HL 27: Photovoltaics: Innovative Material Systems

Time: Tuesday 9:30–11:00 Location: ER 270

HL 27.1 Tue 9:30 ER 270

Iron based photovoltaic devices: $FeSi_2$ and FeS_2 from first principles — •Timo Schena, Pengxiang Xu, Gustav Bihlmayer, Markus Betzinger, Martin Schlipf, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Photovoltaic devices are one of the most attractive power supplies for the future. To expand their proliferation and guarantee long-term power supply, we explore the possibility to move away from CdTe or In-based cells by researching solar cells from abundant materials as, for example, Fe, Si, S, Zr, Cu.

In this talk we present first-principles results for the electronic structure of the semiconductors β-$FeSi_2$ and the pyrite structure of FeS_2. The calculations have been performed with the `FLEUR` code [www.flapw.de], based on density-functional theory using a full-potential linearized augmented-plane-wave basis set. The bulk structure is examined with different exchange-correlation functionals (LDA, PBE, HSE, PBE0, EXX), also including a one-shot GW calculation, carried out with the `SPEX` code, for describing quasi-particle energies, from which the dielectric function can be extracted. To determine the most stable surface configurations for future calculations, various surfaces of different crystallographic orientations and terminations are compared in energy. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

HL 27.2 Tue 9:45 ER 270

Colloidal zinc oxide nanoparticles in organic and hybrid photovoltaic applications — •Sebastian Wilken, Dorothea Scheunemann, Verena Wilkens, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

In recent years, zinc oxide (ZnO) reached much interest in photovoltaics as a low cost, non-toxic and easy to process n-type semiconductor with a large band-gap of about 3.3 eV. Here, we present a detailed study of wet chemically derived colloidal ZnO nanorods (NRs) with a length and width of about 20 nm and 8 nm, respectively. Homogeneous nanoparticular films, deposited by solution-based techniques, were widely characterized using electron microscopy, X-ray diffraction, optical spectroscopy, and cyclic voltammetry.

As one possible application, we present inverted indium tin oxide-free polymer/fullerene solar cells based on poly(3-hexylthiophene) with an electron-selective interlayer of ZnO NRs, incorporated between the cathode and absorber layer. In the case of an aluminum/chromium cathode a strong increase in power conversion efficiency was achieved compared to cells without interlayer. We attribute this result to optimized contact properties and an enhanced symmetry breaking. Furthermore, we show that our ZnO NRs are also suitable as acceptor material in hybrid polymer/nanoparticle solar cells.

HL 27.3 Tue 10:00 ER 270

Insights into the growing mechanism of electrocrystallised ZnO — •Miriam Schwarz, Karolis Parfeniukas, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campusring 1, D-28759 Bremen (Germany)

Hybrid approaches to solar cells, offer the combined advantage of high mobilities of inorganics with tailored design of organic / polymeric materials in one device. A well designed inorganic scaffold is desired in which the organic material can be embedded. This scaffold requires on one hand, a dense inorganic layer as blocking layer at the interface to the cathode, on the other hand, rods of a high aspect ratio and proper spacing on top to offer a large interface to the organic material. Such well designed hybrid solar cells are expected to outperform fully organic photovoltaics by minimizing tortuous pathways for charges to the appropriate electrodes, typical for organic devices. In this context, we report on the morphological control of crystalline ZnO deposited by electrochemistry at low temperatures (< 100 °C). We relate the time dependent deposition current of the main deposition parameters to certain stages of ZnO growth. Since nucleation occurs extremely fast, the first few seconds (< 15 s) are of special interest. Thus, the analysis of the growing mechanism reveals a rather weak voltage and a strong temperature and concentration dependence. Consequently, tuning the temperature and concentration allows to design the crystal density and shape of the ZnO nanostructures for appropriate hybrid solar cell application.

HL 27.4 Tue 10:15 ER 270

Radiative recombination in kesterite Cu2ZnSnS4 single crystals — •Sergej Levcenko[1], Viktor Tezlevan[1], Ernest Arushanov[1], Susan Schorr[2], and Thomas Unold[2] — [1]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, MD 2028, Moldova — [2]Helmholtz Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

Among the quaternary chalcogenides, Cu2ZnSnS4 (CZTS) semiconductor has attracted much attention due to their potential photovoltaic application. A recent record conversion efficiency value of 8.2% has been achieved on CZTS-solar cell devices [1]. Although there are a number of studies discussing the development of thin film CZTS based solar cells, there are only a few reports concerning the basic material properties of CZTS. Here, we report a detailed study on the emission properties of the CZTS single crystals by photoluminescence (PL) spectroscopy. CZTS single crystals were grown by chemical vapor transport technique using iodine as a transport agent. At low temperature the PL spectrum shows one broad asymmetric band peaked at around 1.29 eV. Temperature and excitation intensities dependences of the PL band indicate that it is due to a free to bound recombination type recombination mechanism that involves a free electron and a trapped hole in the acceptor state with an activation energy of 150 meV. We attribute this acceptor level to Cu on Zn antisite defects.

[1] B. Schin, O. Gunawan, Y. Zhu, N.A. Bojarczuk, S. J. Chey, S. Guha, Prog. Photovolt: Res. Appl. (2011).

HL 27.5 Tue 10:30 ER 270

Radiative recombination in Cu_2ZnSnS_4 thin films with varying composition — •Steffen Kretzschmar, Sergej Levcenco, Justus Just, Bjoern Schubert, and Thomas Unold — Helmholtz-Zentrum Berlin, Institut für Technologie, Hahn-Meitner Platz 1, 14109 Berlin

The quarternary compound Cu_2ZnSnS_4 may be used as an absorber material for thin film solar cells. Although current conversion efficiencies are much lower than for $Cu(In, Ga)Se_2$-based solar cells, 8.4% have been demonstrated recently. Currently, little is known about the optical and electronic properties of this materials, in particular about defects and radiatiative recombination behaviour. In this work Cu_2ZnSnS_4 thin films with widely varying composition, grown by co-evaporation, are investigated by photoluminescence spectroscopy. At low temperature shallow and deep transitions are observed. By temperature and intensity dependent measurements the nature of these transitions are identified.

HL 27.6 Tue 10:45 ER 270

Tiefenprofilierung von Fremdphasen in Cu_2ZnSnS_4 mit winkelaufgelöster Röntgenabsorptionspektroskopie — •Justus Just[1,2], Thomas Unold[2], Dirk Lützenkirchen-Hecht[1], Steffen Kretzschmar[2], Ole Zander[2] und Ronald Frahm[1] — [1]Bergische Universität Wuppertal — [2]Helmholtz-Zentrum-Berlin, Institut für Technologie E-I3

Cu_2ZnSnS_4 (CZTS) in Chalkopyrit-verwandter Kesterit-Struktur bietet sich als alternatives Absorbermaterial für Dünnschichtsolarzellen an. Alle enthaltenen Elemente bzw. deren Verbindungen sind ungiftig und zur Genüge in der Erdkruste enthalten. CZTS und dessen strukturverwandte Fremdphasen werden mittels Nahkanten-Röntgenabsorptionsspektroskopie (XANES) bezüglich ihrer elektronischen Struktur nahe der Leitungsbandkante untersucht. Dies ermöglicht u. A. eine quantitative Identifikation von Fremdphasen in den mittels Ko-Verdampfung hergestellten Dünnschichten. Durch Messung der Röntgenabsorptionsfeinstruktur bei unterschiedlichen Einfallswinkeln wird unter Ausnutzung der Selbstabsorption von Röntgenstrahlung in der Probe eine Tiefenprofilierung von Fremdphasen möglich. Messungen an Probenserien unterschiedlichen Fremdphasengehaltes zeigen Oberflächenfremdphasen, die einige nm dick sind und den Heteroübergang zwischen Absorber und Puffer signifikant beeinflussen können.