Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Can Ferroelectric Polarization Explain the High Performance of Hybrid Perovskite Solar Cells?

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Table S1: Parameters used in numerical simulation of perovskite solar cell.

Parameter	Symbol
Concentration (electron; hole)	n; p
Mobility (electron; hole)	μ_n; μ_p
Elementary charge	q
Boltzmann constant	k
Solar cell temperature	T
Dielectric permittivity of the perovskite	ϵ
Bimolecular recombination pre-factor	γ_{pre}
Fill Factor	FF

A Mobility Study

We performed calculations for different charge carrier mobilities in the perovskite solar cell. For all cases, the open-circuit voltage (V_{OC}) remained unchanged and the change in short-circuit current (J_{SC}) was only marginal. The mobility influenced significantly the fill factor (FF) of the solar cell and the results are shown in Figure S1.

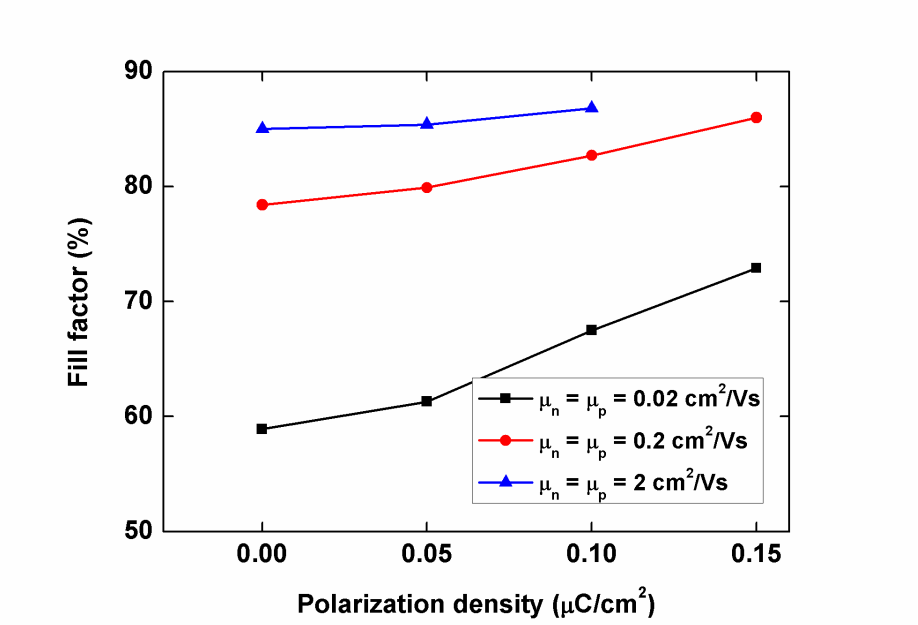

Figure S1: Variation of fill factor (FF) with polarization density for different charge carrier mobilities in the perovskite.

The bimolecular recombination rate expression is given by

$$R = \gamma np, \tag{S1}$$

where the γ is the rate constant, given by [1]

$$\gamma = \gamma_{pre}\frac{q}{\epsilon}(\mu_n + \mu_p), \tag{S2}$$

which scales proportionally with mobility of charge carriers.

The variation of fill factor (FF) for different charge mobilities are compared by keeping the rate constant (γ) fixed. This is made possible by changing the value of γ_{pre} accordingly. The value of γ_{pre} used for mobilities 0.02 cm^2/Vs, 0.2 cm^2/Vs and 2 cm^2/Vs is 1 , 0.1 and 0.01 respectively.

B Idealized Limit for Fill Factor (FF)

The limit for the fill factor (FF) for an idealized solar cell with a given V_{OC} can be calculated by [2]

$$FF = \frac{\upsilon_{oc} - \ln(\upsilon_{oc} + 0.72)}{\upsilon_{oc} + 1} \tag{S3}$$

where υ_{oc} is the open-circuit voltage normalized to kT/q. Hence for a open circuit voltage of $V_{OC} = 0.93$ V, the idealized limit for FF is 88.1%.

References

[1] L. J. A. Koster, O. Stenzel, S. D. Oosterhout, M. M. Wienk, V. Schmidt and R. A. Janssen, *Adv. Energy Mater.*, 2013, **3**, 615–621.

[2] M. A. Green, *Solid-State Electronics*, 1981, **24**, 788–789.