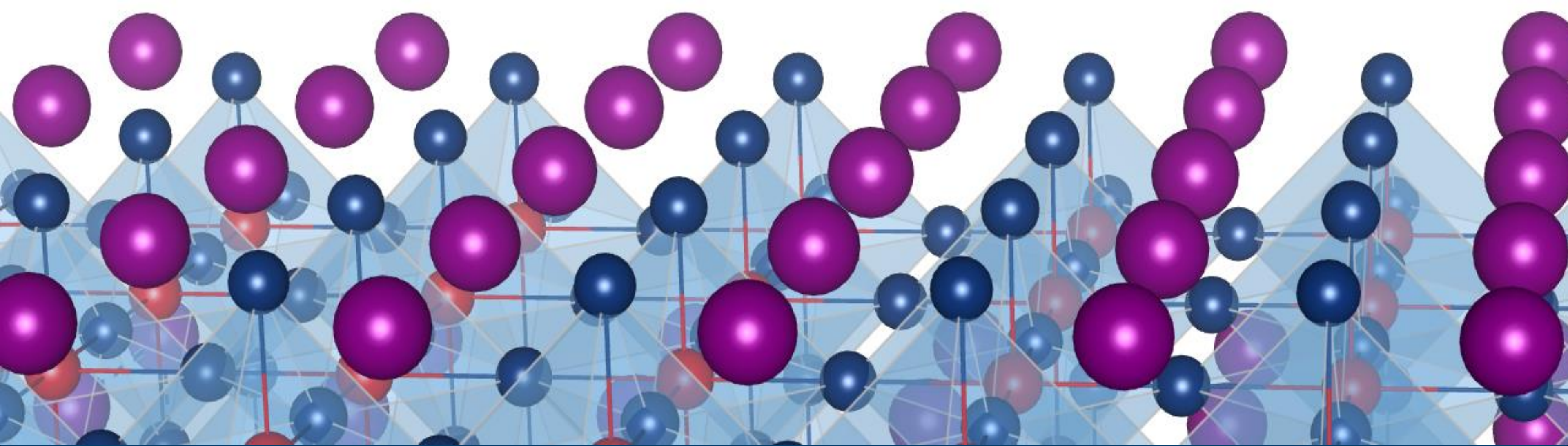


Impact of Defects on Halide Perovskite Solar Cells

Thomas Kirchartz[1,2]

[1]IEK-5 Photovoltaik, Forschungszentrum Jülich,

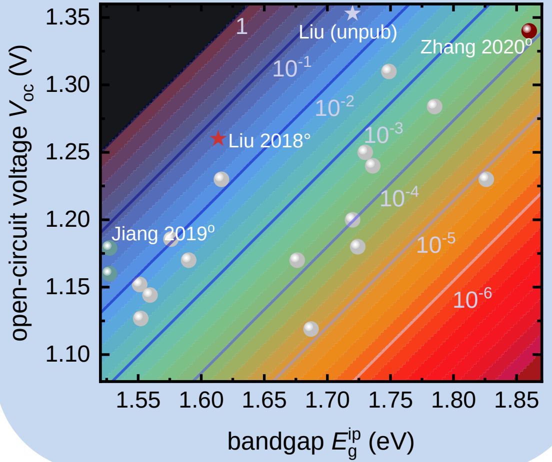
[2]NST and CENIDE, Universität Duisburg-Essen

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

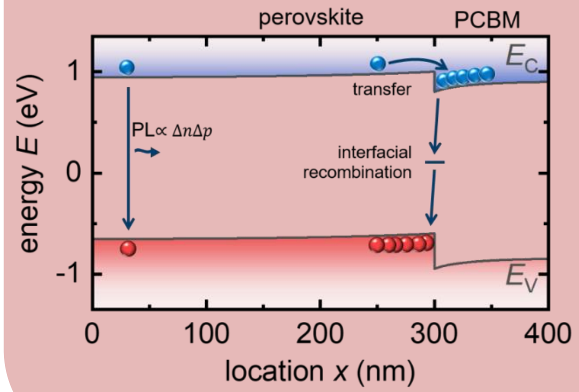
JÜLICH Forschungszentrum

Questions regarding defects in MHPs

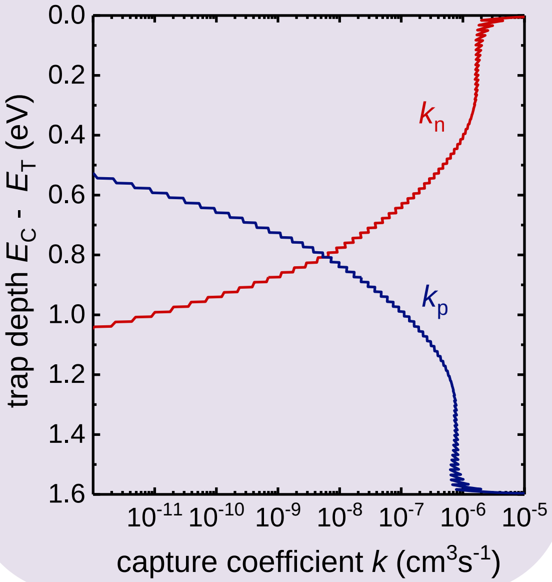
Do defects matter for high η perovskite solar cells?



Where are they in space?

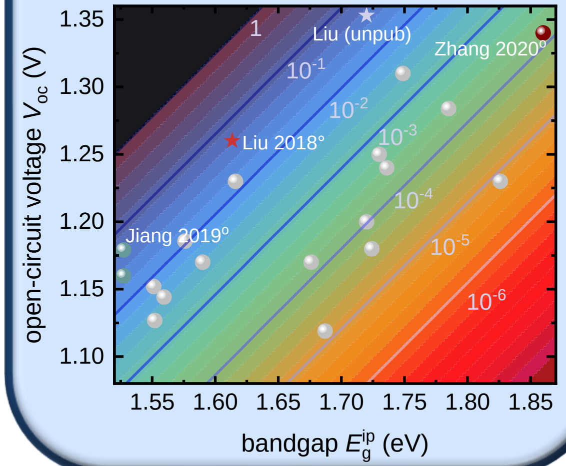


Where are they in energy?

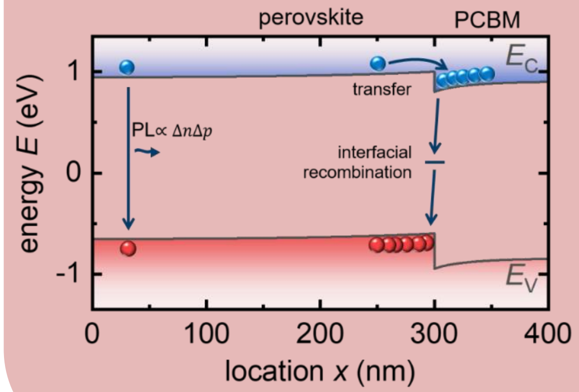


Questions regarding defects in MHPs

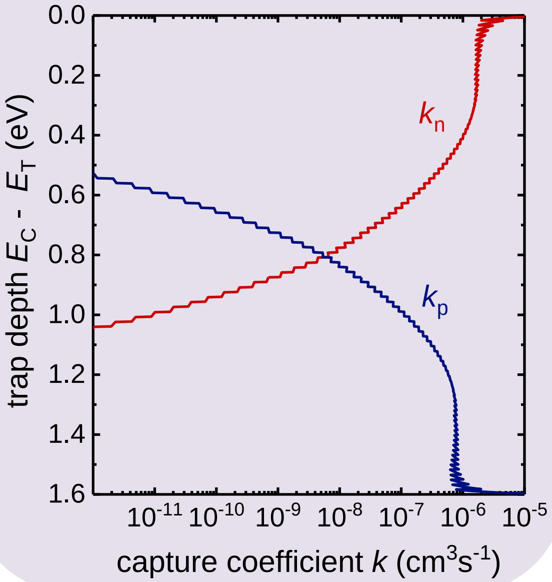
Do defects matter for high η perovskite solar cells?



Where are they in space?

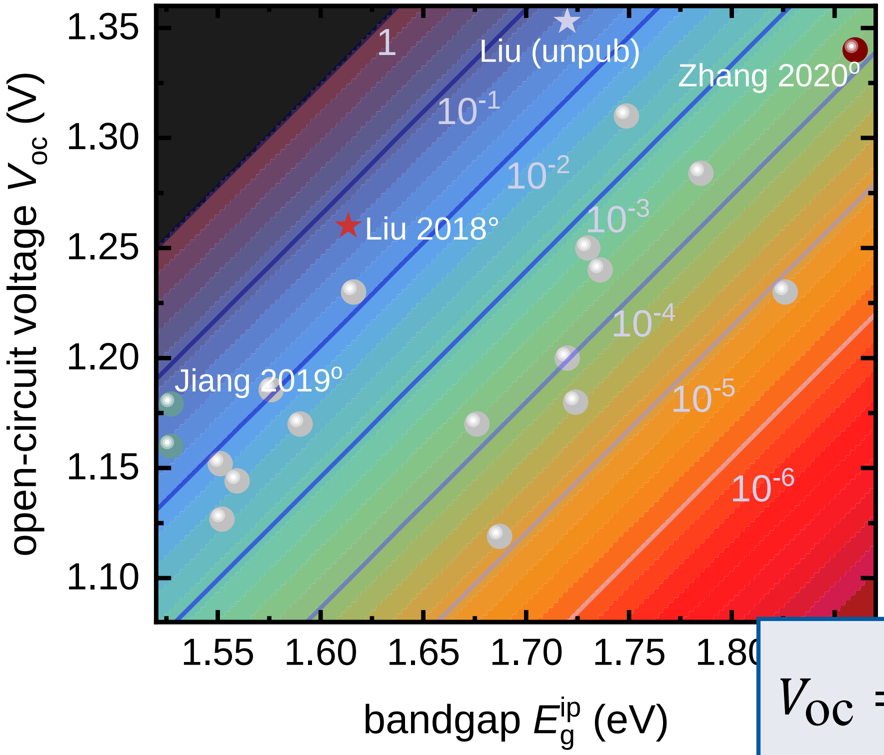


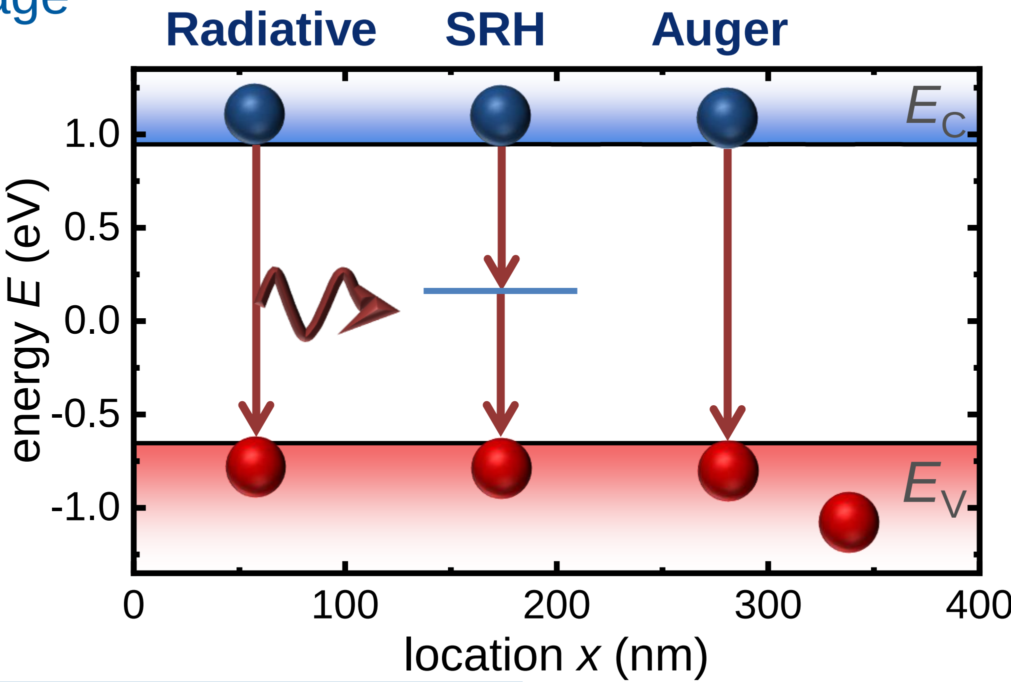
Where are they in energy?



Defect assisted recombination

Luminescence vs. open-circuit voltage

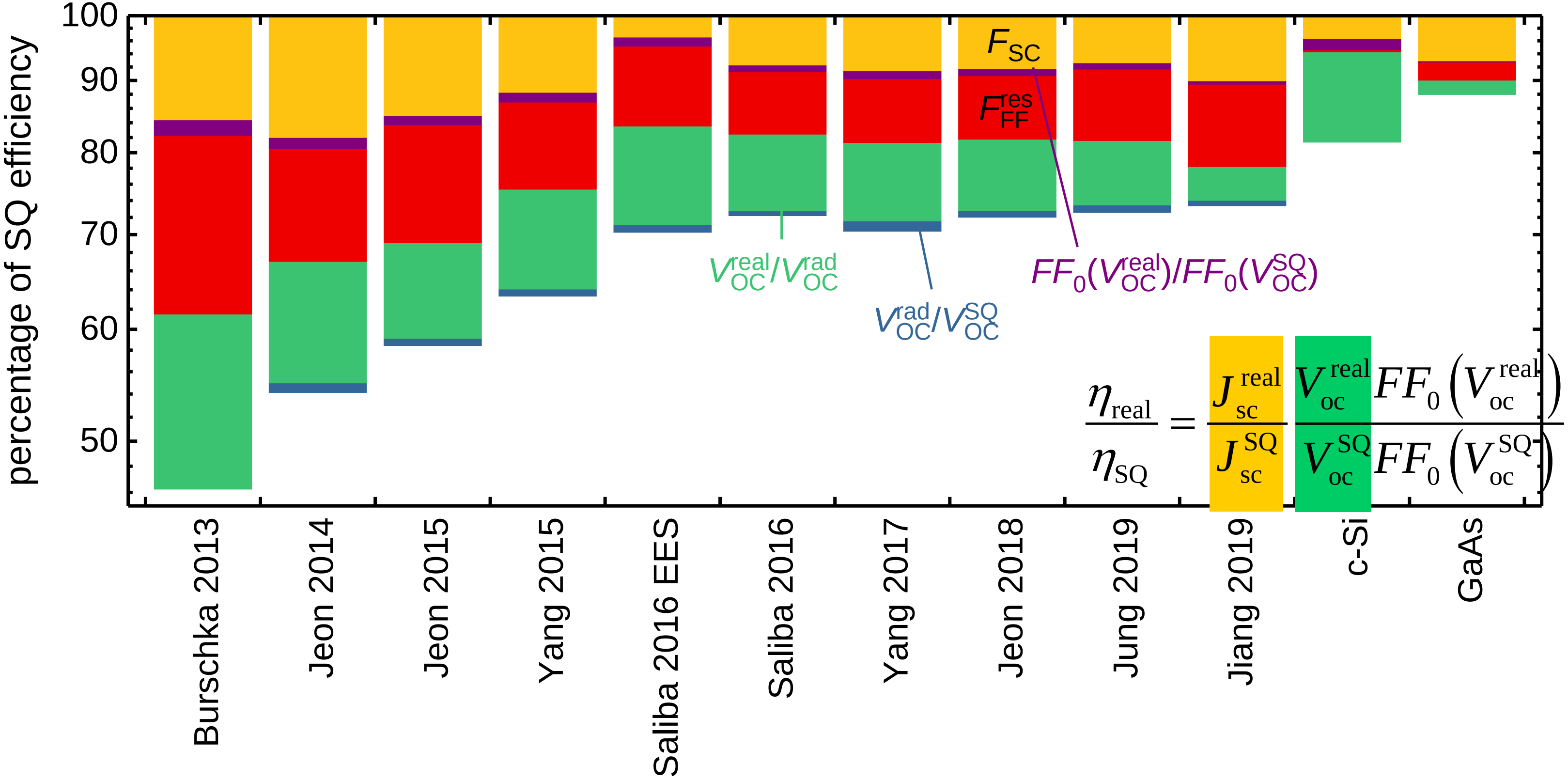




$$V_{oc} = V_{oc}^{rad} + \frac{kT}{q} \ln\left(Q_e^{lum}\right)$$

Do defects matter?

Losses in lead-halide perovskite solar cells over the years



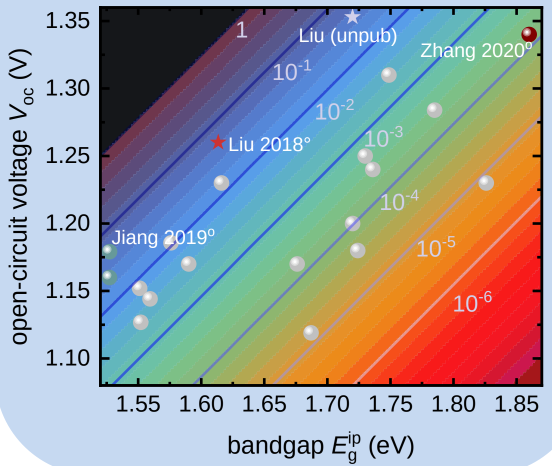
$$\frac{\eta_{real}}{\eta_{SQ}} = \frac{J_{sc}^{real}}{J_{sc}^{SQ}} \, \frac{V_{oc}^{real} FF_0\left(V_{oc}^{real}\right)}{V_{oc}^{SQ} FF_0\left(V_{oc}^{SQ}\right)} \, \frac{FF^{real}}{FF_0\left(V_{oc}^{real}\right)}$$

Krückemeier et al. Adv. Energy Mater. 2019, 10.1002/aenm.201902573

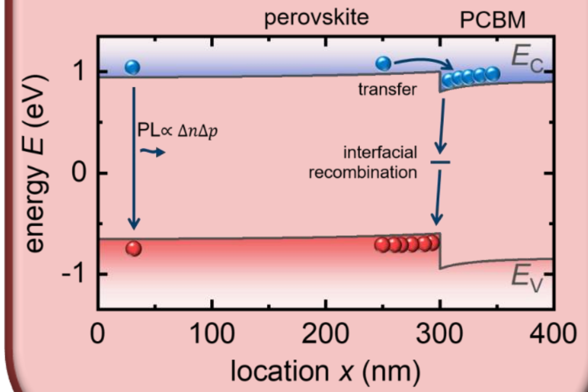
Questions regarding defects in MHPs

Do defects matter for high η perovskite solar cells?

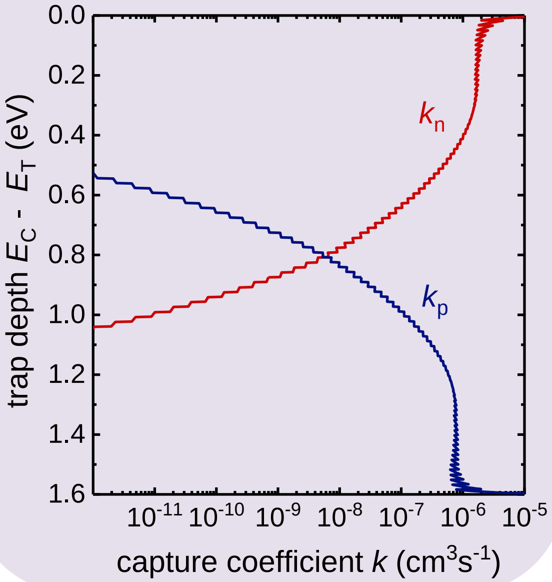
yes



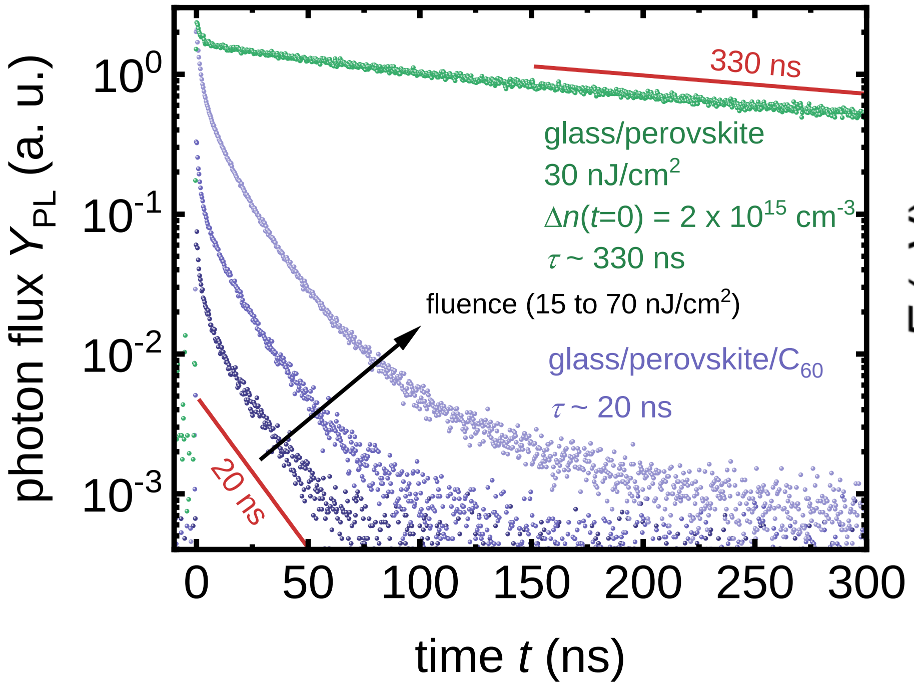
Where are they in space?

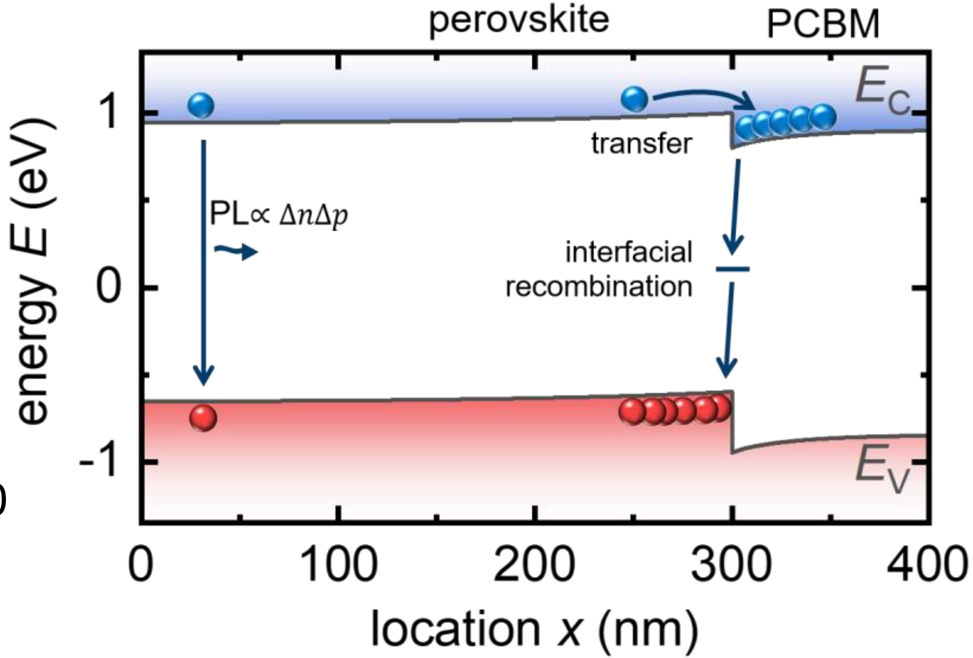


Where are they in energy?



Interface recombination

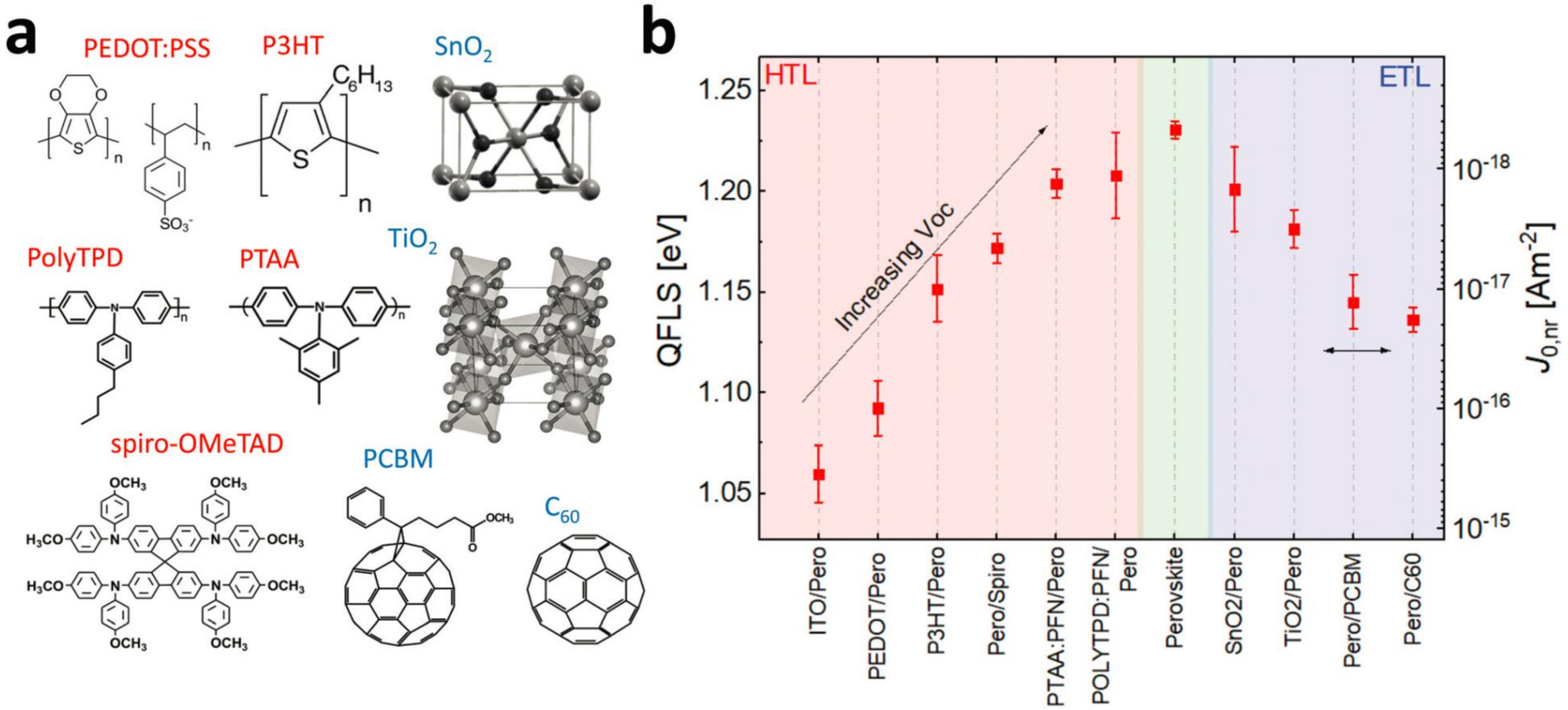




Stolterfoht et al. Nature Energy (2018)
Kirchartz et al. Adv. Energy Mater. (2020), accepted

Screening of contact layers for high V_{oc}

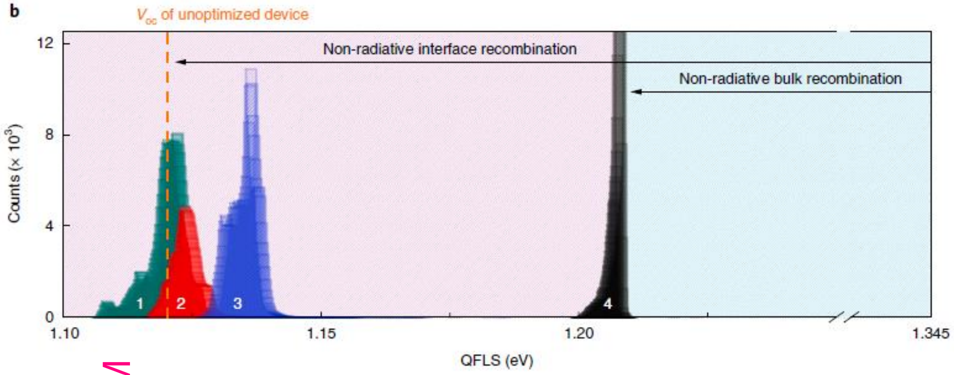
Triple cation recipe from Potsdam University

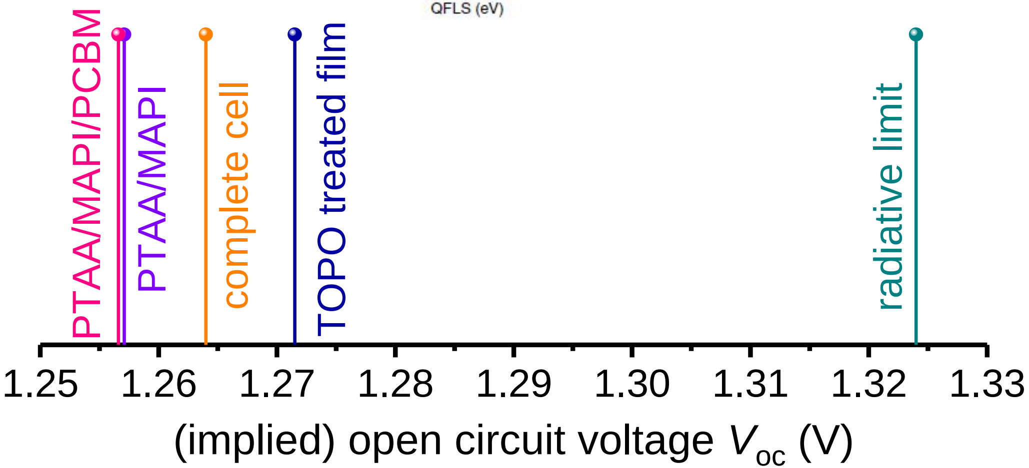


Stolterfoht et al. Energy Environ. Science (2019)

Steady-State PL

Measuring indirectly the quasi-Fermi-level splitting





$$\boxed{kT\ln(10) \approx 60\text{meV}}$$

Stolterfoht et al. Nature Energy (2018)

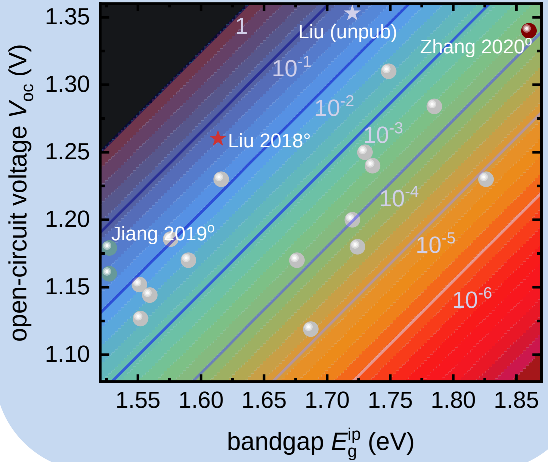
$$\boxed{qV_{oc}^{rad} - qV_{oc} = -kT\ln\left(Q_e^{lum}\right) > 0}$$

Liu et al., ACS Energy Lett. **4**, 110 (2019)

Questions regarding defects in MHPs

Do defects matter for high η perovskite solar cells?

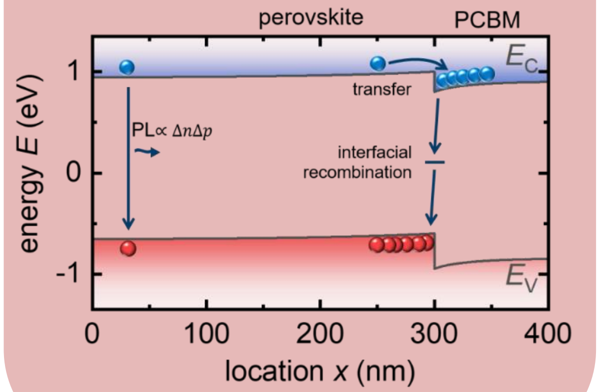
yes



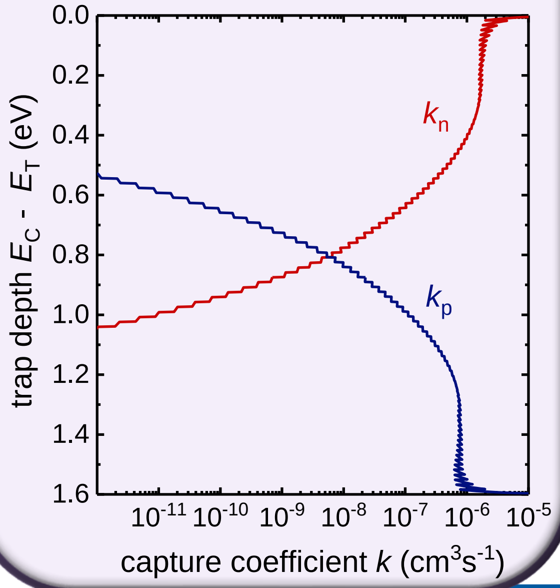
Where are they in space?

Interfaces

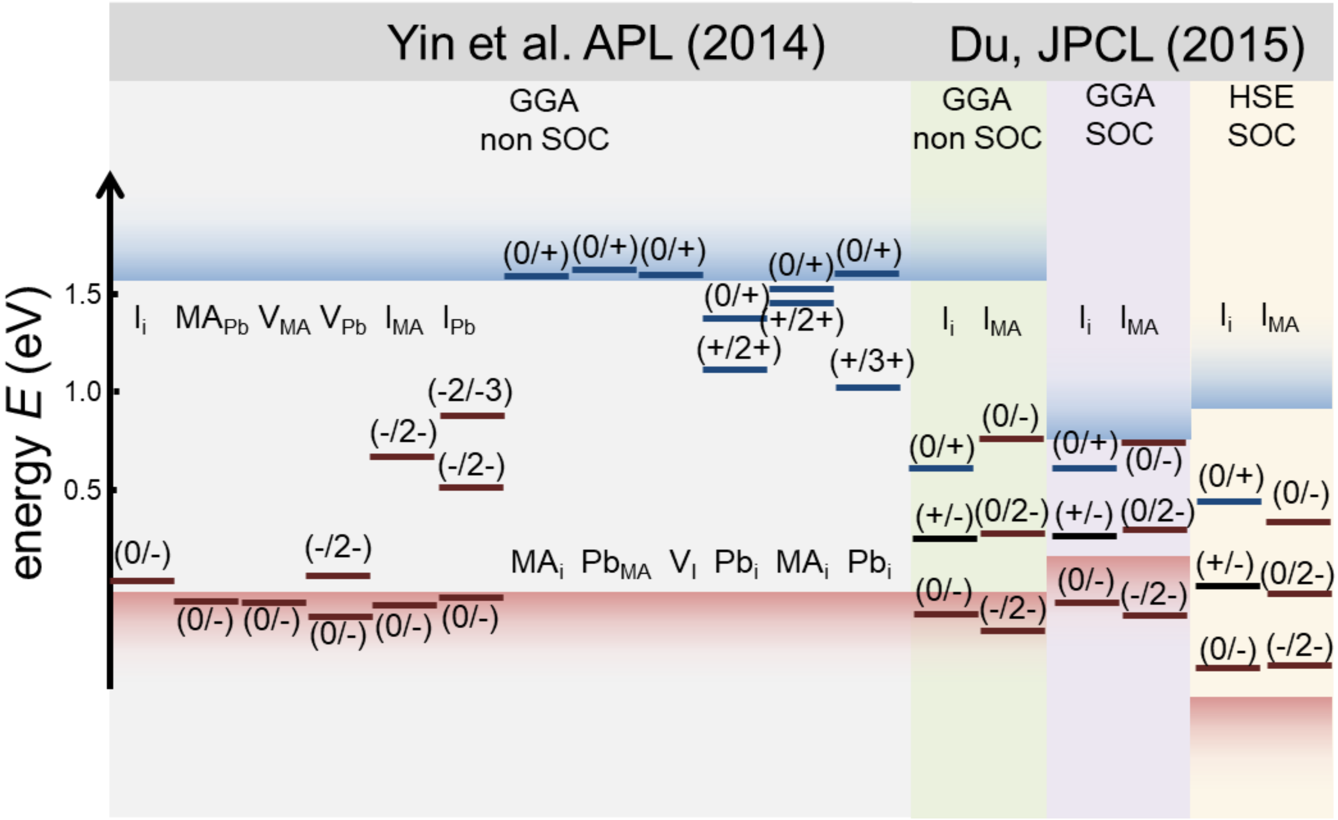
bulk



Where are they in energy?

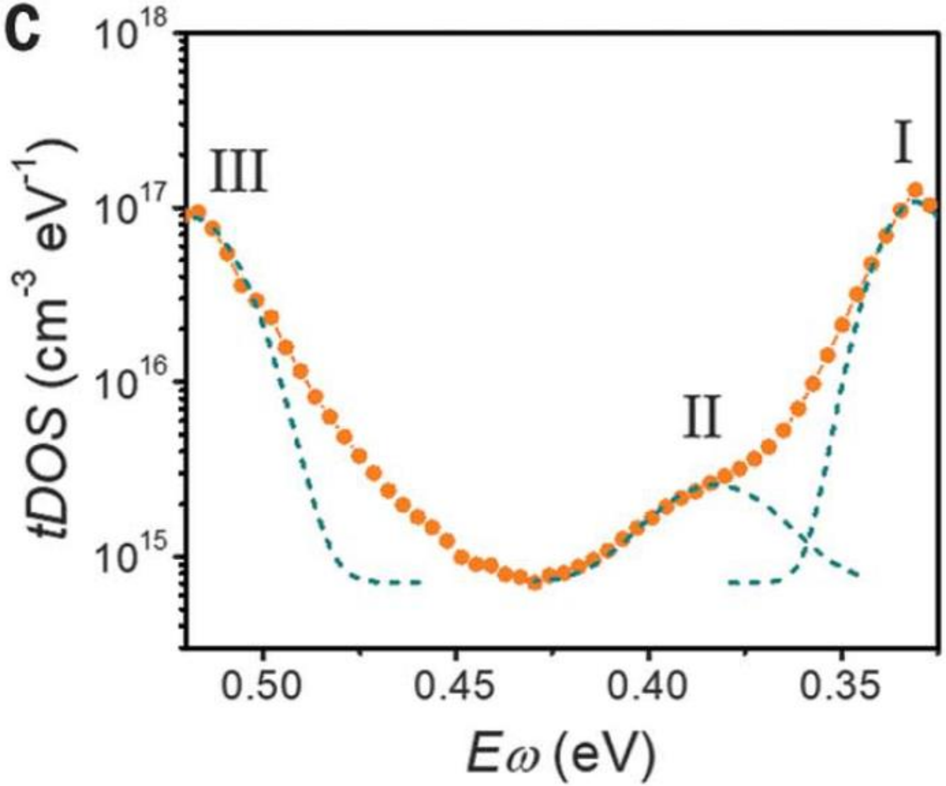


Positions of defects in MAPI - Theory



Kirchartz et al., APL Materials. **6**, 100702 (2018)

Positions of defects in MAPI - Experiment



SOLAR CELLS

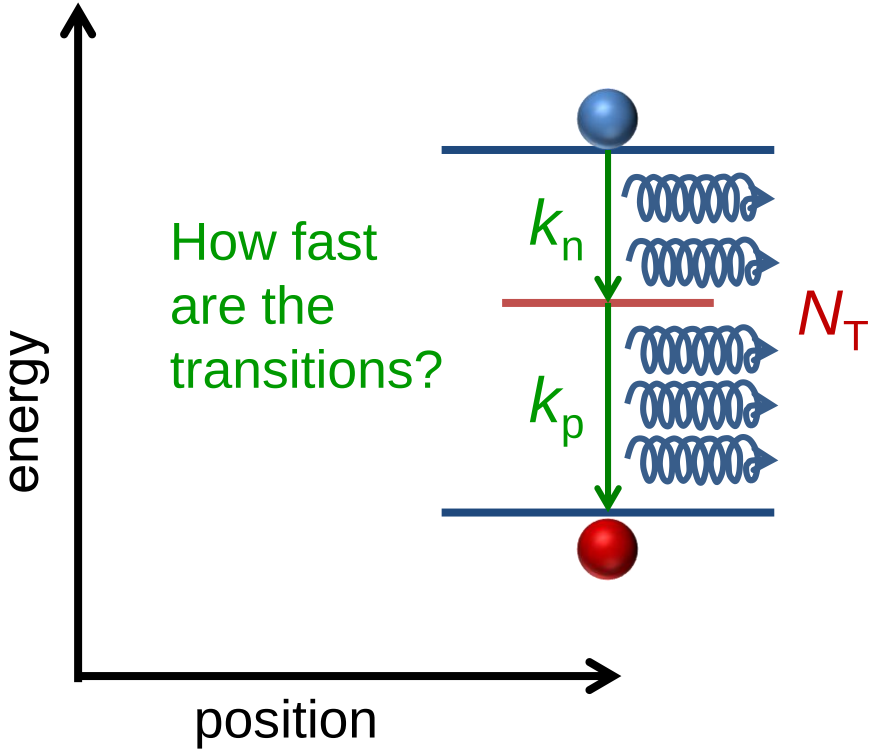
Resolving spatial and energetic distributions of trap states in metal halide perovskite solar cells

Zhenyi Ni[1]*, Chunxiong Bao[2]*, Ye Liu[1,2], Qi Jiang[1], Wu-Qiang Wu[1], Shangshang Chen[1], Xuezeng Dai[1], Bo Chen[1], Barry Hartweg[3], Zhengshan Yu[3], Zachary Holman[3], Jinsong Huang[1,2]†

Ni et al. Science **367**, 1352 (2020)

Recombination Coefficients

For non-radiative recombination



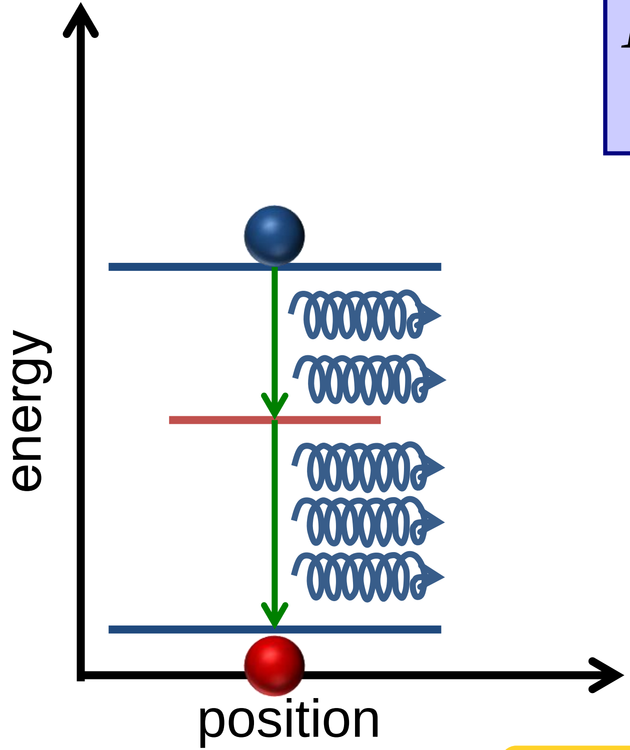
How many defects exist per volume?

$$R_\mathrm{SRH} = \frac{np - n_i^2}{n\tau_p + p\tau_n}$$

$$\tau_\mathrm{n/p} = \left(k_\mathrm{n/p} N_\mathrm{T}\right)^{-1}$$

Recombination Coefficients

For non-radiative recombination



$$R_{\mathrm{SRH}} = \frac{np - n_i^2}{n\tau_p + p\tau_n}$$

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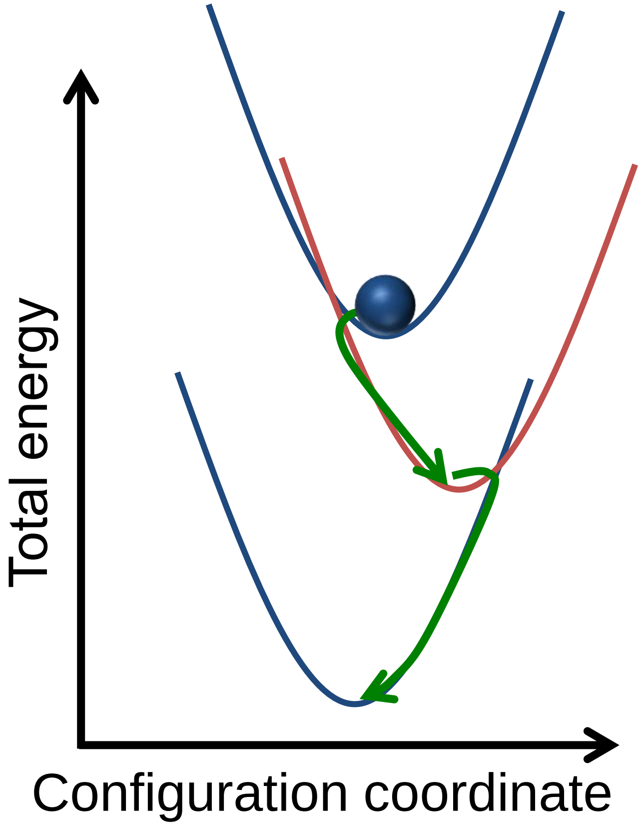
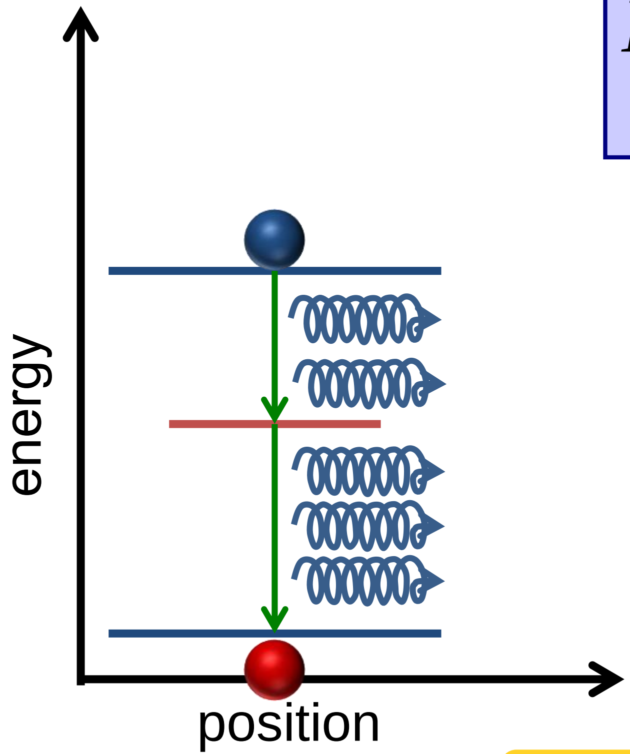
Recombination Coefficients

For non-radiative recombination



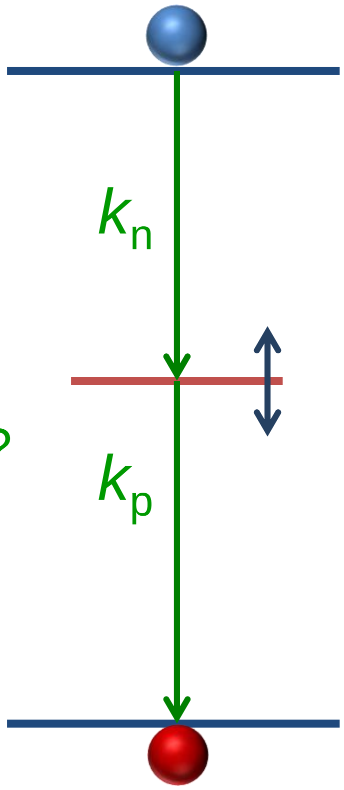


$$\boxed{R_{\mathrm{SRH}} = \frac{np - n_i^2}{n\tau_p + p\tau_n}}$$

$$\boxed{\tau_{\mathrm{n/p}} = \left(k_{\mathrm{n/p}} N_{\mathrm{T}}\right)^{-1}}$$

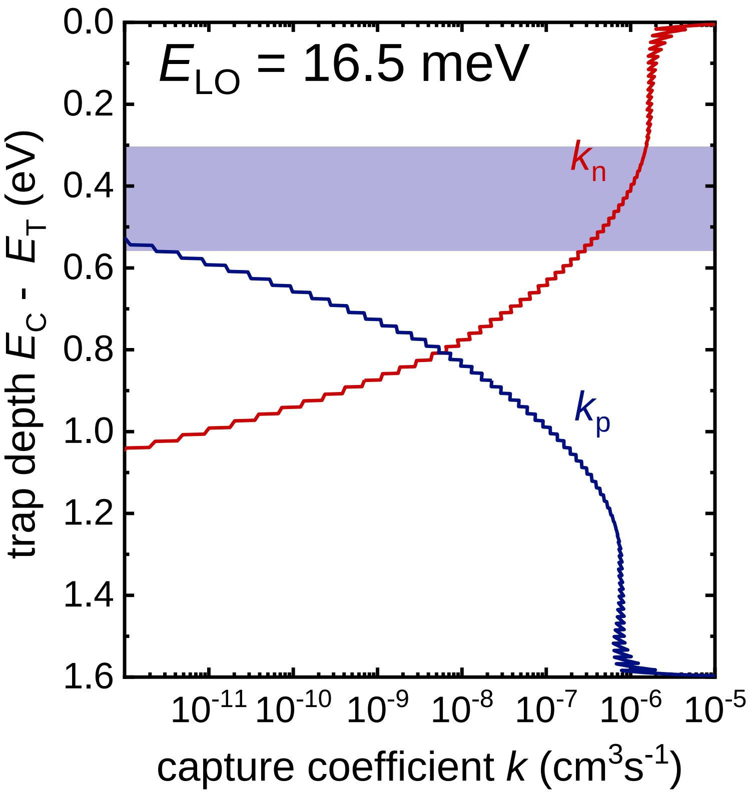
Recombination Coefficients

vs. phonon energy



How fast are the transitions?

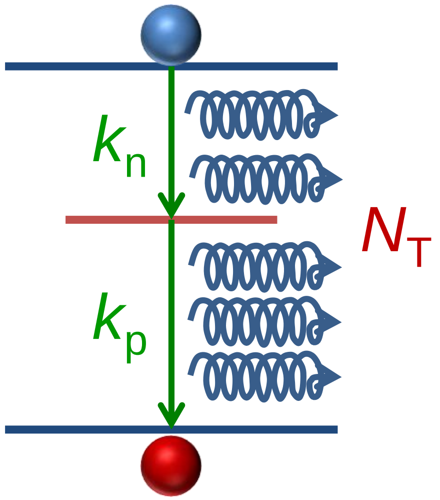
Depends strongly on phonon energy/energetic step ΔE. Low phonon energies are helpful.

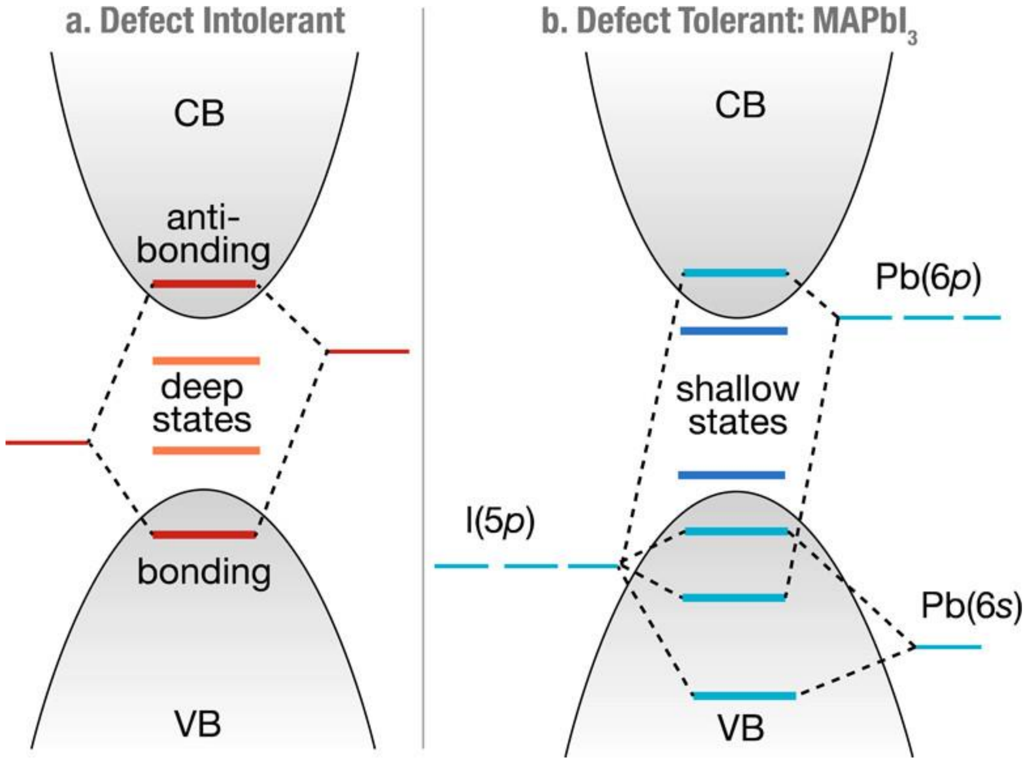


Kirchartz et al., J. Phys. Chem. Lett. **9**, 939 (2018)

Defect Positions

Antibonding valence bands





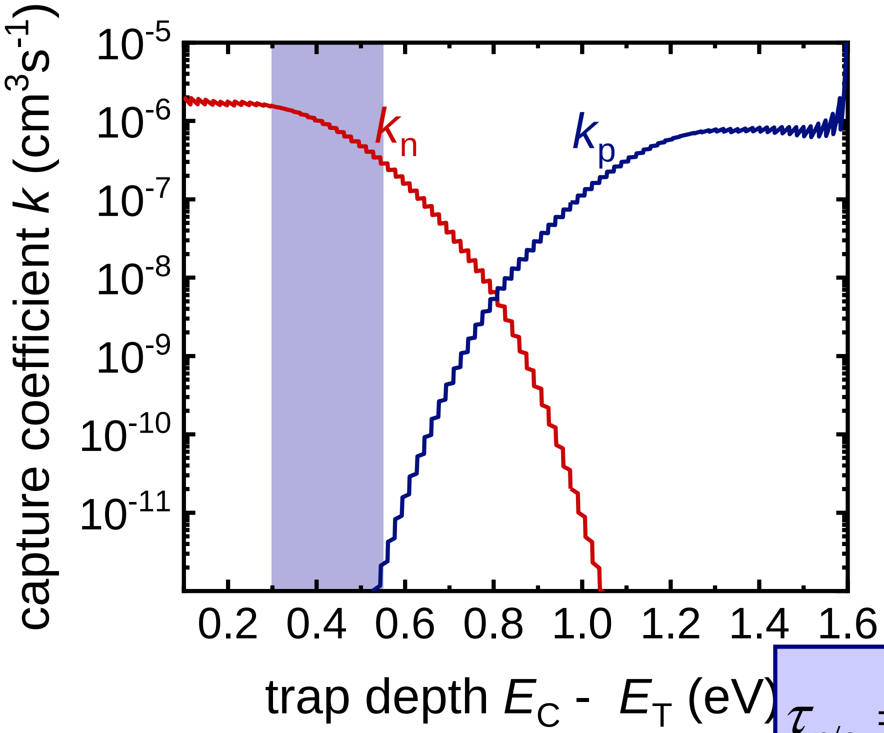
How many defects exist per volume?

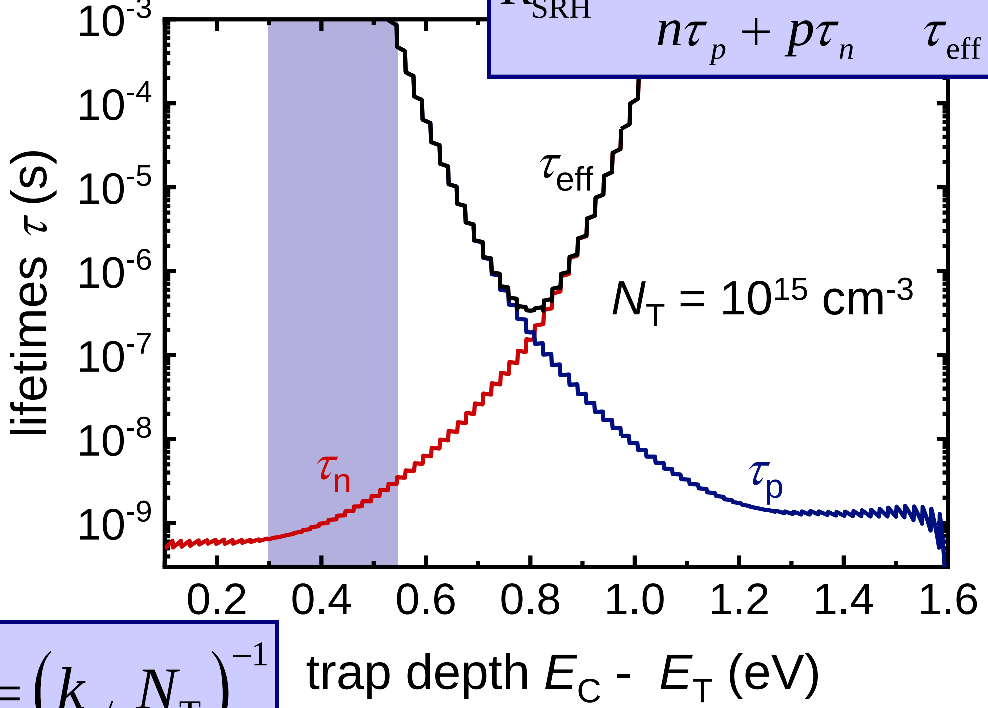
Brandt et al., Chem. Mater. **29**, 4667 (2017)

Theory of Multiphonon Recombination

Applied to $CH_3NH_3PbI_3$

$$R_{\mathrm{SRH}} = \frac{np - n_i^2}{n\tau_p + p\tau_n} = \frac{n}{\tau_{\mathrm{eff}}}$$





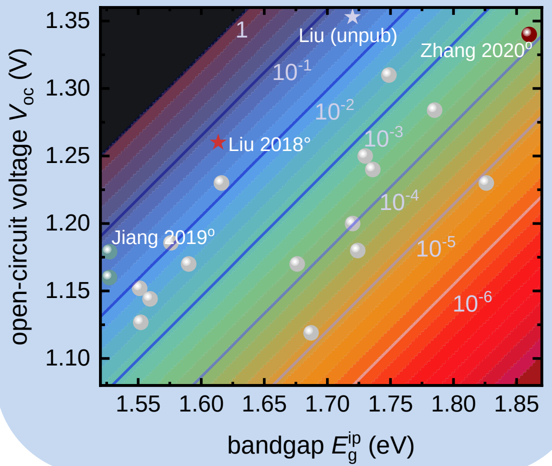
$$\tau_{\mathrm{n/p}} = \left(k_{\mathrm{n/p}} N_{\mathrm{T}}\right)^{-1}$$

Kirchartz et al., J. Phys. Chem. Lett. **9**, 939 (2018)

Conclusions

Do defects matter for high η perovskite solar cells?

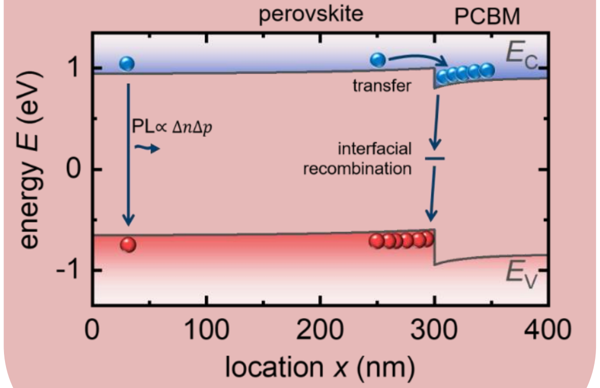
yes



Where are they in space?

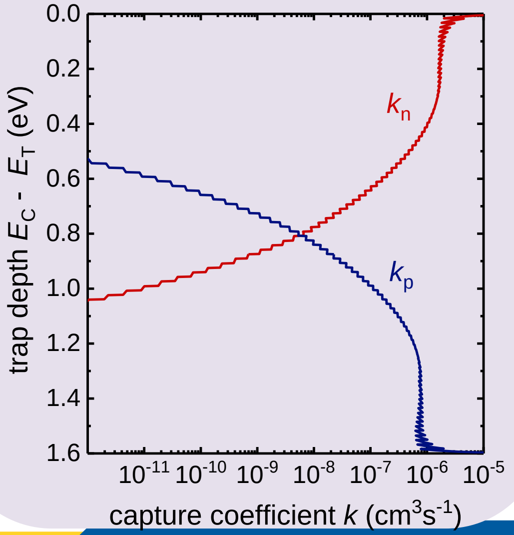
Interfaces

bulk



Where are they in energy?

Close to midgap?



Thank you for your attention

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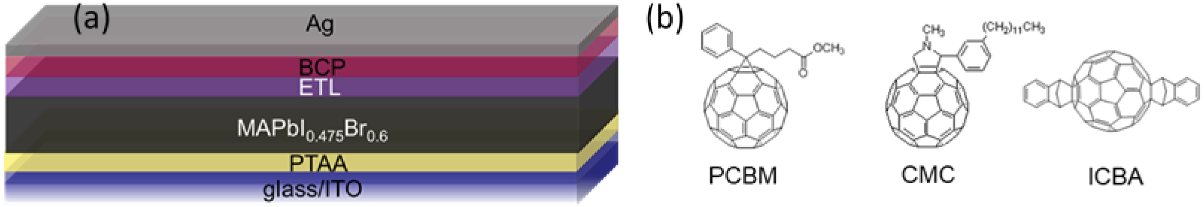
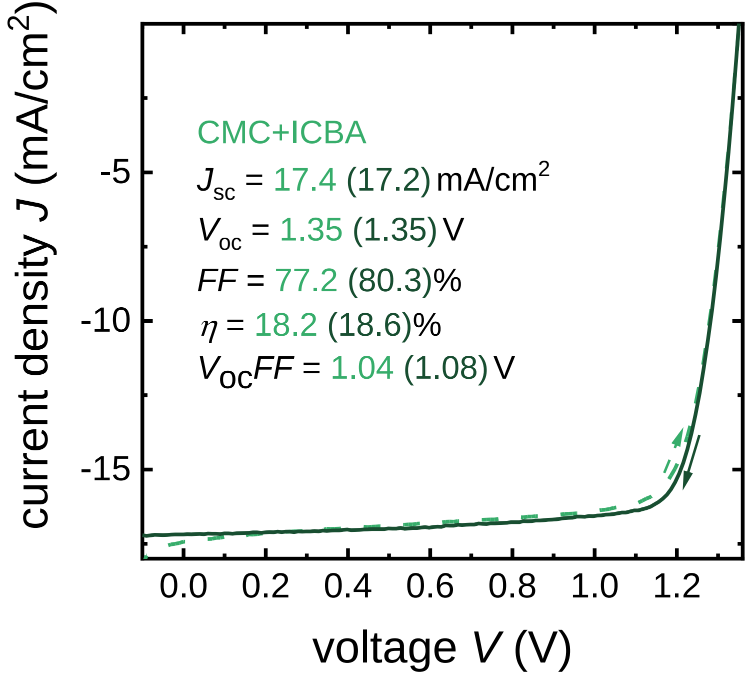
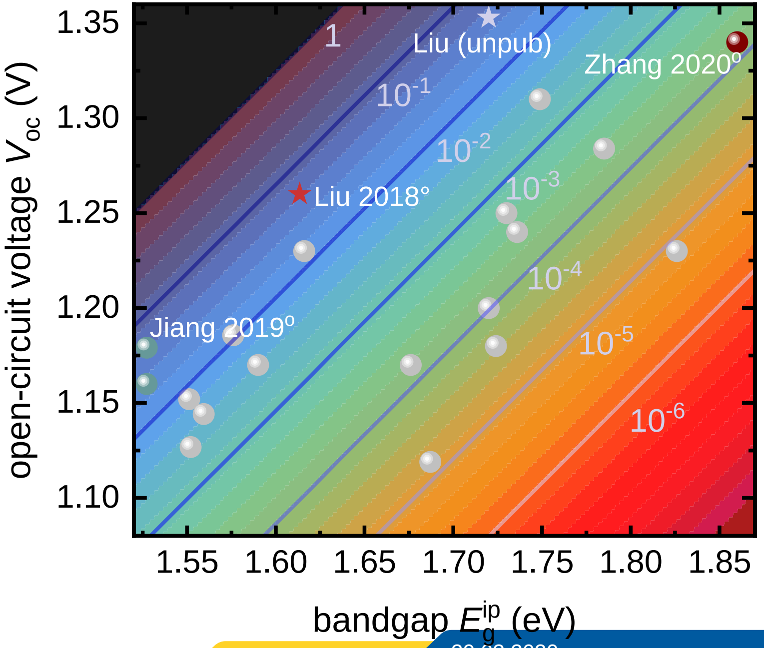
JÜLICH Forschungszentrum

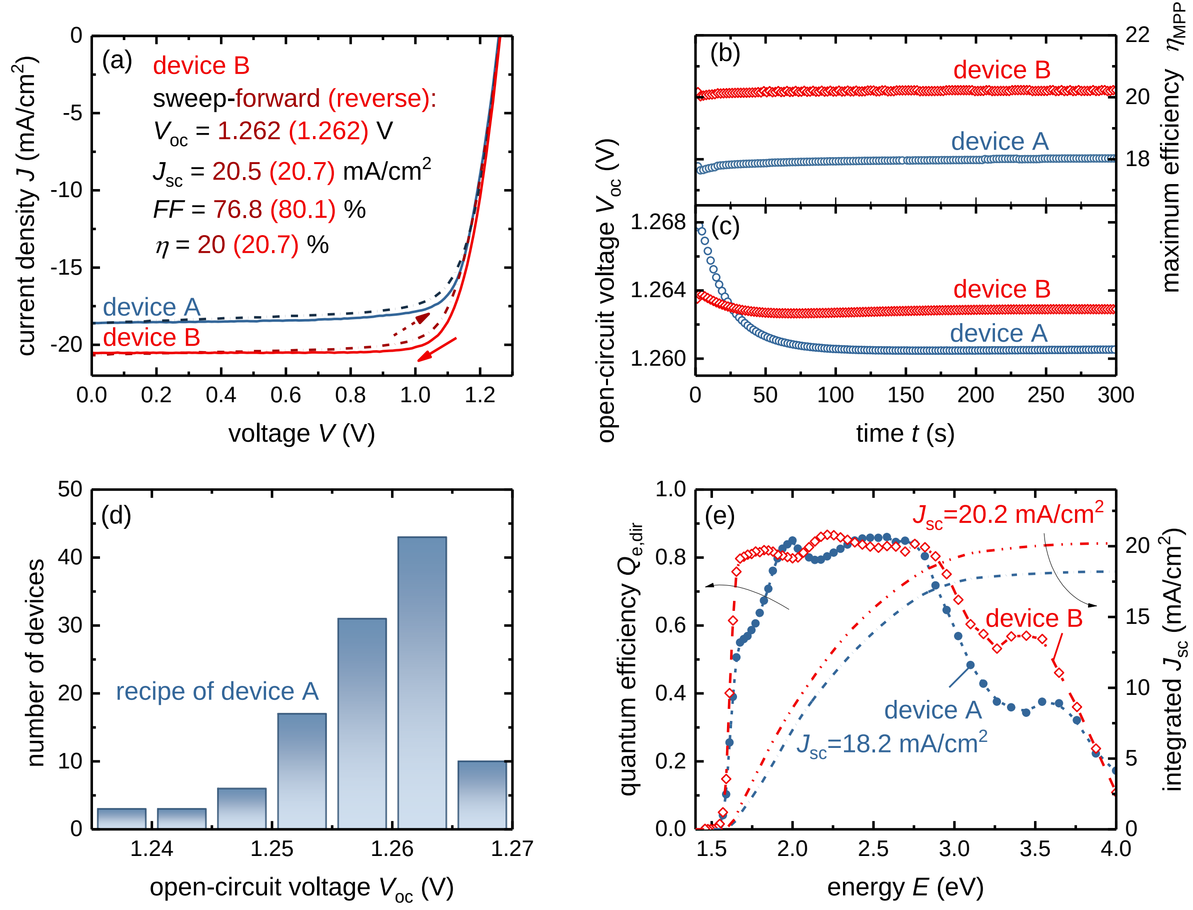
Higher band gap cells

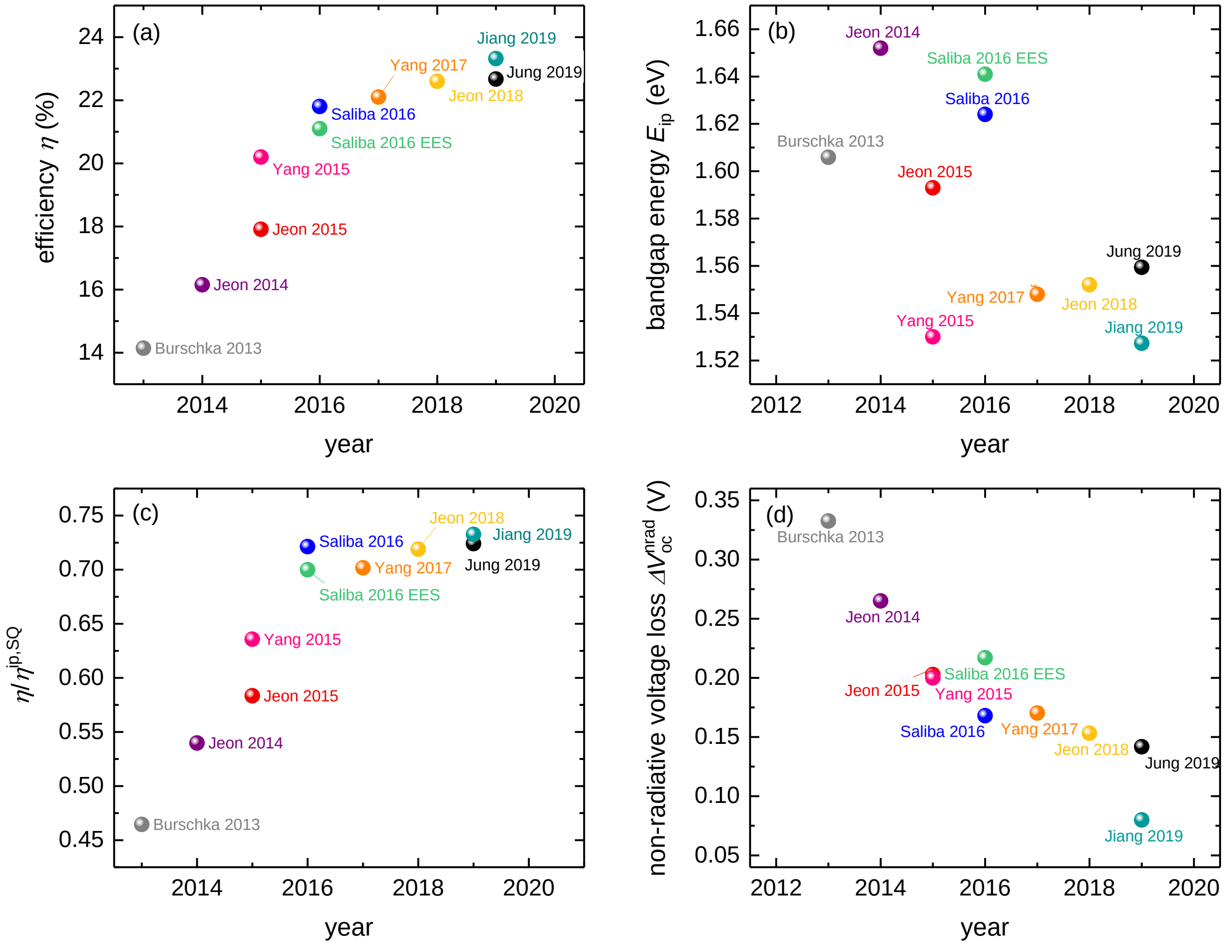






Overview of the Solar Cell Performance

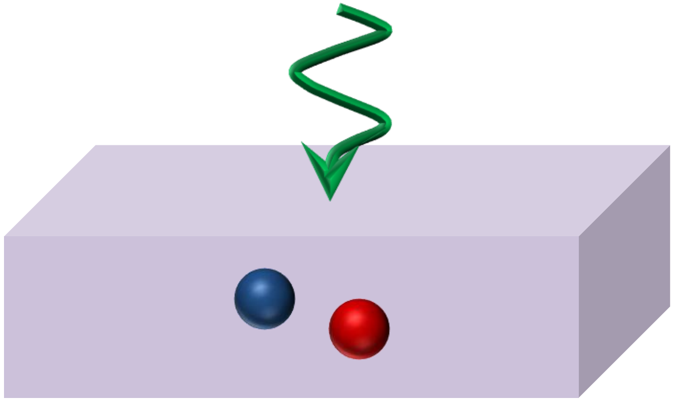


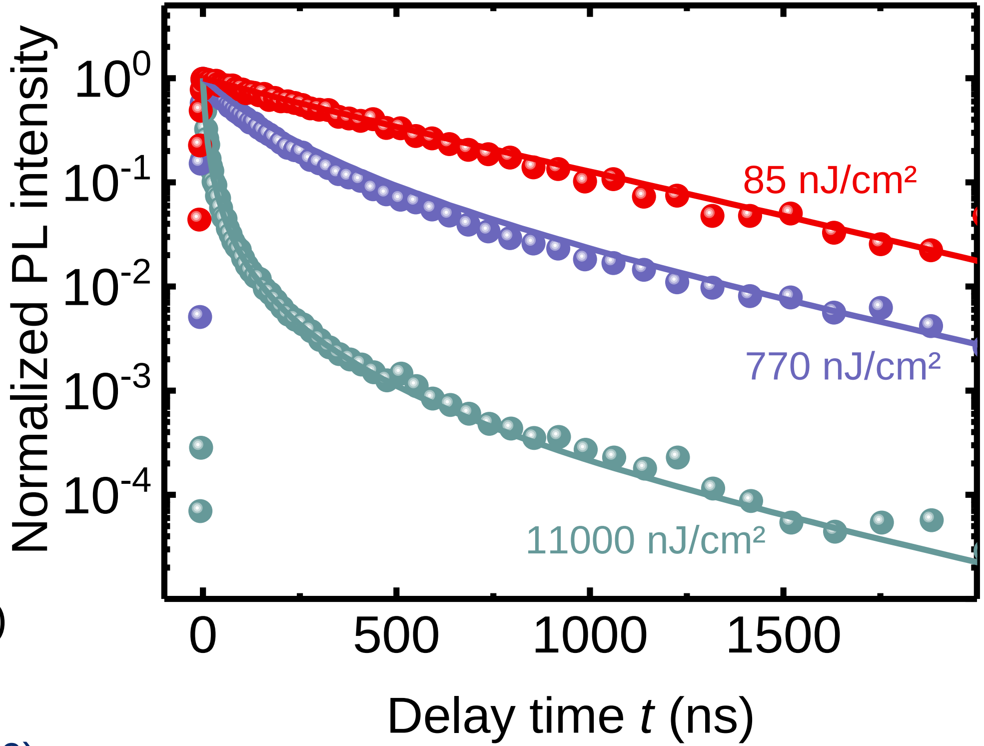


(a)
efficiency η (%)
year
Burschka 2013
Jeon 2014
Jeon 2015
Yang 2015
Saliba 2016
Saliba 2016 EES
Yang 2017
Jeon 2018
Jung 2019
Jiang 2019
(b)
bandgap energy E_{ip} (eV)
year
Jeon 2014
Saliba 2016 EES
Saliba 2016
Burschka 2013
Jeon 2015
Jung 2019
Yang 2017
Jeon 2018
Yang 2015
Jiang 2019
(c)
$\eta/\eta^{ip,SQ}$
year
Saliba 2016
Jeon 2018
Jiang 2019
Yang 2017
Jung 2019
Saliba 2016 EES
Yang 2015
Jeon 2015
Jeon 2014
Burschka 2013
(d)
non-radiative voltage loss ΔV_{oc}^{nrad} (V)
year
Burschka 2013
Jeon 2014
Saliba 2016 EES
Jeon 2015
Yang 2015
Saliba 2016
Yang 2017
Jeon 2018
Jung 2019
Jiang 2019

Transient Photoluminescence

Layer on glass - Data

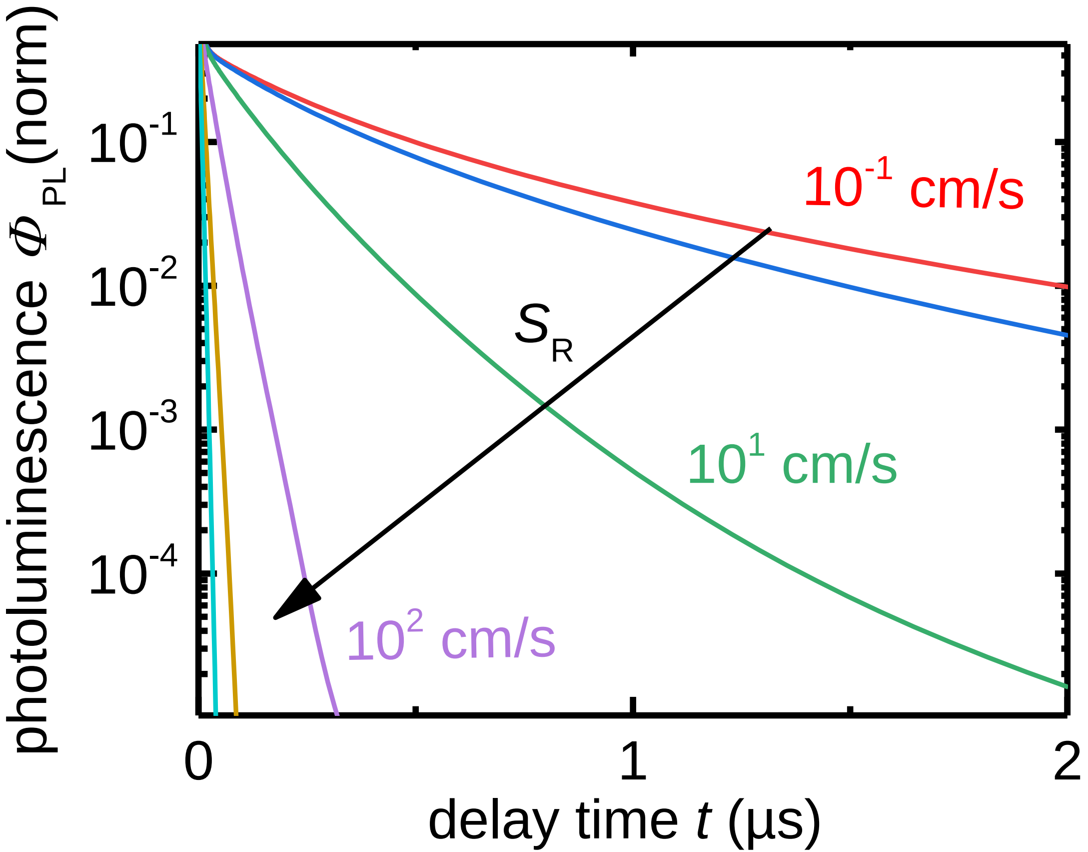




$$\frac{\mathrm{d}n}{\mathrm{d}t} = -knp - \frac{np}{\tau_p n + \tau_n p} - C(np^2 + n^2 p)$$

Staub et al. *Phys. Rev. Appl.* **6**, 044017 (2016)

High fluence behaviour (charge accumulation)



E_L =1000nJ/cm²

high laser fluence