PerTPV – Perovskite thin film photovoltaics

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Report of required perovskite absorber parameters which indicates good PV performance

WP1

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1. Single Junction Cells

To reach the highest efficiency with only absorber material it has been shown before that the bandgap of that material should be around 1.4 eV (Figure 1).

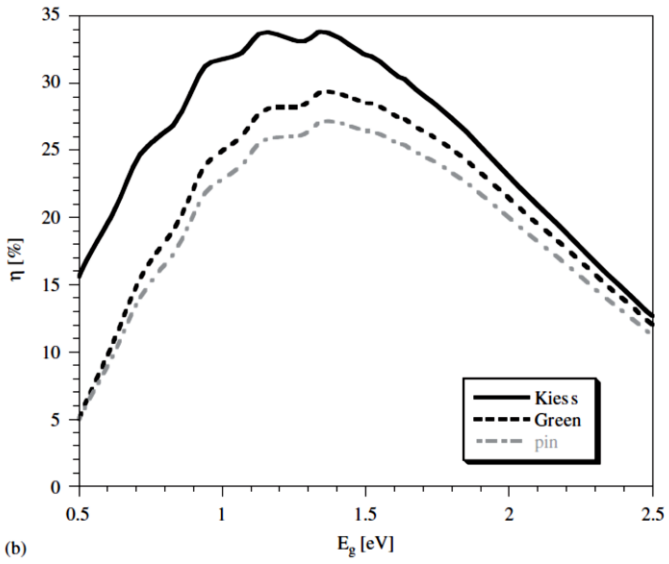


Fig. 1. Upper limits of the efficiency of single junction solar cells, as a function of the gap energy Eg: thermodynamical limit, semi-empiricallimit and p–i–n diode junction limit [adopted from Solar Energy Materials & Solar Cells 90 (2006) 2952].

Perovskite based on formamidium lead iodide ($FAPbI_3$), with a bandgap of 1.48 eV, represents the simplest compositional perovskite close to the targeted value. However, $FAPbI_3$, suffers from phase instabilities if no additional components are added. Therefore, the methylammonium lead iodide ($MAPbI_3$), with a bandgap of 1.55 eV is still a very promising candidate for high efficiency perovskites.

Besides having a bandgap as close to the optimum value, it is also important that the material exhibits additional optoelectronic properties such as high absorbance, high carrier diffusion length, (related) low trap density, as well as thermal stability. The absorbance of perovskite is generally sufficient to use films with a thickness of 500 nm that absorb >90% of the incident light (with an energy higher than the perovskite bandgap).

Thermal stability, preferably in excess of 85 °C, is another desired property for efficient use in photovoltaic applications. Generally, perovskites containing MA are considered less stable to high temperatures, however, some reports indicate that with proper film preparation, passivation or device sealing also MA containing perovskites can have the required thermal stability.

Nevertheless, perovskites using FA mixed with a small amount of Cs have been reported to be more thermally stable. These formulations, however, have a slightly higher bandgap reducing the maximum achievable efficiencies of the solar cells using this type of perovskite material.

Another important requirement for high efficiency solar cells, is to ensure a low trap density. There is up to now no clear relation between trap density and perovskite material composition. In some cases larger grain sizes have led to improved PV performance due to higher open circuit voltages (Voc's). Also the passivation of interfaces with a variety of materials has led to similar effects; however, this cannot yet be translated to a preferred perovskite composition.

There is a clear trend and known relationship between external radiative efficiency (ERE) of the solar cell, and open-circuit voltage, with increasing ERE leading to increased voltage. The very best in class perovskite solar cells today, have an ERE of ~ 2%, which is comparable to silicon PV cells, but inferior to GaAs which stands at ~20%. ERE is a property of the complete solar cell. However, the external photoluminescence quantum efficiency (PLQE) of the absorber layer is also a good indicator as to whether the material will subsequently perform well and deliver a high ERE and subsequent open-circuit voltage in the solar cell. Since there are more losses induced in the construction of the complete solar cell than in the isolated perovskite film, the PLQE is usually higher than the ERE. We therefore deem a thin film PLQE of 5%, for films processed on glass substrates, as the bench mark required for a new absorber layer to be transferred into the cell fabrication work stream.

2. Tandem Cells

For double junction or tandem solar cells, a lot of parameters described for the single junction perovskite absorber materials are the same, with the notable difference of the bandgap for the perovskite used in the front and real cell of the PV device. Hence, also for the tandem cell absorbers it is important that they have a high absorbance, are thermally stable, and have a high carrier diffusion length and low trap density.

Calculations have demonstrated that the highest efficiencies for a two terminal tandem cells using two different absorber materials can be reached if the front cell (in the figure referred to as top cell) and the back cell (in the figure referred to as bottom cell) have absorber materials with a bandgap in the range of 1.65 to 1.85 eV and 1.0 to 1.23 eV, respectively (Figure 2). The lowest reported bandgap for a perovskite absorber leading to good efficiency in single junction cells is 1.2 eV [Science, Snaith et al.] This low bandgap perovskite has the following composition ($FA_{0.75}Cs_{0.25}Pb_{0.5}Sn_{0.5}I_3$). It was recently shown that this composition leads to single junction PV devices with a power conversion efficiency (PCE) of 17 % that exhibit a stability in excess of 95 % at 100 °C over more than 100 hours. Hence, this composition (or similar) is the targeted perovskite for the low bandgap absorber for the back cell in the tandem device.

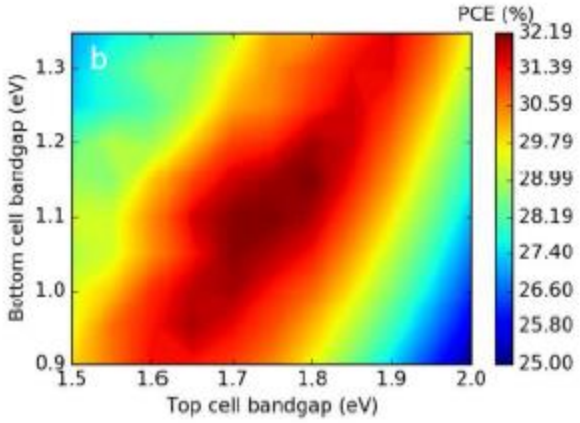
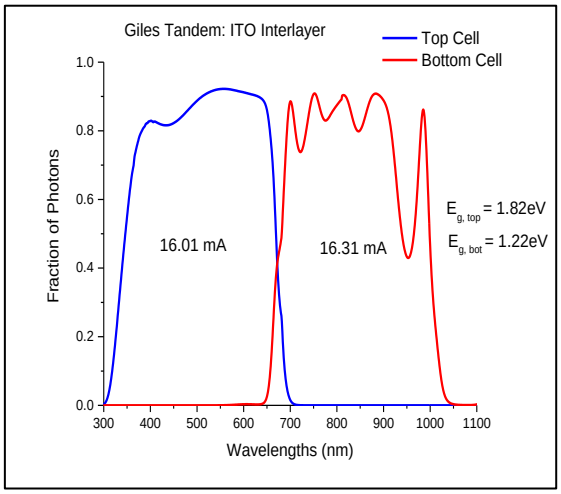


Fig. 2. All-perovskite double junction PCE for varied band-gap combinations of bottom (back) and top (front) absorber.

As mentioned the most promising low bandgap perovskite absorber has a bandgap of 1.2 eV. This implies that, taking into account the calculations leading to Figure 2, the front cell absorber should have a bandgap around 1.8 eV. This bandgap is only slightly above the archetype perovskite absorber employing $MAPbI_3$ and many reports have demonstrated that the bandgap can be increased by substituting a small part of the iodide by bromide ions. For example a promising composition that has led to stable perovskite and single junction solar cells with efficiencies above 18 % is the following: $FA_{0.83}Cs_{0.17}Pb(I_{0.6}Br_{0.4})$. However, this has a band gap of 1.74eV, and hence required further tuning to push towards 1.8eV.

We have recalculated the optimised tandem solar cell efficiency using our presently best in class low band gap perovskite absorber material, $FA_{0.75}Cs_{0.25}Pb_{0.5}Sn_{0.5}I_3$, which has a band gap of 1.22eV. We show the calculated EQE and estimated solar cell performance parameters in Figure 3. Form these calculations we can specify that we need to aim for a top-cell band gap of 1.82eV, and attempt to increase the absorber layer thickness' up towards 1.3 microns.



Layer	Thickness
Top Perovskite (Range: 1000-1500nm)	1301 nm
Bottom Perovskite (Range: 1000-1500nm)	1369 nm
Interlayer (Range: 50-250nm)	203nm

PCE	28.83%
J_{sc}	16.01
V_{oc}	2.18
FF	0.83

Figure 3. Calculated EQE spectrum for a perovskite-perovskite tandem cell (left). Thickness of perovskite absorber layers and ITO intermediate interlayer (top right). Solar cell performance parameters estimated from parametrised diode model.

Naturally, if a perovskite absorber with good stability can be developed with a bandgap below 1.2 eV it is possible to further raise the 2T tandem cell efficiency. However, currently it is not clear what the composition of such very low bandgap perovskite would be. Our best efforts to raise the efficiency should therefore be spent on optimisation of the thickness of each layer, and maximising the open-circuit voltage of each sub cell.

3. Conclusion

A key parameter of a perovskite absorber that determines the achievable efficiency of a single junction and tandem solar cells is its bandgap energy. Besides this very important parameters are that the material has a high absorbance, is thermally stable and has a high carrier diffusion length. The latter is very much influenced by the recombination in the solar cell, and ERE and PLQE are good metrics to quantify non-radiative losses. Therefore the targeted materials are:

1. Band gaps of 1.22eV or lower for bottom cell
2. Band gap of 1.82eV for top cell
3. PLQE of isolated perovskite films > 5%.

For single junction perovskite solar cells we therefore conclude that the most promising absorber composition is one that contains FA, Cs, Pb, I, aiming for a bandgap close to 1.55 eV.

For a 2T tandem perovskite solar cell, we conclude that the most promising compositions for the front and back cell absorbers are:

Low bandgap bottom cell absorber: $FA_{0.75}Cs_{0.25}Pb_{0.5}Sn_{0.5}I_3$

High bandgap top cell absorber: $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ with band gap ~1.8eV