

## DS 2: Fundamentals of Hybrid and Perovskite Photovoltaics (Joint symposium of CPP, DF, DS and HL, organized by CPP)

Time: Monday 9:30–12:15

Location: H1

**Invited Talk** DS 2.1 Mon 9:30 H1  
**Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design** — ●DAVID B. MITZI — Duke University, Edmund T. Pratt Jr. School of Engineering, Durham, NC 27708-0300 USA

Organic-inorganic and related halide-based perovskites (e.g., those based on Pb halide frameworks) have attracted substantial recent interest for solar cell and other optoelectronic technologies, because of the large optical absorption coefficients, high carrier mobilities, long minority carrier lifetimes, and relatively benign defects and grain boundaries. Indeed, these materials have enabled an unprecedented rapid improvement in photovoltaic (PV) performance to levels above 20% power conversion efficiency. Despite the great promise, challenges for the current generation of PV materials include replacing lead with more environmentally benign metals, improving PV device stability (moisture, UV and air) and controlling hysteresis. This talk will explore beyond the current focus on three-dimensional (3-D) lead(II)-based perovskites, to highlight the outstanding structural, chemical and electronic flexibility of the perovskite family. Particular focus will be afforded to systems in which divalent lead is replaced with other metal cations exhibiting a lone pair of electrons, such as Sn, Bi and Sb, since these systems share some of the beneficial electronic structure characteristics of the Pb-based systems. Further discovery within the perovskite structural and chemical space may offer prospects to solve the current technological challenges for perovskite PV and yield important opportunities for energy materials design.

**Invited Talk** DS 2.2 Mon 10:00 H1  
**Perovskite Solar Cells: A new Paradigm in Photovoltaics** — ●MOHAMMAD NAZEERUDDIN — EPFL, GMF, Sion Switzerland

Perovskite solar cells exhibited significant leapfrog in efficiency due to a broad absorption, high optical absorption coefficient, very low exciton binding energy, long carrier diffusion lengths, efficient charge collection, and very high open circuit potential similar to III-IV semiconductors. Unlike silicon solar cells, perovskite solar cells can be developed a variety of low-temperature solution process from inexpensive raw materials. By engineering compositional ratio of perovskite absorber, film formation using anti-solvent, and interface engineering of charge transport materials a remarkable power conversion efficiency of over 21% has been demonstrated, highlighting the unique photovoltaic properties of perovskite materials. In this talk, we present the current progress in perovskite solar cells, various deposition methods for perovskite absorbing layer, synthesis and characterization of novel hole transporting materials, and highlight crucial challenges and prospects

**Invited Talk** DS 2.3 Mon 10:30 H1  
**Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites** — ●LAURA HERZ — University of Oxford, Oxford, UK

Hybrid metal halide perovskites (stoichiometry  $AMX_3$ ) have recently emerged as low-cost active materials in PV cells with power conversion efficiencies in excess of 20%. In addition, hybrid perovskites show prospects for applications in low-cost light-emitting diodes and lasers.

Here we discuss how parameters essential for photovoltaic operation, such as charge carrier recombination and diffusion lengths are altered with substitutions of the organic A cation (e.g. methylammonium versus formamidinium), the metal M cation (e.g.  $Pb^{2+}$  or  $Sn^{2+}$ ) and the halide X anion (I versus Br). We analyze distinct charge-carrier recombination mechanisms, such as trap-mediated, bi-molecular (electron-hole) and Auger recombination, which show different dependences on composition and temperature.

We use these insights to predict charge-carrier diffusion lengths and

radiative efficiencies in the limit of ultra-low trap-related recombination, which could potentially be reached through further advances in material processing. We find that for hybrid lead iodide perovskites with typical charge-carrier mobilities of  $\sim 30\text{cm}^2/(\text{Vs})$ , charge-carrier diffusion lengths under solar irradiation are unlikely to exceed  $\sim 10\mu\text{m}$  even if all trap-related recombination is eliminated. We further show that if high radiative efficiencies are to be obtained for intermediate charge-carrier densities ( $n \sim 10^{14}\text{cm}^{-3}$ ), trap-related recombination lifetimes have to exceed microseconds.

**15 min. break.**

**Invited Talk** DS 2.4 Mon 11:15 H1  
**Photovoltage losses in perovskite solar cells** — ●KRISTOFER TVINGSTED — Experimental Physics VI, Julius Maximilians Universität, Würzburg, Germany

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage (VOC). The VOC of most solar cells is however far from its potential upper limit due to charge carrier recombination of various types, whose origin must be accurately determined. Herein, I summarize what we have learned about these photovoltage losses by studying the radiative part of recombination in Perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far the solar cells are from their own thermodynamic upper limit and further, how they relate to a reference OPV cell. We evaluate the carrier density dependence of the radiative efficiency and associate it to the ideality factor, which in itself represents a uniform figure of merit for the dominant type of recombination. We show that, as the perovskite steady state photoluminescence is strong at open circuit conditions, but substantially quenched only at short circuit, they perform in this respect just as an ideal solar cell should do, and also very different from most OPVs or DSSC cells studied so far. Substantially improving the radiative efficiency to increase the open circuit voltage is a promising route to put these new photovoltaic converters in efficiency parity with the best inorganic counterparts.

**Invited Talk** DS 2.5 Mon 11:45 H1  
**Computational screening of perovskite solar energy materials** — ●KARSTEN W. JACOBSEN — CAMD, Dept. of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In the talk I shall describe computational efforts to identify new materials for efficient light absorption with particular focus on materials in the perovskite structure and water splitting. The materials have to obey a number of criteria in order to work for light absorption and water splitting depending on the particular design of the device. We consider in particular stability, appropriate bandgap and bandstructure for visible light absorption, and an adequate line-up of band edges to the water redox potential. We also identify descriptors to determine defect-sensitivity of the materials.

We have considered several classes of materials with most emphasis on the cubic perovskite structure and derivatives like double perovskites and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with anions O, N, F, or S. Also a range of Sn and Pb based organic and inorganic perovskites have been considered with different combinations of the anions I, Br, and Cl. The possibilities of band gap tuning using atomic-level heterostructures or strain will also be touched upon.

I shall finally mention presently available open databases of relevance for energy materials including the Computational Materials Repository (<https://cmr.fysik.dtu.dk>) where the discussed data are made publicly available.