AKE 4: Renewable Energy - Photovoltaics and Electronic Processes

Time: Monday 15:00–16:45 Location: DÜL

Invited Talk AKE 4.1 Mon 15:00 DÜL

Highly Efficient Monolithic Tandem Devices with Perovskite Top Cells — •Steve Albrecht — Helmholtz-Center Berlin, Young Investigator Group Perovskite Tandem Solar Cells

Integrating metal halide perovskite top cells with crystalline silicon or CIGS bottom cells into monolithic tandem devices has recently attracted increased attention due to the high efficiency potential of these cell architectures. To further increase the tandem device performance to a level well above the best single junctions, optical and electrical optimizations as well as a detailed device understanding of this advanced tandem architecture need to be developed. In this talk, Prof. Albrecht will present the recent results on monolithic tandem combinations of perovskite with crystalline silicon and CIGS, as well as tandem relevant aspects of perovskite single junction solar cells. Finally, it will be shown how utilization of a self-assembled molecular monolayer (SAM) and fine tuning of the perovskite band gap in perovskite/silicon tandem solar cells further improved the efficiency to 27.5% and to 23.3% for perovskite/CIGS tandems, the latter being a certified world record efficiency.

AKE 4.2 Mon 15:30 DÜL

Structural and Electronic Contributions of Organic/Inorganic Cations on Perovskite Solar Cells Band Gap — •Mohammad Moaddeli and Mansour Kanani — Department of Materials Science and Engineering, School of Engineering, Shiraz University

New generation of organic/inorganic perovskite photovoltaics is becoming one of the main players for future solar technology, because of their lower cost and simplicity in synthesis process. The progress has facing various challenges in stability and efficiency since last decay. Many groups have developed appropriate experimental and computational methods to overcome those challenges by proposing different combination of organic and inorganic structures. However, lack of proper knowledge of background mechanisms governing electron transport phenomena via such elemental and molecular substitutions, is limiting developing of predictive models. We use modified density functional approach to investigate lattice parameter and long-range electronic effect of cations on band gap and electronic structure of different perovskites. Since no ionic/covalent bond is realized between cation and lead/halide, the van der Waals (vdW) field around cation controls lattice parameter and therefore the bonding length between lead and halide as well as its performance. Results show dominance of the former one for small lattice parameters while by increasing lattice parameter a correlative behavior of both is observed. This let us to draw a predictive approach for selecting organic (or even inorganic) cation for different structural combinations based on cation long range electronic field evaluation.

AKE 4.3 Mon 15:45 DÜL

Topological semimetal YbMnSb2 toward promising thermoelectric performance — •Yu Pan[1], Chenguang Fu[1], Jeffrey Snyder[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187, Dresden, Germany — [2]Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA

Topological semimetals have attracted a lot of interest due to their exotic properties induced by the topological band structure. However, little is known about the thermoelectric properties of these materials. With extremely high mobility and heavy elements induced low thermal conductivity, topological semimetals can be high-performing thermoelectric materials. In this work, we report the thermoelectric properties of topological semimetal YbMnSb2 single crystal. A large Seebeck coefficient of ~160 μV/K at 300 K is obtained and there is no evidence for large bipolar thermal conductivity. Moreover, topologically protected both in-plane resistivity (~1 mΩ*cm) and cross-plane thermal conductivity (~1.5 W/mK) at 300 K are very close to that of the state-of-the-art (Bi,Sb)2Te3 polycrystalline samples, implying YbMnSb2 as promising thermoelectrics. Further enhancement of the thermoelectric performance relies on decreasing the in-plane thermal conductivity and/or the cross-plane resistivity. Taking YbMnSb2 as an example, we clarify the potential of topological semimetals toward high thermoelectric performance.

AKE 4.4 Mon 16:00 DÜL

Simultaneous CO2 fixation and power generation using aqueous Al-CO2 batteries — •Pan Ding[1], Yanguang Li[2], and Ian Sharp[1] — [1]Walter Schottky Institut, TUM, Munich, Germany — [2]Institute of Functional Nano & Soft Materials, Suzhou, China

The energy crisis and excessive emission of CO2 caused by the sharp depletion of fossil energy are two biggest challenges facing humanity. The capture and fixation of CO2 by metal-CO2 batteries have been proposed as *killing two birds with one stone* devices. Here, we reported that 2D Bi nanosheets could be prepared from cathodic conversion of Bi2S3 nanoribbons. It can enable the efficient and robust CO2 reduction to formate at a peak FE of almost 100% (-0.59 V with an initial current density of up to ~208 mA/cm2). Primary Al-CO2 flow battery with Bi2S3 NRs exhibited high formate selectivity at the cathode during discharging. When working at a short-circuit state (0 V), the Al-CO2 battery will transform into a CO2 electrolyzer, and thus highly efficient electrochemical CO2 conversion to formate is available in a power free manner. Moreover, when using recycled Al foils from beverage cans as the source of anode material and photocathodes, the electrochemical performance could be further enhanced in a hybrid solar-driven AlCO2 battery. Therefore, it provides a new solution to electrochemical fixation and utilization of CO2 in a low-cost and green way.

AKE 4.5 Mon 16:15 DÜL

Impact of Interface Roughness on Thermal Transport in Half-Heusler Superlattices — •Sven Heinz[1,2] and Gerhard Jakob[1,2] — [1]Institut für Physik, Uni Mainz, Deutschland — [2]Graduate School of Excellence MAINZ, Mainz, Deutschland

In periodic multilayer structures a large portion of heat can be transported by so called "coherent" phonons [1]. The periodic multilayer structure leads to the formation of stop-bands: certain wavelength bands are suppressed for phonon transport, thereby potentially reducing thermal conductivity [2]. For these effects to be observed, the roughness of the interfaces has to be as low as possible [2].

Investigations will be presented on multilayer structures, in which the interface quality is purposefully deteriorated in part of the sample series by introducing an artificial intermixing layer. This is done by altering the layer sequence from ABAB to ACBCACBC, where C is a mixture of Material A and B. The thin intermixing layer simulates an increased interface roughness, thus destroying coherent transport. Additionally, the intermixing layer can act as a transition layer, lowering the acoustic contrast between the main layers A and B, acting as a so-called phonon bridge [3]. Both effects are discussed in the presentation.

[1] M.N. Luckyanova et al., Science 338 (2012) 936-939.
[2] M. Maldovan, Nat. Mater. 14 (2015) 667-674.
[3] P. Chakraborty et al., Sci. Rep. 7 (2017) 1-8.

15 Minutes Coffee Break