# HL 8: Photovoltaics

Time: Monday 9:30–11:45                                                                    Location: POT 251

HL 8.1    Mon 9:30    POT 251

**Light enhanced degradation of Cu(In,Ga)Se$_2$ investigated by time-resolved photo-luminescence and X-ray photoelectron spectroscopy** — •Torsten Hölscher, Stefan Förster, Thomas Schneider, Setareh Zahedi-Azad, Eva Maria Zollner, Matthias Maiberg, and Roland Scheer — Martin-Luther-University Halle-Wittenberg, Germany

Cu(In,Ga)Se$_2$ (CIGSe) as absorber material for thin-film solar cells is known to degrade when exposed to air. So far, only little is known about the underlying surface processes. A method of choice for such an investigation is time-resolved photoluminescence (TRPL), which gives insight into the recombination kinetics of minority charge carriers. In our work, we have applied TRPL to CIGSe layers grown on molybdenum covered soda lime glass. The results show a strong decrease of the minority carrier lifetime after 10 till 60 min illumination with white light (1 sun) under ambient conditions. Measurement of X-ray photoelectron spectroscopy reveals an increase of the Na 1s and O 1s peak on the CIGSe surface. The position of the O 1s peak is centered at 531.7 eV, which we refer to the Na–O-CIGSe bonding complex. Based on TRPL and XPS we propose a light enhanced formation of this Na–O-CIGSe complex on the surface as the origin of the degradation. This model may also explain the often observed – "laser degradation" – during TRPL measurements. In the end, we discuss the influence of this degradation effect on the solar cell performance.

HL 8.2    Mon 9:45    POT 251

**Optoelectronic properties of a-Si:H and a-Si:H/c-Si interfaces from first principles** — •Philippe Czaja[1], Urs Aeberhard[1], Massimo Celino[2], and Simone Giusepponi[2] — [1]IEK-5 Photovoltaics, Forschungszentrum Jülich, Germany — [2]ENEA Casaccia, Italy

In order to optimize the optoelectronic properties of novel solar cell architectures, such as the amorphous-crystalline interface (a-Si:H/c-Si) in silicon heterojunction devices, we calculate and analyze the local microscopic structure at the interface and in bulk a-Si:H, in particular with respect to the impact of material inhomogeneities. The microscopic information is used to extract macroscopic material properties, and to identify localized defect states, which govern the recombination properties encoded in quantities such as capture cross sections used in the Shockley-Read-Hall theory.

To this end, atomic configurations for a-Si:H and a-Si:H/c-Si interfaces are generated using molecular dynamics. Density functional theory calculations are then applied to these configurations in order to obtain the electronic wave functions. These are analyzed and characterized with respect to their localization and their contribution to the (local) density of states. GW calculations are performed for the a-Si:H configuration in order to obtain a quasi-particle corrected absorption spectrum. The results suggest that the quasi-particle corrections can be approximated through a scissors shift of the Kohn-Sham energies.

HL 8.3    Mon 10:00    POT 251

**Investigation of the Loss Mechanisms in CuInS$_2$/ZnO Nanocrystal Solar Cells** — •Dorothea Scheunemann, Sebastian Wilken, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

Heterojunction solar cells based on colloidal nanocrystals have shown remarkable improvements in performance in the last decade. This progress was accompanied by a deeper understanding of the underlying physical processes in nanocrystal solids and devices. However, the vast majority of these studies is focused on two materials, PbS and PbSe. In contrast, there is still a lack of such detailed knowledge in case of other materials, as for example copper-based compounds, which show lower power conversion efficiencies when incorporated into solar cells. Here, we present a detailed study on the photocurrent loss mechanisms in nanocrystalline CuInS$_2$/ZnO heterojunction solar cells by combining steady-state characterization methods with transient photocurrent and photovoltage measurements. We demonstrate the presence of two different loss mechanisms: An extraction barrier at the CuInS$_2$/ZnO interface, which can be reduced upon illumination with UV light, as well as significant trap-assisted recombination in the CuInS$_2$ layer. The presented results confirm the potential of heterojunctions made from CuInS$_2$ and ZnO nanocrystals in solution producible solar cells, but also clearly highlight the importance of a substantial reduction of sub-band gap states to improve the performance.

HL 8.4    Mon 10:15    POT 251

**First-principles modeling the alkali-metal post-deposition treatment of CIGS solar cells** — •Maria Fedina, Hannu-Pekka Komsa, Ville Havu, and Martti Puska — Department of Applied Physics, Aalto University, P.O. Box 11000, Espoo, Finland

The efficiency of the Cu(In,Ga)Se$_2$ (CIGS) solar cell has increased significantly during the last few years thanks to the post-deposition treatment (PDT) by alkali metals. The PDT process results in formation of alkali metal impurities inside the CIGS grain interiors (GIs) and near grain boundaries (GB) We have calculated formation energies and migration barriers for Li, Na, K, Rb, and Cs impurities in bulk CuInSe$_2$ (CIS) within the framework of the density-functional theory. We will discuss the interplay between the alkali metal impurities and the native point defects in CIS. Moreover, the most important parameters of the secondary phases, such as lattice constants, band gaps, and heats of formation have been calculated. Mechanisms for secondary phase formation in CIGS will be discussed. Due to low free energies at surfaces and GBs, alkali metal atoms accumulate preferably at GBs and near the CIGS surface resulting in possible formation of secondary phases. We have calculated formation energies of alkali metal impurities also near different types of GBs and close to the surface, and we will discuss the prominent trends between different alkali metal atoms.

**Coffee Break**

HL 8.5    Mon 10:45    POT 251

**Theoretical analysis of an Intermediate Band in Sn-doped Hematite with Wide-spectrum Solar Response** — Wilayat Khan[1] and •Jan Minar[2] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzen*, Czech Republic — [2]Department of chemistry and Center for NanoScience, LMU Munich, Butenandtstra*e 11, 81377 M*unchen, Germany

Hematite $\alpha$-Fe2O3 is exposed to be an efficient photocatalytic material for water splitting process under visible light. We have further improved the photocatalytic activity of Hematite by varying Tin (Sn) concentration substituted for Fe in pristine hematite. Experimental measurements on the Sn doped Fe2O3 and a brief theoretical study on the density of states (DOS) have been reported in the previous studies, but further detail insight into the optoelectronic and spectroscopic properties is still missing. Here we obtained the accurate insulating character and feature the electronic structure and other key properties of pristine and Sn doped Fe2O3 by the combination of on-site Hubbard interaction and generalized gradient approximation within WIEN2k code. The electronic structures explore the engineering of the orbitals around the Fermi level due to increase in the concentration of Sn in Fe2O3, and the expected reduction in the band gap is also attributed to the corresponding contents of Sn. The electronic structure of doped hematite introduces an intermediate band (IB) and absorption edge is shifted to the infrared regime. In addition, the Fe-K edge and Fe-L2,3 edge were also calculated using the SPR-KKR code.

HL 8.6    Mon 11:00    POT 251

**Preparation and Analysis of In$_2$S$_3$:V Intermediate Band Thin-Film Absorbers for Solar Cells** — •Leonard Wägele[1], Tanja Jawinski[1,2], Christoph Bahret[1], Holger von Wenckstern[2], Marius Grundmann[2], and Roland Scheer[1] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany — [2]Institute of Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany

To achieve higher energy conversion efficiencies above the Shockley-Queisser limit, one can use larger band gap materials provided with an intermediate band. This allows the absorption of low energy photons via the intermediate band, while high energy photons can generate charge carriers with reduced thermalization losses. One theoretically suitable material for such a device is In$_2$S$_3$ combined with transition metals. We grow thin-film In$_2$S$_3$:V with physical co-evaporation from the elements. We use SEM, EDX, XRD and Raman spectroscopy to study the structural changes of vanadium variations. We show that

vanadium is successfully incorporated into the $In_2S_3$ structure. Furthermore, UV-VIS-NIR spectroscopy, photoluminescence and photo-conductivity are used to study the electro-optical properties of the material. We find that the absorption increases slightly with incorporated vanadium, while the below band gap photoluminescence decreases. Additionally, we show results from $In_2S_3$:V p-i-n solar cells utilizing both SnO:F and ZnO:Al as n-TCOs and ZnCo2O4 and NiO as p-TCOs. EQE and JV-measurements reveal the formation of functioning solar cells with so far low short circuit currents.

HL 8.7   Mon 11:15   POT 251

**Investigating photocurrents on a micrometer scale: Ultra-broadband reflection microscopy and photo-current imaging of structured thin-film solar cells** — ●Moritz Gittinger[1], Regina-Elisabeth Ravekes[2], Ralf Vogelgesang[1], Martin Vehse[2], Carsten Agert[2], Christoph Lienau[1], and Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Next Energy EWE Research Centre for Energy Technology, Oldenburg, Germany

Silicon thin-film solar cells are promising candidates in the quest for higher quantum efficiencies. Currently, though, they still suffer from an inefficient light coupling due to the thin, sub-$\mu$m thick absorber material. Light trapping using honeycomb-structured ZnO electrodes appear to be a low-cost and large-scale approach to significantly increase the external quantum efficiency (EQE) of the cell [1]. Here, we present a fast optical far-field technique to map simultaneously the locally-induced photocurrent in and the reflected light from these honeycomb-structured films with varying honeycomb dimensions with micrometer resolution and in a broad spectral range. We observe locally varying photocurrents and reflection signals that reflect the peri-odic variation of local optical density of states of the two-dimensional honeycomb pattern of the cell. The local fluctuations are quantitatively analyzed in terms of a one-parameter scaling theory for random light localization [2] and are correlated to the EQE of the cell. [1] R.-E. Nowak et al., IEEE Journal of Photovoltaics 5, 479 (2015) [2]Th. M. Nieuwenhuizen, M.C.W. van Rossum, PRL 74, 2674 (1995)

HL 8.8   Mon 11:30   POT 251

**Many-body effects in X-ray absorption spectra of the sulfur $L_{2,3}$ edge in $Cu_2ZnSnS_4$** — ●Archana Manoharan[1], Lorenzo Pardini[1], and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]European Theoretical Spectroscopic Facility (ETSF)

The kesterite material $Cu_2ZnSnS_4$ (CZTS) is a promising candidate as an absorber layer for solar-cell applications. In the present work, we study its structural, electronic, and X-ray absorption properties using a first-principles approach. We explore the X-ray absorption spectra at the sulfur $L_{2,3}$ edge in CZTS by solving the Bethe-Salpeter equation (BSE) and compare them to corresponding binary phases, i.e., ZnS and $SnS_2$. Special emphasis is put on the spin-orbit coupling between the S $2p_{1/2}$ and $2p_{3/2}$ core states. In comparison to the independent-particle approximation, the inclusion of Coulomb interaction redshifts the absorption edge in all three materials. In case of CZTS, a bound exciton is found. It is formed by transition from the S $2p_{3/2}$ core state. The second peak with excitonic character is due to the mixing of excitation channels of the $L_2$ and $L_3$ edges. In the binary phases, a bound state is observed in $SnS_2$ but not in ZnS. We assign the bound exciton in CZTS to hybridisation of Sn with S. The calculated BSE results are in good agreement with experimental spectra.