

CPP 52: Functional semiconductors for renewable energy solutions II (joint session HL/CPP)

Time: Tuesday 14:00–15:30

Location: POT 151

CPP 52.1 Tue 14:00 POT 151

Small-polaron transport and the role of defects in BiVO₄ photoanodes for solar water splitting — ●TIM F. RIETH, VIKTORIA F. KUNZELMANN, and IAN D. SHARP — Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Photoelectrodes can provide a route to a renewable energy supply by absorbing solar light and, thereby, drive an electrochemical reaction to produce chemical fuels. Bismuth vanadate (BiVO₄) exhibits the necessary properties for solar water splitting, namely visible light absorption, efficient charge carrier separation and well positioned band edges, and is the highest performing oxide photoanode to date [1]. Despite these advantages, the performance of BiVO₄ is inhibited by a low charge carrier mobility caused by small-polaron formation [2]. In our work, we investigate the limiting thermally activated hopping transport of small-polarons by the determination of the associated energy barrier E_h with temperature-dependent conductivity measurements on polycrystalline BiVO₄ thin films. Furthermore, we study how E_h is impacted by intentionally introduced defects such as vacancy defects and hydrogen impurities, which has been shown to greatly enhance the conductivity of BiVO₄ [3]. An improved understanding of charge carrier transport and its modification by defects can help to increase the performance of BiVO₄ and gives insights that aid in the development of new metal oxide photoelectrodes.

- [1] I.D. Sharp et al., ACS Energy Lett. 2, 139 (2017)
- [2] A.J.E. Rettie et al., Appl. Phys. Lett. 106, 022106 (2015)
- [3] J.K. Cooper et al., Chem. Mater. 28, 5761 (2016)

CPP 52.2 Tue 14:15 POT 151

InP(100) surfaces for efficient photoelectrochemical water splitting — ●OLFA DANI¹, MARIO KURNIAWAN², AGNIESZKA PASZUK¹, MANALI NANDY¹, ANDREAS BUND², and THOMAS HANNAPPEL¹ — ¹Institute of Physics, Technische Universität Ilmenau, Germany — ²Institute of Materials Science and Engineering, Technische Universität Ilmenau, Germany

To date, III-V semiconductor device structures enable the highest solar-to-hydrogen efficiencies. In this approach, a detailed understanding of the reactions at the semiconductor-electrolyte interface is essential to design the semiconductor surface for efficient charge transfer [1]. In this work, we studied the atomic structure of InP(100)-based photocathode surfaces before and after exposure to an aqueous electrolyte. The preparation of P- or In-rich surfaces on p-type InP(100) wafers with metal organic vapor phase epitaxy (MOVPE) was monitored in situ with reflection anisotropy spectroscopy (RAS). After contamination-free transfer from an MOVPE reactor to ultra-high vacuum, the surface structures were characterized by photoelectron spectroscopy (PES) and low-energy electron diffraction (LEED). Subsequently, the samples were transferred under nitrogen gas to a sealed photoelectrochemical cell for photocurrent density-potential measurements. In order to resolve changes in the surface chemistry and structure after exposure to the electrolyte, the samples were analyzed again by RAS, PES and LEED. For comparison, the same measurements were performed on InP(100) wafers with a native oxide layer. [1] M. M. May et al., J. Phys. Chem. C 118 (2014) 19032.

CPP 52.3 Tue 14:30 POT 151

Random structure search: Solving the kesterite-stannite puzzle in (Cu,Ag)₂ZnSnSe₄ solid solution — ●DANIEL FRITSCH¹ and SUSAN SCHORR^{1,2} — ¹Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Department of Geosciences, Freie Universität Berlin, Malteserstr. 74–100, 12249 Berlin, Germany

Cu₂ZnSnSe₄ and Ag₂ZnSnSe₄ are both crystallising in the kesterite structure with the structurally similar stannite structure being energetically slightly less favourable. In the solid solution, however, there is experimental evidence that for some intermediate concentrations the stannite structure is energetically favoured. This behaviour is so far not understood.

Here, we're using density functional theory calculations to shed some light into the structure-property relations in (Cu,Ag)₂ZnSnSe₄. In order to simulate the different concentrations within the solid solution, we're employing the supercell approach based on the respective

end members in the kesterite and stannite structure. The Ag and Cu cations are distributed randomly within the supercell, thereby creating several structure models for the solid solutions for further analysis. All random structure models are geometry optimised employing the recently developed SCAN functional. In order to obtain more reliable electronic and optical properties, selected optimised structures are subjected to single-shot calculations employing the more accurate hybrid functional HSE06.

CPP 52.4 Tue 14:45 POT 151

Photocatalytic performance of ALD-functionalized Nanoporous Anodic Alumina Photonic Crystals — ●CARINA HEDRICH¹, SIEW YEE LIM², ABEL SANTOS², ROBERT H. BLICK¹, and ROBERT ZIEROLD¹ — ¹Center for Hybrid Nanostructures (CHyN), Universität Hamburg, 22761 Hamburg, Germany — ²School of Chemical Engineering and Advanced Materials / Institute for Photonics and Advanced Sensing (IPAS) / ARC Centre of Excellence for Nanoscale BioPhotonics (CNBP), The University of Adelaide, South Australia 5005, Australia

Nanoporous anodic alumina (NAA) membranes feature self-organized, highly ordered pores with distinct geometrical characteristics. Modifying the electrochemical anodization parameters and applying pulse-like anodization profiles tailors the pore morphology from straight to modulated structures such as distributed Bragg reflectors or gradient index filters. The photocatalytic performances of these photonic crystals (PCs) can be enhanced by functionalizing the surface with photocatalytically active materials (e.g. TiO₂, ZnO, WO₃) or tuning the photonic stopband of the NAA by adapting the pore morphology. Herein, thickness-controlled surface modifications of NAA-PCs by atomic layer deposition (ALD) are conducted and the photocatalytic properties of these structures are investigated by studying the photodegradation of methylene blue. Optimizing and combining these different preparation strategies to further improve the photocatalytic efficiency and to tune the wavelength selectivity of NAA-PCs could expand their utilization as tailor-made photocatalysts.

CPP 52.5 Tue 15:00 POT 151

Thermoelectric transport properties of mesoporous silicon and mesoporous silicon - poly(3,4-ethylenedioxythiophene) hybrids — ●HAIDER HASEEB^{1,2}, DANNY KOJDA¹, KLAUS HABICHT^{1,2}, and TOMMY HOFMANN¹ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin — ²Universität Potsdam - Institut für Physik, Karl-Liebknecht-Straße 32, 14476 Potsdam

This presentation studies thermoelectric transport in mesoporous silicon (pSi) and mesoporous silicon-poly(3,4-ethylenedioxythiophene) (pSi-PEDOT) hybrids. We comprehensively explain electrochemical etching of pSi and infiltration of PEDOT based polymer blends (PEDOT:PSS, PEDOT:Tos) into pSi by dip- and drop-casting and vapor-phase polymerization. Surface sensitive SEM and volume sensitive nitrogen sorption isotherms probe morphological features such as pore size distributions, specific surfaces and porosities of as-etched pSi and pSi-PEDOT hybrids. Macroscopic transport measurements determine electrical and thermal conductivity, Hall mobility, charge carrier concentration and Seebeck coefficient of pSi, PEDOT, and pSi-PEDOT hybrids. We compare the temperature dependent thermoelectric performance of pSi-PEDOT hybrids with the properties of the corresponding inorganic and organic bulk systems. Our quantitative data analysis of charge and heat transport focuses on effective medium models.

CPP 52.6 Tue 15:15 POT 151

Impact of p-doping on the electronic and optical properties of copper iodide — ●MICHAEL SEIFERT, CLAUDIA RÖDL, and SILVANA BOTTI — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The lack of viable p-type transparent conductors represents a critical bottleneck for future transparent electronics. CuI, with its direct band gap of 3.1 eV and its demonstrated p-type conductivity, is a promising candidate for such a material. Recently, it has raised significant renewed interest due to the production of transparent conducting bipolar CuI/ZnO heterostructure diodes, its applications as hole collection layer in organic electronics, or as promising candidate for a flexible,

transparent thermoelectric material.

The possibility to enhance and tune key properties of the material is a major step towards potential technological applications. One ansatz to achieve this is substitutional doping. In a recent study by Graužinytė *et al.*, PCCP **21**, 18839 (2019), the chalcogen elements have been identified as promising candidates for *p*-type doping of CuI, due

to thermodynamically accessible transition levels to a hole-generating charge state ($q = -1$). Here, the effect of such *p*-doping on the electronic structure and absorption spectrum is explored in the framework of density-functional theory and the properties of the doped material are compared to those of pristine CuI.