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Wide Band-gap Perovskite Solar Cells

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Wide band-gap perovskite solar cells have the potential for a relatively high output voltage and resilience in a degradation-inducing environment. Investigating the reasons why high voltages with adequate output power have not been realized yet is an underexplored part in perovskite research although it is of paramount interest for multijunction solar cells. Methylammonium lead tribromide ($MAPbBr_3$) with a wide band-gap has the potential to generate an open-circuit voltage close to 2.0 V, close to its 2.3 eV band gap. These types of materials suffer from low performance compared to their lower band-gap counterparts and this is due to the high level of non-radiative losses in both the bulk materials and in devices that leads to reduced carrier lifetimes and voltage loss. Three main approaches can improve the V_{OC} of $MAPbBr_3$ PSCs, i.e., (i) interface passivation techniques that reduce the recombination at the perovskite/transport layer interfaces, (ii) reducing the defect density which can be achieved by improving perovskite crystallization by adding dopants, and (iii) using alternative transport layers.

We demonstrated two ultrathin passivation layers consisting of [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) and Poly(methyl methacrylate) (PMMA), that can effectively passivate defects at the TiO_2/perovskite and perovskite/spiro-OMeTAD interfaces, respectively. In addition, perovskite crystallization was investigated with the established anti-solvent method and the novel flash infrared annealing (FIRA) with and without passivation layers. These modifications significantly suppress interfacial recombination, providing a pathway for improved V_{OC}-values and stability of devices over 140 h.

To make a further V_{OC} improvement, high-quality perovskite thin-films with a low concentration of defects was achieved through cation engineering using a Cs halide salt. We reported the application of green, rapid and solvent-free mechanosynthetic ball milling for the incorporation of the otherwise insoluble CsBr into perovskites, to realize wide band-gap PSCs. The results show that the use of a mechanosynthetic strategy to add insoluble dopants to wide band-gap perovskites provides a promising strategy for the formation of high-quality films.

Considering that the stability of PSCs under operating conditions remains a limiting factor to their application, we tried to use supramolecular strategies in controlling wide bandgap PSCs. We employed dibenzo-21-crown-[7] to mitigate ion migration in the perovskite composition through a host-guest interaction. This emerging approach represents a promising strategy to overcome the perovskite crystal structure as well as the resulting device performances and stabilities.

Furthermore, according to the fact that predicting the performance of solar cells though analytical models is important for the theory-guided optimization of photovoltaic devices, we developed a new model to deeply understand the missing physical phenomena in the widely used existing models.

Jury members:

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