More is Different: the Effects of Mobile Ions on the Device Performance of Perovskite Solar Cells

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Overview

Metal halide perovskites are mixed ionic-electronic conducting materials which show great promise for application in next generation solar cells. The presence of mobile ions in perovskite solar cells significantly impacts their device physics as the ions can redistribute in the active layer and thus screen the electric field. Here, we use device simulations and voltage-dependent photoluminescence to show that this ionic field screening leads to electronic carrier accumulation and increased recombination losses at short circuit. By contrast, our simulations suggest that mobile ions can be beneficial at open circuit as they supress surface recombination currents and make the open circuit voltage more tolerant to energetic offsets between the perovskite and its transport layers.

Short Circuit Conditions: the Effects of Built-in Field Screening

Bulk Field Screening by Mobile Ions Under Short-Circuit Conditions

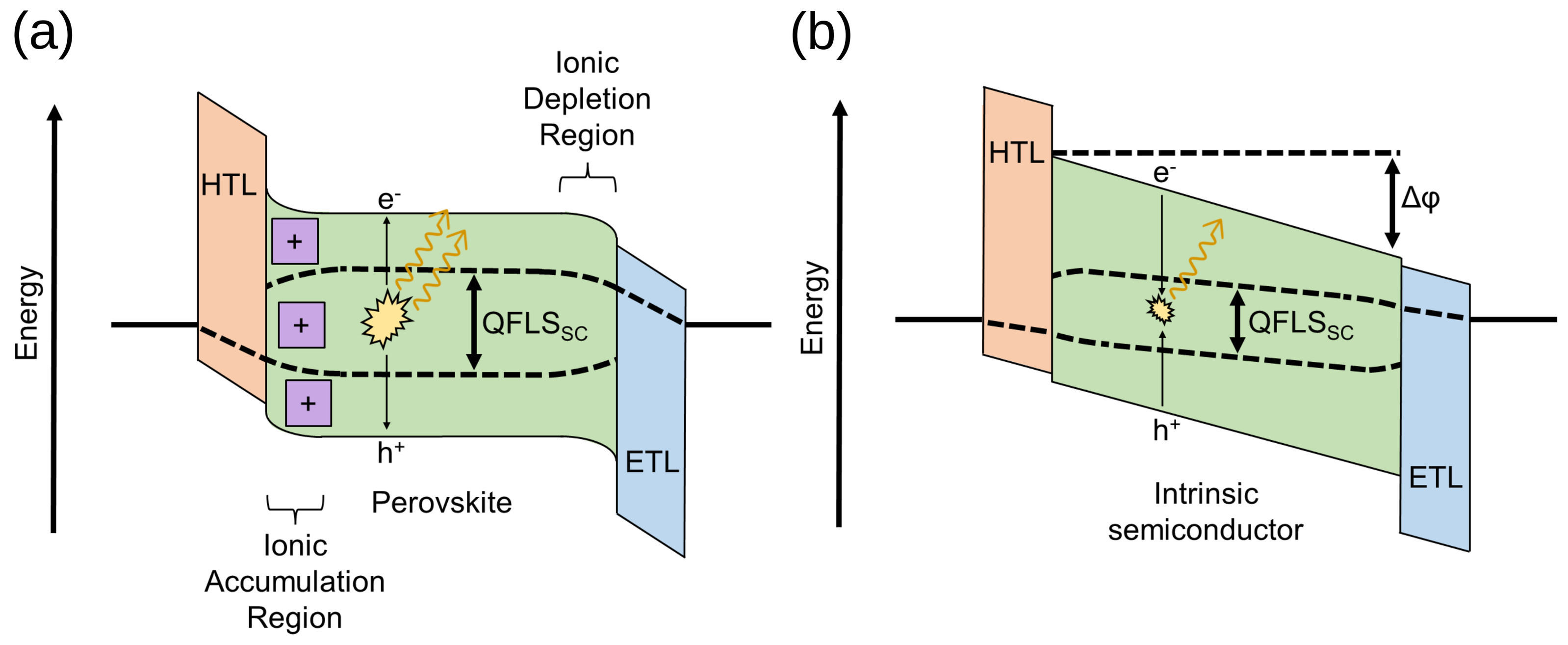
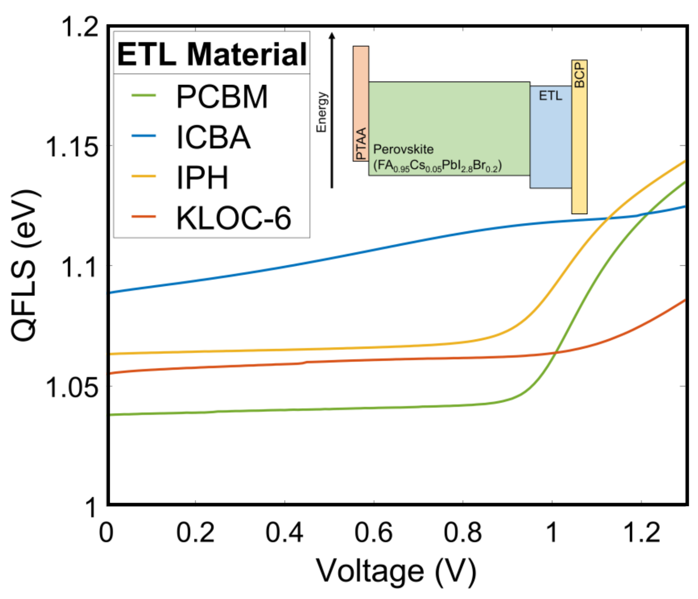


Figure 1: Comparison of the band diagrams for p-i-n devices at short circuit (a) with and (b) without mobile ions. The mobile ions in (a) redistribute and screen the potential drop across the active layer due to the built-in potential, Δφ, reducing electronic carrier extraction efficiency.

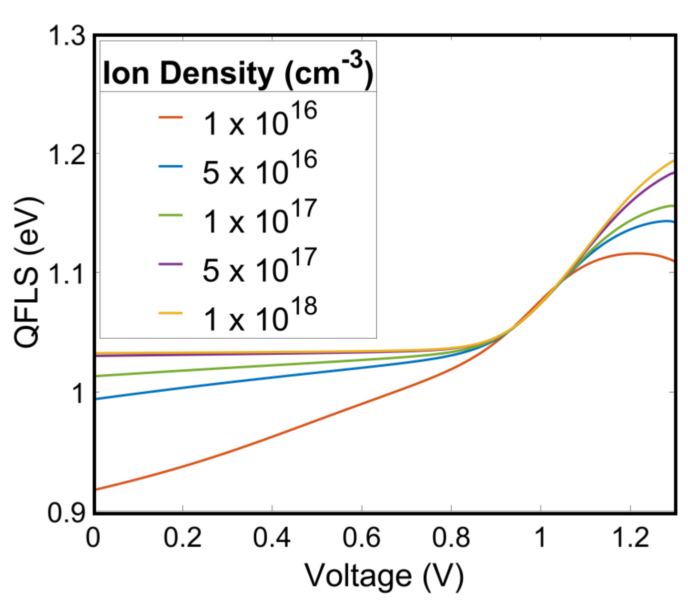
Predicted Consequences of Ionic Field Screening:

1. Increase in short-circuit Quasi-Fermi Level Splitting (QFLS$_{SC}$) and photoluminescence.
2. Reduction in short-circuit current density.

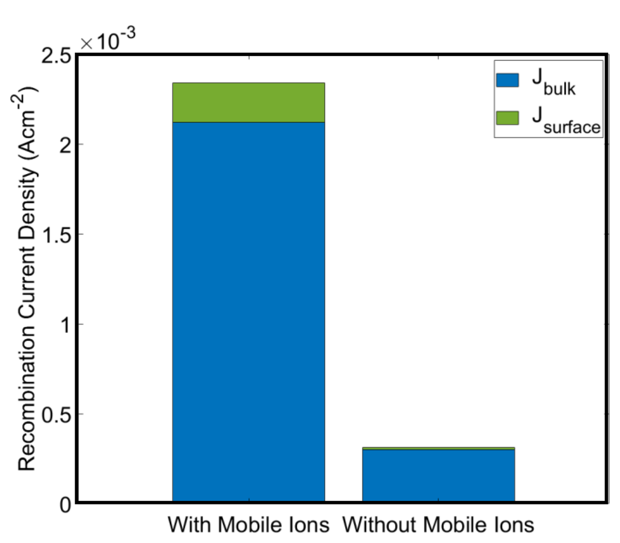
Voltage-Dependent Photoluminescence: Experimental Evidence for Ionic Field Screening



- Measured voltage-dependent photoluminescence on four p-i-n perovskite solar cells with varying electron transport layers (left, device structure shown in inset).
- All four devices had a QFLS$_{SC}$ of over 1 eV.



- Simulated champion device to investigate link between ionic field screening and QFLS$_{SC}$.
- Results indicate a mobile ion density of over 10^{17} cm^{-3} is necessary to match experimental values of QFLS$_{SC}$ (right).



- Presence of mobile ions in the simulated device reduced the average extraction velocity by an order of magnitude.
- Led to increased recombination losses at short circuit (left) and a reduction in short circuit current density of ~ 2 mA cm^{-2}.

Acknowledgements

We thank ATIP for funding this research and also thank the Durrant and Barnes groups for their support and guidance.

Open Circuit Conditions: Ionic Modulation of Surface Recombination Currents

Ionic Modulation of Interfacial Electronic Carrier Densities Improves Open Circuit Voltage

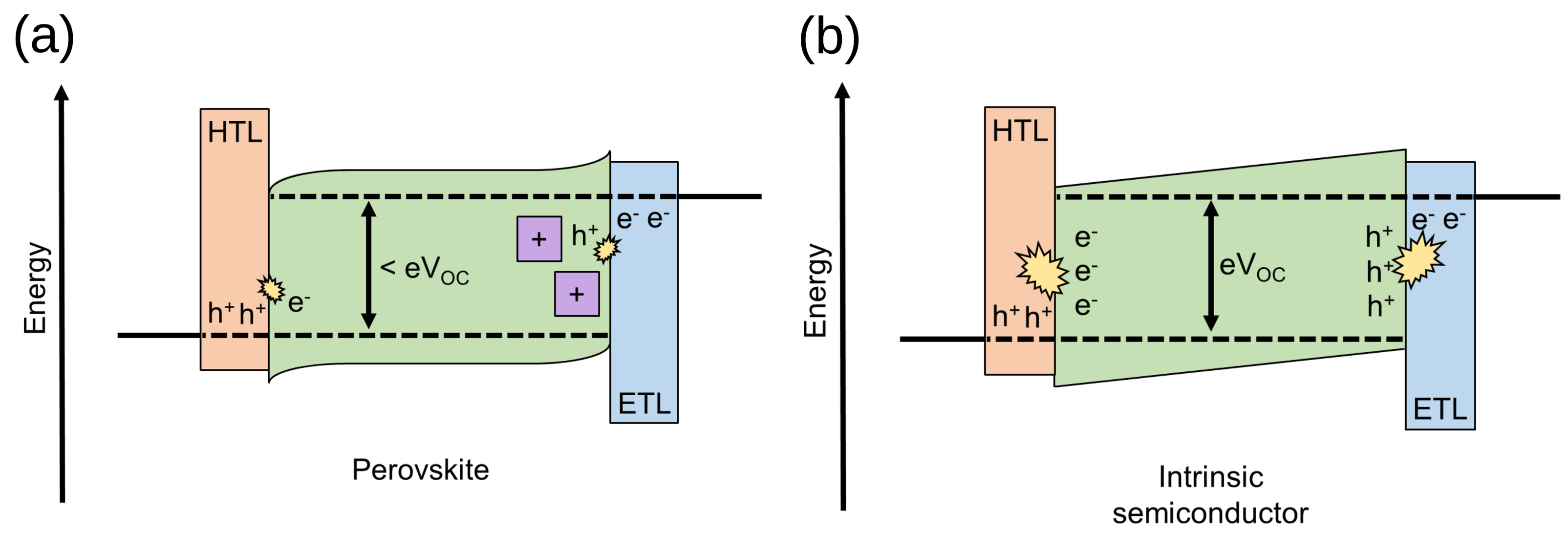
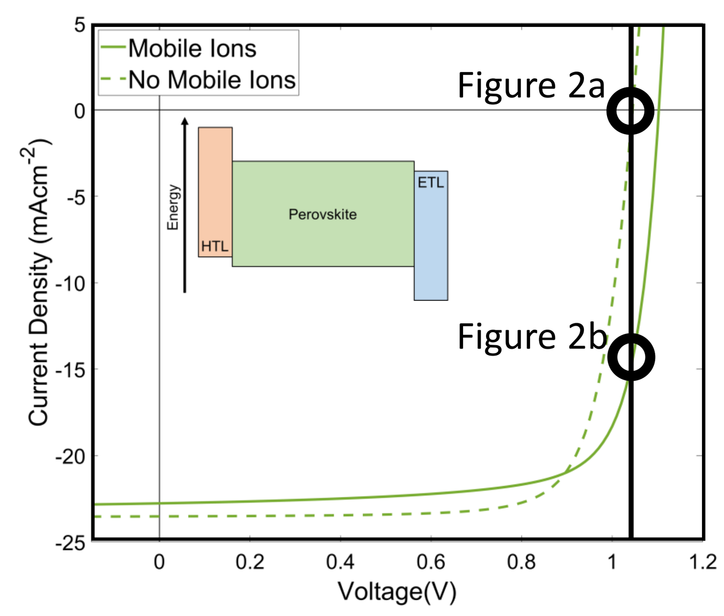


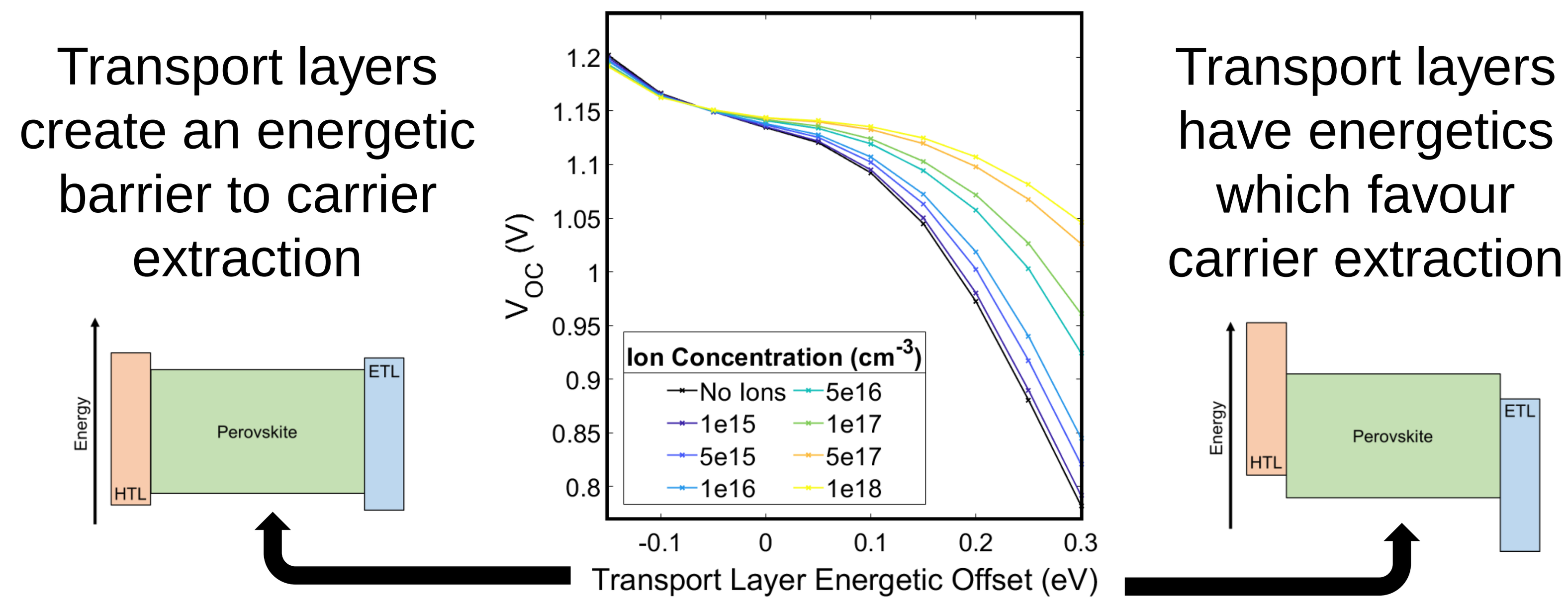
Figure 2: Band diagrams (a) with and (b) without mobile ions drawn under open circuit conditions for the intrinsic semiconductor (see J-V curves, below). This is below the open circuit voltage (V_{OC}) for the perovskite, since the presence of mobile ions reduces the rate of surface recombination losses at a given QFLS. Band bending in the transport layers has been neglected for clarity.



- Figure shows simulated J-V curves for the p-i-n perovskite device structure shown in the inset.
- Device including mobile ions has better performance due to its significantly higher V_{OC}.

Presence of Mobile Ions Makes Open Circuit Voltage More Tolerant to Transport Layer Energetic Offsets

- Investigated how the magnitude of the ionic improvement to V_{OC} depends upon the energetic offsets to the transport layers.
- Found that presence of mobile ions increases V_{OC} in all devices where there is an energetic offset to the transport layers which favours carrier extraction.



Conclusions

- Field screening by mobile ions reduces short circuit current density.
- Mobile ions can lead to a significant increase in V_{OC} when there is an imperfect energetic alignment between the perovskite and its transport layers.
- Overall impact on PCE is a competition between these two factors (right).