

HL 2: Organic-inorganic perovskite semiconductors (with O)

Time: Monday 9:30–11:00

Location: ER 164

HL 2.1 Mon 9:30 ER 164

Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites — ●SILVIA PICOZZI¹, ALESSANDRO STROPPA¹, DOMENICO DI SANTE¹, PAOLO BARONE¹, MENNO BODKAM², GEORG KRESSE², CESARE FRANCHINI², and MYUNG-HWAN WHANGBO³ — ¹CNR SPIN L'Aquila (IT) — ²Univ. Vienna, Fac. Physics Wien (AT) — ³North Carolina State Univ. Raleigh (USA)

Ferroelectricity is a potentially crucial issue in halide perovskites, breakthrough materials in photovoltaic research. Using density functional theory simulations and symmetry analysis, we show [1] that the lead-free perovskite iodide (FA)SnI₃, containing the planar formamidinium cation FA, (NH₂CHNH₂)⁺, is ferroelectric (FE). In fact, the perpendicular arrangement of FA planes, leading to a "weak" polarization, is energetically more stable than parallel arrangements of FA planes. Moreover, we show that the "weak" and "strong" FE states with polar axis along different crystallographic directions are energetically competing. Therefore, at least at low temperatures, an electric field could stabilize different states with the polarization rotated by 45 degrees, resulting in a highly tunable ferroelectricity appealing for multi-state logic. Intriguingly, the relatively strong spin-orbit coupling in non-centrosymmetric (FA)SnI₃ gives rise to a coexistence of Rashba and Dresselhaus effects and to a spin-texture that can be induced, tuned and switched by an electric field.

[1] A.Stroppa, D.Di Sante, P.Barone, M.Bodkam, G.Kresse, C.Franchini and S.Picozzi, Nature Comms. (in press)

HL 2.2 Mon 9:45 ER 164

In situ XRD monitoring of phases formed during growth of co-evaporated perovskite thin films — ●JULIANE BORCHERT¹, PAUL PISTOR¹, WOLFGANG FRÄNZEL¹, RENÉ CSUK², and ROLAND SCHEER¹ — ¹Martin-Luther-University Halle-Wittenberg, Physics Department, Halle, Germany — ²Martin-Luther-University Halle-Wittenberg, Organic Chemistry Department, Halle, Germany

Currently, information on the phases and crystal structures, which form during the growth and annealing of (CH₃NH₃)Pb(I,Cl)₃ perovskite films is scarce. To gain an insight into these, we studied thin films during their growth. Films were grown through co-evaporation of (CH₃NH₃)I and PbCl₂ or PbI₂. In situ x-ray diffraction (XRD) was utilized to study phase formation in real time. Films grown by evaporation of PbCl₂ and MAI exhibited a cubic crystal structure and two different (CH₃NH₃)Pb(I_xCl_(1-x))₃ phases could be distinguished for varying (CH₃NH₃)I to PbCl₂ flux ratios. They differed in their crystal structure observed by XRD, optical absorption properties and I/I+Cl ratio (either above 0.95 or below 0.5). For films grown with PbI₂ and MAI a tetragonal structure was observed. To monitor thermally induced changes and decomposition, we studied the films during heating. Below 200°C, recrystallization was observed. The chlorine free films additionally showed a transition from tetragonal to cubic structure. Above 200°C decomposition was observed. These results show the strong dependence of the phase formation on varying growth conditions. The formed structures can be monitored and adjusted in real time with the help of in situ XRD.

HL 2.3 Mon 10:00 ER 164

Electroabsorption spectroscopy investigation and hysteresis study of perovskite solar cells — ●CHENG LI¹, STEFFEN TSCHESCHNER², TANAJI GUJAR¹, JOHANNES KIESSLING¹, ANNA KÖHLER², MUKUNDAN THELAKKAT¹, and SVEN HÜTTNER¹ — ¹Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — ²Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany

Solution-processed organic-inorganic perovskite solar cells (e.g. CH₃NH₃PbI_{3-x}Cl_x and CH₃NH₃PbI₃) currently show the highest and most promising performances. However, the hysteresis in the J-V curve, i.e. the history dependence of the applied voltage, is still not sufficiently understood. This hysteresis is related to the way how perovskite solar cells are processed. This process exhibits significant influence on the electronic properties of these photovoltaic devices. In this respect, we study the temperature dependent dynamic processes in these perovskite solar cells by characterizing their current-voltage behaviour. Through this method, we can elucidate the migration of

ions and the origin of the hysteresis behaviour. Furthermore, we also use electroabsorption (EA) spectroscopy, a unique non-invasive characterization approach, to investigate the built-in potential in the working device. In this way, we can understand the interaction at the interface between the perovskite active layer and electrodes, providing guideline to optimize the device architecture.

HL 2.4 Mon 10:15 ER 164

Rutherford Backscattering Spectroscopy of Mass Transport by Transformation of PbI₂ into CH₃NH₃PbI₃ within np-TiO₂ — ●FELIX LANG¹, ALBERT JUMA^{1,2}, VORANUCH SOMSONGKUL^{1,3}, THOMAS DITTRICH¹, and MARISA ARUNCHAHA³ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Tallinn University of Technology, Department of Materials Science, Ehitajate tee 5, Tallinn 19086, Estonia — ³Department of Materials Science, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

A key technique in methylammonium lead iodide (CH₃NH₃PbI₃) thin film preparation is the sequential transformation of an inorganic precursor layer such as PbI₂, infiltrated in nanoporous TiO₂ to the final CH₃NH₃PbI₃ by dipping into an organic precursor solution containing CH₃NH₃I. Here, we present an investigation on the mass transport during transformation by Rutherford backscattering spectroscopy (RBS). Energy dispersive X-Ray (EDX) spectroscopy mapping of cross sections first, revealed a homogenous PbI₂ infiltration in nanoporous TiO₂ before transformation and second, an accumulation of Pb and I at the surface after transformation. Quantitative depth profiles of Pb and I were obtained from RBS analysis. An instant degradation of CH₃NH₃PbI₃ upon ⁴He⁺ ion radiation was found. The concentration profiles of Pb could be simulated with a one dimensional diffusion model taking into account an effective diffusion coefficient of Pb in the nanocomposite (about 1.5 · 10⁻¹¹ cm²/s) as well as a parameter considering frazzling at the surface due to formation of crystallites.

HL 2.5 Mon 10:30 ER 164

Fluorescence studies on organometal halide perovskite nanoparticles — ●NIKLAS MUTZ^{1,2}, CARLOS CÁRDENAS-DAW^{1,2}, MING FU^{1,2}, VERENA HINTERMAYR^{1,2}, MATHIAS VOLLMER^{1,2}, JACEK STOLARCZYK^{1,2}, ALEXANDER URBAN^{1,2}, and JOCHEN FELDMANN^{1,2} — ¹Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Amalienstr. 54 80799 München, Germany — ²Nanosystems Initiative Munich Schellingstraße 4 80799 München, Germany

During recent years organometal halide perovskite based solar cells have shown a significant rise in power conversion efficiency. Despite this improvement in fabricating efficient perovskite solar cells, the underlying photophysical properties are not yet fully understood. An important insight into processes such as charge generation and separation can be obtained by studying single particles instead of disordered films. In this project we investigate the morphology and photoluminescence properties of individual lead halide perovskite particles by varying the chemical synthesis procedure. In particular we investigate their temperature dependent photoluminescence signal and in addition have performed electric field-dependent studies to get insight into the charge separation process.

HL 2.6 Mon 10:45 ER 164

Band structure and optical absorption of halide organometal perovskites from first principles — ●MENNO BODKAM, TOBIAS SANDER, CESARE FRANCHINI, and GEORG KRESSE — University of Vienna, Faculty of Physics, Sensengasse 8, A-1090 Vienna, Austria

The high efficiency of lead halide organic perovskite solar cells has raised many questions on the mechanisms at work here. An accurate description of the macroscopic dielectric properties is essential for understanding the origin of the materials ability to convert light to electricity. In this talk, we present an accurate account of the electronic, optical and excitonic properties of twelve halide organometal perovskites ABX₃ (A = CH₃NH₃⁺, HC(NH₂)₂⁺; B = Pb, Sn; X = Cl, Br, I) by means of many-body first principles methods. We use optimized structures obtained at room temperature using parallel tempering molecular dynamics. Quasi particle band structures and absorption spectra are calculated at the GW₀ level. Electron-hole interactions

have been included in the dielectric function by solving a Bethe-Salpeter equation for the polarizability. We demonstrate that a description beyond independent particles is necessary to describe the onset of the optical absorption. The calculated degree of localiza-

tion of the excitons in k-space indicates Wannier-Mott type excitons with binding energies ranging from 30 meV (ABl_3) and 100-200 meV (ABC_3). To validate our predictions, we compare the results with available experimental data (band gap and optical absorption).