DF 4: Photovoltaics (HL with DF)

Time: Monday 14:45–18:30 Location: H2

Invited Talk DF 4.1 Mon 14:45 H2

Surface chemistry of colloidal semiconductor nanocrystals — •Zeger Hens — Physics and Chemistry of Nanostructures, Ghent University, Krijgslaan 281-S3, B9000 Gent, Belgium

Colloidal semiconductor nanocrystals or quantum dots are hybrid nano-objects composed of an inorganic, crystalline core capped by organic surface ligands. This talk addresses recent advances in the understanding of this ligand shell. First, solution NMR will be introduced as a unique, in-situ analysis technique for identifying and quantifying these ligands and for analysing ligand exchange reactions. This has recently led to the classification of nanocrystal/ligand nanocrystals based on the ligand binding motif, where use is made of the covalent bond classification scheme that was originally introduced for the classification of metal complexes. It is shown how this classification enables ligand exchange reaction to be rationalized and predicted and how this now provides researchers with an extensive toolbox to tweak nanocrystal properties at will by changing their surface chemistry. In the last part of the talk, the extension of the approach to metal oxide nanocrystals is addressed. It is shown that these feature a markedly different surface chemistry, which enables for example their use as colloidal nanocatalysts.

DF 4.2 Mon 15:15 H2

Combined Black Silicon Textures for Advanced Antireflective Surfaces — •Maria Gaudig[1,2], Jens Hirsch[1,3], Alexander N. Sprafke[2], Dominik Lausch[3], Norbert Bernhard[1,3], and Ralf B. Wehrspohn[2,4] — [1]Anhalt University of Applied Sciences, Technologies of Photovoltaics Group, Bernburger Str. 55, D-06366 Köthen — [2]Martin Luther University Halle-Wittenberg, Institute of Physics, Group microMD, Heinrich-Damerow-Str. 4, D-06120 Halle (Saale) — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeldt-Straße 12, D-06120 Halle (Saale) — [4]Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, D-06120 Halle (Saale)

Black silicon (b-Si) promises with its extremely low reflectivity to become a real alternative to wet chemical textured silicon in the PV industry. In this work, the nano texturing is realized with a maskless SF6/O2 plasma etch process. Compared to the wet chemical texturing, this method provides benefits like reduced silicon waste, independence of prior surface treatment and crystal orientation and the variation of the texture forms by different plasma processes by different plasma processes. We showed two different plasma textures with absorption about 95 %: (I) a needle like texture (needle height/width ~ 500/100-200 nm) with a strong antireflection and (II) parabolic pits (height/width ~ 2/1 micron) with improved light trapping. In this contribution, we want to go one step further and combine these two techniques to exploit the optical benefits of both textures. For this purpose, the two etch processes are applied successively on the wafer. The experimental data will be discussed and advantages will be highlighted.

DF 4.3 Mon 15:30 H2

Improved light harvesting and carrier collection using transparent nano-textured back contacts in sub-micron chalcopyrite absorber solar cells — •Wiebke Ohm[1,2], Wiebke Riedel[1,2], Ümit Aksünger[2], Martha Ch. Lux-Steiner[1,2], and Sophie Gledhill[1,2] — [1]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — [2]Institut für Heterogene Materialsysteme, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

We investigate bifacial $Cu(In,Ga)Se_2$ (CIGS) solar cells on glass/F:SnO_2 substrates with ZnO nanorods (NR) at the back contact and a reduced absorber thickness ($<1\,\mu m$). Optical simulations of reflection and depth resolved absorption were used to show the potential of ZnO NR in bifacial sub-micron CIGS solar cells to increase the short-circuit current J_{SC}. Next to anti-reflection properties a shift of the absorption closer to the pn-junction was identified for back side illumination enhancing charge carrier collection resulting in an overall J_{SC} increase by up to 30 %. The anti-reflection effect of ZnO NR at the solar cell back contact was observed using optical measurements and the anti-reflection enhancement was estimated resulting in a maximum photo current increase of 2 %. An overall 5 % increase in J_{SC} with NR was achieved, identified in I-V measurements for back side illumination. The external quantum efficiency, however, show that parasitic absorption in the NR-based back contact limits the photo current enhancement, whereas in a wide wavelength range 20 % J_{SC} increase is demonstrated.

DF 4.4 Mon 15:45 H2

Hybrid charge transfer excitons at ZnMgO/P3HT interfaces — •Moritz Eyer, Sergey Sadofev, Joachim Puls, and Sylke Blumstengel — Institut für Physik, Humboldt-Universität zu Berlin

The performance of hybrid photovoltaic devices is strongly related to the efficiency of the charge separation process. In photovoltaic operation excitons generated in the organic and inorganic part diffuse to the interface of the heterojunction. It is suggested that prior to full charge separation a hybrid charge transfer exciton (HCTE) is formed i.e. a coulombically bound charge pair residing on both sides of the interface. Only after dissociation of such a pair a photocurrent is generated.

The formation of HCTE is experimentally verified in planar ZnMgO/poly(3-hexylthiophene) (P3HT) heterojunction devices via electroluminescence (EL) measurements [1]. Radiative recombination across the interface produces EL in the near infrared spectral region. The energy offset ΔE_{IO} between the conduction band minimum of ZnMgO and the P3HT highest unoccupied molecular orbital is tuned systematically by varying the Mg content. Combined analysis of radiative properties and the open circuit voltage V_{OC} in photovoltaic operation shows a clear correlation to the HCTE transition energy.

Investigation of the properties of HCTE yields valuable input for the optimization of the charge separation process at inorganic/organic semiconductor interfaces in order to fully exploit the potential of hybrid devices.

[1] M. Eyer et al., Appl. Phys. Lett. **107**, 221602 (2015).

DF 4.5 Mon 16:00 H2

VUV Pump-Probe Magneto-optical Ellipsometry at ELI Beamlines — •Shirly J. Espinoza-Herrera[1], Bastian Besner[2], Jakob Andreasson[1], and Michael A. Ruebhausen[2] — [1]ELI Beamlines Project, Institute of Physics of the ASCR, 252 41 Dolní Břežany, Czech Republic — [2]Institut fuer Nanostruktur- und Festkoerperforschung, Center for Free-Electron Laser Science, Advanced Study Group APOG, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

A new ellipsometer that is capable of measuring in one run the dielectric function of solid states samples from the IR and the VUV spectral range is being set up at ELI beamlines. ELI is a pillar of the transnational European Extreme Light Infrastructure (ELI) that will hold some of the most intense lasers in the world. The Center for Free Electron Laser in Hamburg is joining this European effort and the work presented here is the development of the pump-probe VUV ellipsometer that will allow the study of materials out of the Fermi level, testing the established tradition of condensed matter physics where most of the phenomena observed are driven the physics close to the Fermi level. Results showing the coupling between the low and high energy levels of freedoms on the case of STO and LAO will be presented.

DF 4.6 Mon 16:15 H2

Synchrotron-based spectroscopy study of the conduction band development in Cu2ZnSn(S,Se)4 with different [S]/([S]+[Se]) ratios — •Tetiana Olar[1], Iver Lauermann[1], Archana Manoharan[2], Lorenzo Pardini[2], Karsten Hannewald[2,3], Claudia Draxl[2,3], Haibing Xie[4], Edgardo Saucedo[4], Binoy Chacko[1], and Martha Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH,Albert-Einstein-Str. 15, 12489 Berlin,Germany — [2]Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, 12489 Berlin, Germany — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [4]Catalonia Institute for Energy Research- IREC, Jadinsde les Dones de Negre 1, 08930 Sant Adrià de Besòs (Barcelona), Spain

Cu2ZnSn(S,Se)4 absorber layers with different [S]/([S]+[Se]) ratios were studied using XPS, UPS, HIKE and NEXAFS. To investigate the band gap transition from the pure sulfide to the pure selenide compound, the valence band maximum (VBM) and conduction band minimum (CBM) were probed. In UPS and HIKE measurements, the relative distance between Fermi level and VBM for the pure sulfide sample was 130 meV larger than for the pure selenide. Using NEX-

AFS to probe the CBM, a systematic study of the positions of K- and L-absorption edges was done and the observed shifts are proportional to the relative shifts in the CBM. The experimental findings are further validated and analyzed by performing corresponding ab initio calculations using the full-potential all-electron code exciting.

30 min. Coffee Break

DF 4.7 Mon 17:00 H2

Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites — Menno Bokdam[1], Tobias Sander[1], Alessandro Stroppa[2], Silvia Picozzi[2], •D.D. Sarma[3], Cesare Franchini[1], and Georg Kresse[1] — [1]Faculty of Physics, Computational Materials Physics, University of Vienna, Austria — [2]Consiglio Nazionale delle Ricerche - CNR-SPIN, L'Aquila, Italy — [3]Indian Institute of Science, Bangalore, India

The development of high efficiency perovskite solar cells has sparked a multitude of measurements on the optical properties of these materials. For the most studied methylammonium(MA)PbI_3 perovskite, a large range (6-55 meV) of exciton binding energies has been reported by various experiments. The existence of excitons at room temperature is unclear. For the MAPbX_3 perovskites we report on relativistic GW-BSE calculations. This method is capable to directly calculate excitonic properties from first-principles. At low temperatures it predicts exciton binding energies in agreement with the reported 'large' values. For $MAPbI_3$, phonon modes present in this frequency range have a negligible contribution to the ionic screening. By calculating the polarisation in time from finite temperature Molecular Dynamics, we show that at room temperature this does not change. We therefore exclude ionic screening as an explanation for the experimentally observed reduction of the exciton binding energy at room temperature.

DF 4.8 Mon 17:15 H2

Stable single-phase Zn-rich $Cu_2ZnSnSe_4$ through In doping — Stefan Hartnauer[1], •Sabine Körbel[2,3], Miguel A L Marques[1,3], Silvana Botti[2,3], and Roland Scheer[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France

Alloying in the system $Cu_2ZnSnSe_4$–$CuInSe_2$–ZnSe (CZTISe) is investigated experimentally and with *ab initio* calculations. The goal is to distinguish stable (single-phase) and unstable (multi-phase) regions within the pseudo-ternary phase diagram. Thin CZTISe films are prepared by co-evaporation of the chemical elements and are investigated in real-time during growth using in-situ angle dispersive X-ray diffraction (XRD). *Ab initio* calculations with density-functional theory are performed to determine the thermodynamic stability of the alloy with respect to the formation of secondary phases. Both in experiment and calculation, we find a surprisingly large single-phase region in the phase diagram for Zn-rich $Cu_2ZnSnSe_4$ if a small amount of In is present, from which we conclude that In doping may help avoiding secondary phase formation under Zn- rich conditions and open up new possibilities for the application of CZTISe thin films in solar cells.

DF 4.9 Mon 17:30 H2

Optical characterization of Cu(In,Ga)Se2 with highly spatially, spectrally, and time resolved cathodoluminescence — •Martin Müller[1], Mathias Müller[1], Frank Bertram[1], Jürgen Christen[1], Torsten Hölscher[2], Setareh Zahedi-Azad[2], Matthias Maiberg[2], and Roland Scheer[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University, Germany — [2]Martin-Luther-University Halle-Wittenberg, Germany

Potential fluctuations and transport parameters are important factors to further improve efficiencies of Cu(In,Ga)Se2 (CIGSe)solar cells. Optical properties of CIGSe absorbers have been studied by means of highly spatially and spectrally resolved cathodoluminescence (CL) to investigate lateral fluctuations and transport parameters. The measurements were performed from low temperature (T = 4.5 K) up to room temperature. CL spectra recorded at 4.5 K, exhibit a dominant emission at 1.06 eV (1170 nm). A shoulder at 1.14 eV (1090 nm) on the low energy side and at 0.99 eV (1250 nm) on the high energy side were observable. In excitation density dependent CL measurements, a blue shift of 25 meV/decade is observed. Additionally, ps-time resolved CL was performed. A dependence of the initial lifetime of more than one order of magnitude from the emission energy could be observed, illustrating relaxation of charge carriers in potential fluctuations. Investigation of panchromatic temperature dependent initial lifetimes reveals a pronounced increase up to 50 K and a subsequent decrease caused by non-radiative recombination. A concept for optical investigations of transport parameters and first results will be presented.

DF 4.10 Mon 17:45 H2

Investigation of shallow defects in $Cu(In,Ga)Se_2$ with time-resolved photoluminescence — •Torsten Hölscher, Matthias Maiberg, Setareh Zahedi-Azad, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle(Saale), Germany

Time-resolved photoluminescence (TRPL) is a powerful method to observe the recombination kinetics of minority carriers in solar cell materials like $Cu(In,Ga)Se_2$ (CIGSe). The influence of a shallow defect (traps) close to the conduction band leads to bi-exponential and curved TRPL-transients due to trapping of minority carriers. TRPL-measurements under increased device temperatures revealed a strong reduction of the second longer decay time, which is may be attributed to the temperature enhanced restitution of the trapped carriers to the conduction band. Saturation of shallow and deep defects became observable by varying the excitation of excess carriers. With Synopsys TCAD® we simulated the recombination behavior of minority carriers in CIGSe as a function of temperature and excitation in the presence of shallow defects. In comparison with the experiments, we obtained in the simulations $E_C - E_t \approx 200$ meV for the energy level, $\sigma_n \approx 10^{-13}$ cm^2 for the electron capture cross-section and $N_t \approx 10^{16}$ cm^{-3} for the density as significant parameters of the trap-state. These trap parameters closely match the N1 admittance signature detected previously - a signature which explanation has been heavily disputed. Our findings now support the explanation of the N1 defect as due to a minority carrier trap. We will discuss the influence of this trap on the solar cell performance.

DF 4.11 Mon 18:00 H2

Plasma-enhanced atomic-layer-deposited MoO_x emitters for silicon heterojunction solar cells — •Johannes Ziegler[1], Thomas Schneider[1], Alexander N. Sprafke[1], Kai Kaufmann[3,4], and Ralf B. Wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg, *μMD Group*, Institute of Physics, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM Halle, Walter-Hülse-Str. 1, 06120 Halle, Germany — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeld-Strasse 12, 06120 Halle, Germany — [4]Hochschule Anhalt Köthen, University of Applied Sciences, Bernburger Str. 55, 06966 Köthen

A method for the deposition of molybdenum oxide (MoO_x) with high growth rates at temperatures below 200 °C based on plasma-enhanced atomic layer deposition (PE-ALD) is presented. The stoichiometry of the of the over-stoichiometric MoO_x films can be adjusted by the plasma-parameters. First results of these layers acting as hole-selective contacts in silicon heterojunction (SHJ) solar cells are presented and discussed.

DF 4.12 Mon 18:15 H2

In-Situ XRD Analysis of the structural Evolution of CZTS Nanoparticles during an Annealing Process — •Marco Brandl[1], Mohamed Sayed[2], Levent Gütay[2], and Rainer Hock[1] — [1]Chair for Crystallography and Structural Physics, Friedrich-Alexander-University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany — [2]Laboratory for Chalcogenide Photovoltaics (LCP), Energy and Semiconductor Research Laboratory (EHF), Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Str. 9-11, 26111 Oldenburg, Germany

A potential method for Kesterite (Cu2ZnSnS4, CZTS) based solar cell production is the synthesis of CZTS nanoparticles by a low temperature wet chemical process. Powders of nanoparticles produced by this process are analysed by X-ray powder diffraction. Initially, these particles have a cubic disordered structure with potential hexagonal stacking faults. With the method of in-situ XRD during an annealing process up to 550°C the recrystallisation to a tetragonal structure of the CZTS as well as the healing of the hexagonal defects can be observed. Furthermore, by mixing the CZTS particles with Selenium powder, the incorporation of Se into CTZS can be studied. The time and temperature resolved observation of the change in unit cell parameters can directly be connected to the Se content in the resulting CZTSSe phase via Vegard's law.