and TiO_2 bulk composition. We observe precursor-dependent differences in contaminant species in the TiO_2 bulk, at the surface, and at the TiO_2/III-V heterointerface, while their concentration is strongly influenced by deposition temperature and post-growth annealing. Finally, we correlate precursor choice and initial surface condition with TiO_2 layer stability in aqueous electrolytes under PEC-relevant conditions.

HL 12.5 Mon 17:45 POT/0051

Lab-Based NAP-XPS for Probing Photoelectrochemical Interfaces: The Case of $CuBi_2O_4$ — •Katarina S. Flashar[1,2], Miriam Fehrenbach[1,2], Gaurav Anand[3], Dominic Rapf[1,2], Barbara A. J. Lechner[3], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Chemistry Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Understanding complex (photo)electrochemical conversion processes at functional interfaces requires in situ and operando characterization. A tool enabling such investigations is near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS). In this contribution, we discuss the implementation of an open liquid cell for (photo)electrochemical measurements at our recently installed, lab-based NAP-XPS system (SPECS). As a photoelectrochemical case study, we examine sputter-deposited copper bismuthate ($CuBi_2O_4$) thin film photocathodes in contact with water-based electrolytes. We thereby extend previous NAP-XPS studies on light- and gas-dependent changes in surface chemistry of $CuBi_2O_4$ [1] to the solid|liquid interface under illumination. These investigations demonstrate the capability of our lab-based NAP-XPS to probe functional interfaces of energy materials under working conditions, offering an accessible and flexible alternative to synchrotron-based measurements. [1] F. E. Oropeza et al., ACS Appl. Energy Mater. 2019, 2, 6866 - 6874.

HL 12.6 Mon 18:00 POT/0051

Correlative Atomic Force Microscopy to Understanding Local Charge Transport in Photoanodes — •Sven Doll and Johanna Eichhorn — Technical University of Munich, Garching, Germany

Efficient photosystems for solar-to-chemical energy conversion are often based on nanostructured semiconductor architectures. In these material systems, the nanoscale properties frequently dominate the performance at the macroscale. Therefore, local understanding of their charge transfer and transport properties is decisive for optimizing their efficiency and stability.

To this end, we correlate Kelvin probe force microscopy (KPFM) and (photo)conductive atomic force microscopy (AFM) to study the local band bending, charge accumulation, as well as variations in the generated surface photovoltage and (photo)conductivity. However, analyzing nanostructured materials with complex morphologies is not trivial, because effects such as topographic crosstalk can significantly influence the results obtained. To overcome these issues, we leverage 2nd eigenmode and heterodyne KPFM measurements with improved resolution and sensitivity compared to conventional tapping mode KPFM techniques. For $BiVO_4$, one of the most extensively studied metal oxide photoanode materials, we compare different KPFM modes and correlate the results with local conductivity measurements to gain insights into local semiconductor properties at grain boundaries or different crystal facets. Overall, the gained nanoscale insights will put forward the development of rational design strategies to enhance the macroscale durability and efficiency of solar energy conversion systems.

HL 12.7 Mon 18:15 POT/0051

Persistent UV-Induced Work Function Control at Atomic Layer Deposited TiO_2 /Ta_2O_5 Bilayer Interfaces — •Julius Kühne[1,2], Tim Rieth[1,2], Katarina S. Flashar[1,2], Johannes Dittloff[1,2], Lukas Wolz[2], Johanna Eichhorn[2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching

While atomic layer deposition (ALD) enables precise fabrication of ultrathin metal-oxide films, the mechanisms governing charge-carrier dynamics and band alignment at their interfaces often remain poorly understood. Oxide bilayers grown by ALD offer a versatile platform to characterize and tune defects that dictate interface energetics and charge transfer. Here, we examine the optical tuning of interface energetics in ultrathin ALD TiO_2/Ta_2O_5 bilayer films. A persistent -0.4 eV work-function (WF) shift is observed via contact potential difference (CPD) measurements after 275 nm illumination, with polarity reversal upon bilayer sequence inversion. This response arises from long-lived deep-trap filling, suggesting oxygen-vacancy migration. Capacitance-voltage (C-V) profiling, in-plane transport, and Kelvin probe force microscopy (KPFM) confirm vertical and lateral charge redistribution, while X-ray photoelectron spectroscopy (XPS) probe defect states. The results indicate that WF modulation originates from charge trapping by deep-trap states at the interface, offering insight into defect-driven effects in oxide heterointerfaces.