HL 10: Photovoltaics: Kesterites and less widely used materials (with DF)

Time: Monday 11:15–13:00   Location: ER 164

HL 10.1 Mon 11:15 ER 164

Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW and the Bethe-Salpeter equation — •Sabine Körbel[1,2], David Kammerlander[2], Rafael Alejandro Sarmiento Pérez[2,3], Miguel Alexandre Lopes Marques[1], and Silvana Botti[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Université Claude Bernard Lyon 1, France — [3]Friedrich-Schiller-Universität Jena, Germany

Self-consistent GW and the solution of the Bethe-Salpeter equation are currently the best approaches to accurately simulate electronic excitations in a vast class of materials, ranging from molecules to solids. However, numerical instabilities, caused by a vanishing band gap in density-functional theory, make it impossible to use the common implementations of these techniques to calculate optical absorption spectra of the best-known thin-film absorbers for solar cells: $Cu(In,Ga)(S,Se)_2$ chalcopyrites and $Cu_2ZnSn(S,Se)_4$ kesterites/stannites. Here we solve this problem by using a finite-difference method in k-space to evaluate the otherwise diverging dipole matrix elements, obtaining excellent agreement with experiment. Having established the validity of this approach, we use it then to calculate the optical response of the less-studied, but promising, $Cu_2ZnGe(S,Se)_4$ compounds, opening the way to predictive calculations of still unknown materials.

HL 10.2 Mon 11:30 ER 164

Formation of Single-Phase Cu_2ZnSnS_4 Thin Films by Control of Secondary Phases in a Solid State Reaction — •Justus Just[1,2], Jan-Christoph Hebig[1,2], Roland Mainz[1], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Bergische Universität Wuppertal, Gaußstraße 20, 42109 Wuppertal, Germany

The conversion efficiency of Cu_2ZnSnS_4(CZTS) based solar cells significantly depends on deposition conditions and specifically the composition of the material. Although best material qualities are observed for Cu-poor and Zn-rich conditions, it has been shown that the compositional region of single phase CZTS is rather small, inevitably leading to a segregation of secondary phases, especially ZnS for Zn-rich material. To overcome this, but still maintain Cu-poor and Zn-rich growth we have developed a two stage co-evaporation process including a thermal treatment. In this process CZTS is formed by a cation interdiffusion process during a solid state reaction of ZnS with ternary Cu_2SnS_3. By oversupplying ZnS the chemical potential of Zn is higher than needed for stoichiometric CZTS, while an uncontrolled segregation of ZnS within the CZTS layer is avoided. This method allows the synthesis of single phase CZTS as shown by X-ray absorption spectroscopy. The final absorber layers show a homogenous distribution of atoms indicating that the solid state reaction is fully completed. To investigate the diffusion kinetics as well as the recrystallization mechanism in-situ real-time X-ray diffraction measurements were performed.

HL 10.3 Mon 11:45 ER 164

Reversible band gap changes in $Cu_2ZnSn(S,Se)_4$ solar cells induced by post-annealing — •Christoph Krämmer[1], Christian Huber[1], Christian Zimmermann[1], Mario Lang[1], Thomas Schnabel[2], Tobias Abzieher[1,2], Erik Ahlswede[2], Heinz Kalt[1], and Michael Hetterich[1] — [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

The absence of the environmentally problematic and expensive metals indium and gallium makes the kesterite $Cu_2ZnSn(S,Se)_4$ (CZTSSe) material system a promising alternative to the established $Cu(In,Ga)Se_2$. Recent publications demonstrated that the amount of $Cu_{Zn}+Zn_{Cu}$ antisite defect pairs can be influenced by post-annealing experiments. This has a direct impact on the band gap E_g of the material. We demonstrate that this effect can be used to reversibly tune E_g within a range of over $100\,meV$ – even in finished solar cell devices. These reversible band gap shifts are detected using electroreflectance. We demonstrate that the band gap of the material is directly correlated to the amount of Cu–Zn disorder and follows the stochastic Vineyard model.

HL 10.4 Mon 12:00 ER 164

Effect of post-annealing on $Cu_2ZnSn(S,Se)_4$ solar cells studied by photoluminescence spectroscopy — •Christian Zimmermann[1], Christoph Kraemmer[1], Christian Huber[1], Mario Lang[1], Thomas Schnabel[2], Tobias Abzieher[1,2], Erik Ahlswede[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

In contrast to the established absorbers for thin-film solar cells such as $Cu(In,Ga)Se_2$ and CdTe, thin-film solar cells based on kesterite absorbers like $Cu_2ZnSn(S,Se)_4$ (CZTSSe) require less toxic and scarce constituents. Recently it has been shown by Scragg *et al.*, that a thermal processing can lead to a change in the ordering of the kesterite Cu–Zn planes (Appl. Phys. Lett. **104**, 041911 (2014)), which could lead to a change in the density of the defect pair $Cu_{Zn}+Zn_{Cu}$. The density and nature of intrinsic defects have a huge influence on the recombination characteristics of kesterites. Hence we use photoluminescence spectroscopy to investigate the influence of post-annealing of solar cells based on solution-processed CZTSSe. Our results lead to the conclusion, that electrostatic potential fluctuations still play a major role in CZTSSe solar cells regardless of the Cu–Zn ordering.

HL 10.5 Mon 12:15 ER 164

Theoretical and experimental approach to optoelectronic study of Nb3O7(OH) — •Wilayat Khan[1], Sophia Betzler[2], Christina Scheu[2], and Jan Minar[1,3] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic — [2]Department of Chemistry, Ludwig-Maximilians-Universität and Center for NanoScience (CeNS), Butenandtstraße 11, 81377 Munich, Germany — [3]Dept. of Chemistry, University of Munich, Germany

Recently, Nb3O7(OH) single crystal has been recommended as a high performing Dye-Sensitized Solar Cell. Theoretical and experimental studies of the Nb3O7(OH) single crystals are performed. The theoretical study were performed by using the full potential linearized augmented plane wave (FP-LAPW) method to calculate the electronic properties The experimental studies were carried out by characterizing this material by EELS [1]. We also performed theoretical calculations using the multiple-scattering Spin-Polarized Relativistic-KKR (SPR-KKR) code to investigate Ok and NbL2,3 egde, in order to support the EELS spectroscopy. The calculated band using the modified Becke Johnson approximation (mBJ) is 2.32 eV which is in comparison to the experimental band gap. The electronic density of states around the Fermi level is dominated by the H-1s and Nb-4p states (VB) and Nb-5d states (CB), which play an important role in optical transition resulting in maximum peaks in the imaginary part of dielectric function. [1] Sophia B. Betzler et al., J. Mater. Chem. A, 2014,2, 12005-12013.

HL 10.6 Mon 12:30 ER 164

Modelling of octahedral tilts in NBT by first-principles — •Kai-Christian Meyer, Melanie Gröting, and Karsten Albe — TU Darmstadt, Jovanka-Bontschits-Str 2, 64287 Darmstadt

In this work we deal with the structural configuration of Sodium Bismuth Titanate (NBT) on a atomistic level by first-principles studies and we link our results to the experimentally observed dielectric properties. NBT is a lead-free relaxor ferroelectric with interesting physical properties around the temperature range from 100-200 °C, where it shows a broad frequency dependent peak in the dielectric constant. Around 200°C the tetragonal and rhombohedral (and octahedral) phase are simultaneously present. We believe that a connection between polar nanoregions (PNR) and planar octahedral defects in a rhombohedral matrix exist. We show among other things that certain chemical orders enhance the probability for PNRs to occur.

HL 10.7 Mon 12:45 ER 164

Formation of n-type defect levels in 1.0 eV GaInNAs layers and their influence on GaInNAs solar cell performance — •Fabian Langer, Svenja Perl, Sven Höfling, and Martin Kamp — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, University of Würzburg, Am Hubland,

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The semiconductor material GaInNAs can be grown lattice matched to GaAs/Ge by molecular beam epitaxy (MBE) with a broad degree of freedom in its bandgap. Besides emerging applications like telecommunication light sensing requiring bandgaps below 0.95 eV, GaInNAs material with a 1.0 eV wide bandgap is of increasing interest for the solar cell industry. Up to now the market for space or concentrator photovoltaic (CPV) is dominated by solar cells made of the material combination GaInP/(In)GaAs/Ge. However, this type of solar cell has reached its practical average efficiency limit. But further improvement by the integration of a 1.0 eV GaInN(Sb)As junction could already be shown. In this presentation we report on the investigation of n-type defects formed during the GaInNAs growth and analyze their influence on the performance of 1.0 eV GaInNAs solar cells. Utilizing these defects we achieved very high internal quantum efficiencies above 90 % due to a compensation effect of the background p-doping in the GaInNAs layer. However, this comes along with a strongly increased dark current generated by the defect states within the bandgap and results in reduced open-circuit voltages of about 0.2 V.