CPP 44: Functional semiconductors for renewable energy solutions I (joint session HL/CPP)

Time: Tuesday 9:30–12:00 Location: POT 151

Invited Talk CPP 44.1 Tue 9:30 POT 151

Ionic Defects in Hybrid Perovskite Solar Cells — •Carsten Deibel[1], Sebastian Reichert[1], Qingzhi An[2], and Yana Vaynzof[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [2]Technische Universität Dresden, Institut für Angewandte Physik and Centre for Advancing Electronics Dresden (cfaed), Nöthnitzer Straße 61, 01069 Dresden

Hybrid perovskite semiconductors are an interesting material system to build low-cost solar cells with high efficiency. However, processing them can be challenging: minimal and unintentional sample-to-sample variations during the fabrication process affect the ionic defects and thus the device performance. Here, I will present a joint study on the defect properties in perovskite solar cells consisting of methylammonium lead iodide ($MAPbI_3$) in dependence of the precursor solution stoichiometry. We applied impedance spectroscopy and deep-level transient spectroscopy. Our results show different ion species, and each of them features a distribution of the diffusion coefficients. The ion migration activation energies vary systematically with stoichiometry, which might explain the wide range of activation energies in the literature. I will show that the ionic defect properties we observed can be categorised using the Meyer–Neldel rule.

CPP 44.2 Tue 10:00 POT 151

Ferroelectric Materials for Photocatalytic Water Splitting - Strained Mixed Anion Perovskites — •Nathalie Vonrüti and Ulrich Aschauer — University of Bern, Switzerland

Polarity, for example in ferroelectric materials, can significantly increase a catalyst's performance by improving charge-carrier separation. However, polar distortions also increase the band gap as shown for epitaxially strained SrTiO3 (1). While this band-gap increase is small for oxides, our density functional theory calculations show a much larger increase for oxynitrides: The enhanced covalency due to reduced electronegativity of nitrogen compared to oxygen results in larger strain-induced polar distortions and therefore more strongly increased band gaps by up to 1.5 eV. The reduced electronegativity, which leads to a higher valence band in oxynitrides and therefore a band gap in the visible that is attractive for photocatalysis, thus also has a detrimental effect on photo absorption when polar distortions are present. This results in a trade-off between small band gaps and polarity. We will discuss different strategies on how to overcome this trade-off with mixed anion perovskite compounds, which have not yet been considered for photocatalytic water-splitting. (1) RF Berger et al. PRL 107.14(2011):146804

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CPP 44.3 Tue 10:15 POT 151

Preparation of $Mg_xZn_{1-x}O$ Photoanodes for Increased Photovoltage in Dye-sensitized Solar Cells — •Andreas Ringleb[1], Tsukasa Yoshida[2], and Derck Schlettwein[1] — [1]Justus Liebig University Gießen, Institute of Applied Physics — [2]Yamagata University (Yonezawa, Japan), Graduate School of Science and Engineering

ZnO is an n-type semiconductor and a promising candidate for applications in various types of optoelectronic devices due to its wide direct bandgap of about 3.3 eV and a high electron mobility. The targeted substitution of Zn with magnesium enables a tunable band gap of $Mg_xZn_{1-x}O$ in the ZnO wurtzite structure between 3.3 and 4.0 eV through control of the Mg-content. The tunability of the bandgap can be used to minimize losses during electron injection in dye-sensitized solar cells (DSCs). $Mg_xZn_{1-x}O$ nanoparticles have been prepared from acetate precursors in ethanol through a wet chemical route. Thin films have been deposited on quartz and FTO-coated glass substrates by screen-printing of pastes and subsequent annealing. SEM has been used to study the morphology of these films, while XRD was used to detect changes in the crystal lattice caused by Mg. The modulation of the band gap has been confirmed by UV-Vis spectroscopy. A focus has been put on the homogeneity and porosity of the resulting films. DSCs were prepared and analyzed to investigate the effect of the shifted band edge on the solar cell characteristics.

15 min. break.

CPP 44.4 Tue 11:00 POT 151

Reactive sputtering of tantalum nitride for photoelectrochemical energy conversion — •Laura Wagner, Chang-Ming Jiang, and Ian Sharp — Walter Schottky Institut, Technische Universität München

Nitride semiconductors have gained increasing attention for photoelectrochemical (PEC) energy conversion. Traditionally, oxides have been widely investigated as photoelectrodes due to their chemical stability and versatile synthesis pathways; however oxide materials that simultaneously fulfill the efficiency and stability requirements have yet to be found. Many nitrides compounds are theoretically predicted to be semiconducting, though only a small fraction of these materials have been synthesized. Given their higher covalency compared to oxides, these nitrides may be promising candidates for PEC applications. Among transition metal nitrides, Ta3N5 has 2.1 eV bandgap and suitable valence band position for driving the water oxidation. While most studies perform nitridation on Ta or TaOx in order to obtain Ta3N5 thin films, we prepare Ta3N5 on various substrates by reactive magnetron sputtering deposition, which allows a wide range of control of chemical composition, crystallinity, and defect concentration. Additional to Ta3N5, this work also obtained a rarely reported Ta2N3 phase that adopts the Bixbyite structure. Detail characterization of structural, optical, and electrical properties of Ta2N3 are reported. Optimization of PEC performances of Ta3N5 and Ta2N3 thin films as photoanodes is achieved by adjusting deposition parameters. Improvement strategies for these emerging nitrides will also be discussed.

CPP 44.5 Tue 11:15 POT 151

Atomic-Layer-Deposited TiO_2 protection layers for InP photocathodes — •Matthias Kuhl[1], Oliver Bienek[1], Alex Henning[1], Agnieszka Paszuk[2], Thomas Hannappel[2] und Ian D. Sharp[1] — [1]Walter Schottky Institut, Technische Universität München — [2]Institut für Physik, Technische Universität Ilmenau

InP has gained increased interest as a photocathode for solar fuels generation due to its suitable band gap of 1.34 eV, a conduction band edge slightly above the water reduction potential and a high incident photon to charge conversion efficiency (IPCE). While it has been found that a TiO_2 passivation layer, grown by atomic layer deposition (ALD), improve the InP/TiO_2 photocathode stability, the influence of the TiO_2 optoelectronic properties on surface reactions and interfacial charge transfer is not yet understood.

Here we investigate the role of ultrathin TiO_2 (<10nm), grown by plasma-enhanced ALD, its phase, as well as defect type and concentration for the photoelectrochemical (PEC) performance of InP/TiO_2 photocathodes. Tetrakis(dimethylamino)titanium (TDMAT) and titanium isopropoxide (TTIP) as precursors as well as H_2O and O_2-Plasma as oxidants are used to grow ALD TiO_2 films with different oxidation states and defect levels. X-Ray photoelectron spectroscopy of TiO_2 grown by PE-ALD revealed only trace amounts of impurities and stoichiometric TiO_2 consistent with a lower defect density measured by photothermal deflection spectroscopy. This work provides insights into how electronic properties of photocathode protection layers affect interfacial charge injection.

CPP 44.6 Tue 11:30 POT 151

Photoanode protection by atomic-layer-deposited TiO_2 thin films — •Oliver Bienek, David Silva, and Ian D. Sharp — Technische Universität München, Walter Schottky Institut, Germany

In the development of artificial photosystems, significant effort has been devoted to preventing the degradation of photoanodes under harsh electrochemical reaction environments. A promising solution is the deposition of highly conformal protective coatings by atomic layer deposition (ALD). While the application of TiO_2 protection layers to improve the stability of photoanodes has been demonstrated successfully, questions remain regarding the mechanisms of charge carrier transport across the interface and the critical role of defects on performance characteristics. In this work, TiO_2 thin films are fabricated by plasma-enhanced ALD using different precursors and oxidizing agents on n-type Si substrates to vary both defect concentration and crystallinity of the films. In addition, the defect concentration, which is typically dominated by oxygen vacancies, is manipulated by post-annealing treatments in oxidizing atmosphere. The successful re-

moval of defects is confirmed by analysis of sub-bandgap absorption using photothermal deflection spectroscopy. Grazing incidence X-ray diffractometry and Raman spectroscopy further prove changes in the film structure from amorphous to anatase phase upon annealing. Supplementing the optical and structural characteristics, the role of film structure and defect concentration on charge injection across the interface into the electrolyte during water oxidation is investigated using photoelectrochemical methods.

CPP 44.7 Tue 11:45 POT 151

Pseudo-dreidimensionales schwerioneninduziertes Single-Event-Effect Mapping an Hochvolt Silizium Super-Junction-MOSFETs (SJ-MOS) — •Marcel Gerold[1], Michael Rüb[1], Günther Dollinger[2], Judith Reindl[2], Matthias Sammer[2] und Andreas Bergmaier[2] — [1]Ernst-Abbe-Hochschule Jena, SciTec, Carl-Zeiss-Promenade 2, 07747 Jena — [2]Universität der Bundeswehr München, LRT 2, Werner-Heisenberg-Weg 39, 85577 Neubiberg

Vertikale SJ-MOS sind weit verbreitete Halbleiterbauelemente, die in der Energiewandlung eingesetzt werden. SJ-MOS zeichnen sich durch eine komplexe drei dimensionale innere Struktur aus, welche einen niedrigen Einschaltwiderstand bei gleichzeitig hoher Spannungsfestigkeit ermöglichen. Dabei zeigt sich durch eine breite Driftzone, eine Empfindlichkeit gegenüber Partikelstrahlung. Bereits die Wirkung eines einzigen Partikels kann zu Single Event Burnout führen. Wir berichten über Ergebnisse zur Analyse der Empfindlichkeit von SJ-MOS auf Höhenstrahlung durch orts- und tiefenaufgelöste Bestrahlung mit hochenergetischen Kohlenstoffionen (E<=55 MeV, Mikrostrahlanlage "SNAKE", Maier-Leibnitz-Laboratorium, Garching). Während der Bestrahlung wird eine definierte Sperrspannung eingestellt und die Bauelementreaktion erfasst. Es werden Ladungs-Positions-Maps mit einer Auflösung von ca. 1 μm erstellt. Es zeigen sich charakteristische, mit dem Bauelementlayout korrelierbare Bereiche unterschiedlicher Sensitivität. Diese Arbeit demonstriert die Abbildung sensibler Volumina auf mikroskopischer Skala, mit dem Ziel das Verständnis von Ausfallsmechanismen bei Single-Event-Effekten zu verbessern.