

CPP 45: Photovoltaics (joint session HL/CPP)

Time: Wednesday 15:00–17:30

Location: H36

CPP 45.1 Wed 15:00 H36

Revisiting the electronic structure of vanadium doped In_2S_3 — ●ELAHEH GHORBANI¹, PAUL ERHART², and KARSTEN ALBE¹ —
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Transition metal impurities often have noticeable impacts on the electronic and optical properties of the host material. Recently, they have been suggested as intentional dopants for the purpose of creating intermediate metallic bands within the band gap of parent semiconductor. These intermediate bands (IB), if partially filled and optimally placed between valence and conduction bands, can collect photons of sub-band gap energies and enhance the photocurrent density. In this context, the formation of an IB in V-doped In_2S_3 ($\text{In}_2\text{S}_3:\text{V}$) was predicted by first-principles calculations. In this contribution, we revisit $\text{In}_2\text{S}_3:\text{V}$, using a band gap corrected method (hybrid functional) and show that V^{3+} (with $3t_{2g}^2 e_g^0$ configuration) substituting for octahedral In^{3+} is a Jahn-Teller active ion. The aroused Jahn-Teller distortion necessitates removing the degeneracy of t_{2g} levels through splitting it into filled e and empty a sublevels, which reside at the top of the valence band and bottom of the conduction band, respectively. Consequently, no IB forms, when both V and In are in 3+ oxidation state. To give a fuller picture of $\text{In}_2\text{S}_3:\text{V}$, we studied the rehybridization of V d orbitals with S p orbitals for different oxidation numbers of V. Our results show that in the presence of a reducing agent, like H^+ , a totally filled t_{2g} level can form inside the gap.

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Angle-resolved electroreflectance spectroscopy on CIGS solar cell absorber and buffer layers — ●JASMIN SEEGER¹, JONAS GRUTKE¹, WOLFRAM WITTE², DIMITRIOS HARISKOS², OLIVER KIOWSKI², HEINZ KALT¹, and MICHAEL HETTERICH^{1,3} — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — ³Light Technology Institute, KIT, 76131 Karlsruhe, Germany

Thin-film $\text{Cu}(\text{In,Ga})\text{Se}_2$ (CIGS) solar cells can be further improved by replacing the standard CdS buffer layer with an alternative material, which leads to less absorption losses and therefore higher efficiencies. We employ electroreflectance spectroscopy (ER) for the destruction-free determination of the bandgap energies of different buffer materials grown by chemical bath deposition and to get insights into potential interdiffusion processes at the buffer/absorber interface. In this contribution, a new ER technique called angle-resolved electroreflectance spectroscopy (ARER) is presented, which allows the determination of the buffer's bandgap energy. This is possible despite interference effects occurring due to the layered structure and despite the low signal due to the small buffer thickness. To demonstrate the applicability of ARER, results for absorber and CdS buffer layers are shown and compared to results from other ER measurement methods. Additionally, ARER is applied to solar cells with $\text{Zn}(\text{O,S})$ buffer layers, enabling the determination of the sulfur to oxygen ratio of the $\text{Zn}(\text{O,S})$ buffer and yielding hints for the possible formation of mixed phases.

CPP 45.3 Wed 15:30 H36

Spatially resolved composition and functionality of high efficiency $\text{Cu}(\text{In,Ga})\text{Se}_2$ thin film solar cells — ●CHRISTIAN PLASS¹, MAURIZIO RITZER¹, PHILIPP SCHÖPPE¹, SVEN SCHÖNHERR¹, PHILIP JACKSON², ROLAND WUERZ², CLAUDIA S. SCHNOHR¹, and CARSTEN RONNING¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Stuttgart, Germany

$\text{Cu}(\text{In,Ga})\text{Se}_2$ solar cells yield one of the highest efficiencies among all thin film photovoltaics. Compositional variations of the absorber elements as well as incorporated alkali elements significantly affect the conversion efficiency. Hence there is a strong need to determine the composition spatially resolved.

High resolution synchrotron based methods like X-ray fluorescence analysis (XRF) and X-ray beam induced current (XBIC) enable insight into such compositional and functional variations. Simultaneous XRF and XBIC measurements of complete solar cells were conducted

in plan-view geometry: The highly focused X-ray nanobeam at the ID16B-NA station of the European Synchrotron Radiation Facility scanned the solar cell and by analyzing the emitted X-Ray fluorescence radiation together with the corresponding induced current correlating maps are obtained. As the spatial resolution is about 50 nm, we can show how different elemental compositions, grains and grain boundaries influence the measured current.

CPP 45.4 Wed 15:45 H36

Intrinsic point defects in kesterite-type $\text{Cu}_2\text{ZnGeSe}_4$ compound semiconductors — ●DANIEL FRITSCH¹ and SUSAN SCHORR^{1,2} — ¹Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Department of Geosciences, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany

In recent years, kesterite-type compound semiconductors such as $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnSe}_4$ (CZTSSe) received a lot of attention due to their possible application as absorber layers in low-cost thin-film solar cells. However, substituting Ge^{4+} for Sn^{4+} in CZTSSe kesterite-type absorber layers has been shown to improve the optoelectronic properties [1].

Here, we address the computational modelling of intrinsic point defects in kesterite-type $\text{Cu}_2\text{ZnGeSe}_4$ employing density functional theory together with the PBE and the more accurate hybrid functional HSE06. Details of the intrinsic defects' characteristics will be discussed, as well as their influence on the electronic and optical properties.

This work made use of computational resources provided by the North-German Supercomputing Alliance (HLRN), and the Soroban and Dirac HPC facilities of the Freie Universität Berlin and the Helmholtz-Zentrum Berlin, respectively.

[1] R. Gunder, J. A. Márquez-Prieto, G. Gurieva, T. Unold, and S. Schorr, *Cryst. Eng. Comm.* **20**, 1491 (2018).

15 min. break

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2D Sb_2S_3 periodic structure induced absorption enhancement — ●WEI WANG, PATRICK PFEIFFER, and LUKAS SCHMIDT-MENDE — Konstanz University

Sb_2S_3 is a promising candidate for solar cell absorbers due to its high absorption coefficient, suitable band gap and earth-abundant constituents. Here we present the fabrication of 2D Sb_2S_3 structures by direct laser interference method and direct electron beam lithography method. The periodic structure induced absorption enhancement can be observed by UV-VIS absorption spectrum and verified by finite difference time domain (FDTD) simulation.

CPP 45.6 Wed 16:30 H36

Numerical and experimental analysis of the time resolved photo-luminescence method at the buffer-absorber interface of CIGS thin film solar cell — ●ASHWIN HARIHARAN, IEVGENIIA SAVCHENKO, JÖRG OHLAND, HIPPOLYTE HIRWA, and STEPHAN HEISE — LCP, University of Oldenburg, Oldenburg, Germany

The minority carrier lifetime is an important second level parameter which affects the primary parameters of the solar cell. To study the minority carrier lifetime - or more generally, the carrier dynamics -, time-resolved photoluminescence (TRPL) method is a powerful technique. The main result obtained from TRPL is the luminescence decay time (or in some cases more than one decay constant), after which two questions follow: (i) under which circumstances is the decay time a direct indicator of minority carrier lifetime, and (ii) is the correlation between minority carrier lifetime and open-circuit voltage valid across all cases. The primary objective of this research is to understand the first correlation in a more perfect manner by studying the charge carrier separation near the heterojunction of CdS/CIGSe . The study includes both experimental analysis and simulation using, Synopsys TCAD. Experimentally, the main analysis involves wavelength-dependent pulsed illumination through which one gains control of the carrier injection density at different depths inside the absorber layer.

For simulation, accurate representation of material parameters in the space charge region of the junction will be done. Based on the baseline model, dependence between physical parameters must be found in order to establish the agreement between numerical and experimental decay curves.

CPP 45.7 Wed 16:45 H36

The impact of solar cell layer variations on the temperature coefficient of CIGS thin film solar cells — ●HAMSA AHMED¹, JANET NEERKEN¹, JÖRG OHLAND¹, IEVGENIIA SAVCHENKO¹, HIP-POLYTE HIRWA¹, ALFONS WEBER², ROBERT LCHNER², JÜRGEN PARISI¹, and STEPHAN HEISE¹ — ¹University of Oldenburg, D-26111 Oldenburg, Germany — ²Avancis GmbH, Munich, Germany

One of the most promising alternatives in photovoltaic technologies is Cu(In,Ga)(S,Se)₂ (CIGS)-based thin film solar cells, mainly because it has reached over 22% efficiency during the recent years, its high energy yield production, and relatively low temperature coefficients (β_x). The temperature coefficients quantify how the solar cell performance changes with temperature and they play a significant role to maximize the energy yield. In order to investigate the impact of the individual solar cell layers on the temperature coefficients, in this study a systematic characterization was performed on various CIGS solar cells with different layer variations such as the absorber, back contact, and buffer layer. The temperature coefficients were extracted from IV (current-voltage) measurements indoor at different illumination intensities in the range of (20*50)°C. Low temperature IV measurements were accomplished in order to assess the activation energies, and to compare them with the band gap values from glow-discharge optical emission spectroscopy (GDOES) and external quantum efficiency (EQE) measurements. Further analyses were accomplished to examine the recombination; such as thermal admittance spectroscopy (TAS) to correlate it with the diode parameters n and J_0 .

CPP 45.8 Wed 17:00 H36

The impact of solar cell layer variations on the temperature coefficient of CIGS thin film solar cells — ●HAMSA AHMED¹,

JANET NEERKEN¹, JÖRG OHLAND¹, IEVGENIIA SAVCHENKO¹, HIP-POLYTE HIRWA¹, ALFONS WEBER², ROBERT LCHNER², JÜRGEN PARISI¹, and STEPHAN HEISE¹ — ¹University of Oldenburg, D-26111 Oldenburg, Germany — ²Avancis GmbH, Munich, Germany

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CPP 45.9 Wed 17:15 H36

2D Sb₂S₃ periodic structure induced absorption enhancement — ●PATRICK PFEIFFER, WEI WANG, and LUKAS SCHMIDT-MENDE — Konstanz University

Sb₂S₃ is a promising candidate for solar cell absorbers due to its high absorption coefficient, suitable band gap and earth-abundant constituents. Here we present the fabrication of 2D Sb₂S₃ structures by direct laser interference method and direct electron beam lithography method. The periodic structure induced absorption enhancement can be observed by UV-VIS absorption spectrum and verified by finite difference time domain (FDTD) simulation.