Bandgap engineering of metal halide perovskite semiconductors

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Metal halide perovskite semiconductors are interesting for stand-alone optoelectronic device applications and may also catalyse the development of large area low-cost hybrid tandem photovoltaics based on commercial silicon technology.[1,2] One prerequisite for efficient hybrid tandem devices is matching the band gaps of the top and bottom cell semiconductor absorber. In Metal halide perovskites (ABX_3), band gaps can be feasibly tuned over a wide range chemical engineering. In regard to hybrid tandem device technology based on bottom absorber materials such as silicon or CIGS, photo-stable higher band gap metal-halide perovskite materials are available that will enable the realization of high efficiency hybrid tandem device technology with efficiencies approaching 30% power conversion efficiencies.[5]

We recently compared many available published experimental data sets of vast compositional variation highlighting the tremendous progress in perovskite photovoltaics in the past years with a particular focus on the state-of-the-art of ABX_3 semiconductors in band gap ranges interesting hybrid tandem devices.[3] This data set comparison gave a more abstract picture of general trends and possible in ABX_3 alloys. As an example, many of the experimental data sets exhibit limited performance enhancements for band gaps larger than 1.7 eV for mixed Br/I perovskites as photo-induced phase segregation, first described by Hoke et al.[4], cause lower energy sites that limit the open circuit voltage and hence power conversion efficiency. We will here present an in-depth analysis of factors determining the energy and dynamic formation of low-energy emitting sites in mixed halide perovskite semiconductors and a reflection on why these low energy sites might be favorable formed during synthesis and whether or not these limitations can be overcome.

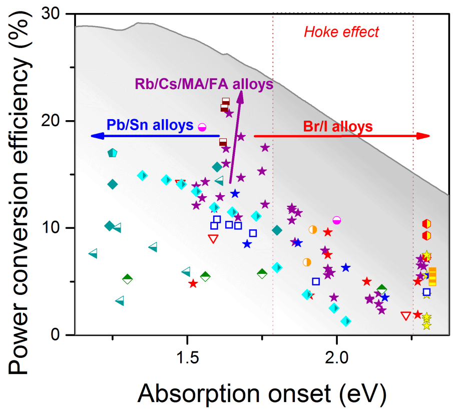

Figure: Visualization of progress and challenges in metal halide perovskite semiconductors with variable band gaps for solar energy conversion.

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