

# Understanding the Efficiency Limits of Perovskite Solar Cells

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# Motivation

- Numerous literature reports on the existence of mobile ions in perovskites
- Causes certain phenomenon such as hysteresis in IV scans
- Widely studied on their impact if the cell is in transient state
  
- What about steady state?
- How do ions interact with other cell parameters, such as traps in bulk material?

# Methodology

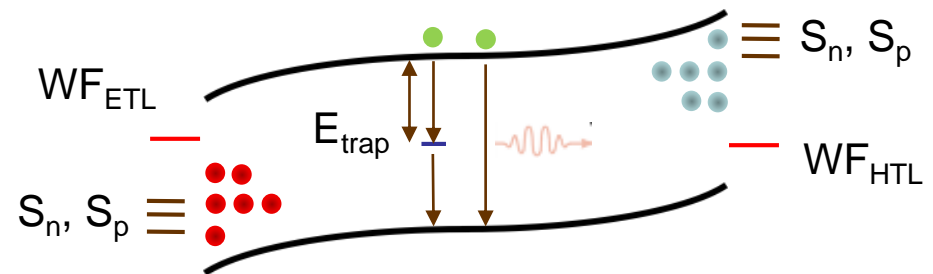
## Simulation is performed using Quokka



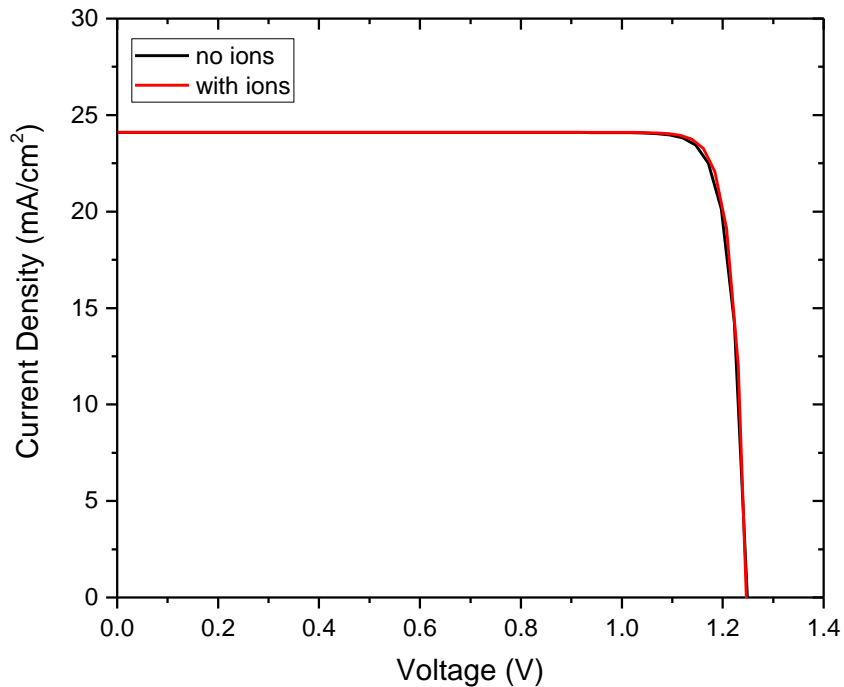
- 1D drift and diffusion model
- Incorporation of mobile ions as free charged particles
- Transport materials are modelled as fixed work function materials

## Perovskite cell setup

- Symmetrical band alignment on ETL and HTL sides
- Band offset of 0.2eV at the interface
- Mobile ion mobility does not matter here



# Impact of mobile ions with only radiative recombination

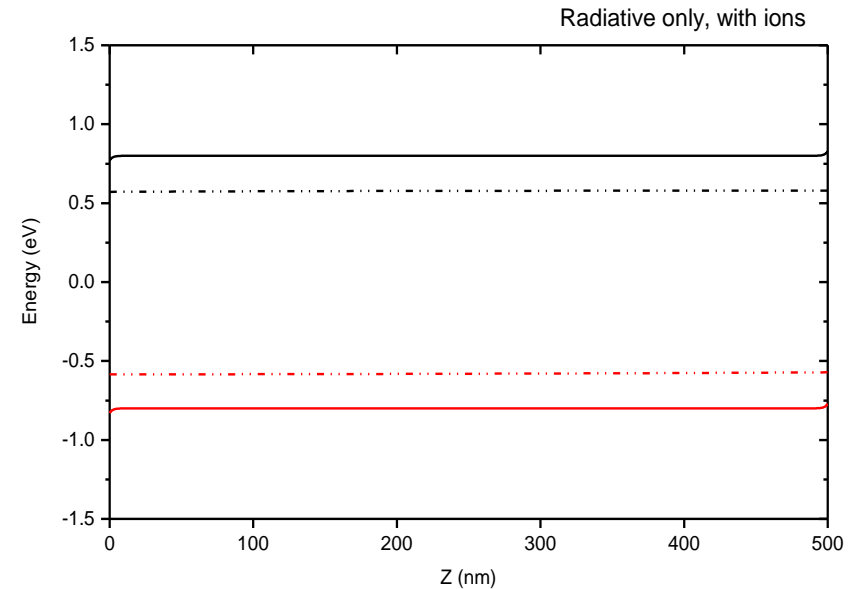
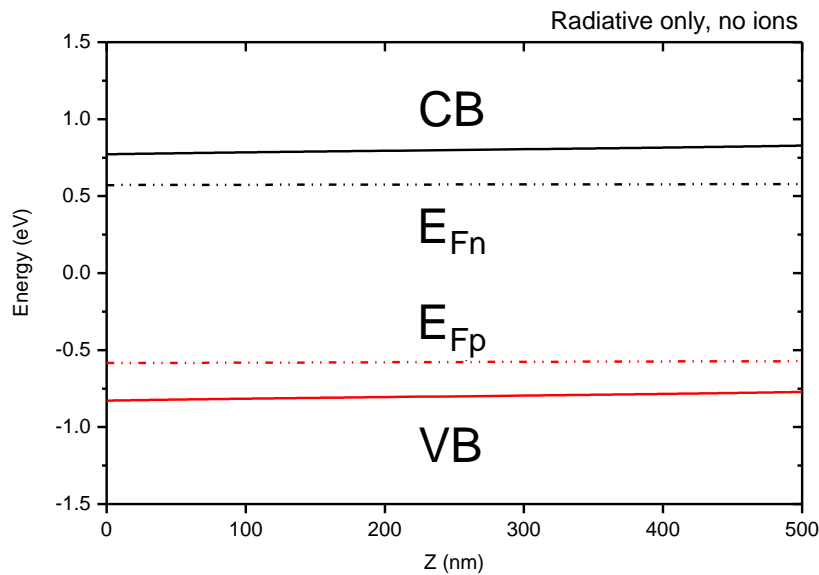


Mobile ion concentration:  $5 \times 10^{18} \text{ cm}^{-3}$

Carrier mobility:  $1 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$

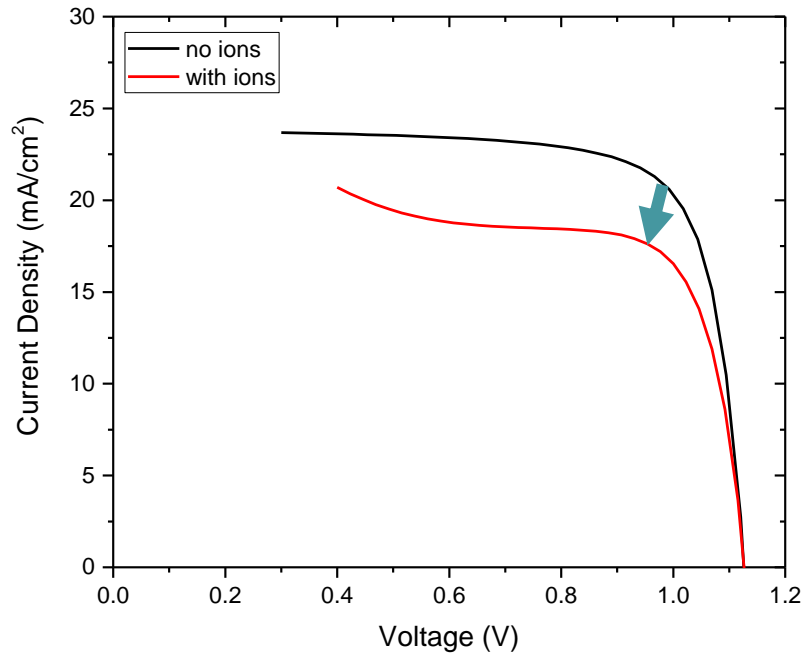
	No ions	With ions
$V_{OC}$ (V)	1.249	1.247
$J_{SC}$ (mA/cm <sup>2</sup> )	24.10	24.08
FF	89.31%	89.10%
$\eta$	26.87%	26.76%

# Impact of mobile ions with only radiative recombination – at MPP



- Flattened CB and VB due to mobile ions – removal of internal electric field
- No change in qFL due to loss of electric field
- Diffusion length > device thickness

# Impact of SRH recombination with mobile ions

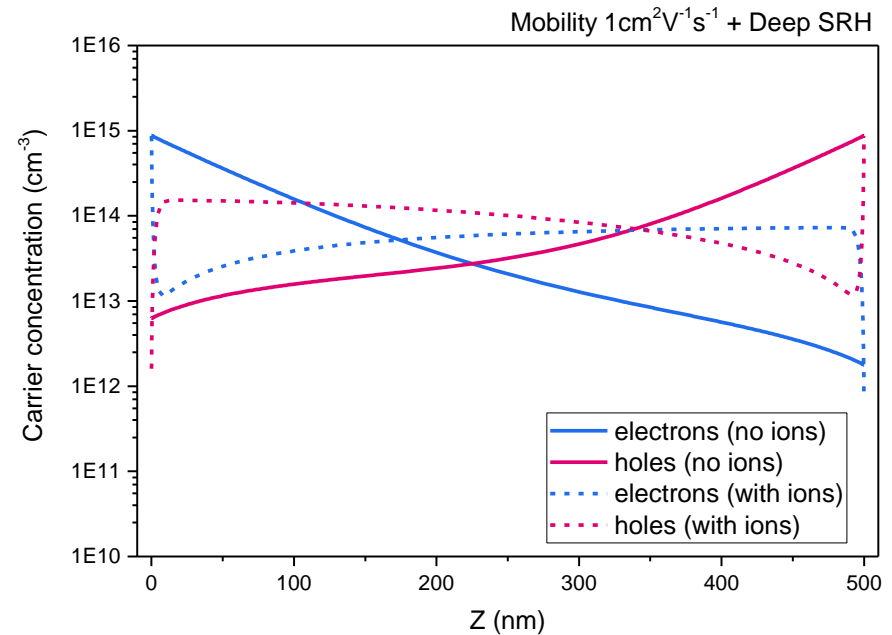
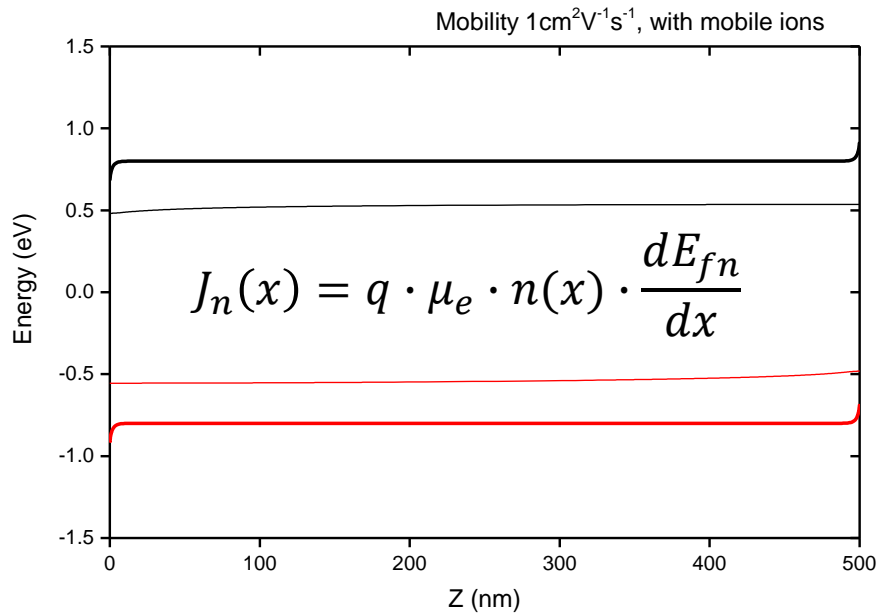


Introduced mid-band traps to both cases:

	No ions	With ions
$V_{OC}$ (V) *	1.126	1.126
$J_{SC}$ (mA/cm <sup>2</sup> )	23.68	23.67
FF	77.18%	63.15%
$\eta$	20.58%	16.83%

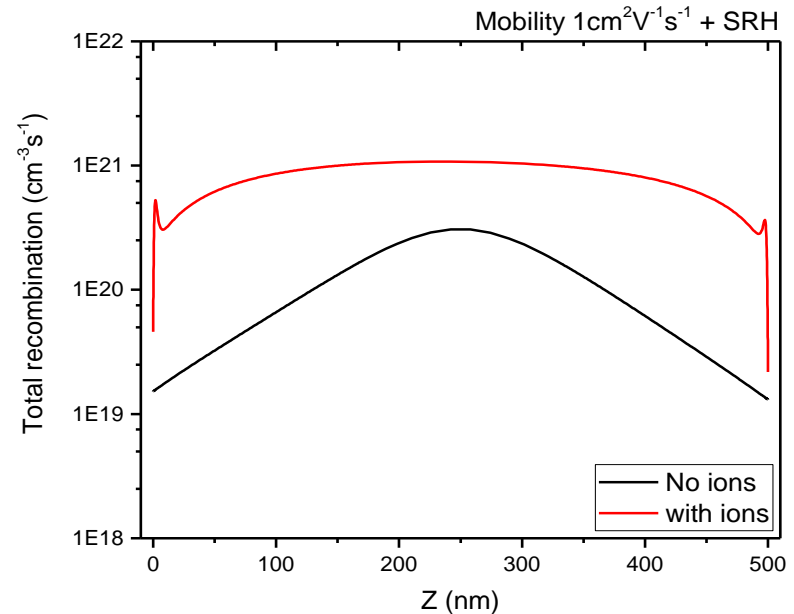
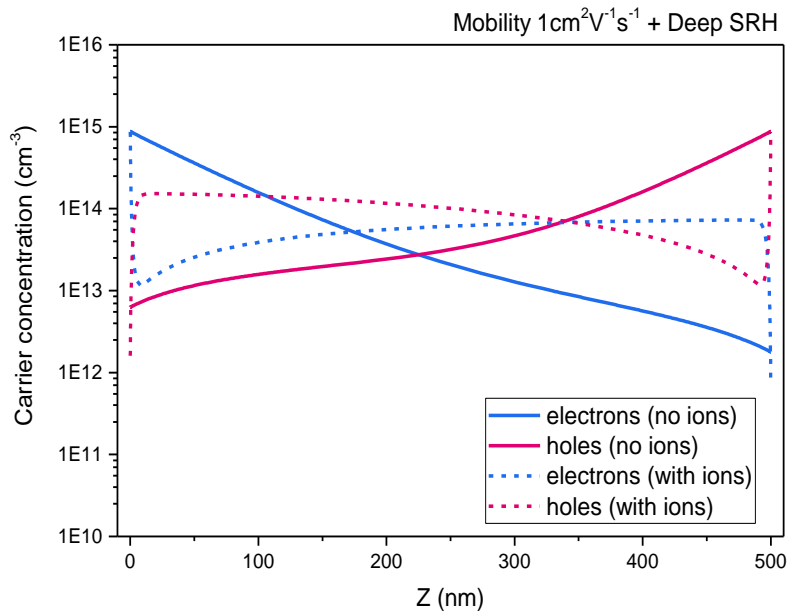
\*SRH concentration were set to match  $V_{OC}$

# Impact of SRH recombination with mobile ions



- Reduction in majority carrier concentration near the interface
- Such drop in quasi-Fermi levels are required for carrier extraction

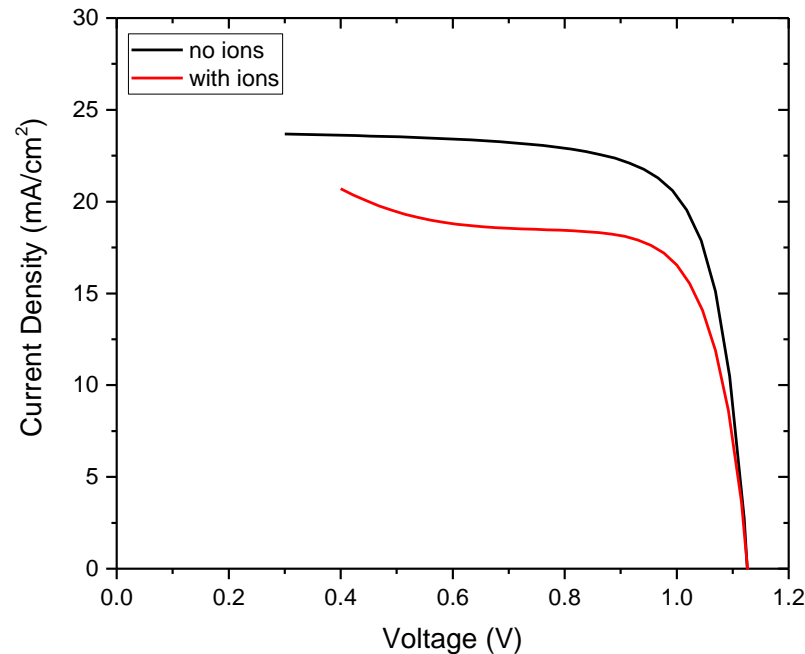
# Impact of SRH recombination with mobile ions



- Elevated minority carrier concentration in the bulk
- Increased rate of SRH recombination
- Collection efficiency is lower for diffusion current compared to drift current

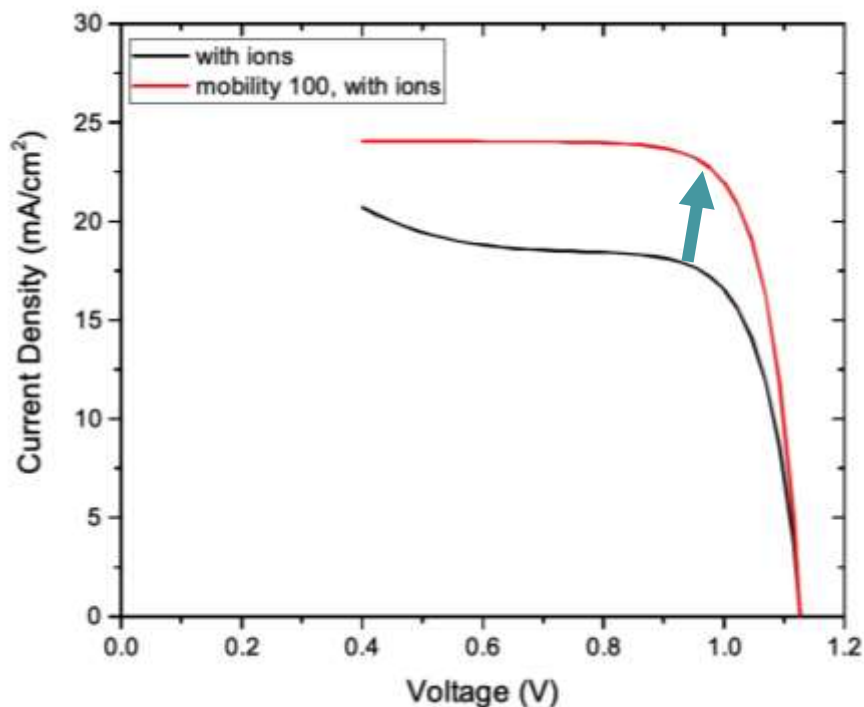


# Impact of SRH recombination with mobile ions



- Qualitatively mobile ions in combination with parasitic recombination will result in poor cell performance
- But we cannot quantitatively determine how much exactly yet

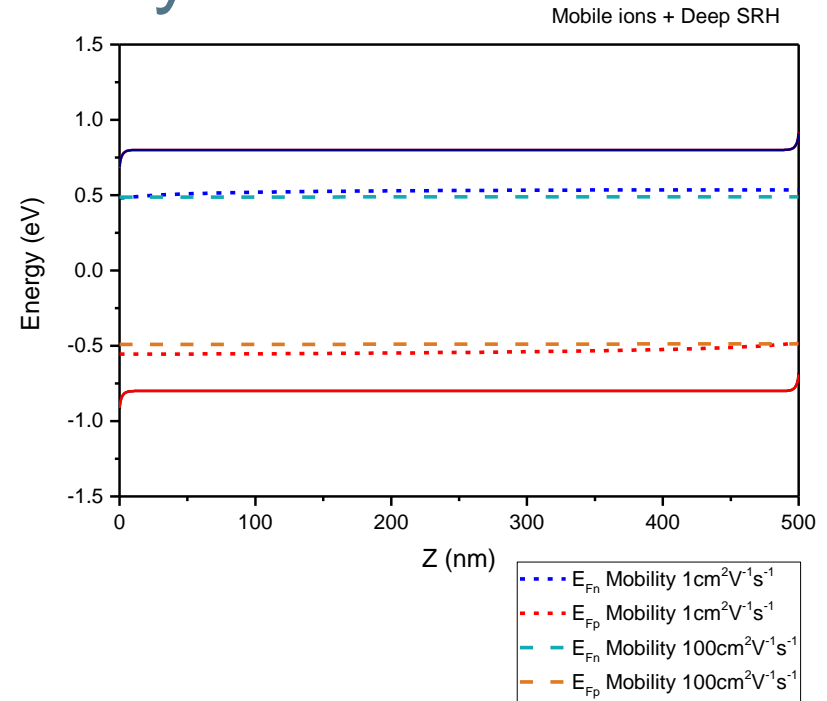
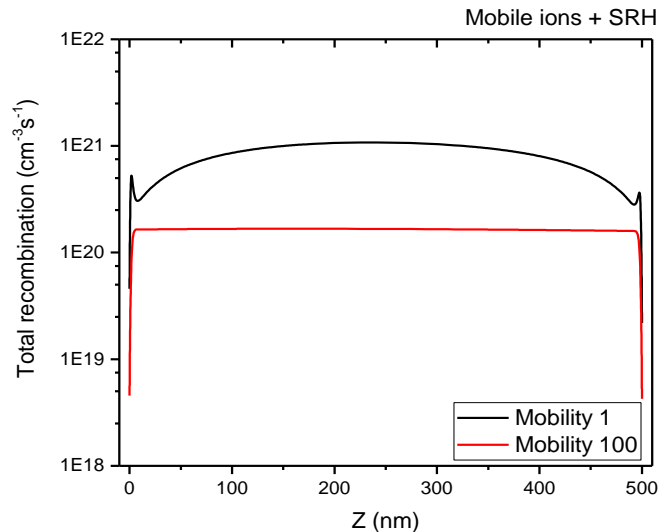
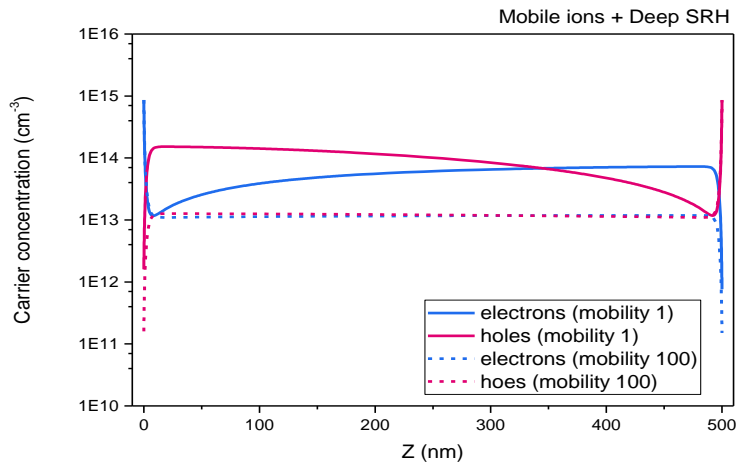
# The effect of carrier mobility



Carrier mobility	1cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>	100cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup>
V <sub>OC</sub> (V)	1.126	1.126
J <sub>SC</sub> (mA/cm <sup>2</sup> )	23.67	24.06
FF	72.18%	81.89%
η	16.83%	22.18%

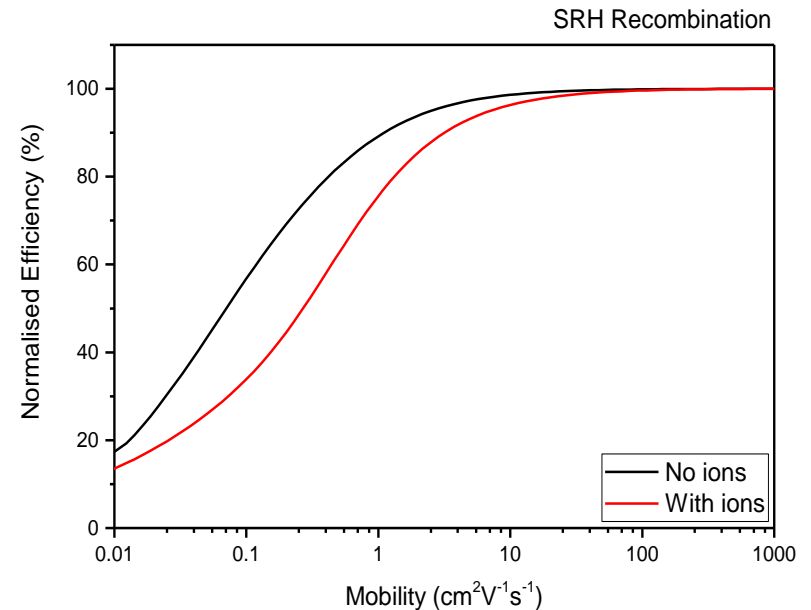
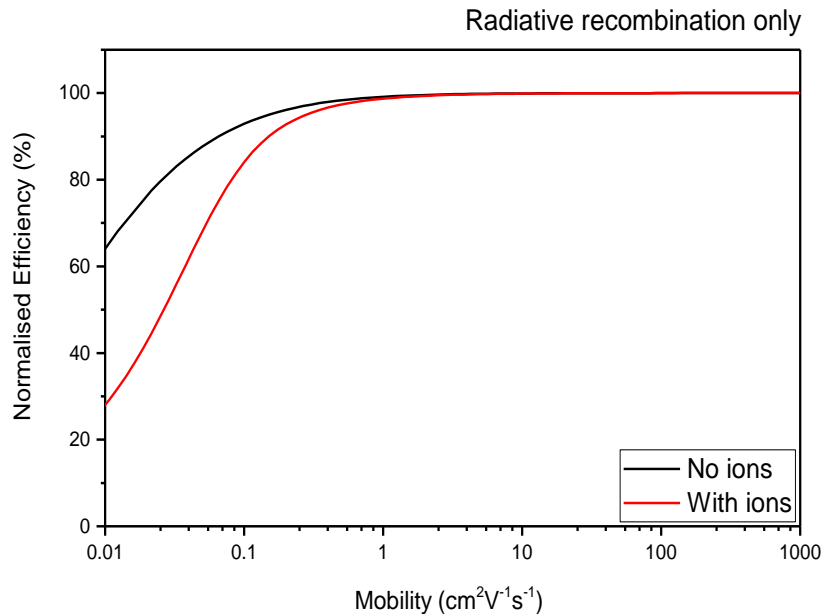
- Device is no longer transport limited
- Efficiency loss is now due to recombination dynamics

# The effect of carrier mobility



- No drop in qFL, and lowered qFL separation
- Reduced recombination across the bulk
- Transport barrier disappeared

# The effect of carrier mobility



- Ions are always detrimental to device performance
- SRH lowers carrier concentration, therefore higher mobility is required to prevent transport limitations

# Conclusion

- Mobile ions screen the internal electric field, and therefore result in a diffusion only carrier transport
- The removal of drift current component increases the carrier concentrations in the perovskite bulk, which is needed for current extraction
- Higher carrier concentration leads to higher recombination and reduces current at MPP
- With improved carrier mobility, device performances can be significantly boosted.

Thank you!