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Understanding the Efficiency Limits of Perovskite Solar Cells

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Perovskite solar cells have demonstrated great potential over recent years with rapid increase in device efficiency through modifications in transport layers, perovskite composition, and interface engineering. To obtain further improvements, it is useful to develop a better understanding of where in the device the efficiency reductions occur – is it the bulk properties, the interfaces or the transport layer properties?

Through modelling it is possible to develop an understanding of the efficiency limits imposed on a device as a result of the basic properties of the absorber and interfaces with transport layers. This can allow us to understand how much further a device based on a particular absorber material can be pushed, or to what extent the absorber properties need to be improved.

In this work we use a numerical drift and diffusion solver incorporating mobile ions to investigate the change in device efficiency with respect to carrier mobility, for different recombination schemes and recombination lifetime. We also investigate the impact of mobile ions on the efficiency limits for each of the cases. To determine the efficiency limits, we assume ideal transport layers with bands that are optimally aligned to the absorber.

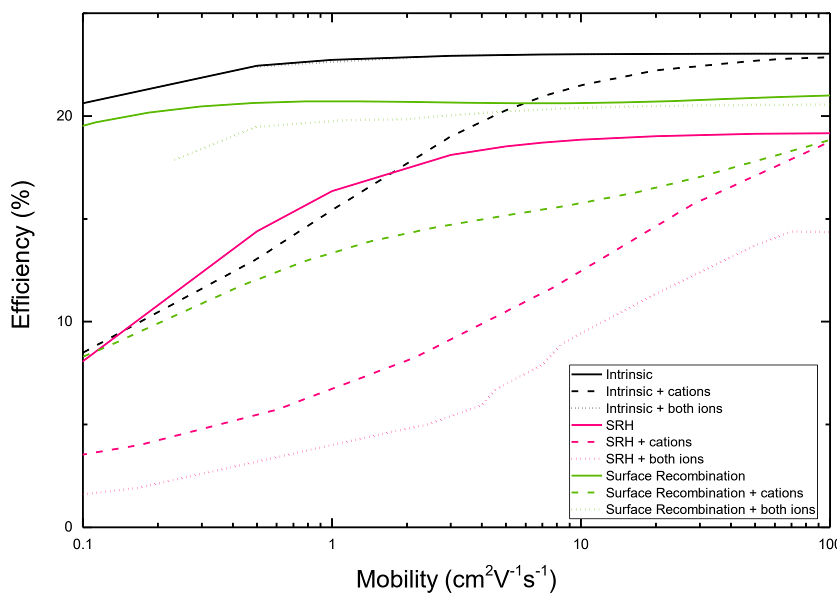

Figure 1 Simulated device efficiency as a function of carrier mobility assuming ideal band alignment and transport layers. Black line represents a device that is only limited by radiative recombination, pink lines represent devices with mid-gap bulk Shockley-Read-Hall recombination at a concentration of $5x10^{15}$ cm^{-3}, and green lines represent devices with no bulk SRH recombination, but a high surface recombination velocity of 1x106 cm /s for both carriers.

We demonstrate that for a perovskite material with only radiative recombination, only at low mobility levels will the device performance be impacted, but once past a certain mobility level, the efficiency plateaus and further increase will not result in performance improvement, which is consistent with the work of Kirchartz and Rau.[1] Such a plateau still exists when Shockley-Read-Hall recombination is added into the equation, but the device is now somewhat more sensitive to carrier mobility, and a high mobility is required to reach the efficiency limit. Here, we simulated mid-gap defects with a density of $5x10^{15}$ cm^{-3}, which reduces V_{OC} in the high mobility limit by 130mV.

The presence of mobile ions generally results in a substantial decrease in device performance, particularly when only one type of ion is present. In addition, the presence of ions leads to a greater sensitivity of device performance on the carrier mobilities in the absorber, with substantially higher mobilities being required to reach the limiting efficiencies. In the case of two types of mobile ions of equal concentration but opposite character (one anion and one cation) the impact of the mobile ions is greatly reduced.

These results show that the impact of mobile ions on device performance is generally, but not always, detrimental. Under certain conditions, their impact is minimal. The results also suggest that mobilities of at least $10cm^2/V$-s in the absorber should be targeted to ensure the carrier mobility does not limit device efficiency.

References

[1] Kirchartz, T. and U. Rau, 201, 'Decreasing Radiative Recombination Coefficients via an Indirect Band Gap in Lead Halide Perovskites', *The Journal of Physical Chemistry Letters*, 8(6), p1265-1271.