HL 90: Inhomogeneous Materials for Solar Cells

Time: Friday 11:30–13:00 Location: POT 81

HL 90.1 Fri 11:30 POT 81

Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnS_x matrices — •Emilio Scalise[1], Stefan Wippermann[1], Giulia Galli[2], and Dmitri Talapin[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]The University of Chicago, Chicago, Illinois, USA

Recent advances in wet chemical techniques enable the facile synthesis of nanocrystals (NCs) and their assembly into complex solid structures (NC-solids), offering exciting prospects for solar energy conversion, light emission and electronic applications. The properties of these composites are strongly determined by structural details at the NC/matrix interface and the composition of the embedding matrix. We carried out a systematic study of the interaction between InAs NCs and SnS_x matrices using a grand canonical *ab initio* thermodynamics approach to identify general trends for the stability of structural motifs possibly occurring at the NC/matrix interface. The resulting models have been used as a basis for *ab initio* molecular dynamics calculations to investigate the impact of different mass densities and stoichiometries on the internal matrix structure and the NC-solids' electronic properties. We demonstrate that both the NC-matrix interface and the internal regions of the matrix show complex structural features, depending on specific synthesis conditions. Thus to obtain a detailed understanding of experimental data it is necessary to take into account such complex interfacial and matrix-internal structures beyond simplified NC-solid models. S. W. acknowledges BMBF NanoMatFutur grant 13N12972.

HL 90.2 Fri 11:45 POT 81

Formation process of the CIGSe absorber layers in a sequential process — •Sven Schönherr, Philipp Schöppe, Michael Oertel, Udo Reislöhner, and Carsten Ronning — Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

$Cu(In,Ga)Se_2$ (CIGSe) solar cells processed in a sequential process lead to high efficiencies of light conversion. However, the formation of the CIGSe absorber layer in such a process is still not completely clarified. In our process, the metallic precursor on top of a molybdenum back contact was reactively annealed in two steps in a selenium vapour atmosphere where it is typically converted to a CIGSe absorber layer. For a better understanding of the CIGSe formation process we varied the substrate temperature in the first step and aborted the selenization prematurely. X-ray diffraction measurements at the partly selenized layers were taken to indicate binary and chalcopyrite phases. For a detailed characterization, 200 nm thick lamellas were prepared with a focused ion beam. The thin cross sections lead to a high spatial resolution which is mainly limited by the diameter of the electron beam. Energy dispersive X-ray spectroscopy measurements were taken to measure the local element composition. Additionally, cathodoluminescence measurements at the lamellas were used to locate CIGSe chalcopyrite phases and to show where these phases arise during the selenization.

HL 90.3 Fri 12:00 POT 81

Band gap changes in $Cu_2ZnSn(S,Se)_4$ solar cell absorbers with varying Cu concentration — •Mario Lang[1], Tobias Renz[1], Niklas Mathes[1], Markus Neuwirth[1], Thomas Schnabel[2], Simon Woska[1], Heinz Kalt[1], and Michael Hetterich[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — [3]Light Technology Institute, KIT, 76131 Karlsruhe, Germany

The efficiency of $Cu_2ZnSn(S,Se)_4$ solar cells highly depends on the composition of the absorber layer. A Cu-poor and Zn-rich composition is crucial for highly efficient devices. This is due to the fact that unwanted and harmful secondary phases and defects are reduced in this case. The effect of the Cu content is not only relevant for the efficiency but also for certain optical device parameters as, e.g., the band gap. In this contribution we analyse the influence of the Cu content of Cu-poor $Cu_2ZnSn(S,Se)_4$ solar cell absorbers on several optical properties and device parameters. We find an increase in band gap with decreasing Cu content whereas the band tailing does not change. Furthermore, the defect luminescence shifts in parallel to the band gap but does also not change its nature.

HL 90.4 Fri 12:15 POT 81

Effect of buffer layer cations on absorber dopant profiles of Cu(In,Ga)Se2 thin film solar cells — •Florian Werner, Michele Melchiorre, Hossam Elanzeery, and Susanne Siebentritt — Laboratory for Photovoltaics, Physics and Materials Science Research Unit, University of Luxembourg, 41 rue du Brill, L-4422 Belvaux, Luxembourg

The correct interpretation of apparent dopant profiles obtained by capacitance-based techniques on chalcopyrite thin film solar cell absorbers is still debated. We have recently shown that Cd in-diffusion into the absorber might in part explain the observed dopant profiles. We expand on this study by comparing frequency-dependent capacitance-voltage measurements of different buffer/window stacks, e.g. CdS/ZnO, Zn(O,S)/ZnO, and MgF2, on the same absorber. Deconvolution of the measured impedance spectra allows to separate the capacitance of the main junction from parasitic elements. We find parasitic capacitances which agree reasonably well with the geometric capacitance of the respective buffer layer. Dopant profiles constructed from the extracted voltage-dependent junction capacitance exhibit significant differences between different buffer/window configurations and are consistent with cation in-diffusion reducing the surface-near acceptor concentration. This in-diffusion gives rise to a depth-dependent dopant profile and is more pronounced for Cd than for Zn. The MgF2 layer in contrast appears to be stable and we obtain depth-independent dopant concentrations close to 1017 cm-3, comparable to the free hole concentration obtained by Hall measurements on similar absorbers.

HL 90.5 Fri 12:30 POT 81

Charge Carriers Dynamics in Kesterite Band Tails: From Ultra-fast Trapping via Hopping Transport to Cryogenic Microsecond Recombination — •Hannes Hempel[1], Rainer Eichberger[2], and Thomas Unold[1] — [1]Department structure and dynamics of energy materials, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109, Berlin, Germany — [2]Institute for solar fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Kesterite solar cells are known to exhibit band tails originating from atomic disorder. We investigate how these tails affect the dynamics of photo-excited charge carrier by applying transient absorption, time resolved THz spectroscopy and photoluminescence spectroscopy to co-evaporated $Cu_2ZnSnSe_4$ thin film. 100 fs after excitation with 1.5 eV photons the carriers form a hot (>1100 K) Boltzmann distribution in the band states. Within 2 ps they thermalize to lattice temperature and reach simultaneously band edge and tail states. After 10 ps up to 10^{17} cm^{-3} carriers are additionally captured into deeper defect states. Then the carriers are distributed in bands, tails and defects and exhibit in average a localized AC-mobility with a DC-value of 100 cm^2/Vs. Their transport can be described by a sequence of trapping and detrapping between extended band and localized tail states. At low temperatures the carriers further localize into these tail states which slows down their hopping transport to the recombination sites and increases the measured lifetime from nano to microseconds.

HL 90.6 Fri 12:45 POT 81

Intermediate gap states in core/shell nanoparticles for solar energy conversion — •Musa Alaydrus[1], Marton Vörös[2], Gergely Zimanyi[3], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Argonne National Lab, Chicago, USA — [3]University of California, Davis, USA

Multi-exciton generation (MEG) and intermediate band (IB) transitions in semiconducting nanoparticles (NPs) are promising paths towards surpassing the Shockley-Queisser limit in solar energy conversion devices. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk. However, quantum confinement effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum. We propose to introduce intermediate states inside the gap to lower the optical absorption threshold and possibly provide additional

pathways for multi-exciton processes at energies lower than the fundamental NP gap. We investigate the formation of such intermediate states in core/shell NPs from first principles.