HL 45: Functional semiconductors for renewable energy solutions II

Time: Thursday 15:00–17:15 Location: POT 6

HL 45.1 Thu 15:00 POT 6

Engineering interfaces in multilayer photoanodes for stable and efficient solar energy conversion — •Katarina-Sophie Flashar, Matthias Kuhl, Gabriel Grötzner, Laura Wagner, Lukas Wolz, Alex Henning, Ian D. Sharp, and Johanna Eichhorn — Walter Schottky Institute and Physics Department, Technical University Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical (PEC) energy conversion is a promising approach for the direct conversion of solar energy into storable chemical fuels. In this context, tantalum nitride (Ta_3N_5) has attracted considerable interest due to a theoretical photocurrent density limit of 12.9 mA*cm^{-2} and a theoretical solar-to-hydrogen conversion efficiency of 15% under AM 1.5G illumination. However, currently Ta_3N_5 photoelectrodes suffer from poor stability, such as oxidative decomposition, under the harsh PEC operation conditions. To overcome these limitations, we investigate the protection of Ta_3N_5 photoelectrodes with ultra-thin catalyst layers deposited via plasma-enhanced atomic layer deposition. In these multilayer architectures, the metal oxide catalyst decreases the activation energy, provides active sites for water oxidation, and promotes charge extraction of photogenerated holes. Here, we use a combination of spectroscopic and microscopic methods to elucidate the impact on interfacial energetics, defect properties, charge transport, recombination, and catalytic reactions. The gained understanding of interfacial properties is applied to design efficient interfaces between semiconductor photoelectrodes and functional catalyst coatings for the realization of highly stable and efficient PEC systems.

HL 45.2 Thu 15:15 POT 6

Discovery of multi-anion antiperovskite as promising thermoelectric materials by computational screening — •Dan Han[1], Bonan Zhu[2], Kieran B. Spooner[2], Stefan S Rudel[1], Wolfgang Schnick[1], Thomas Bein[1], David O. Scanlon[2], and Hubert Ebert[1] — [1]Department of Chemistry, University of Munich, Germany — [2]Department of Chemistry, University College London, United Kingdom

The thermoelectric performance of existing perovskites lags far behind the state-of-the-art thermoelectric materials such as SnSe, PbTe and Bi2Te3. Despite halide perovskites showing promising thermoelectric properties, namely, high Seebeck coefficients and ultralow thermal conductivities, their thermoelectric performance is significantly restricted by low electrical conductivities. Here, we explore new multi-anion antiperovskites by global structure searches, and demonstrate their phase stability by first-principles calculations. Ca6NFSn2 and Sr6NFSn2 exhibit decent Seebeck coefficients and ultralow lattice thermal conductivities (< 1 W m-1 K-1). The weak chemical bonding between the heavy-atom cage-rattler Sn and alkaline-earth metal (Ca and Sr) inducing low-frequency optical modes coupling with heat carrying acoustic phonons in combination with strong bond anharmonicity give rise to ultralow lattice thermal conductivities. Notably, Ca6NFSn2 and Sr6NFSn2 show remarkably larger electrical conductivities compared to halide perovskite CsSnI3. Our exploration of multi-anion antiperovskites X6NFSn2 (X = Ca, Sr) realizes the "phonon-glass, electron-crystal" concept within perovskite structures.

HL 45.3 Thu 15:30 POT 6

Template realized well-defined nanostructures for energy storage and conversion — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Template-based technique provides a perfect approach to realize well-defined arrayed nanostructures within large-scale. We have developed nanostructuring techniques mainly using anodic aluminum oxide templates for fabricating functional nanostructures. The obtained well-defined nanostructures possess large-scale arrayed configuration, high structural density, perfect regularity and cost-effectiveness, and are highly desirable for constructing different nano-devices especially for energy storage and conversion applications, including rechargeable sodium-ion and potassium-ion batteries, supercapacitors, and photo electrochemical devices. The device performances demonstrated that the obtained nanostructures benefit these applications through the precise control over the structural features enabled by the geometrical characteristics of the templates. Refs: Nat Commun, 2022, 13 (1), 2435; Adv Energy Mater, 2021, 11 (15), 2001537. Nat Commun 2020, 11 (1), 299; Nat Nanotechnology, 2017, 12 (3), 244.

HL 45.4 Thu 15:45 POT 6

Optical and Photocatalytic Properties of $BiVO_4$ Nanoplatelets — •Philipp Bootz[1], Bharati Debnath[1], Kilian Frank[2], Markus Döblinger[3], Bert Nickel[2], Jacek Stolarczyk[4], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich, Physics Department, Ludwig Maximilians Universität (LMU), 80539 Munich, Germany — [2]Chair for Soft Condensed Matter, 80539 Munich, Germany — [3]Chair for Functional Nanosystems (Prof. Bein), Department Physical Chemistry, 81377 Munich, Germany — [4]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland

Bismuth vanadate ($BiVO_4$) with a bandgap of about 2.4 to 3.1 eV is known as one of the best water-oxidizing semiconductors in the field of photocatalysis. It is a material which can crystallize in three different phases - orthorhombic, tetragonal and monoclinic - and is often used as thin films or micron-sized crystals. In this study, we report a novel solvothermal synthesis method to obtain colloidal BiVO4 nanoplatelets with a lateral size of less than 30 nm. We have performed X-ray diffraction and transmission electron microscopy measurements for their structural characterization. We compare the linear optical properties of the nanoplatelets with their three-dimensional pendants and discuss the microscopic origins for the observed differences. Finally, we present the results of photocatalytic experiments, where a gas chromatograph is used to measure the produced oxygen from water during illumination with light.

30 min. break

HL 45.5 Thu 16:30 POT 6

beneficial impact of KF post-deposition treatment on optical diode factor and non-radiative recombination of CIGSe absorbers — •Sevan Gharabeiki, Mohit Sood, Valentina Serrano Escalante, Taowen Wang, and Susanne Siebentritt — Department of Physics and Materials Science, University of Luxembourg, 4422 Belvaux, Luxembourg

The efficiency of the solar cells depends on the open circuit voltage (VOC), short circuit current (JSC), and fill factor (FF) which in turn depends on the diode factor. The quasi-Fermi level splitting (QFLS) is the upper limit for VOC and the optical diode factor (ODF) is the lower limit of the diode factor. It has been long known that post-deposition treatment (PDT) with heavy alkalis has a beneficial impact on CIGSe solar cells. An increase in the hole concentration, decrease in non-radiative recombination, and surface passivation have been reported by many studies. We present the effect of the KF PDT on the CIGSe absorbers with different deposition temperature. Our study shows that the KF PDT increases the (QFLS) and decreases non-radiative recombination for the samples deposited on soda lime glass with high deposition temperature. For the samples with low deposition temperature, the improvement in QFLS is mainly due to an increase in doping level. A combination of QFLS, lifetime and capacitive-voltage measurements were conducted to separate the doping effect from the non-radiative recombination effect. We propose that high concentration of Na is required to get the full effect of KF PDT, i.e. increase in the doping and decrease in the non-radiative recombination.

HL 45.6 Thu 16:45 POT 6

Tuning optical properties of graphitic carbon nitrides for photocatalytic applications — •Julian Hirschmann[1], Bharati Debnath[1], Matthias Kestler[1], Kilian Frank[2], Bert Nickel[2], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig Maximilians Universität (LMU) — [2]Chair for Experimental Physics Prof. Rädler, Department of Physics, Ludwig Maximilians Universität (LMU)

In the field of photocatalysis, graphitic carbon nitrides have proven to be a promising and cost-effective material. The organic graphene like material built from heptazine or triazole rings enable various photocatalytic applications such as hydrogen evolution and ammonia production.

Graphitic carbon nitrides have a two-dimensional sheet-like structure, which is advantageous for photocatalytic applications. Our refined synthesis process provides a simple way to obtain nanosheets of different thicknesses and varying π-conjugation areas. Their impact on the optical properties such as absorption and photoluminescence are presented. The results are compared with recently published electronic band structure calculations and with more molecularly based exciton models. Finally, photocatalytic measurements have been carried out and the obtained efficiencies are compared with our data from time-integrated and time-resolved optical experiments.

HL 45.7 Thu 17:00 POT 6

Functionalization of TiO2 thin films with gold nanoparticles aiming at plasmonic photocatalysis — •Narmina O. Balayeva[1,2], Lu He[1], Dietrich R.T. Zahn[1,2], and Teresa I. Madeira[1,2] — [1]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Reichenhainer Str. 70, 09126 Chemnitz, Germany — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Rosenbergstraße 6, 09126 Chemnitz, Germany

Developing novel photocatalytic systems with improved charge separation that can exploit visible light is of great interest. Here, we investigated the functionalization of anatase TiO2 thin films with gold nanoparticles (Au NPs) for enhanced photocatalytic activity. The LSPR effect of Au NPs is studied by depositing them either on top of or embedding them beneath TiO2 thin films or mixing them homogeneously into the precursor solution before the films are prepared using the spin-coating technique. An amount of Au NPs relative to TiO2 (0.01 wt% -1 wt%) was employed to study the effect of photocatalytic degradation of acetone using an FTIR-based gas photo-reactor chamber with a set of 6 cool white light-emitting diodes (LED). The structure and morphology of the Au/TiO2 films were characterized with different techniques, i.e., Raman spectroscopy and X-ray diffraction (XRD), X-ray reflectivity (XRR), scanning electron microscopy (SEM), as well as atomic force microscopy (AFM). Spectroscopic ellipsometry (SE) was used for a complementary analysis of thickness, roughness, and, in addition, dielectric properties of the thin films.