Carnegie Mellon University

It's all about that Bayes:

Data-driven insights into energy devices without the black box

PASC MINISYMPOSIUM ON INTERDISCIPLINARY CHALLENGES IN MULTISCALE MATERIALS MODELING

JUNE 27, 2023

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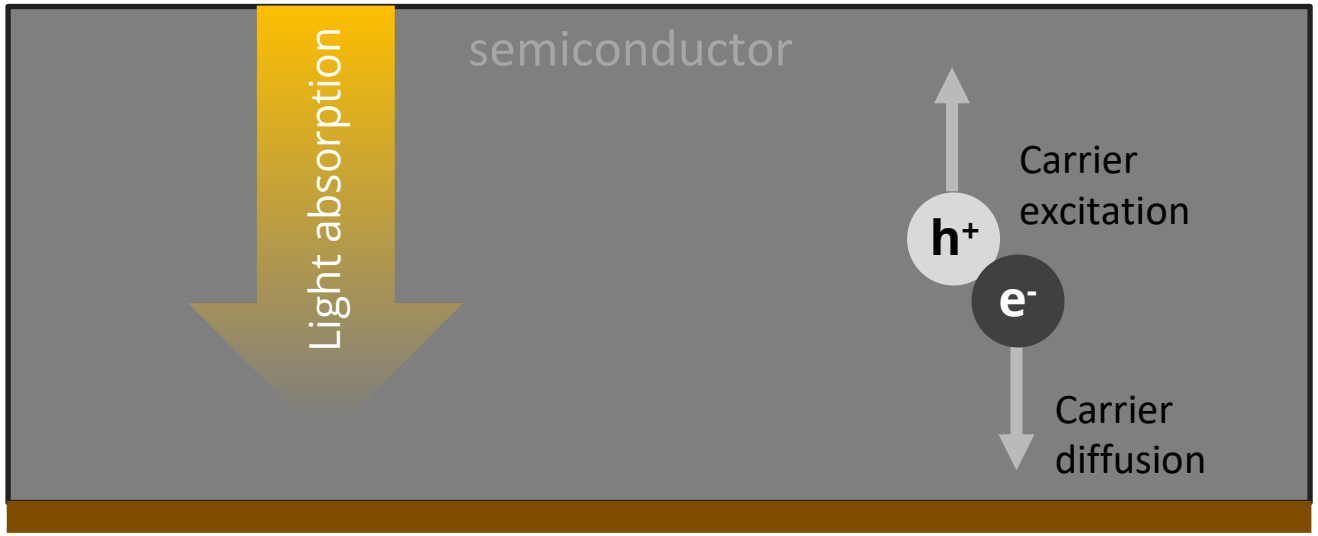
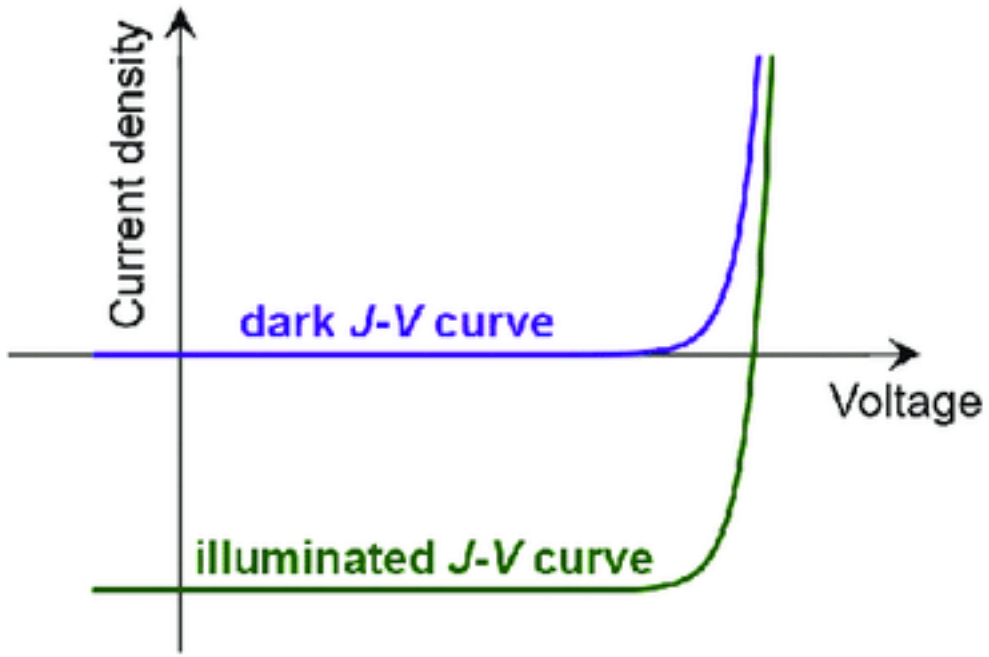
Multiscale processes in photovoltaic devices



…including across interfaces and in the presence of defects (scattering!)
…and in nonequilibrium conditions!

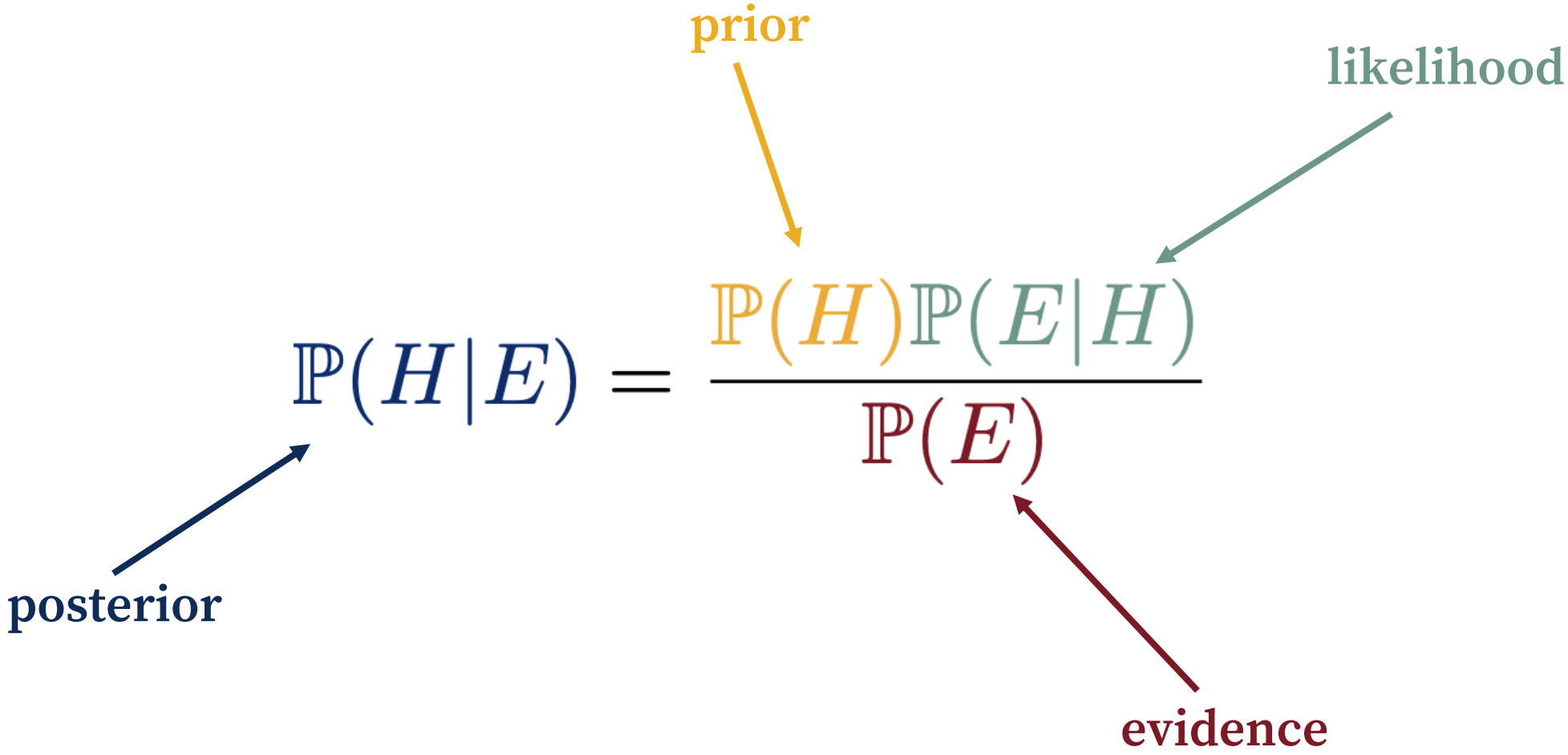
Electrical Characterization of Solar Cells



We can measure current as a function of voltage, light intensity, temperature, …

…each of these “knobs” probes different processes in the device, and hence depends differently on its materials properties.

Bayes' Theorem



Bayes' Theorem

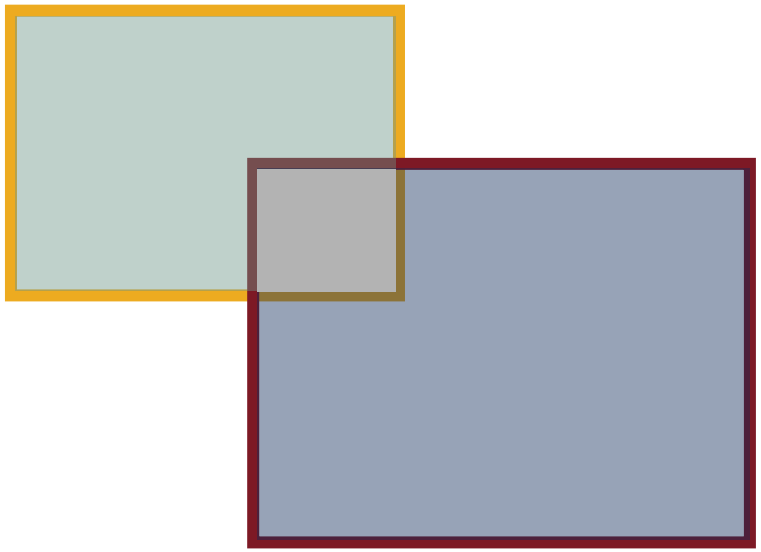
$$\mathbb{P}(H|E) = \frac{\mathbb{P}(H)\mathbb{P}(E|H)}{\mathbb{P}(E)}$$

prior

likelihood

posterior

evidence

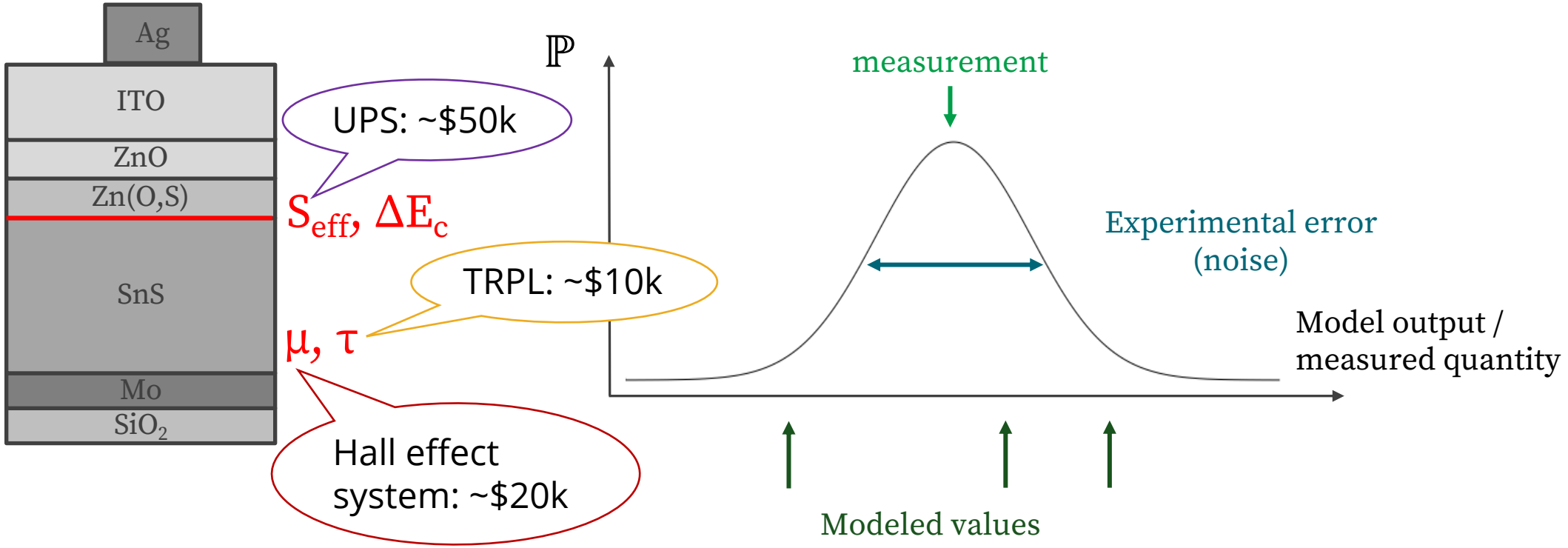


Bayesian parameter estimation

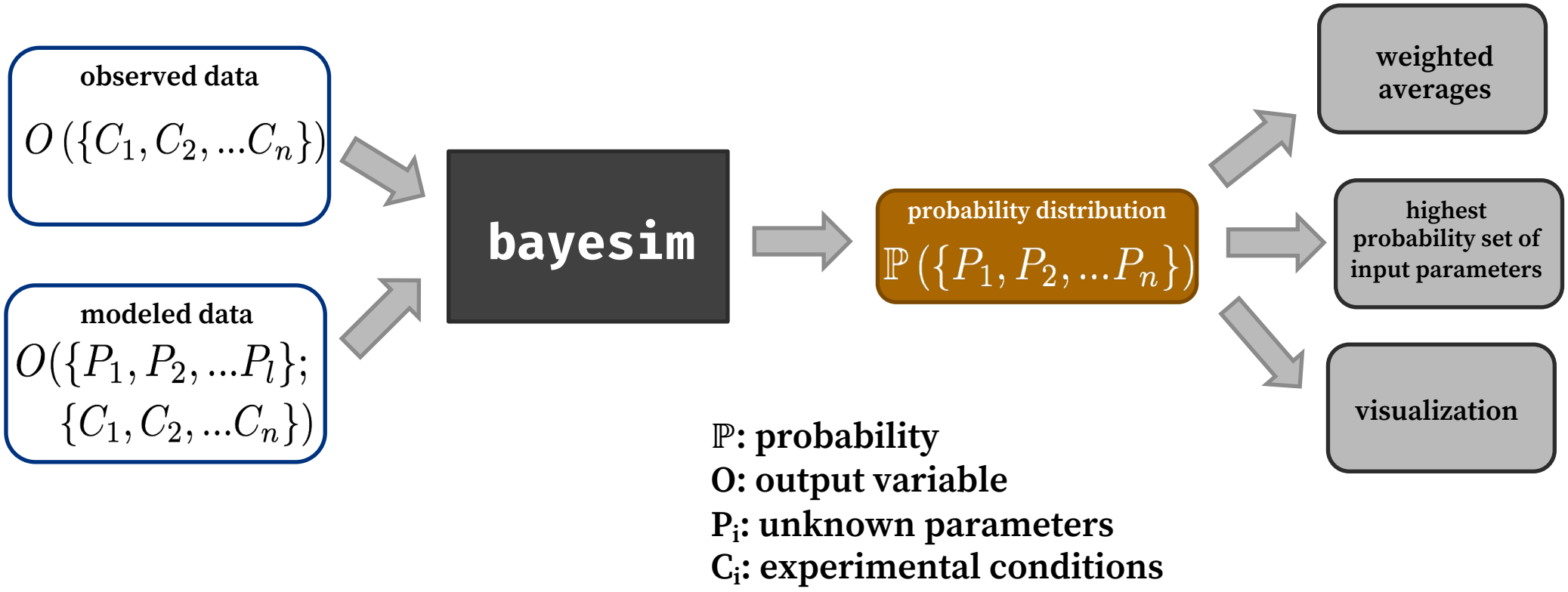
SnS solar cell:

(with some unknown) materials/interface properties)

Likelihood function comes from a **forward model** that tells us what we would measure *if* parameters took particular values…

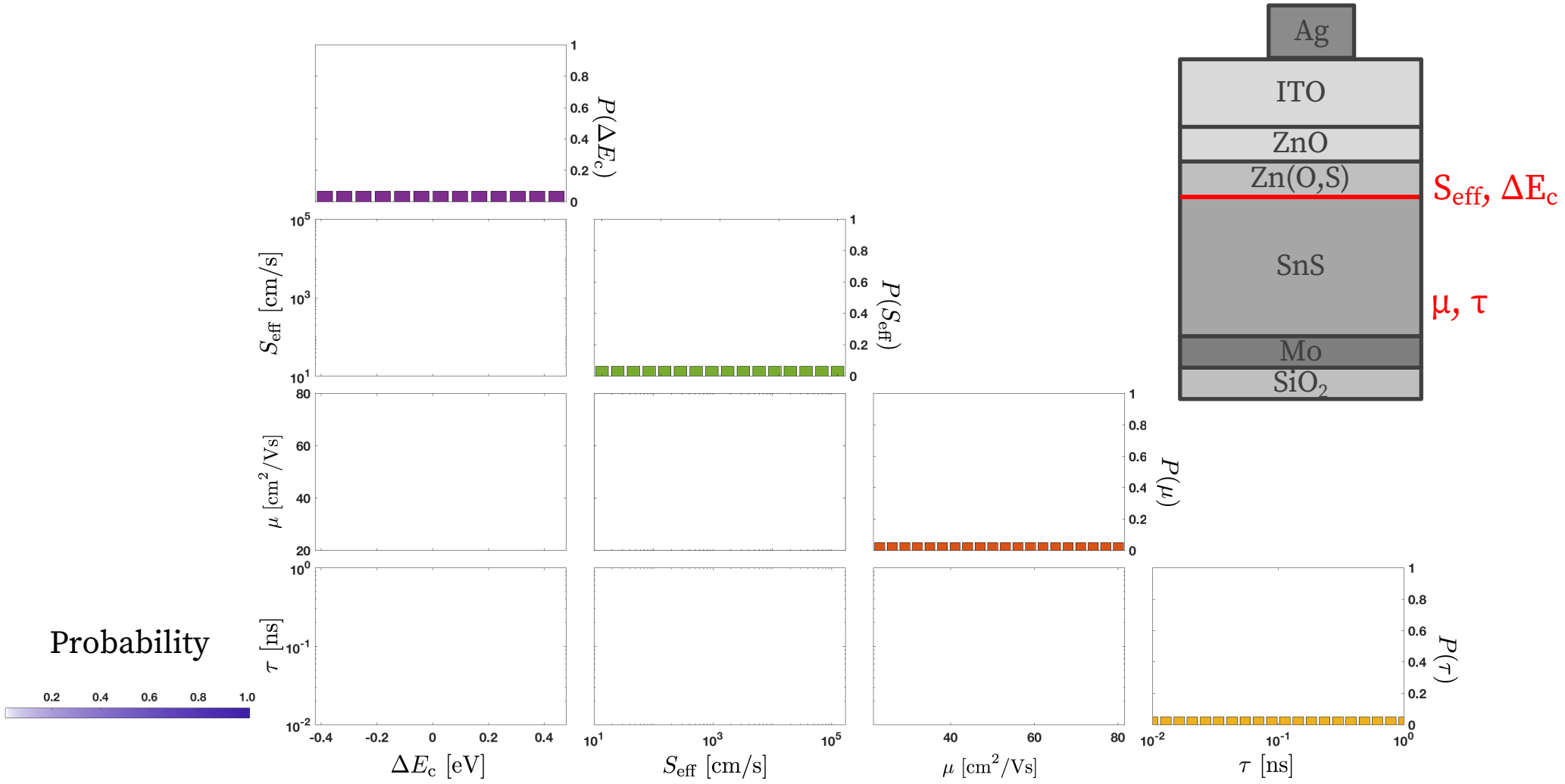


Bayesim: open-source BPE for expensive models



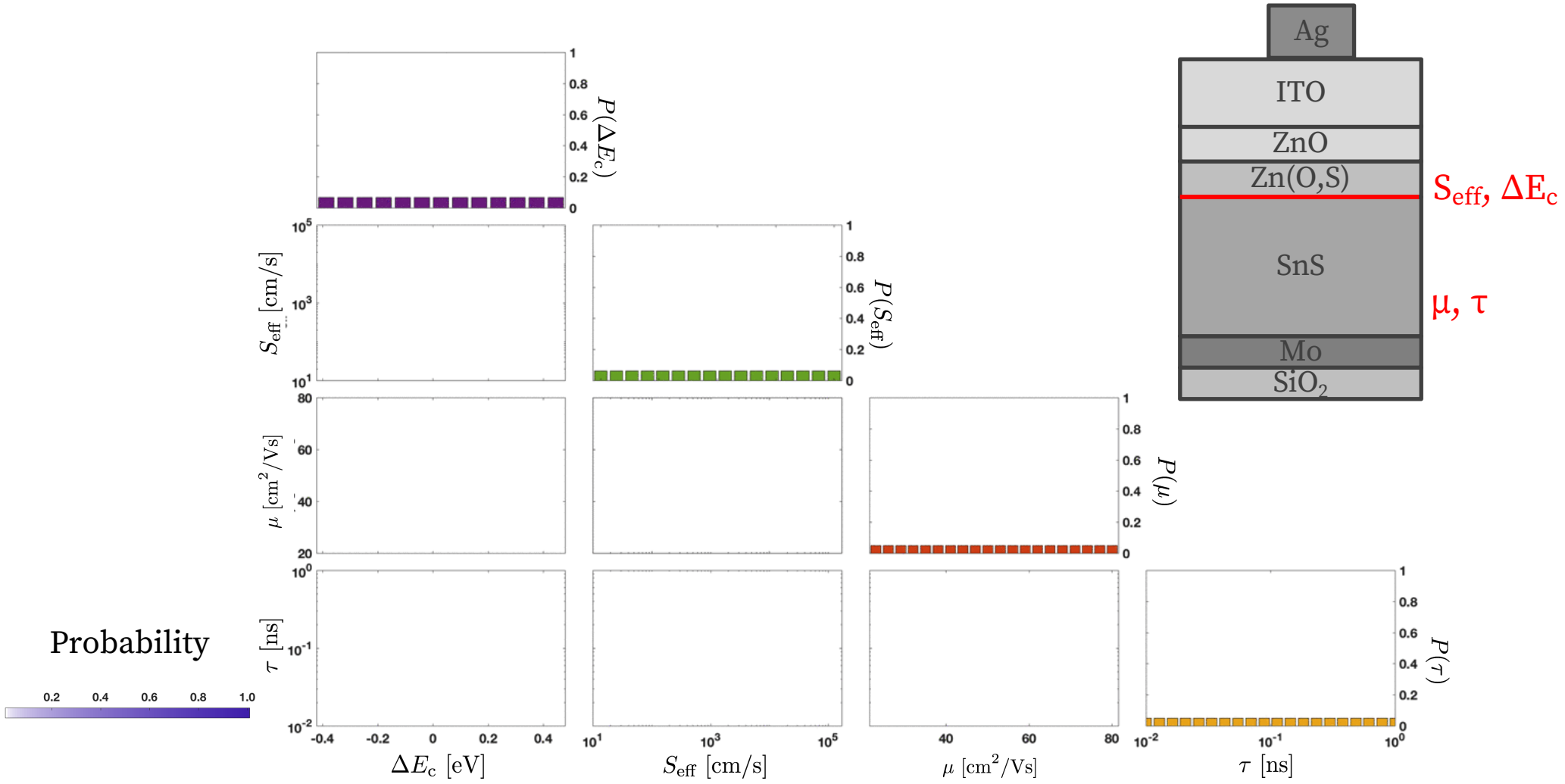
R. Kurchin, G. Romano, and T. Buonassisi. *Computer Physics Communications* **2019**, 239, 161. 10.1016/j.cpc.2019.01.022

Tin Sulfide (SnS) Photovoltaics



R. E. Brandt, **R. C. Kurchin,** et al. *Joule* **2017**, 1(4), 843. 10.1016/j.joule.2017.10.001

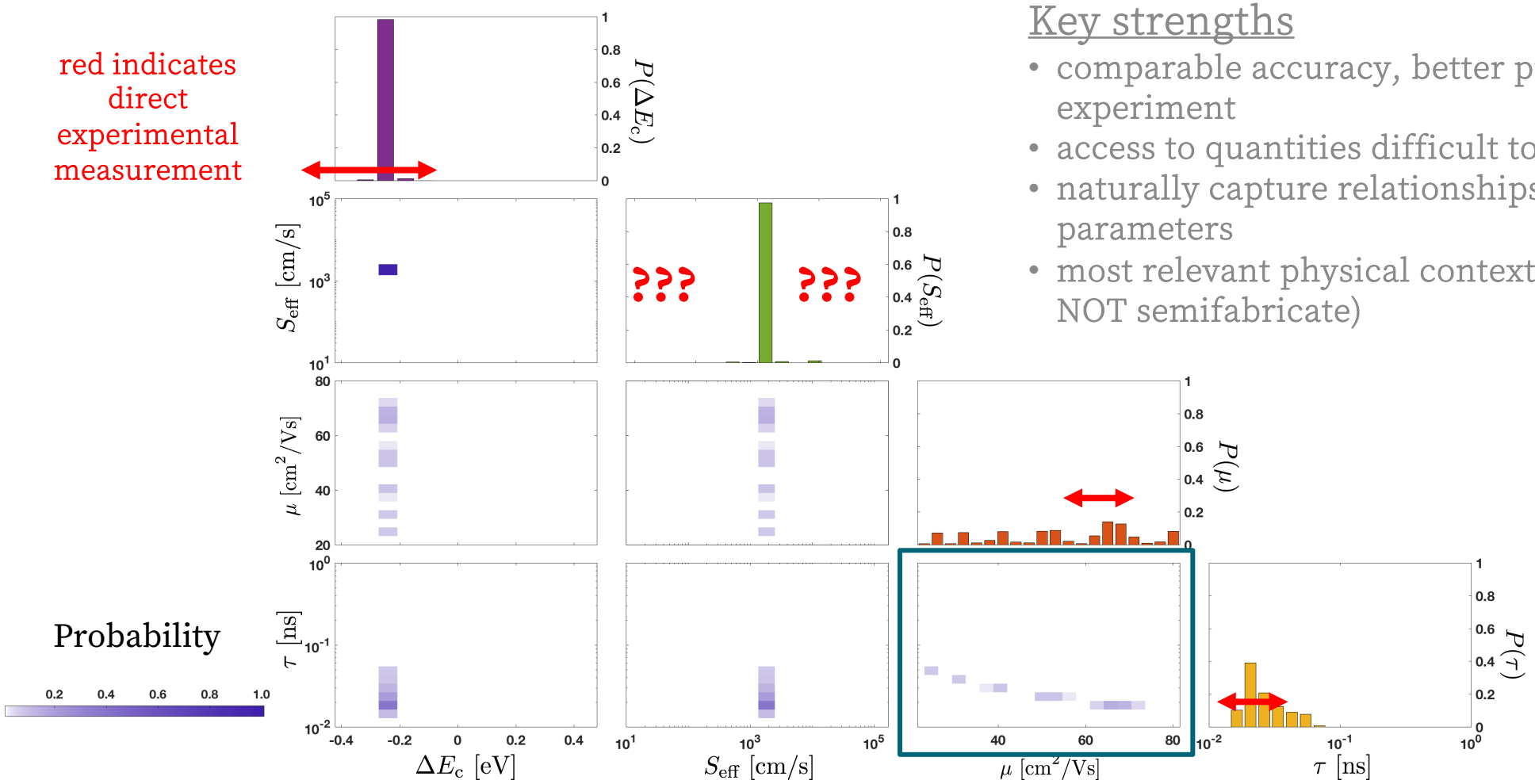
Tin Sulfide (SnS) Photovoltaics



R. E. Brandt, **R. C. Kurchin,** et al. *Joule* **2017**, 1(4), 843. 10.1016/j.joule.2017.10.001

Tin Sulfide (SnS) Photovoltaics

red indicates direct experimental measurement



Key strengths

- comparable accuracy, better precision vs. experiment
- access to quantities difficult to probe directly
- naturally capture relationships between parameters
- most relevant physical context (in device, NOT semifabricate)

constant product → diffusion length!

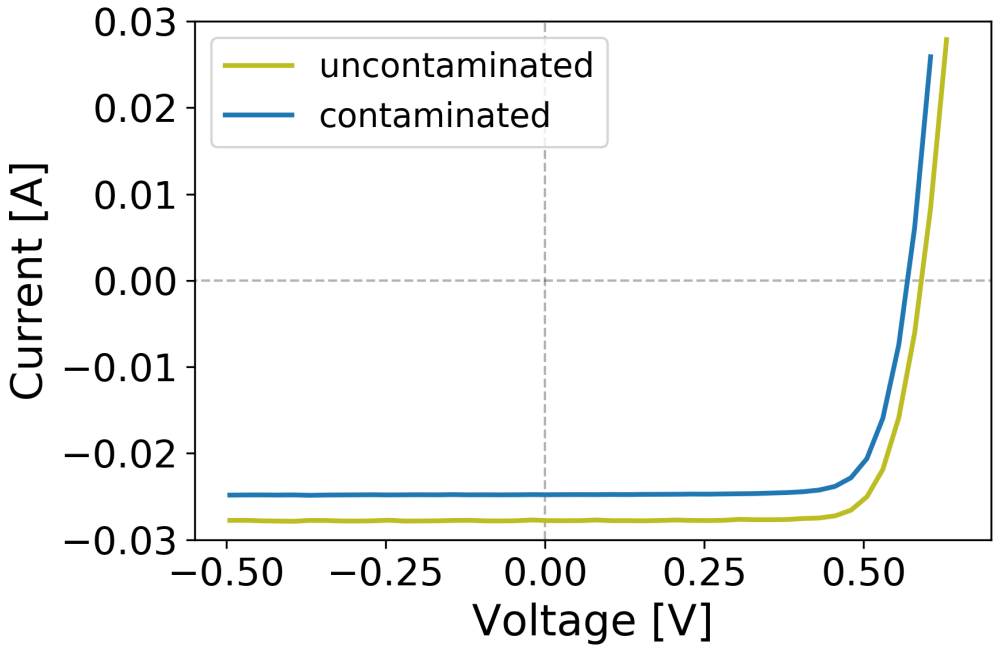
R. E. Brandt, **R. C. Kurchin,** et al. *Joule* **2017**, 1(4), 843. 10.1016/j.joule.2017.10.001

Let's make this a little harder…

- Core intuition: anything that affects experimental measurement must have a *signal* in that measurement…so how much can we get?

- Properties of point defects are notoriously difficult to characterize…yet they can have dramatic effects on PV performance!

Contamination by
1 part in 250 billion
of interstitial iron!



R. C. Kurchin et al. *IEEE Journal of Photovoltaics* **2020**, 10(6) 1532. 10.1109/JPHOTOV.2020.3010105

Defect-Assisted Recombination

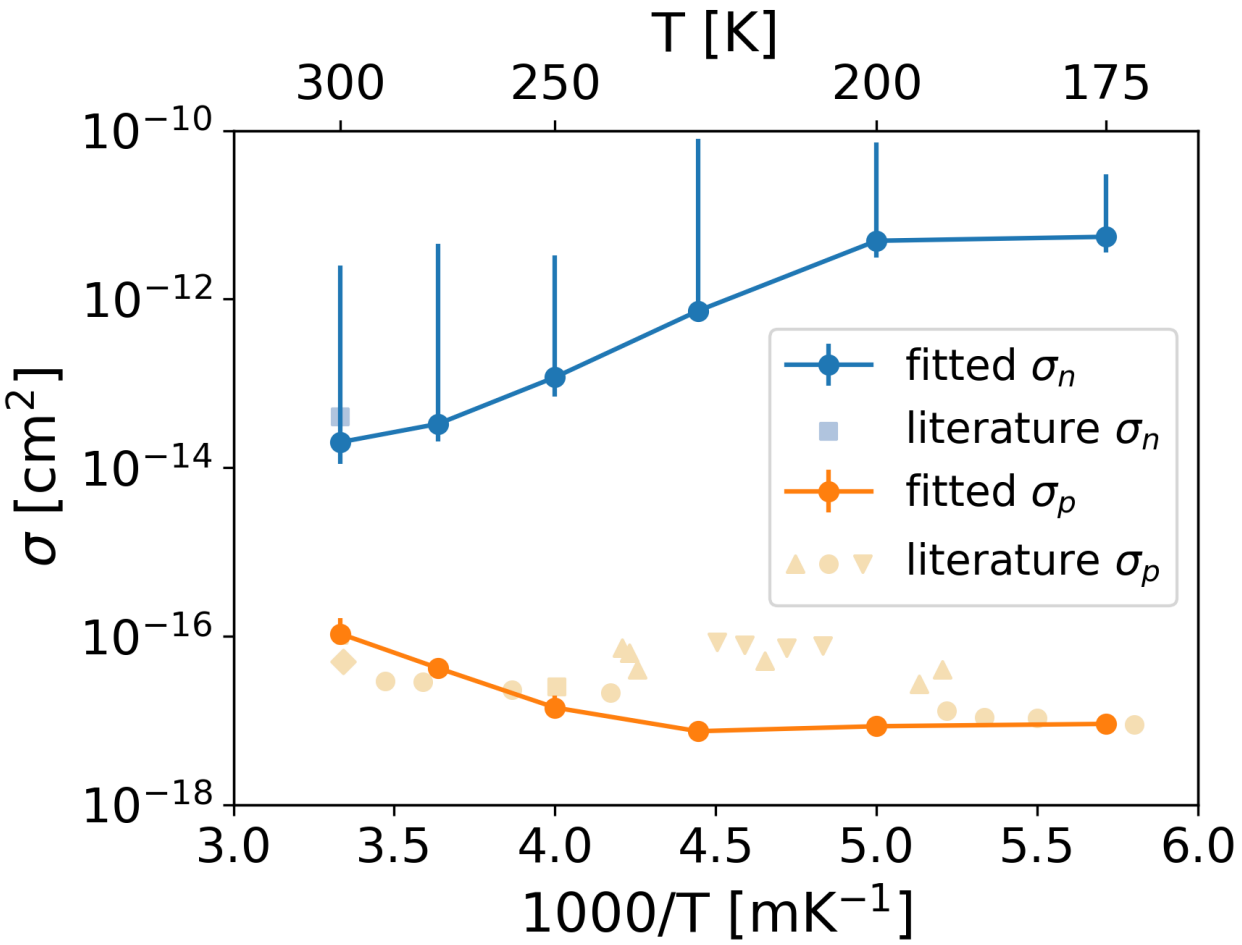
$$\frac{1}{\tau_{\mathrm{SRH}}} \sim \frac{np - n_i^2}{\tau_p \left(n + n_i \exp\left(\frac{E_t - E_\mathrm{i}}{k_B T} \right) \right) + \tau_n \left(p + n_i \exp\left(\frac{E_\mathrm{i} - E_t}{k_B T} \right) \right)}$$

fitting parameters
functions of experimental conditions (ill., T)

$$\tau_p = \frac{1}{N_t \sigma_p v_{\mathrm{th}}}$$

W. Shockley and W. Read. *Phys. Rev.* 1952, 87(46), 835. 10.1103/PhysRev.87.835
R. N. Hall. *Phys. Rev.* 1952, 87(2), 387. 10.1103/PhysRev.87.387
R. C. Kurchin et al. *IEEE Journal of Photovoltaics* 2020, 10(6) 1532. 10.1109/JPHOTOV.2020.3010105

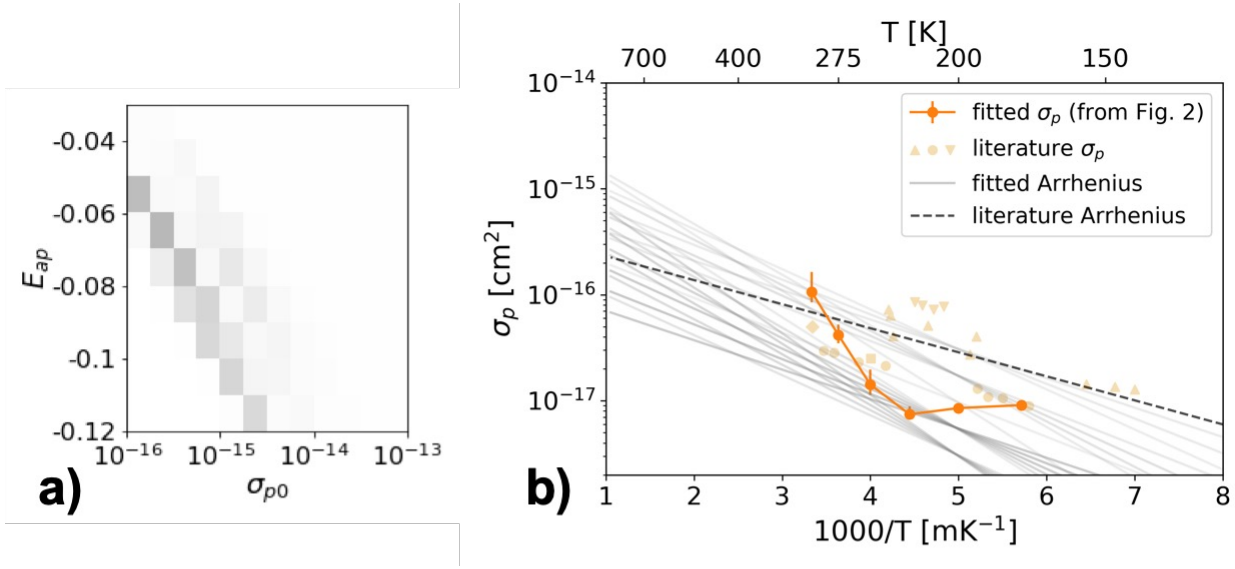
Capture Cross-Sections vs. literature



R. C. Kurchin et al. *IEEE Journal of Photovoltaics* **2020**, 10(6) 1532. 10.1109/JPHOTOV.2020.3010105

Temperature Dependence of σ

$$\sigma_p = \sigma_{p0} \exp\left(\frac{E_{ap}}{k_B T}\right)$$



condition on known activation energy…

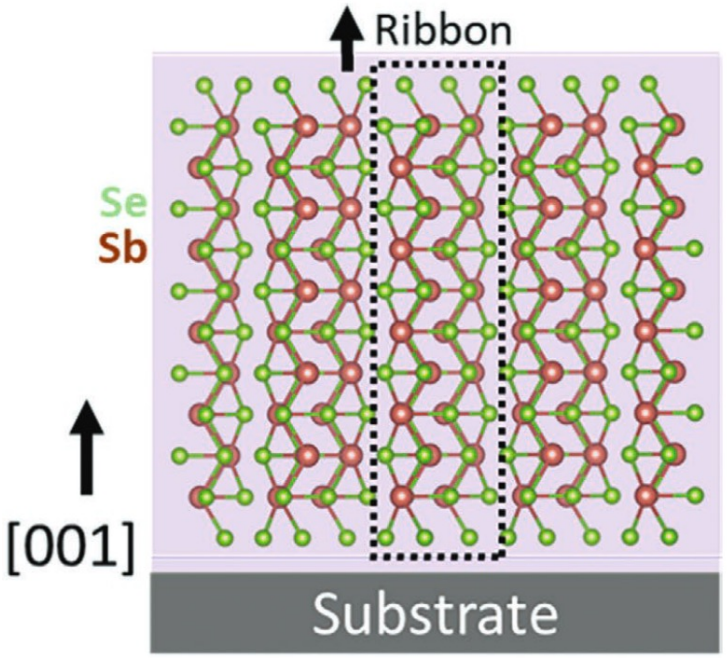
R. C. Kurchin et al. *IEEE Journal of Photovoltaics* **2020**, 10(6) 1532. 10.1109/JPHOTOV.2020.3010105

Summary so far…

- Validated a novel BPE-based approach to measuring materials properties from simple, automatable electrical measurements of solar cells
- Allows us to “trade off” expensive experimental effort for cheap(er) computations
- Redundantly good fits emerge naturally
- We can measure the most relevant “versions” of properties in most relevant context

Ongoing Work

$Sb_2(S,Se)_3$:
a promising class of novel Earth-abundant thin-film PV absorbers



S. Rijal et al. *Adv. Funct. Mater.* **32** 10, 2022.

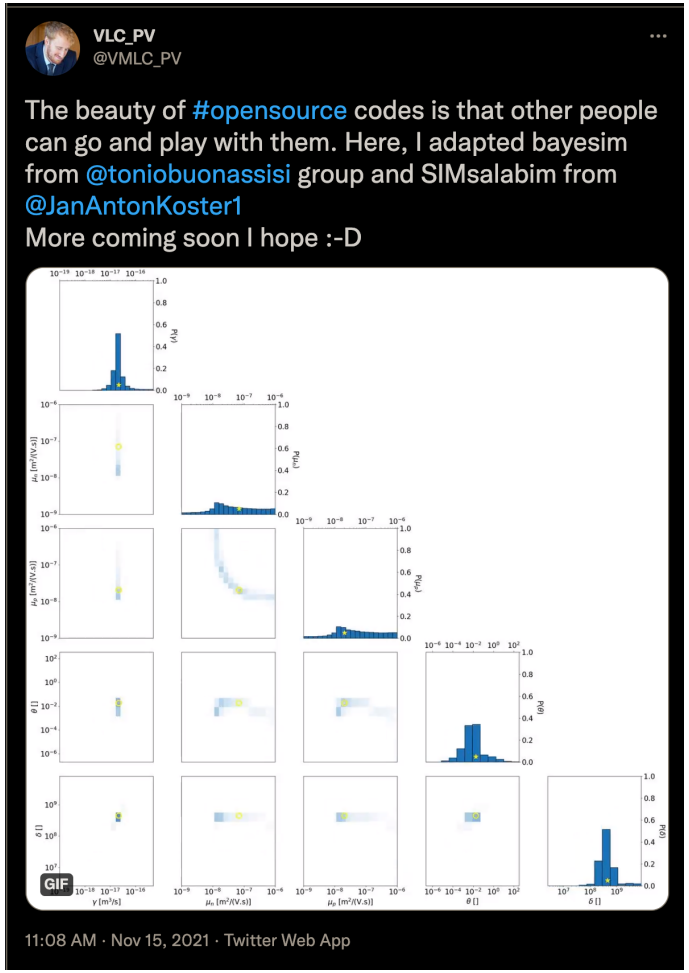
Experimental collaborators:
Prof. Yanfa Yan, Alisha Adhikari

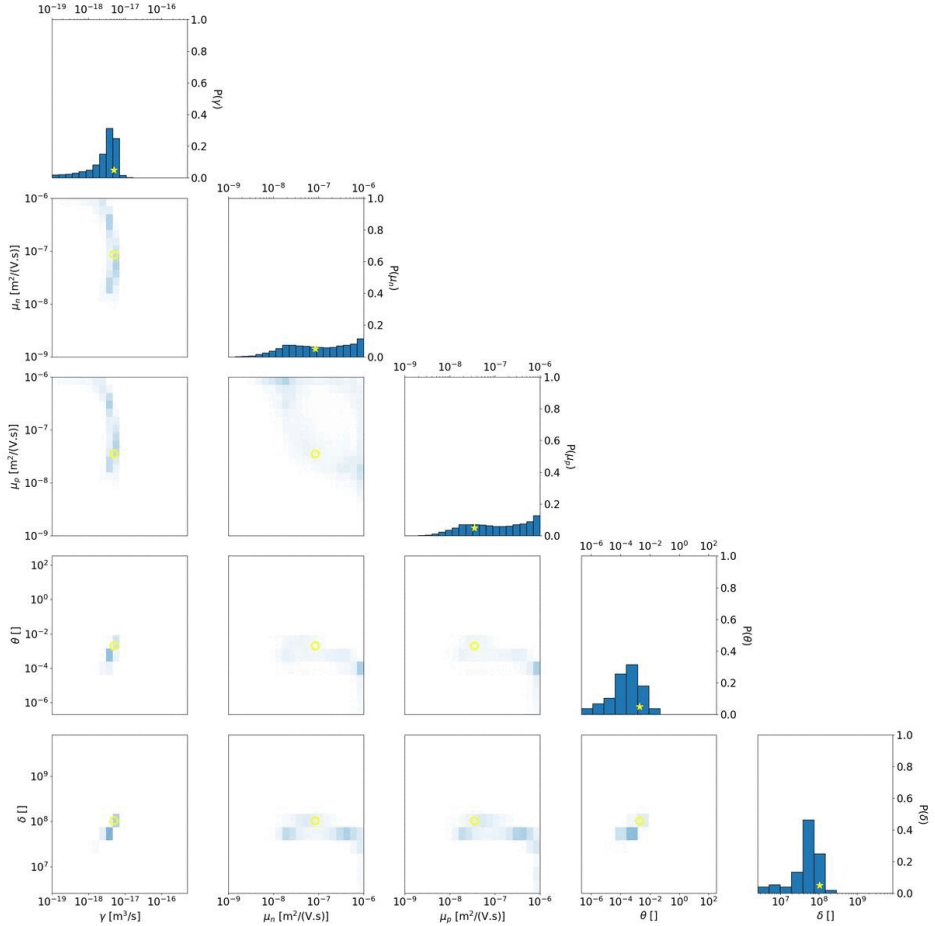
Goal: use BPE to accelerate not only the *characterization* of these materials/devices, but also their *engineering!*

What's next?

- Incorporate better sampling approaches to expand number of parameters we can afford to fit (e.g. VBMC)
- Extend beyond photovoltaics – interested in using this approach in your system of interest? **Please come and chat!**

The beauty of open-source software!





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group website: https://https://acme-group-cmu.github.io/

and of course to
Michael Herbst
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