# DS 17: Focus Session: Thin Film Photovoltaic Materials and Solar Cells I

Thin film photovoltaics based on inorganic materials such as Si, CdTe and chalcopyrites has received much attention during the last decades, yielding good progress in the understanding of the physical properties and device physics of these materials and solar cell structures, although there are still many open questions remaining. Currently there is much interest in expanding the photovoltaic materials spectrum to include earth abundant and nontoxic elements, with high absorption coefficients, tunable band gaps, large charge carrier mobilities and low defect densities, and also to explore nanostructure configurations. This focused session is intended to highlight some of the state-of-the-art research and challenges encountered in thin film photovoltaics using different materials, and also to bring in views from related energy research areas such as thermoelectrics and photoelectrochemical water splitting, which are on first sight distinct topics, but in fact share many commonalities. (Organizer: Thomas Unold, Helmholtz-Zentrum Berlin)

Time: Wednesday 9:30–12:45 Location: H32

**Invited Talk** DS 17.1 Wed 9:30 H32

**Meso-Superstructured Perovskite Solar Cells** — •Henry J. Snaith — University of Oxford, Parks Road, Oxford, OX13PU, UK

Combining both ultimately low cost materials and production with a high efficiency solar technology has thus far been elusive. Low cost materials, such as organics and oxides, tend to suffer from fundamental energy losses required to separate excitons and collect free charge carriers in electronically disordered semiconductors. For organic and dye-sensitized solar cells this energy loss, defined as the difference between the optical band gap and the open-circuit voltage, is typically 0.65 to 0.8 eV, but for a "perfect" single junction solar cell the theoretical minimum losses, as determined by the Shockley Quasar limit are in the region of 0.25 eV. Here I will present a new hybrid solar cell concept based on a printable mesoporous superstructured perovskite absorber combined with an organic hole conductor, which we term a "meso-superstructured solar cell" (MSSC). The minimal fundamental losses are as small as 0.45 eV, and the full sun power conversion efficiency is in excess of 10% in a single junction device. I will describe the concept, operating principles, recent progress.

**Invited Talk** DS 17.2 Wed 10:00 H32

**Thermoelectric perovskite-type oxides and Heusler phases** — •Anke Weidenkaff[1,2], Sascha Populoh[1], Leyre Sagarna[2], Gesine Saucke[1], Andrey Shkabko[1], and Nina Vogel[1] — [1]Empa — [2]Uni Bern

Solar energy can be converted by photovoltaic and photocatalytic processes or by high temperature conversions using concentrated solar radiation. Metal oxides and oxynitrides with perovskite-type structure show substantial potential for thermoelectric conversion processes using concentrated solar radiation as power source. Dense and highly nanostructured thin films are produced by chimie douce [1] and plasma methods [2]. Compositions and morphologies are changed in order to tune the band structure and defects. The thin films provide an alternative way to receive suitable samples to determine the phonon and charge carrier transport and thermoelectric properties. Advanced analytical tools are applied to unravel the structure-property relationships. References [1] Alfaruq, Dimas S., Otal, Eugenio H, Aguirre, Myriam H., Populoh, Sascha, Weidenkaff, Anke, Thermoelectric properties of CaMnO3 coatings and thin films obtained by soft chemistry synthesis routes, Journal of Materials Research, 27, (2012) 985-990. [2] Vogel-Schäuble, N., Romanyuk, Y.E., Yoon, S., Saji, K.J., Populoh, S., Pokrant, S., Aguirre, M.H., Weidenkaff, A., Thermoelectric properties of nanostructured Al-substituted ZnO thin films, Thin Sold Films, 520 (2012) 6869-6875

**Topical Talk** DS 17.3 Wed 10:30 H32

**Photoelectrochemical Water Splitting with Complex Metal Oxides: the Role of Defects** — •Roel van de Krol — Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Transition metal oxides are promising candidates for the conversion of solar energy to chemical fuels. They combine reasonable semiconducting properties with excellent chemical stability and low cost. As such, they can bridge the gap between conventional PV semiconductors and molecular/biological systems. Although exciting progress has been made in the past 5 years on e.g. Fe2O3 and Cu2O, further improvement of these binary oxides is severely hampered by intrinsic materials limitations. To broaden the scope of suitable materials, research efforts are currently shifting towards multinary (complex) oxides such as InVO4 and BiVO4. In InVO4, ionic point defects are found to enhance the visible light absorption, but they also cause extensive recombination. In contrast, BiVO4 is found to be a much more defect-tolerant material, showing internal QEs above 90% when prepared with a low-cost spray pyrolysis technique. We will discuss how photo-electrochemical measurements can be used to determine the performance-limiting factors in this material. This provide valuable guidelines to improve the photoresponse, resulting in a stand-alone water splitting device based on a BiVO4 photoanode and a thin film double-junction a-Si cell with a solar-to-hydrogen efficiency of 4.3%.

**Coffee break (15 min)**

**Topical Talk** DS 17.4 Wed 11:15 H32

**Intrinsic point defects in $CuInSe_2$ and $CuGaSe_2$ studied by screened-exchange hybrid density functional theory** — •Karsten Albe und Johan Pohl — TU Darmstadt, Institut für Materialwissenschaft, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt

$Cu(In,Ga)Se_2$ is one of the most promising absorber material for solar cells. However, the presence of intrinsic point defects can be detrimental to the device properties, because of intrinsic doping and the formation of trap levels. These may act as recombination centres and therefore limit the device efficiency. Therefore, an in-depth understanding of the role of point defects in these devices is essential for optimizing the solar cell efficiency. In this talk, we discuss all relevant intrinsic point defects in terms of their defect formation energies, their charge transition levels and their localized single-particle states in the band gap, where applicable. First, the role of copper vacancies and interstitials for copper diffusion and Fermi-level pinning in the material will be discussed. Then $Cu_{In}$ and $Cu_{Ga}$ antisites are investigated and identified as hole traps with two distinct levels within the band gap, one of which can be attributed to the experimentally observed N2 level. $Ga_{Cu}$ is confirmed as a deep defect in $CuGaSe_2$ and complex formation of antisites with copper vacancies is found not to be decisive for explaining the favourable properties of $CuInSe_2$, since $In_{Cu}$ is already shallow by itself. The results also raise doubts about the relevance of selenium vacancies and DX centers for experimentally observed metastabilities.

**Topical Talk** DS 17.5 Wed 11:45 H32

**Energy Band Alignment in Thin Film Solar Cells** — •Andreas Klein — Technische Universität Darmstadt, Institut für Materialwissenschaft

The energy band alignment at interfaces between covalently bonded semiconductors like Si and GaAs can be well described using the charge neutrality level concept. The electrostatic potential distribution across an interface of such materials can be directly obtained once the band alignment and the doping profiles are known. In contrast to such ideal semiconductor interfaces, thin film solar cells employ more ionic compounds, combination of dissimilar materials, and (low temperature) film deposition techniques being far from equilibrium. As a consequence, deposited films may contain a high concentration of defects, which can prevent a variation of the Fermi energy. Such a bulk Fermi level pinning limits the evolution of band bending at an interface and can even lead to a large variation of energy band alignment. These effects may be a natural explanation for the sensitivity of solar cell efficiency on the selection of material combinations and deposition

techniques and therefore enable new optimization strategies. It further suggests that simulation of electrical cell characteristics assuming ideal semiconductor behaviour may not be adequate.

**Topical Talk** DS 17.6 Wed 12:15 H32

**Nanowire device concepts for thin film photovoltaics** — •Silke Christiansen — Max-Planck-Institute for the Science of Light, Erlangen, Germany — Institut of Photonic Technology, Jena, Germany

Large-area aligned SiNW arrays are fabricated on Si wafers and multicrystalline layers on glass substrates via metal-catalyzed wet chemical etching (WCE) or dry etching processes with or without prior lithographic patterning the use of densely packed well organized polystyrene (PS) spheres as a mask. The diameter, length, packing density, and even the shape of SiNWs could precisely be controlled and tuned by adjusting either plasma etching duration or chemical etching conditions and the diameter and pitch of the PS spheres. The anti-reflective properties of SiNWs and thus the extremely high absorption in thin SiNW layers are essential for NW based next generation solar cells. Several cell concepts with SiNWs are realized including most interesting ones: a hybrid organic/inorganic solar cell using SiNWs as absorber and PEDOT:PSS as a conducting polymer, a semiconductor-insulator-semiconductor (SIS) cell concept with SiNWs as absorbers and a tunneling barrier for charge carrier separation. The thin tunneling oxide is Al2O3 with a thickness of only a few Å and a transparent conductive oxide (TCO here: Al:ZnO) are both grown conformally around the SiNWs using atomic layer deposition (ALD).The first solar cell prototypes of 1-2cm2 area on glass substrates reached (i) open-circuit voltage of 625 mV, a short-circuit current density of 20 mA/cm2 and efficiencies >7% and (ii) an open-circuit voltage of 550 mV, a short-circuit current density of 33 mA/cm2 and efficiencies >10%.