HL 21: Photo-voltaics II

Time: Tuesday 14:00–15:15 Location: EW 202

HL 21.1 Tue 14:00 EW 202

First principles carrier lifetimes, effective masses, and mobilities in $MAPbI_3$ — •Martin Schlipf, Samuel Ponce, and Feliciano Giustino — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Electron-phonon coupling (EPC) fundamentally limits the mobility of charge carriers in halide perovskites. A comprehensive study of all EPC effects has not been conducted fully from *ab initio*, because the organic molecule leads to a large number of atoms in the primitive unit cell. We performed a detailed analysis of the prototypical methylammonium (MA) lead iodide ($MAPbI_3$) in its orthorhombic ground state structure. This contribution assesses the relative impact various scattering channels on the lifetime, mass renormalization, and carrier mobility. A breathing mode of the octahedra emerges as the dominant scattering channel, but two further polar phonon modes exhibit a significant contribution to lifetime and mass renormalization. The coupling to acoustical and transversal phonon modes is weak. The relaxation time of carriers due to this scattering mechanism is below 10 fs at room temperature. The calculated mobilities of the electron and the hole are very similar due to their comparable effective masses and agrees with experimental observations over a wide temperature range. We expect the possibility of higher mobility devices by selective engineering of the identified relevant scattering processes.

HL 21.2 Tue 14:15 EW 202

The application of Direct Laser Interference Pattern (DLIP) on antimony sulfide hybrid solar cell — •wei wang, shaista andleeb, eugen zimmermann, thomas möller, johannes boneberg, and lukas schmidt mende — Department of Physics ,University of Konstanz

Antimony sulfide (Sb2S3) is a promising candidate for hybrid thin film solar cells due to its various favorable properties, such as suitable optical band gap (1.75 eV), high dielectric constant and good band alignment in combination with many organic hole transport materials. In our study, thin layer amorphous Sb2S3 were first spin-coated on the substrates. Then the Sb2S3 film were patterned by direct laser interference. Thin film hybrid solar cells were made by using annealed Sb2S3 film as absorber and P3HT as hole transporter. The photovoltaics performances of the solar cells fabricated from laser patterned Sb2S3 film were superior to the unpatterned ones. Light intensity-dependent current-voltage measurements, transient photocurrent and photovoltage decay measurements, external quantum efficiency measurement as well as total absorption measurement were utilized to characterize the underlying physical mechanisms and measure the photovoltaic device performance.

HL 21.3 Tue 14:30 EW 202

Effect of transition metals on the optoelectronic properties of Nb3O7(OH) — •Wilayat Khan[1], Christina Scheu[2], Lotsch Bettina[3], Ondrej Sipr[1], and Jan Minar[1] — [1]Technologies-Research Center, University of West Bohemia, Univerzitn 8, 306 14 Plzen, Czech Republic — [2]Max-Planck-Institut fr Eisenforschung GmbH, Max-Planck-Strae 1, Dusseldorf, Germany — [3]Department of chemistry and Center for NanoScience, Butenandtstrae 11, 81377 Munchen, Germany

Nb3O7(OH) has a vital role in the water splitting research due to its remarkable efficiency. However, despite this progress, the performance of the Nb3O7(OH) photoelectrode could be substantially increased through doping. Density functional theory, full-potential linearized augmented plane wave method based WIEN2k code was employed to study the effect of doped transition metals in Nb3O7(OH) for the first time. The analysis of the formation energies of doping atoms confirmed that they substitute the Nb atoms within the crystal structure. The electronic structure of the doped- Nb3O7(OH) has also been derived and explained on the basis of relative concentrations of the dopants. The electron energy loss spectra and energy loss near the edge of the structure were calculated and compared with the experimental data, which confirmed the presence of impurity.

HL 21.4 Tue 14:45 EW 202

Thermal Conductivity in Kesterite Crystals — •Martin Handwerg[1,2], Rüdiger Mitdank[1], Laura-Elisa Valle-Rios[2,3], Sergej Levcenco[2], Thomas Unold[2], Susan Schorr[2,3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [3]Free University Berlin, Institute of Geological Sciences, 14195 Berlin, Germany

The kesterite materials Copper-Zinc-Tin-Sulfide (CZTS) and -Selenide (CZTSe) are of huge interest for future solar cell applications, due to the ideal band gap and high absorption rate. Insight in the thermal conductivity of a solar absorption material is important for the thermal management of the cell and therefore for the temperature-dependent efficiency. However, thermal conductivity investigations are rare.
Here we used the 3ω-method to investigate the thermal conductivity of CZTS and CZTSe macro-crystals. The crystal thicknesses were in the range of several hundred micrometers. The metal heater lines with a width of 10 μm were deposited on the polished crystal surface. The measured thermal conductivity is about $3-5$ $Wm^{-1}K^{-1}$. The measured temperature dependence of the thermal conductivity allows conclusions concerning the transport process. Phonon-phonon-Umklapp-scattering dominates the thermal conductivity for $T > 180$ K and point-defect-scattering occurs for $T < 180$ K. With these two scattering processes there is a maximum of the thermal conductivity at $T = 100$ K with increased conductivity values up to 8 $Wm^{-1}K^{-1}$.

HL 21.5 Tue 15:00 EW 202

Exceeding the Shockley-Queisser limit within the detailed balance framework — •Marnik Bercx, Rolando Saniz, Bart Partoens, and Dirk Lamoen — EMAT & CMT groups, Department of Physics, University of Antwerp

The Shockley-Queisser limit is one of the most fundamental theoretical results in the field of photovoltaics. Based on the principle of detailed balance, it defines an upper limit for a single junction solar cell that uses an absorber material with a specific band gap. More recently, Yu and Zunger introduced a more refined selection metric, the Spectroscopic Limited Maximum Efficiency (SLME), which includes the absorptivity of the material in the calculation of the efficiency. We use first-principles DFT calculations based on the HSE06 functional to determine the SLME of the CuAu-like phase of a selected list of I-III-VI_2 compounds, and find several materials with a calculated efficiency above the corresponding chalcopyrite material. Moreover, we find materials for which the calculated efficiency is above the Shockley-Queisser limit. Although it is possible to surpass the Shockley-Queisser limit using several mechanisms, none of these are implemented in the SLME. We show that it is possible to exceed the Shockley-Queisser limit within the detailed balance approach, related to the fact that Shockley and Queisser's assumption of optimal absorption properties also maximizes the recombination current. We conclude that considering a finite thickness for the absorber layer allows the efficiency to exceed the Shockley-Queisser limit, and that this is more likely to occur for materials with small band gaps.