Semiconductor parameter extraction via current-voltage characterization and Bayesian inference methods

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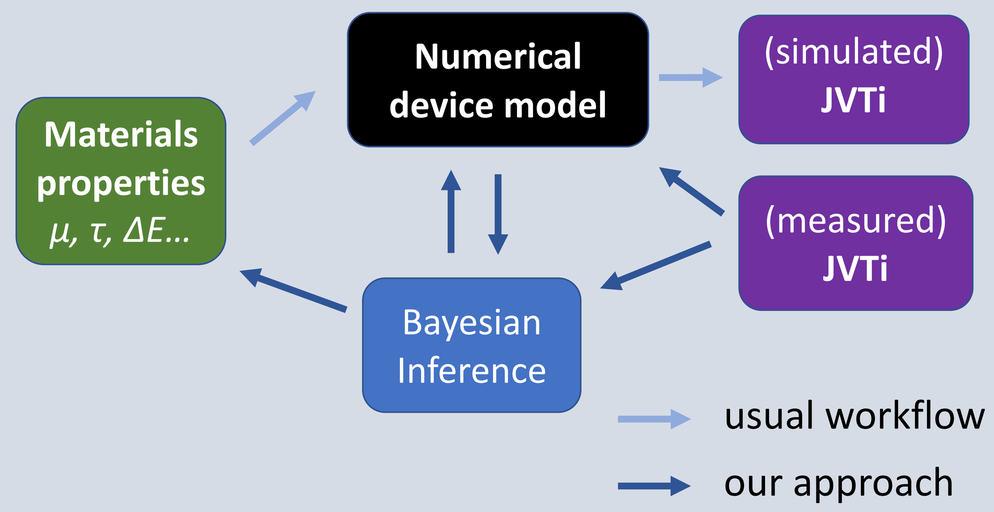
Introduction

- There is a need to accelerate diagnosis of limiting factors in early-stage photovoltaic materials and devices
- Direct measurement of relevant quantities (e.g. carrier mobility, trap energy level, etc.) can be difficult and/or subject to assumptions/models that may not apply in the materials under consideration
- However, by definition, **all materials/device parameters that affect device performance have a measurable (*and modelable*) impact on *JV* characteristics** – in our approach, we exploit this fact



How Does it Work?

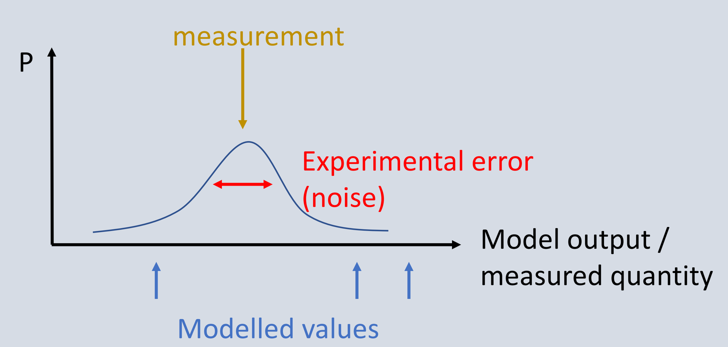
Bayes' Theorem

$$\underbrace{P(H|E)}_{\text{Posterior}} = \frac{\overbrace{P(H)}^{\text{Prior}}\overbrace{P(E|H)}^{\text{Likelihood}}}{\underbrace{P(E)}_{\text{Normalizing Constant (evidence)}}}$$

Bayes' theorem is a relation between conditional probabilities that tells us how to update our beliefs about the likelihood of something given a new piece of evidence about it.

Constructing a Likelihood

In order to apply Bayes' theorem on a discrete set of simulated parameters, we must account for experimental error when computing likelihoods.



Iterating...

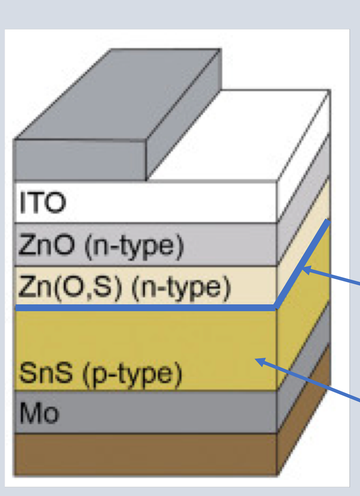
Finally, we iterate this process to update our posterior probability for each piece of observed evidence.

$$P(H|\{E_1, E_2, \dots E_n\}) = \frac{P(H|\{E_1, E_2, \dots E_{n-1}\})P(E_n|H)}{P(E_n)}$$

In this case, each hypothesis *H* is a particular combination of values of parameters and the evidence *E* is *J(V, T, i)*

Tin Sulfide (SnS) solar cells

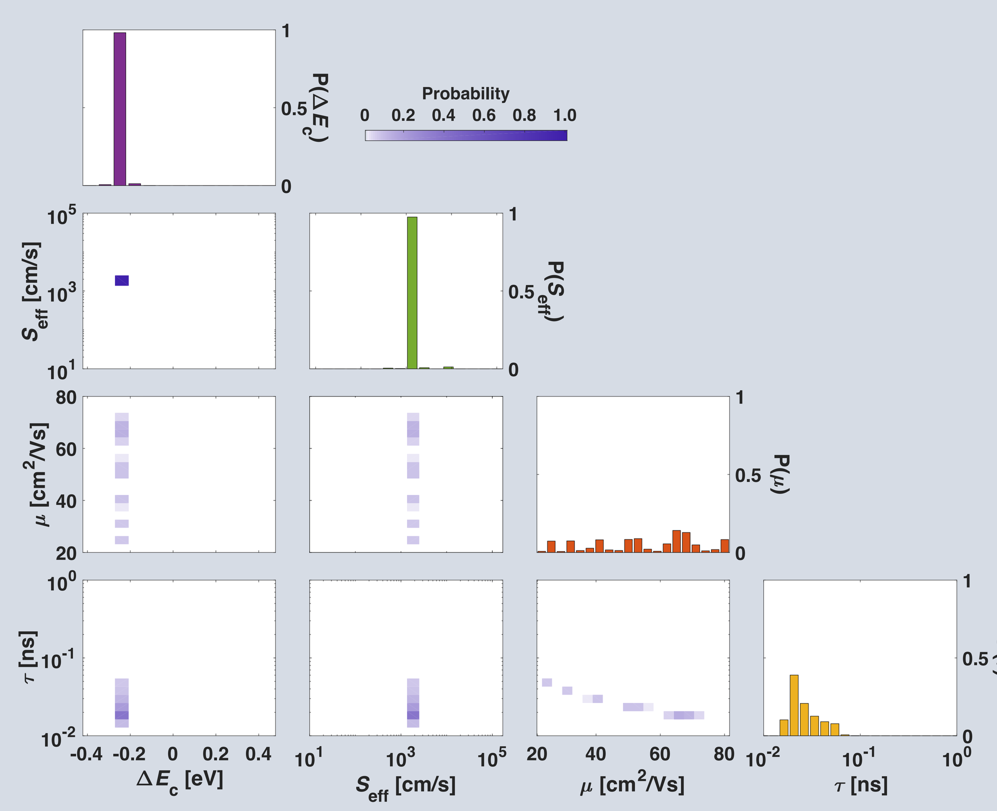
- We first apply this approach to SnS solar cells [1] (device stack shown to the right), modeled using SCAPS-1D [2]
- Band offset is consistent with previous direct measurement and SRV had never before been measured



ΔE_c, S_{eff} at SnS/Zn(O,S) interface

μ_e, τ_e in SnS bulk

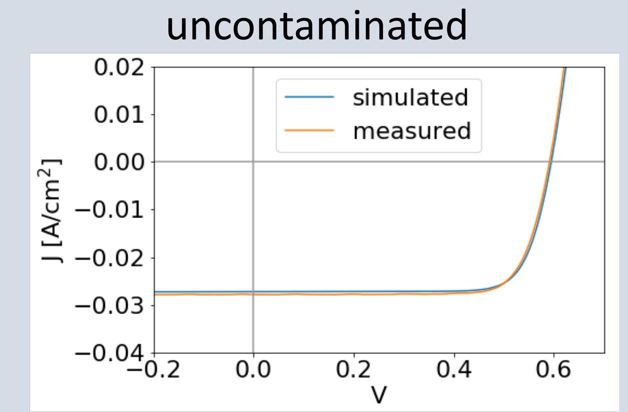
- Diffusion length (mobility-lifetime product) is well-constrained by fit



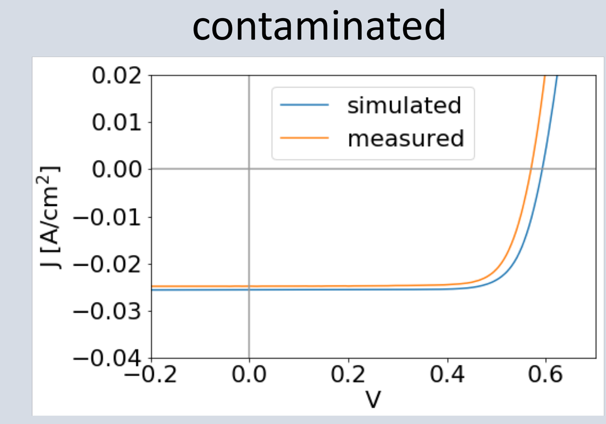
Iron in Silicon

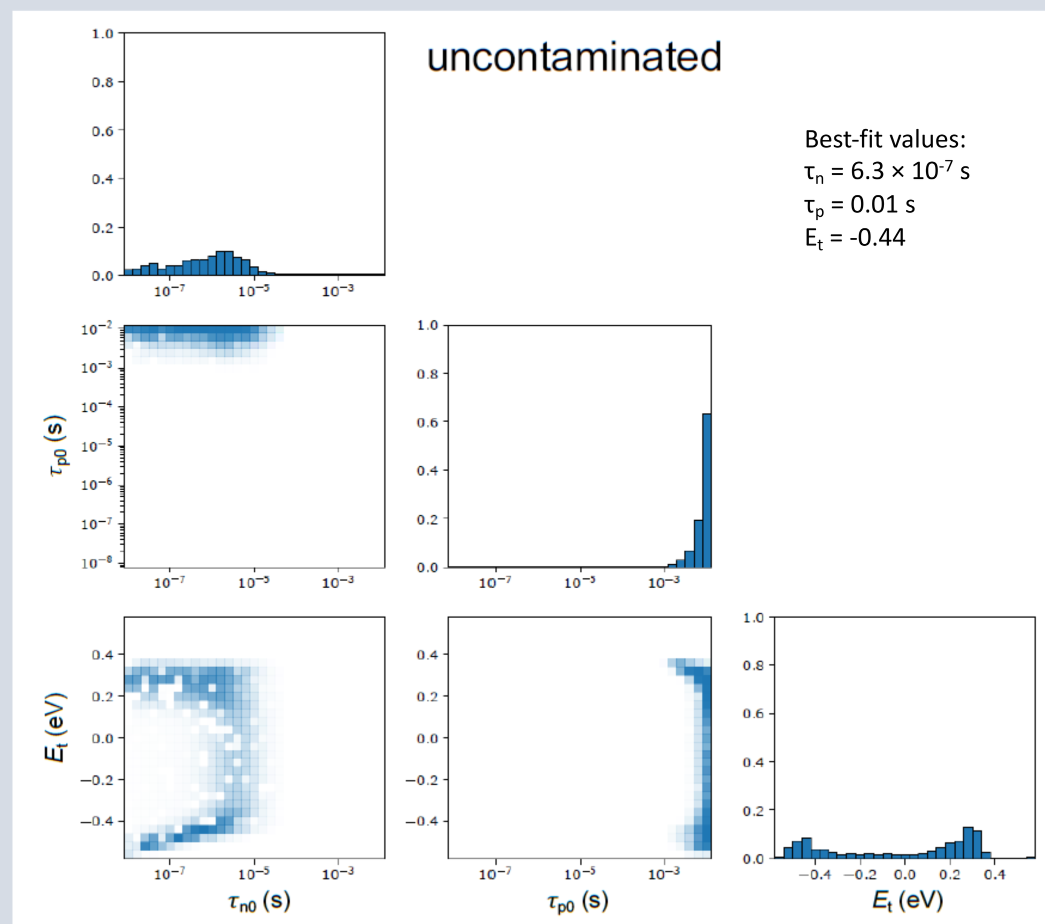
- Defect parameters (e.g. trap level and capture cross-sections) are notoriously difficult to measure directly
- To demonstrate the efficacy of the Bayesian approach, we demonstrate this initially for iron in silicon, an extremely well-characterized system
- Modeling the devices using PC1D [3], we fit one uncontaminated sample and one sample intentionally contaminated with a known level of interstitial iron, characterized in previous work [4]
- Further refinements could be made by including temperature dependence of capture cross-sections and resistances
- Work is ongoing to further subdivide the grid squares and run the inference on more measured data to further converge the fitted parameters

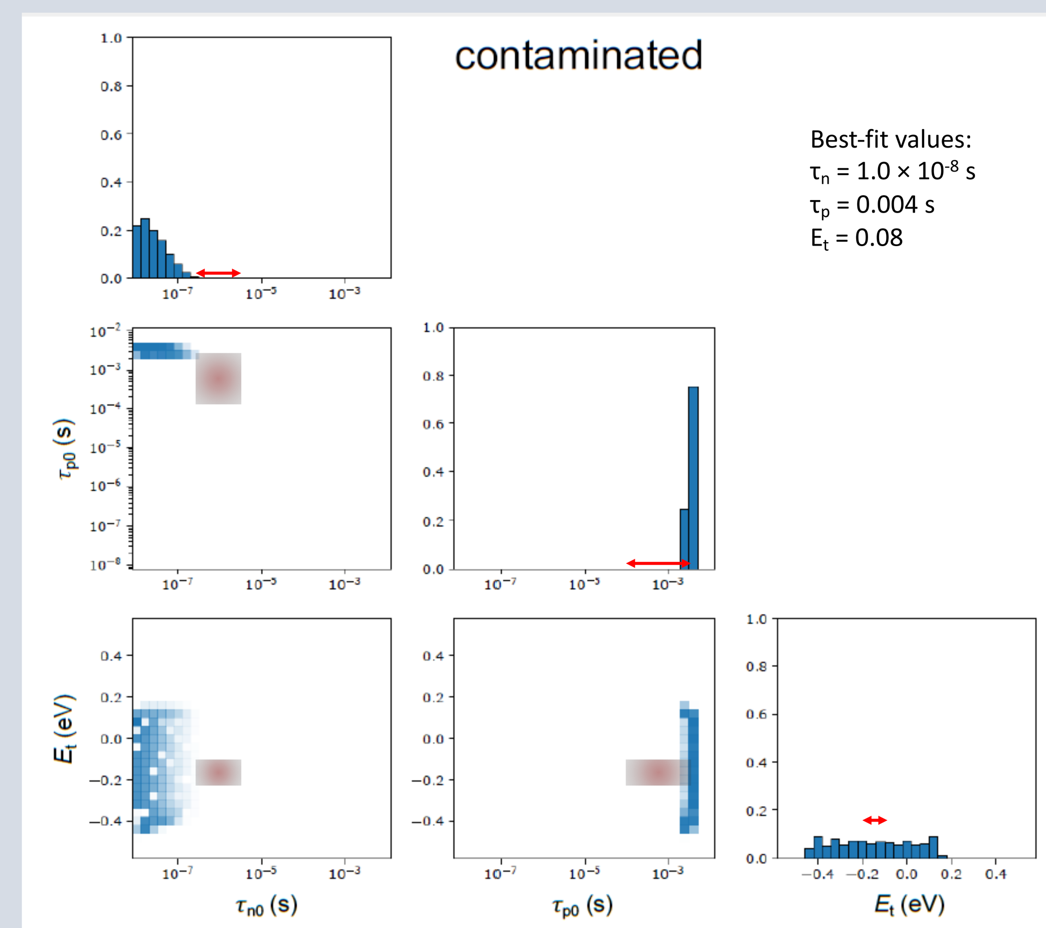
uncontaminated



contaminated







Literature-reported ranges [5] for each parameter are shown in red for the contaminated sample (right).

Conclusions/Acknowledgements

- Bayesian inference is a promising approach to invert numerical device models and use simple, automated JVTi measurements to infer values of underlying physical parameters
- It offers the most physically relevant versions/components of these parameters (e.g. minority carrier mobility in the through-film direction)
- We demonstrate application of this approach to fit bulk and interface properties in SnS devices and SRH parameters of interstitial iron in Si devices
- This method has potential to dramatically accelerate the identification of performance-limiting factors in early-stage photovoltaic materials and devices and reduce the time and cost required to characterize and remedy them

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