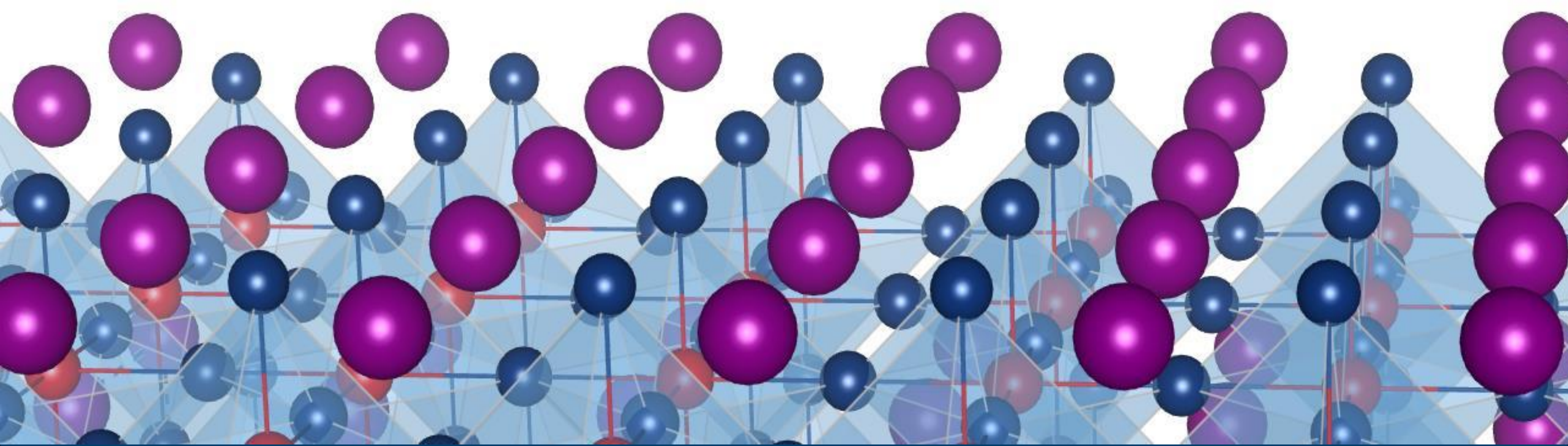


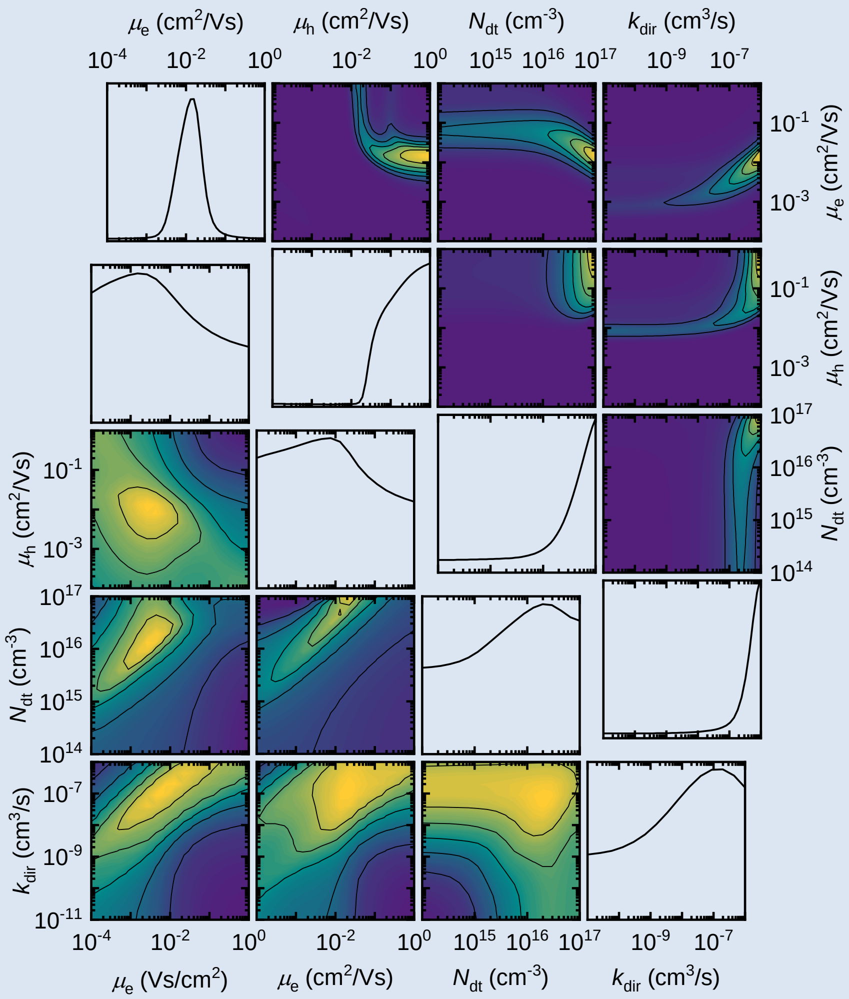
TRANSFORMING CHARACTERIZATION DATA INTO INFORMATION IN EMERGING SOLAR CELLS

Thomas Kirchartz, Paula Hartnagel, Leonard Christen

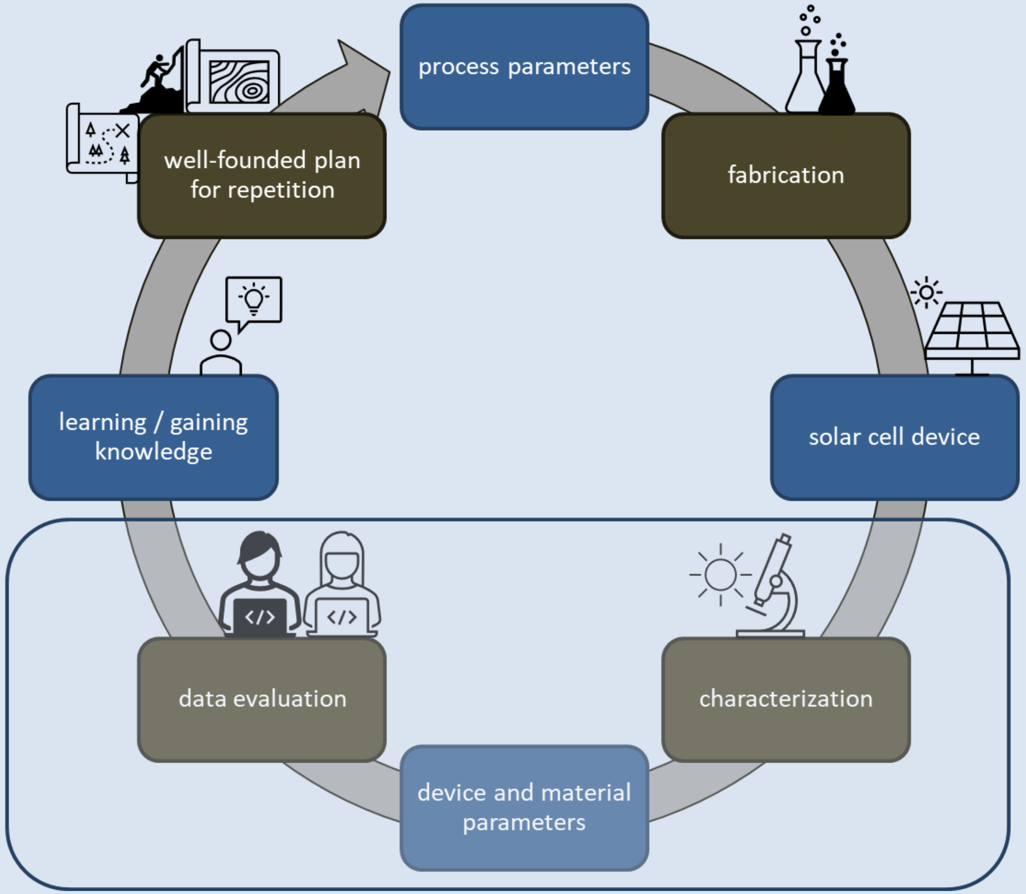
IEK-5 Photovoltaik, Forschungszentrum Jülich

Outline

1) Inferring Parameters

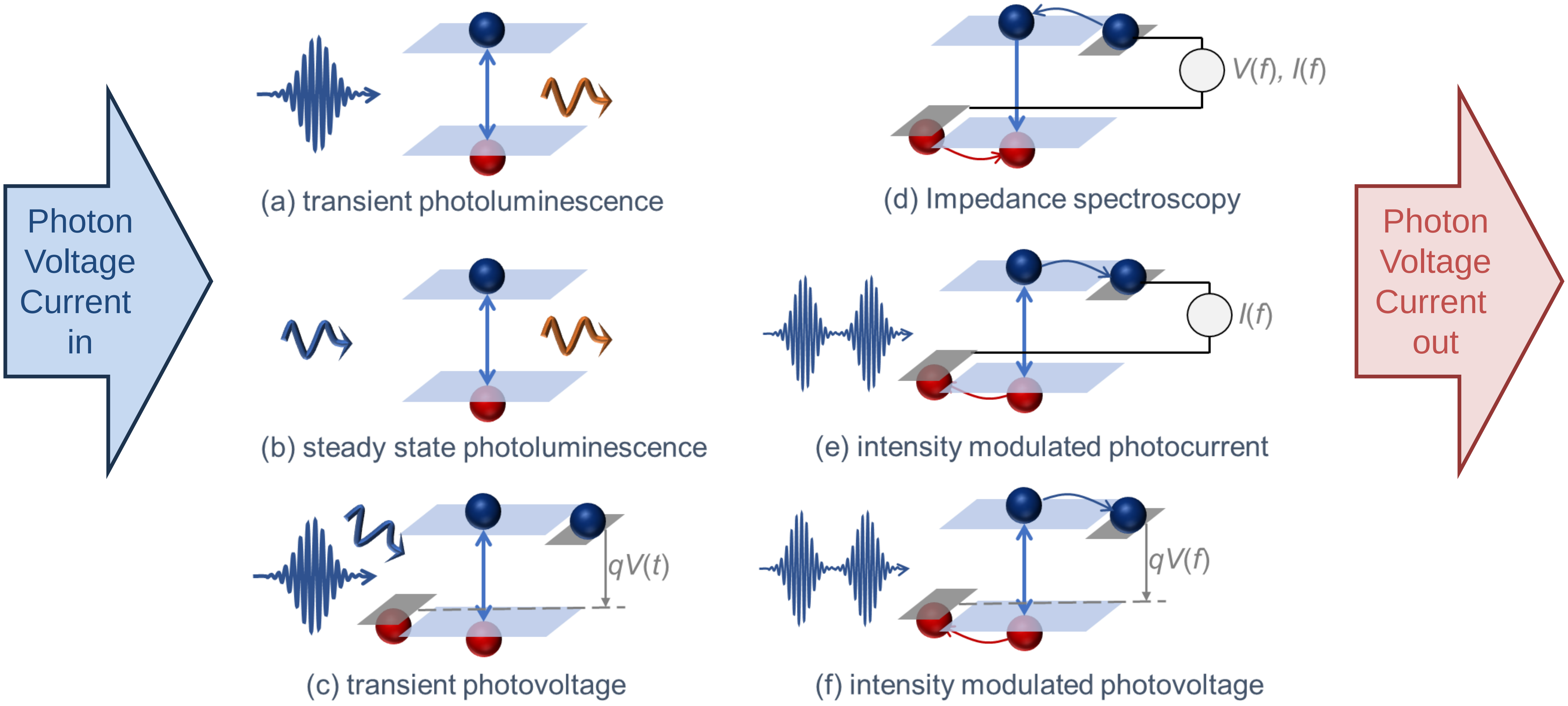


2) Value of Device Characterization



The Challenge

Interpreting methods to infer electronic properties



Kirchartz & Das J. Phys. Energy 2023, **5**, 031001

The Challenge

Interpreting methods to infer electronic properties

(a) Forward Problem

Material parameters, e.g. μ, τ, α, S…

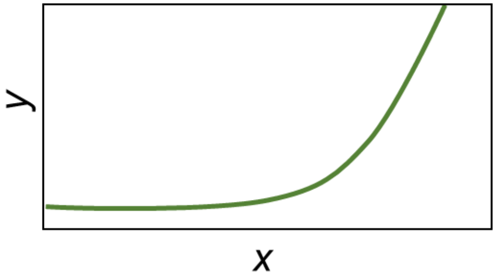
$$\frac{dn}{dt} = G - R + D_n \frac{d^2 n}{dx^2} + \mu_n F \frac{dn}{dx}$$

$$\frac{dp}{dt} = G - R + D_p \frac{d^2 p}{dx^2} - \mu_p F \frac{dp}{dx}$$

$$\frac{d^2 \varphi}{dx^2} = -\frac{\rho}{\varepsilon}$$

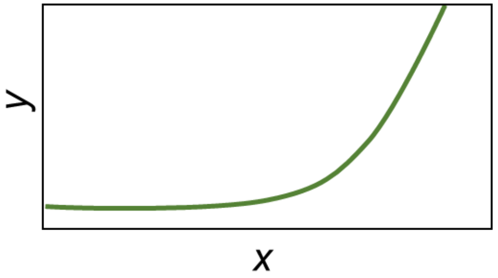
& appropriate boundary conditions

Simulated experimental data



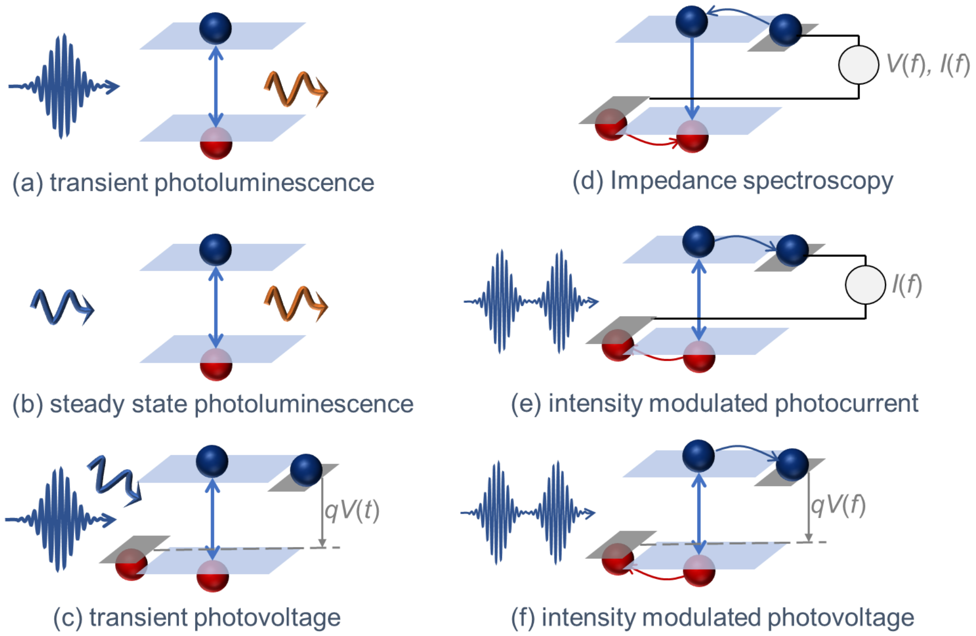
(b) Inverse Problem

Measured experimental data



Algorithm searching for suitable material parameters to explain the experimental data using simulations.

Material parameters, e.g. μ, τ, α, S…



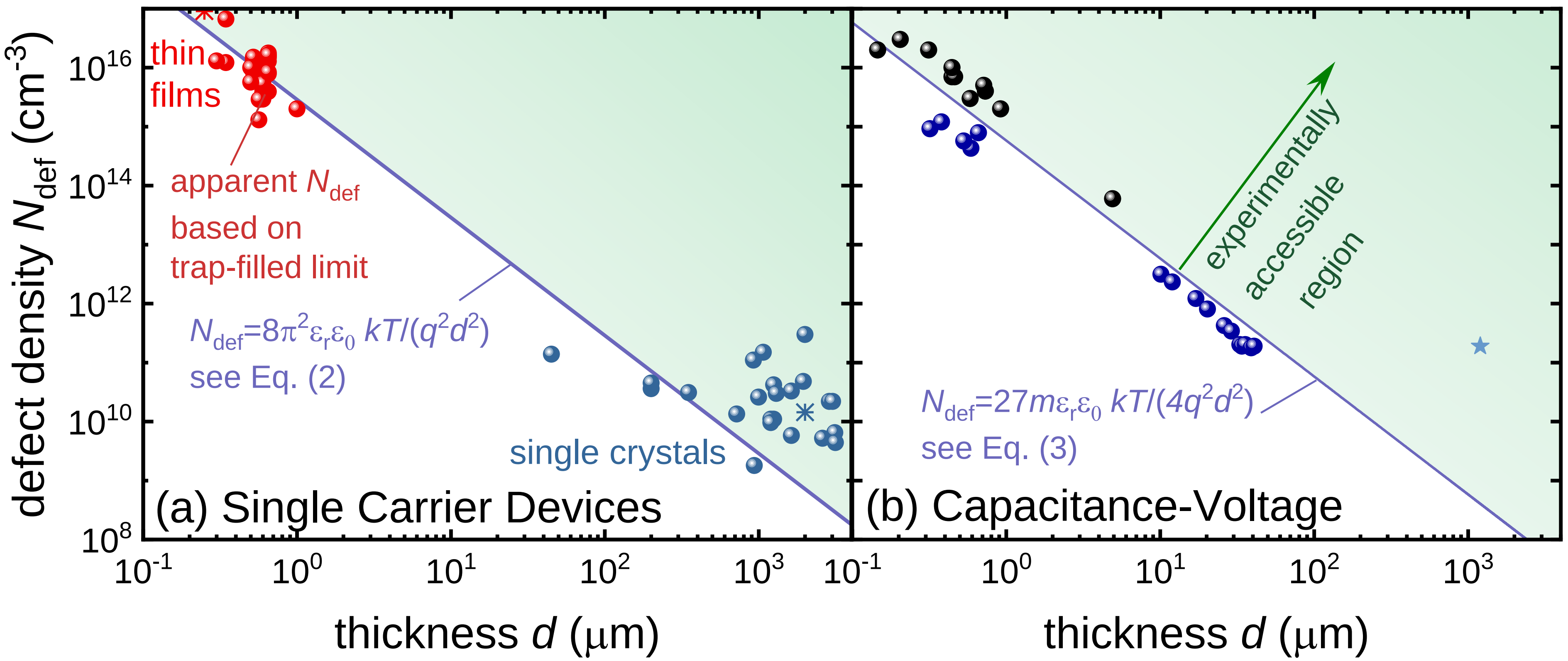
Kirchartz & Das J. Phys. Energy 2023, **5**, 031001

What could possibly go wrong?

Trap densities

Observation:
Trap density scale with ε/d^2

Problem:
Detection limits given by Poisson equation cause the ε/d^2 trend.



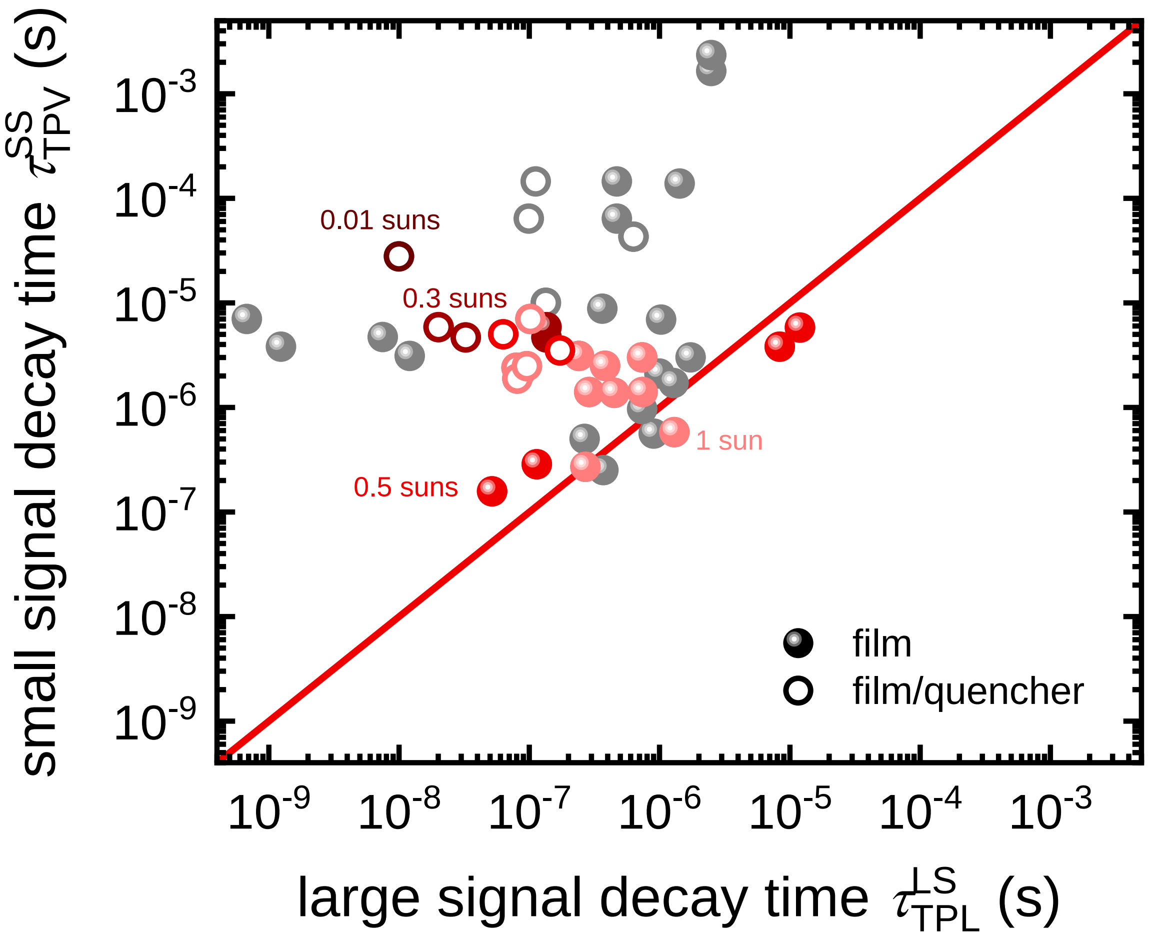
Siekmann et al. ACS Energy Lett. 2021, **6**, 3244

What could possibly go wrong?

Lifetimes

Observation:
Lifetimes depend on the method and sample type

Problem:
Lifetimes are not actual recombination lifetimes but decay times that are affected also by e.g. capacitive discharge of electrodes.



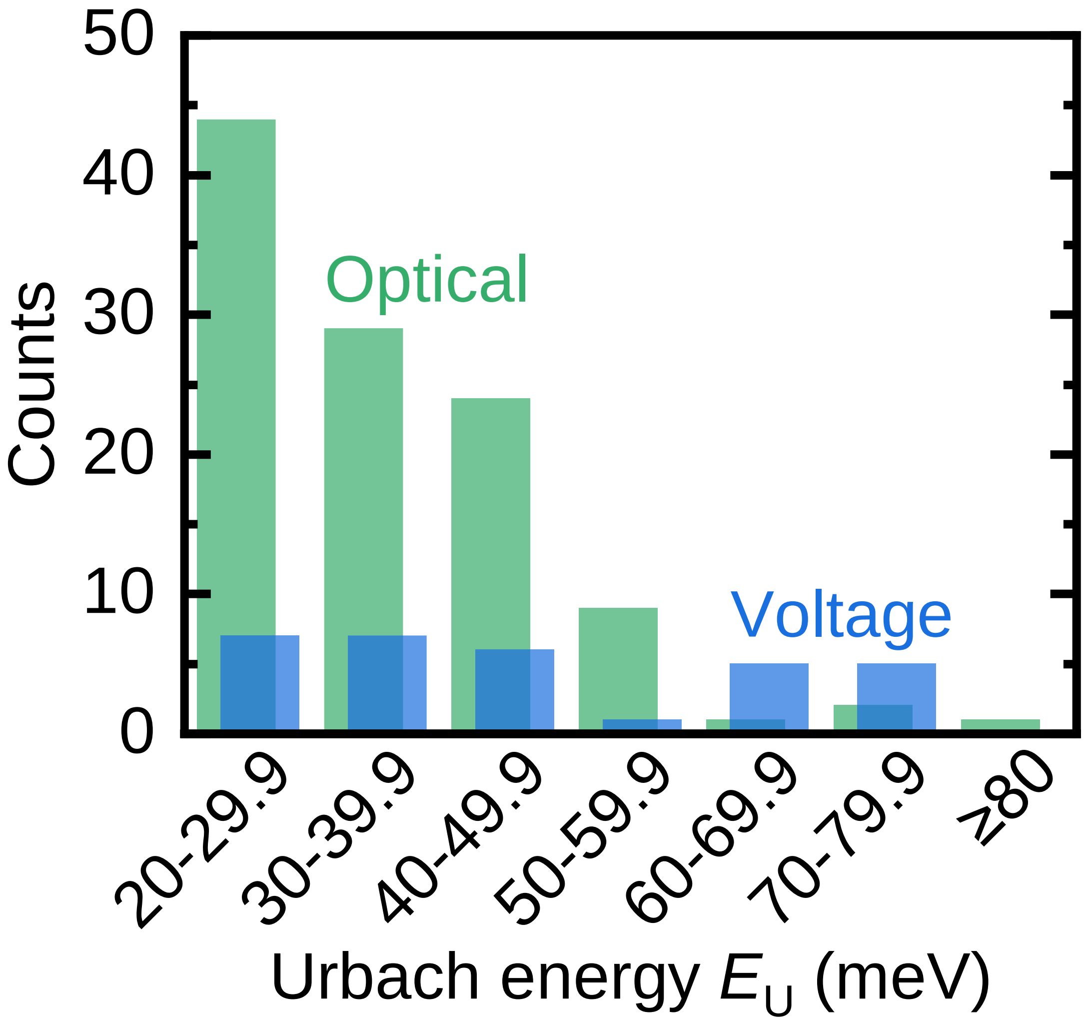
Krückemeier et al. Adv. Energy Mat. 2021, **11**, 2102290

What could possibly go wrong?

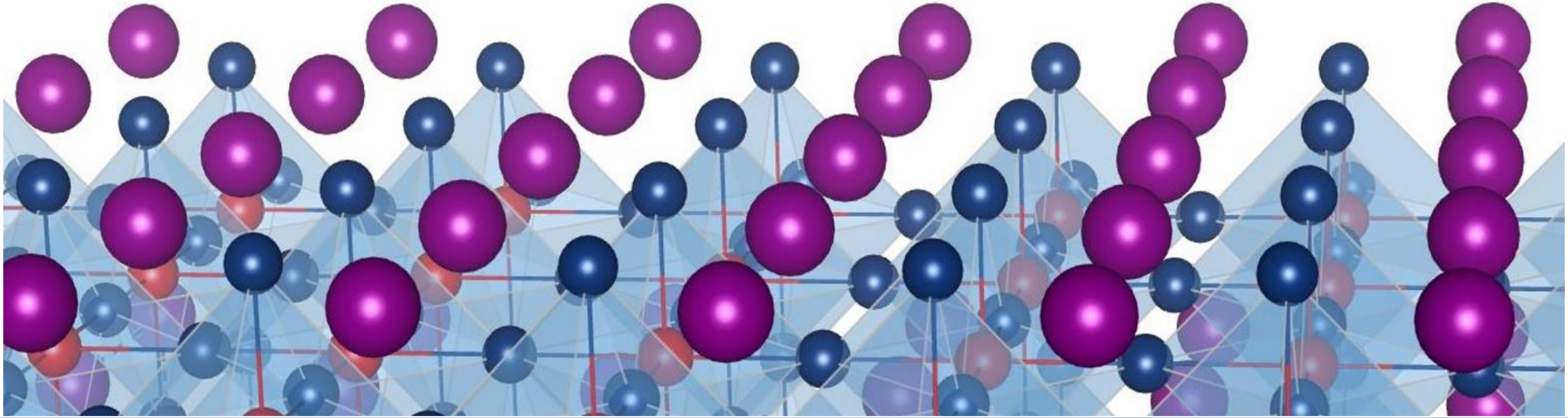
Urbach energies

Observation:
Method-dependent Urbach tail

Problem:
Electrical methods are often affected by low mobilities (resistive effects) and show artificially large Urbach tails



Hartnagel et al. Adv. Energy Mat. 2023, **13**, 2300329



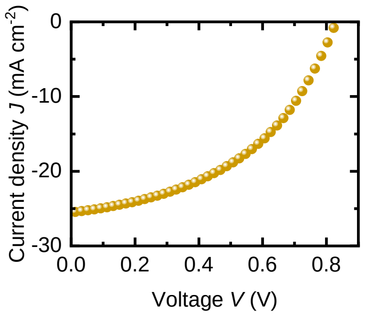
Part 1: Inference of Electronic Properties

Thickness and Light Intensity Dependent Data

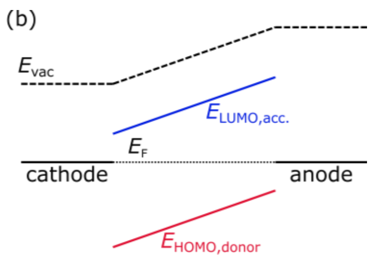
Bayesian Inference

Method

Experimental Data



Device model

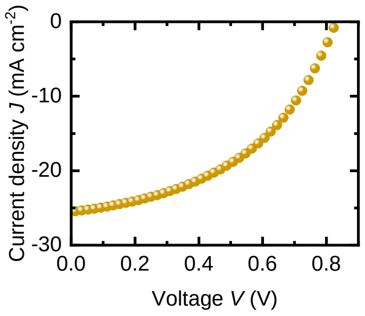



```
variables: mu, tau, …
lower boundaries: 1e-9, 1e-7, …
upper boundaries: 1e-6, 1e-5 , …
```

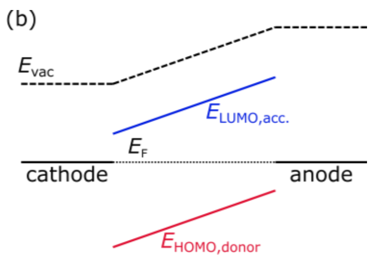
Bayesian Inference

Method

Experimental Data



Device model




```
variables: mu, tau, …
lower boundaries: 1e-9, 1e-7, …
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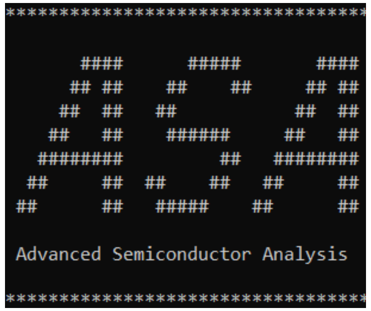
```

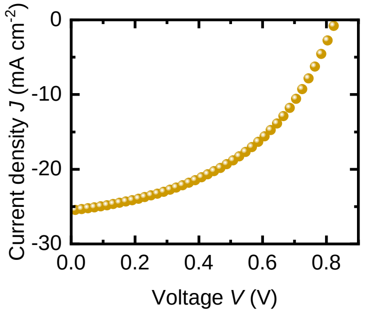
Generate Training Data



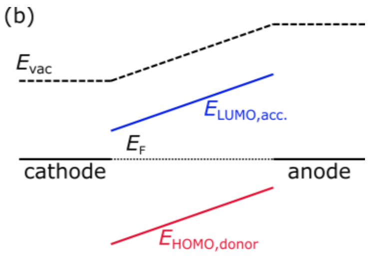
Bayesian Inference

Method

Experimental Data



Device model

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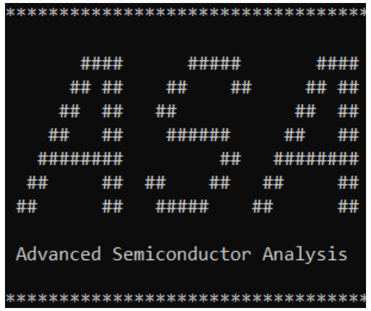
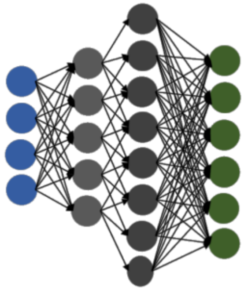


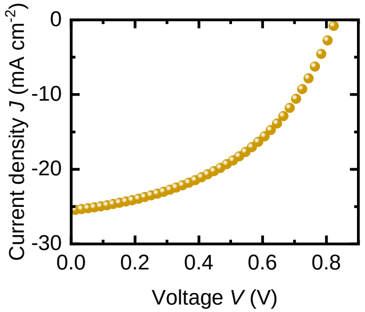
Train Neural Network (NN)



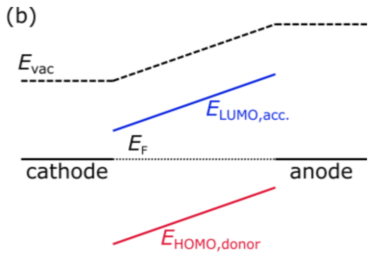
Bayesian Inference

Method

Experimental Data



Device model

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```

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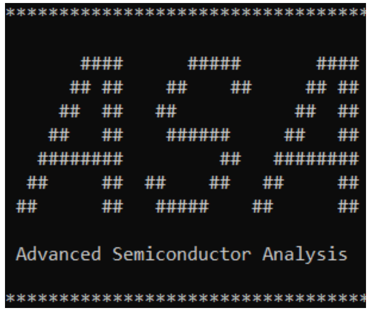

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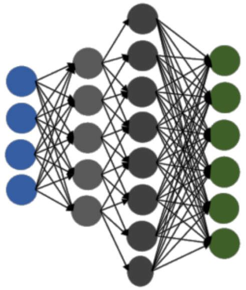
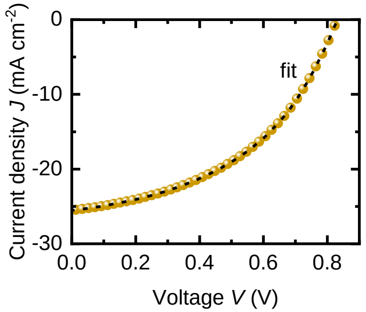


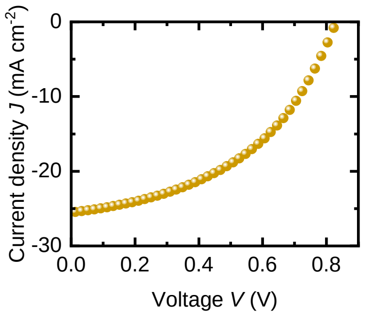
Find Best Fit



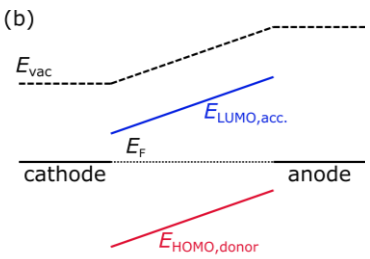
Bayesian Inference

Method

Experimental Data



Device model

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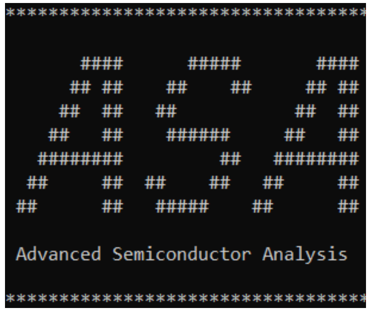

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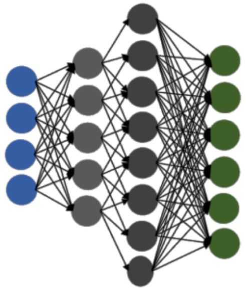
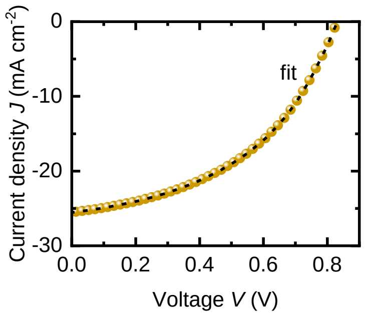
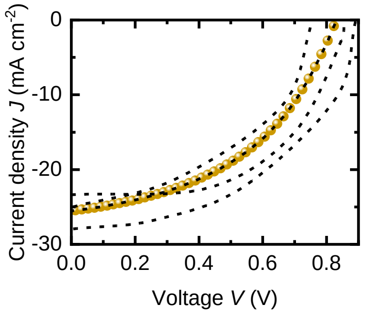


Find Best Fit



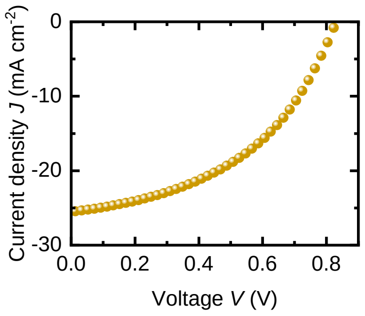
Sample Parameter Space



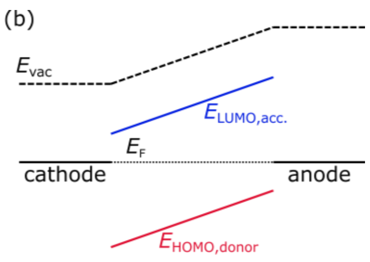
Bayesian Inference

Method

Experimental Data



Device model

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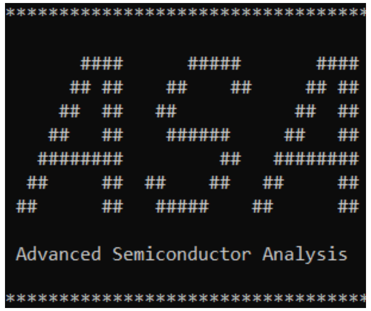
Generate Training Data



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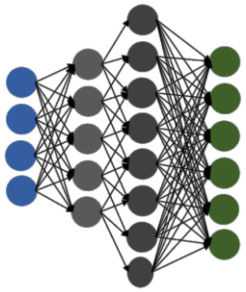
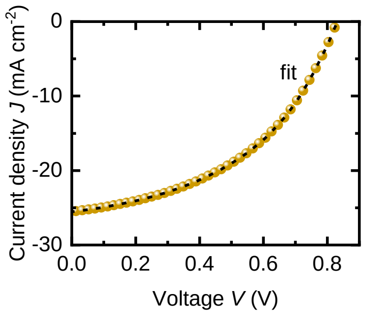
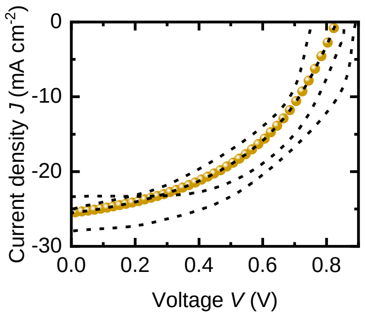


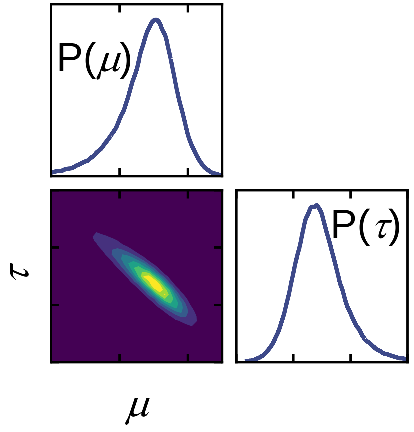
Find Best Fit



Sample Parameter Space

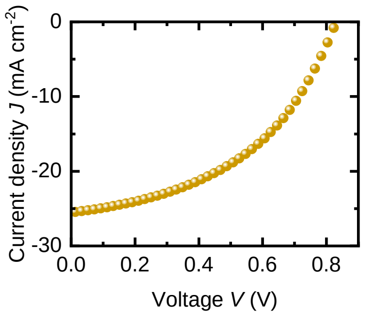


Calculate Probabilities

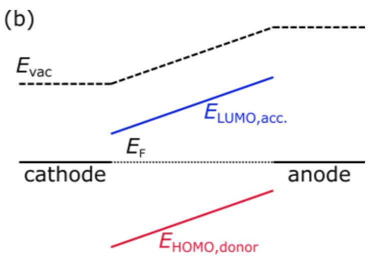


Bayesian Inference
Method

Experimental Data

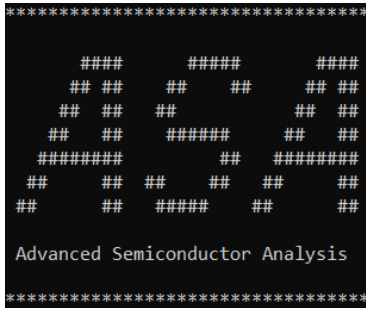


Device model

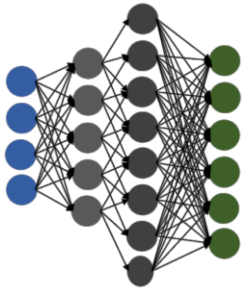


variables: mu, tau, …
lower boundaries: 1e-9, 1e-7, …
upper boundaries: 1e-6, 1e-5 , …

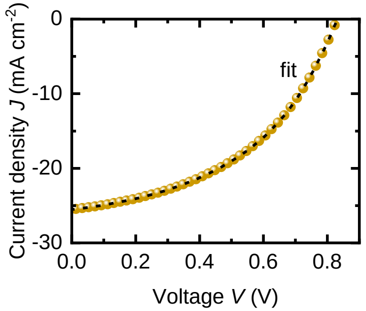
Generate Training Data



Train Neural Network (NN)



Find Best Fit

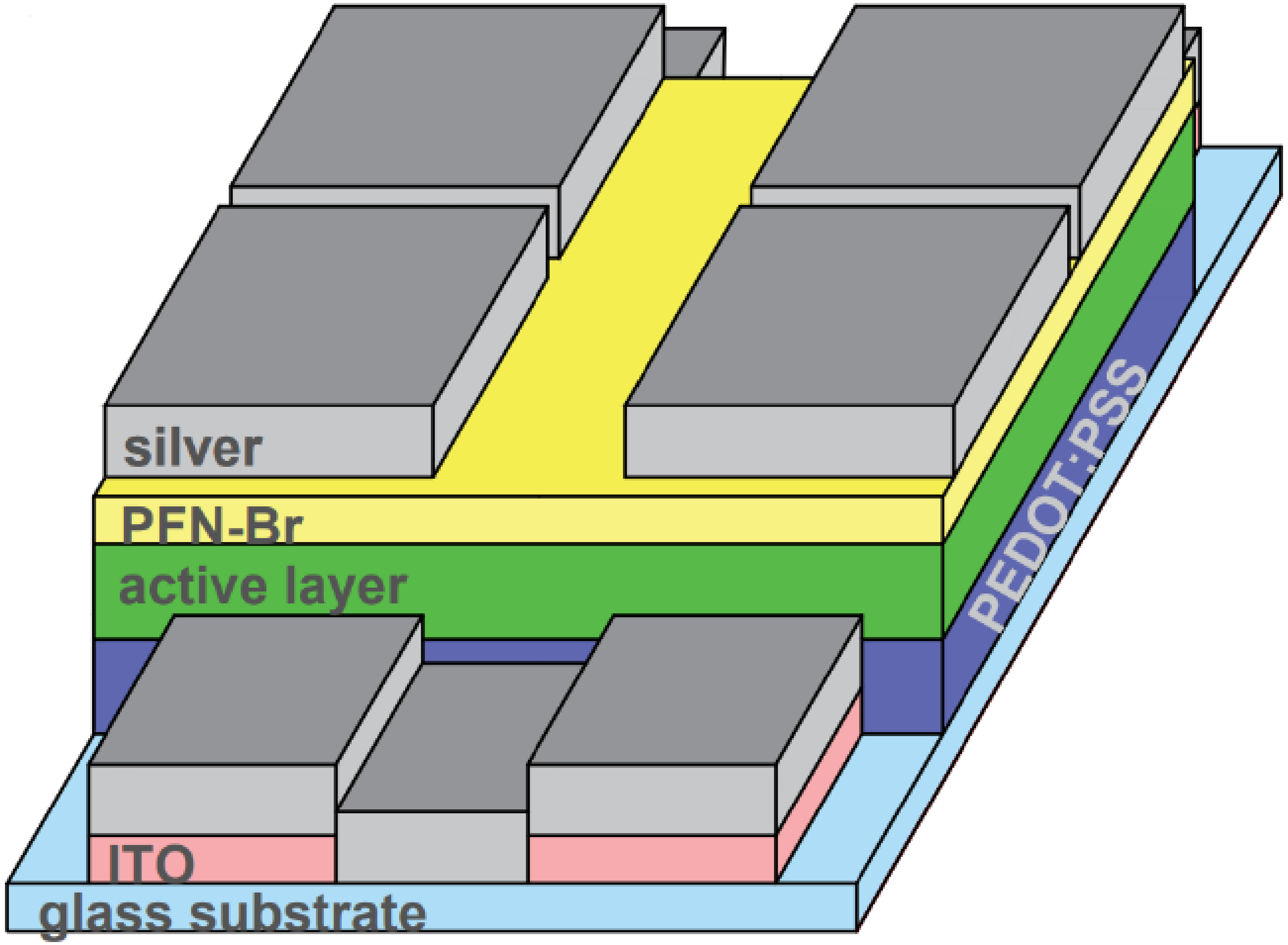


Sample Parameter Space

Calculate Probabilities

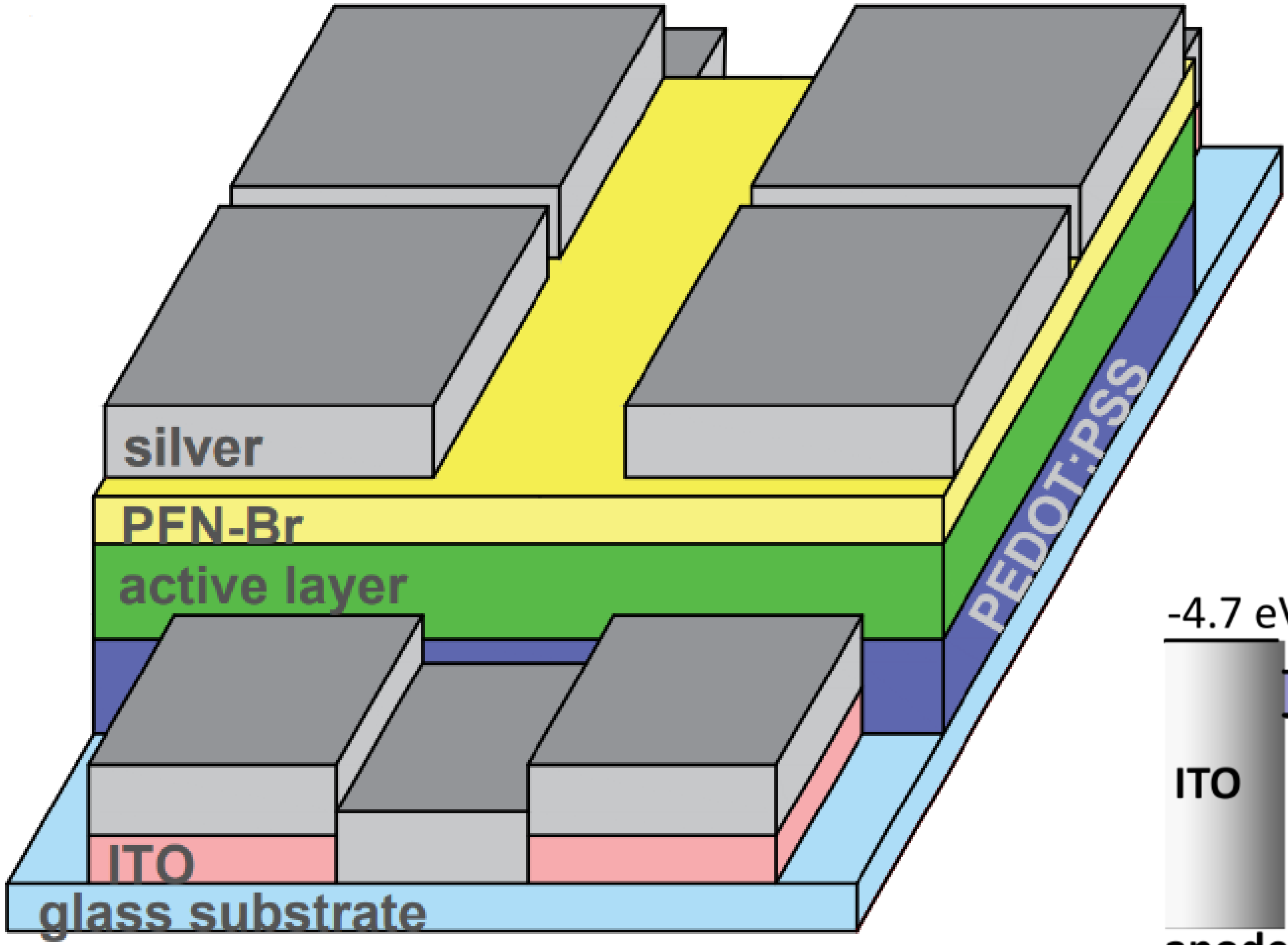
Experimental Data

Device Architecture



Experimental Data

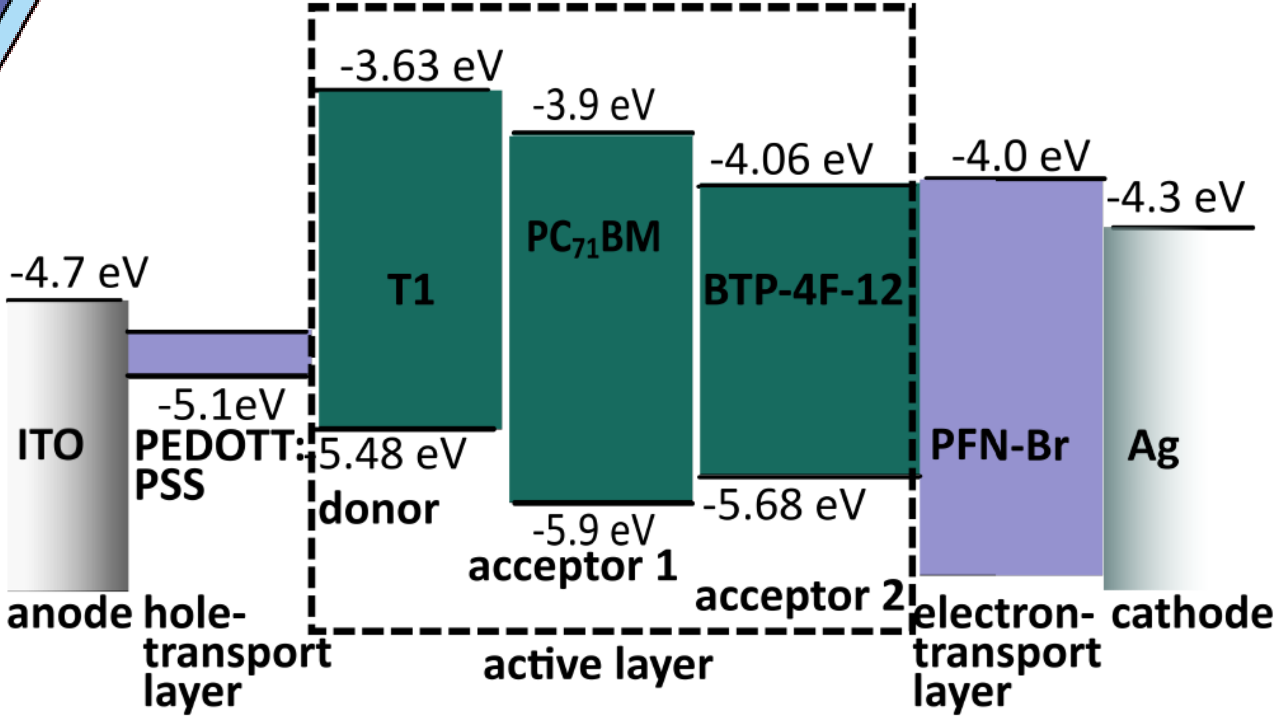
Device Architecture



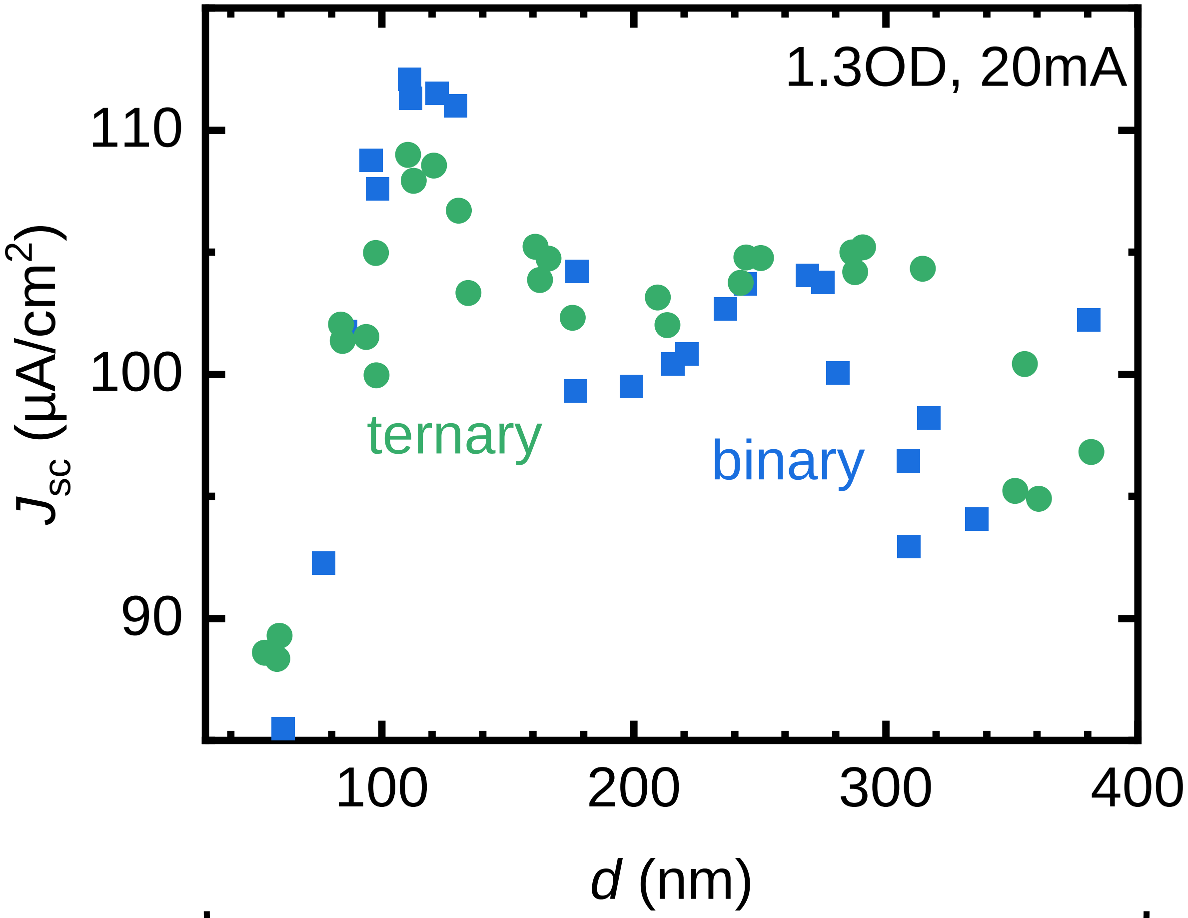
Cell area: 0.16 cm²

Active layers:

- Binary blend (BTP-4F-12: PBDB-TF-T1)
- Ternary blend (BTP-4F-12: PBDB-TF-T1:PC71BM)

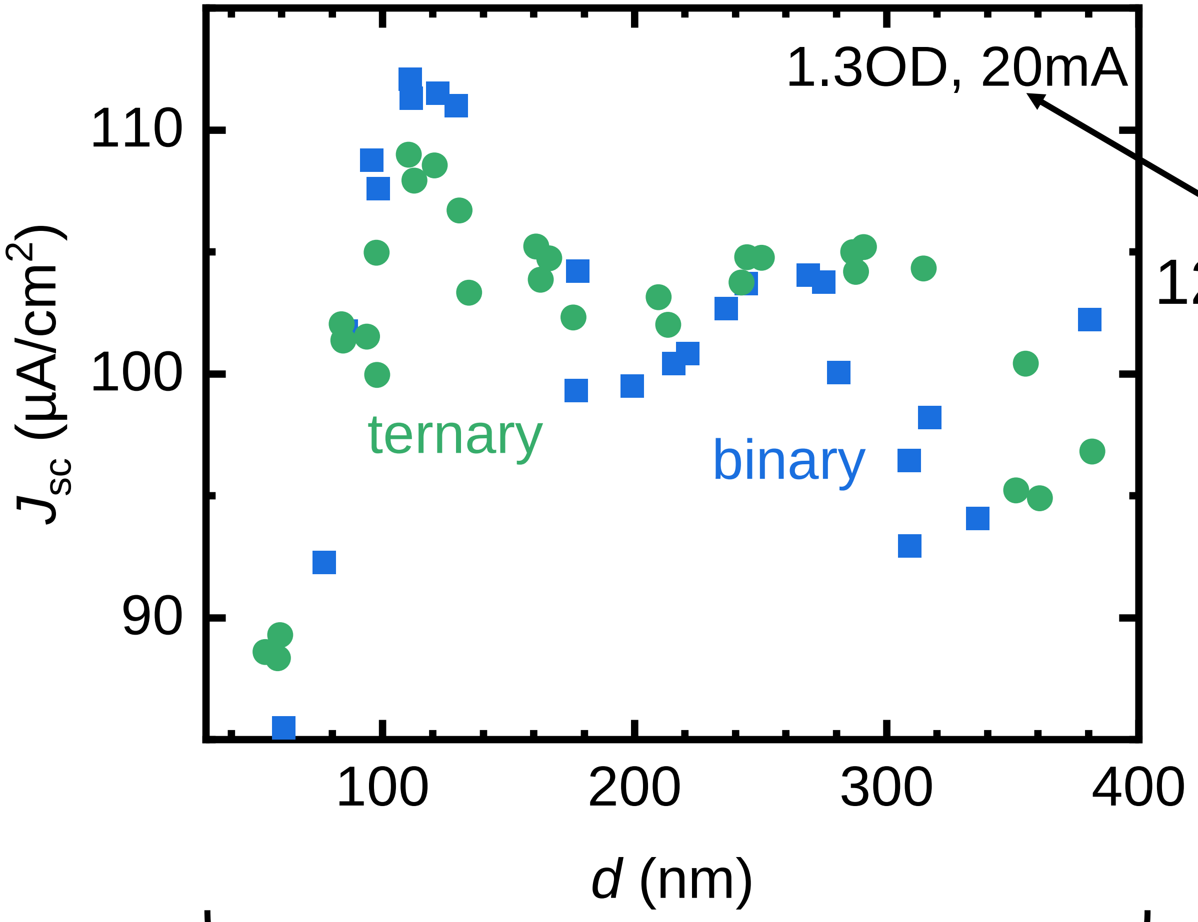


Experimental Data



Wide range of thicknesses

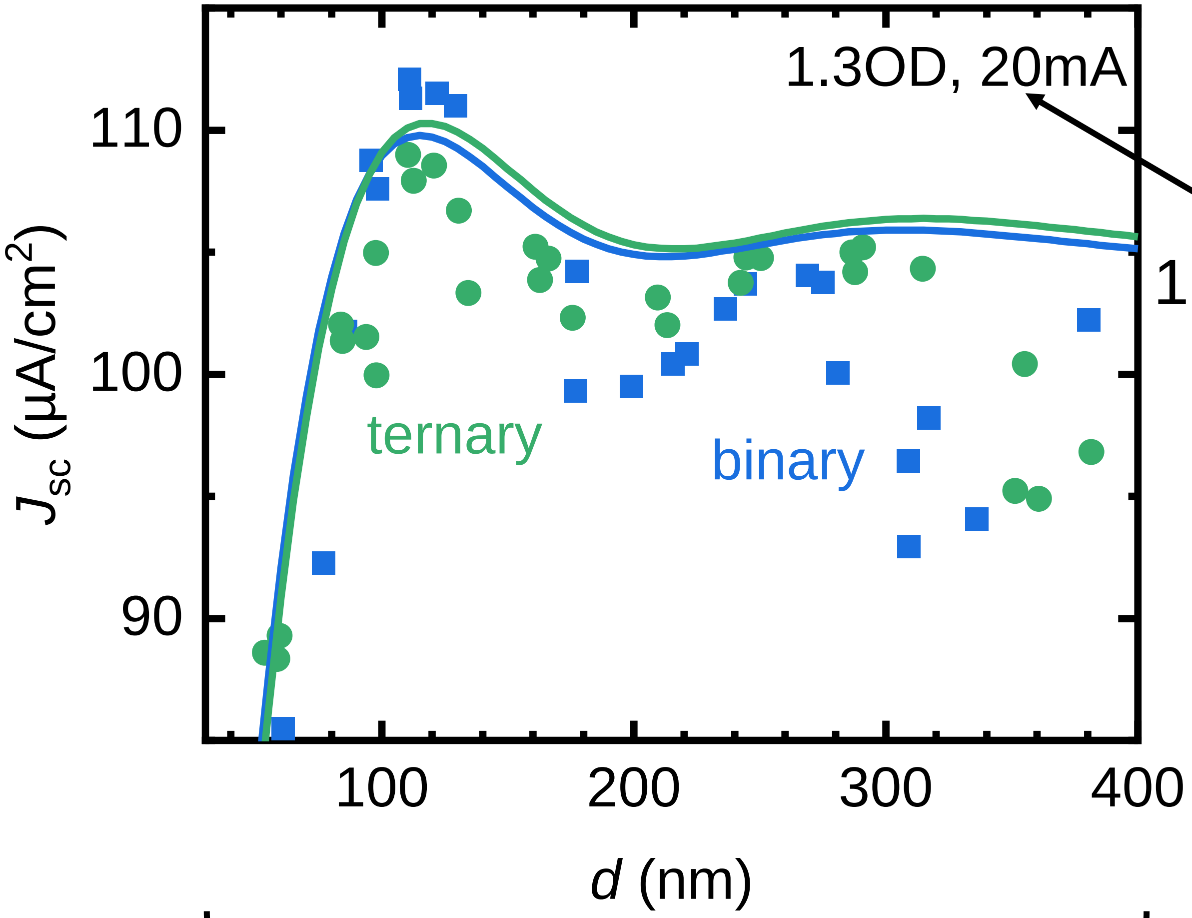
Experimental Data



12 different light intensities

Wide range of thicknesses

Experimental Data

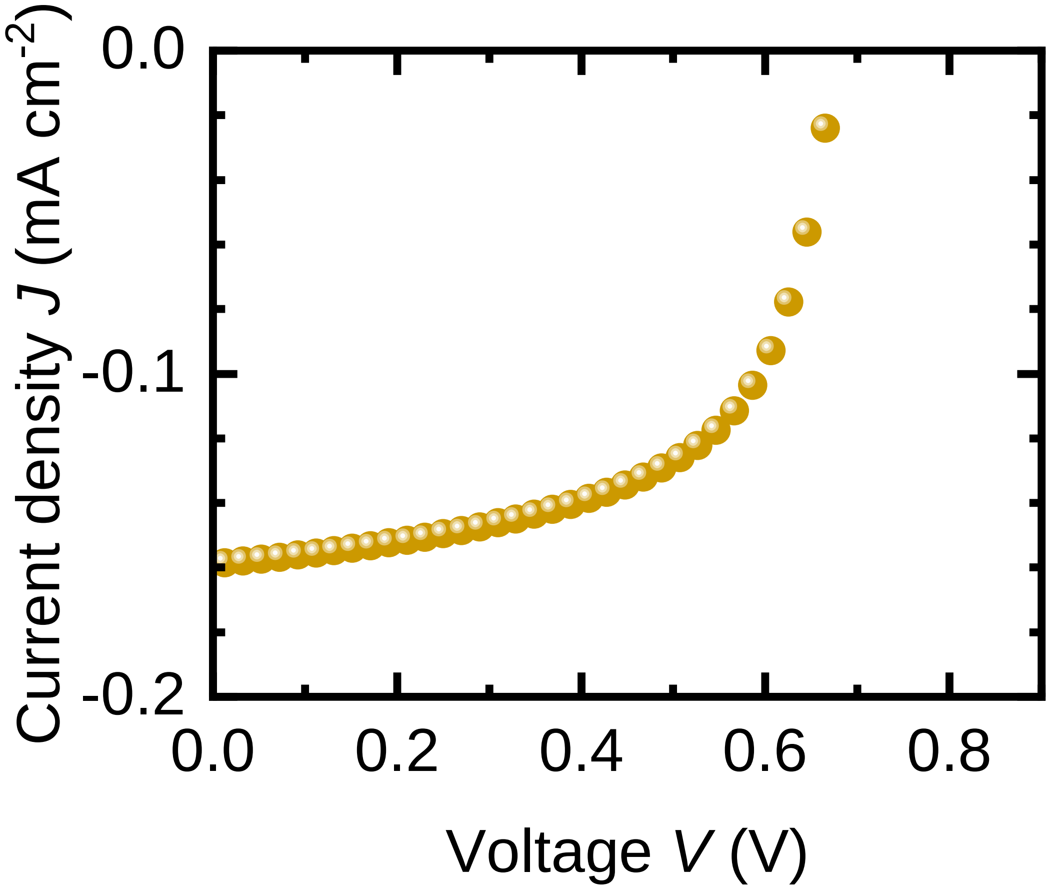


12 different light intensities

Wide range of thicknesses

Experimental Data

What Do We Fit?

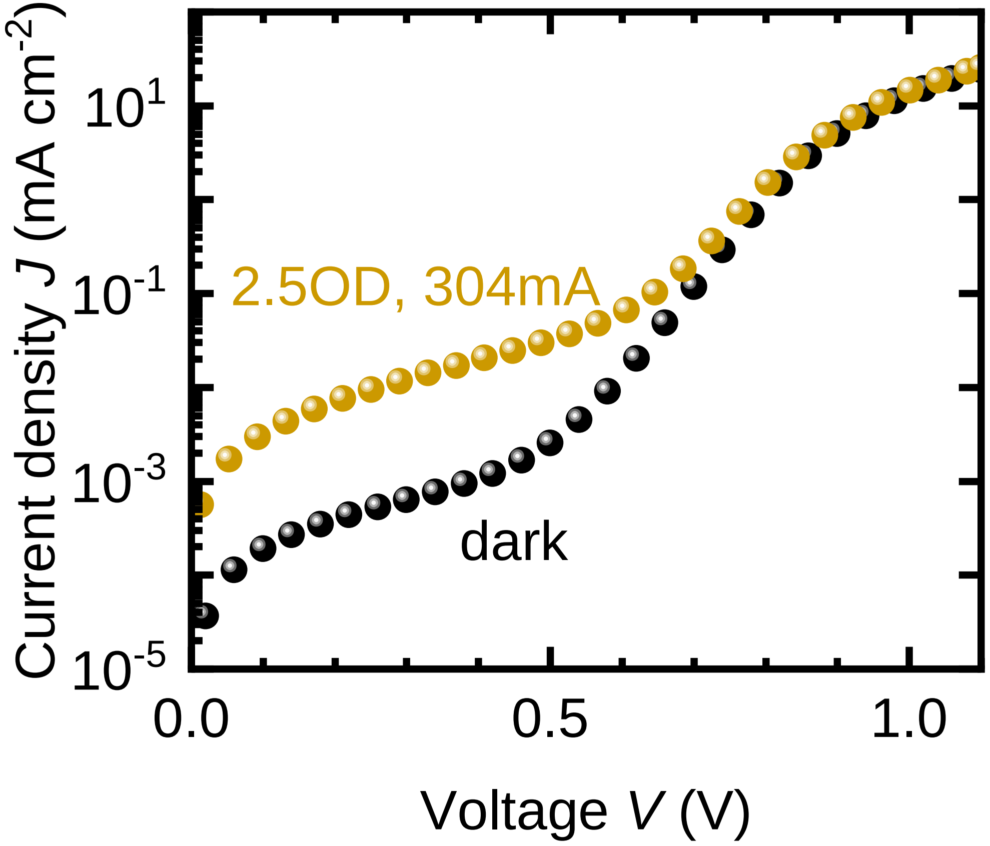


$$\Delta J_{\mathrm{rec}}(V,\Phi) = J_{\mathrm{illu}}(V,\Phi) - J_{\mathrm{sc}}(\Phi)$$

Experimental Data

What Do We Fit?

- Independence of inaccuracies in optical model

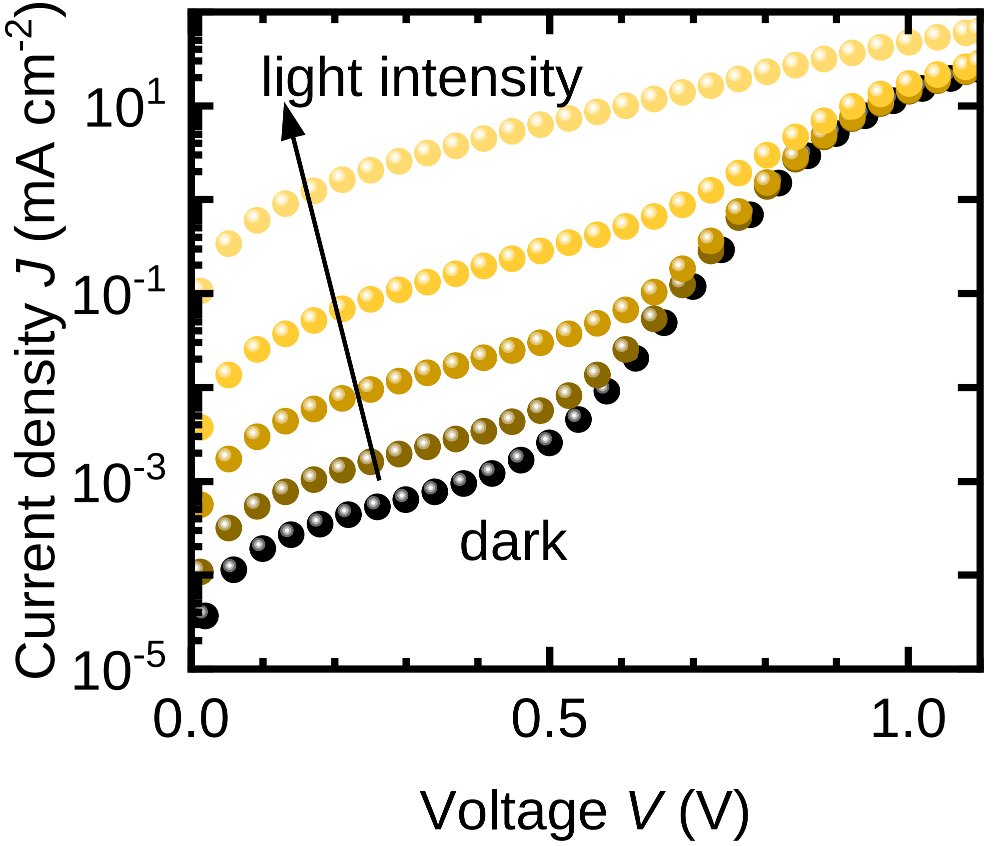


$$\Delta J_{\mathrm{rec}}(V,\Phi) = J_{\mathrm{illu}}(V,\Phi) - J_{\mathrm{sc}}(\Phi)$$

Experimental Data

What Do We Fit?

- Independence of inaccuracies in optical model
- Emphasis on light-intensity dependent recombination current density

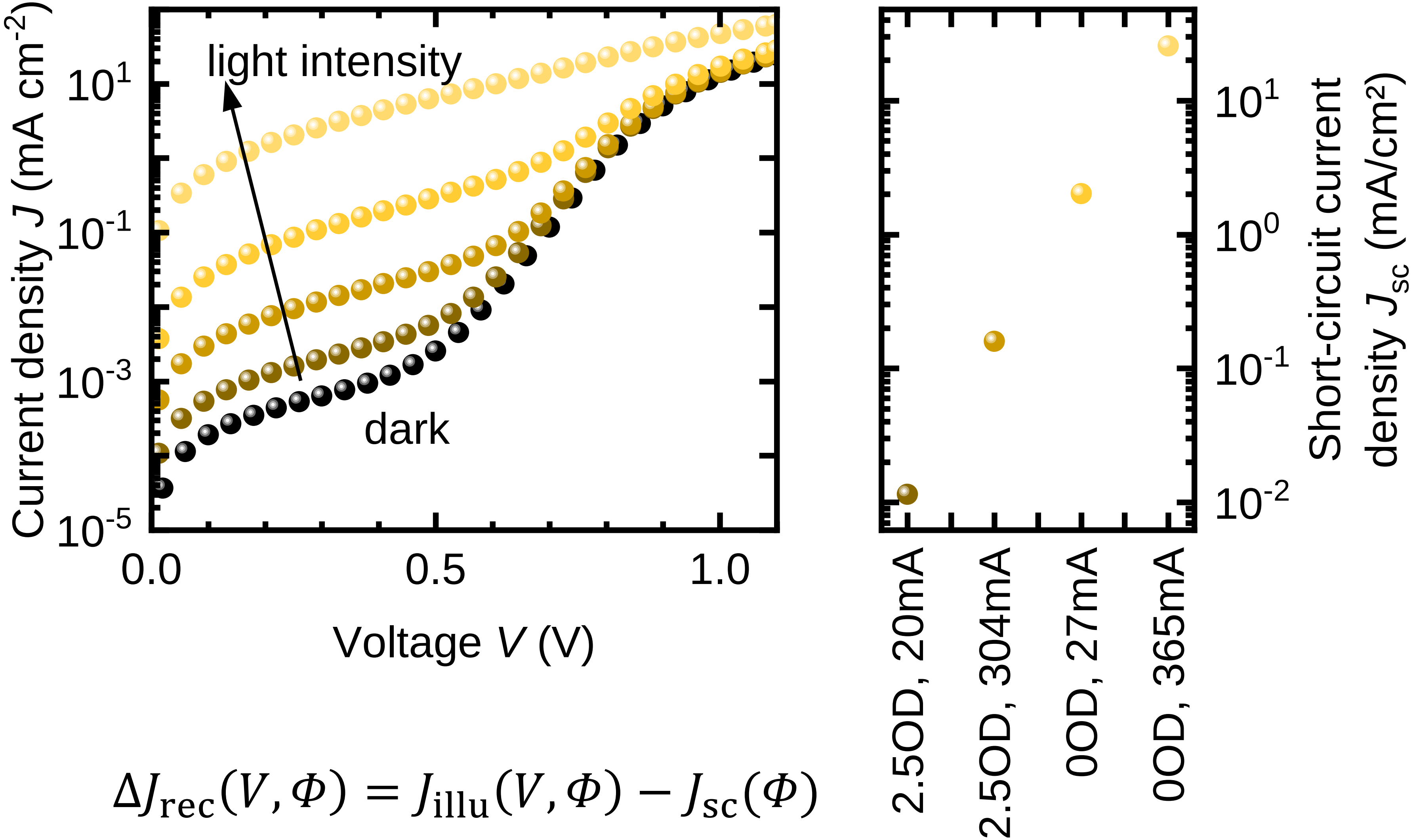


$$\Delta J_{\mathrm{rec}}(V,\Phi) = J_{\mathrm{illu}}(V,\Phi) - J_{\mathrm{sc}}(\Phi)$$

Experimental Data

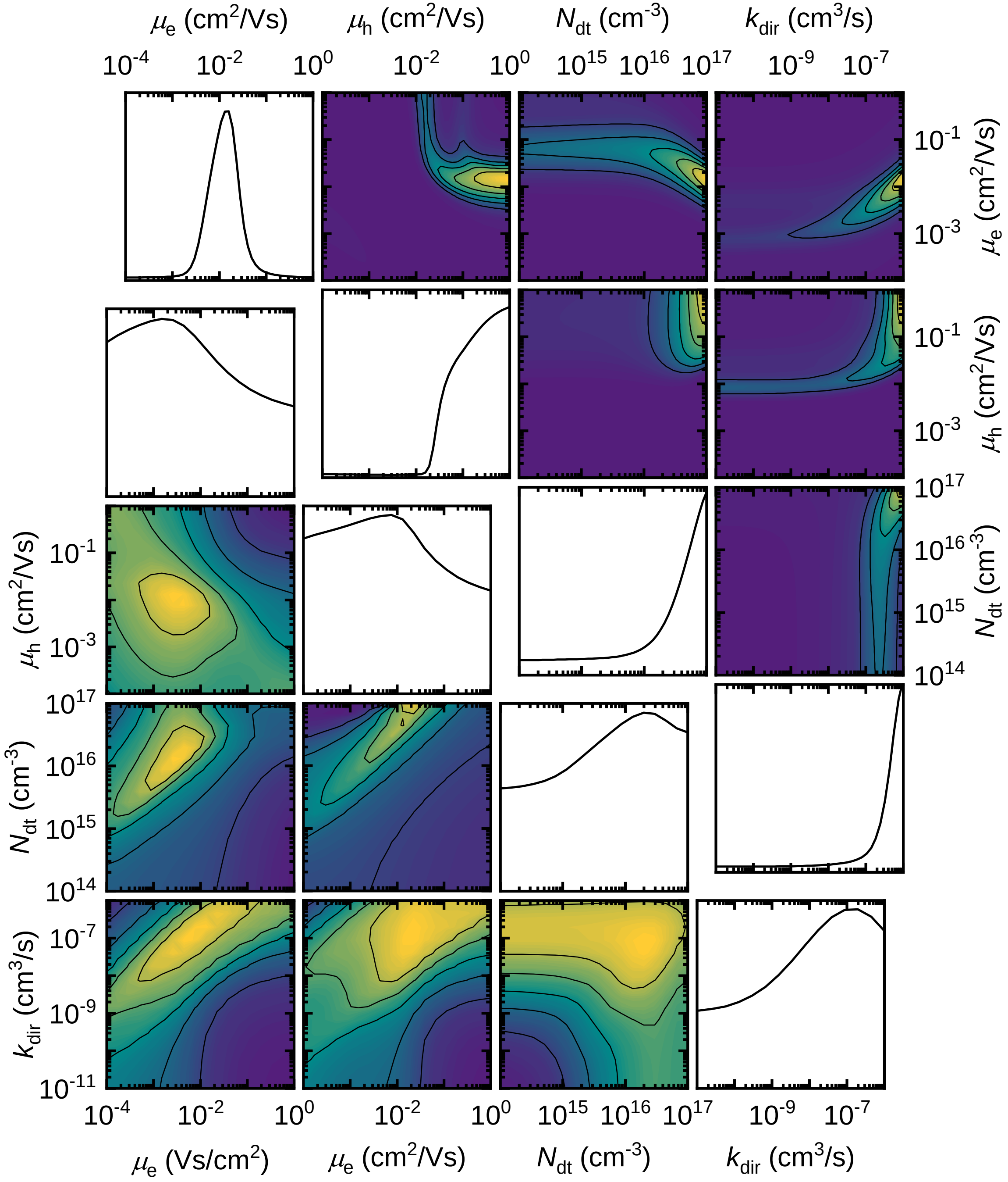
What Do We Fit?

- Independence of inaccuracies in optical model
- Emphasis on light-intensity dependent recombination current density
- Use J_{sc} in fitting procedure to penalize fits that are too far off

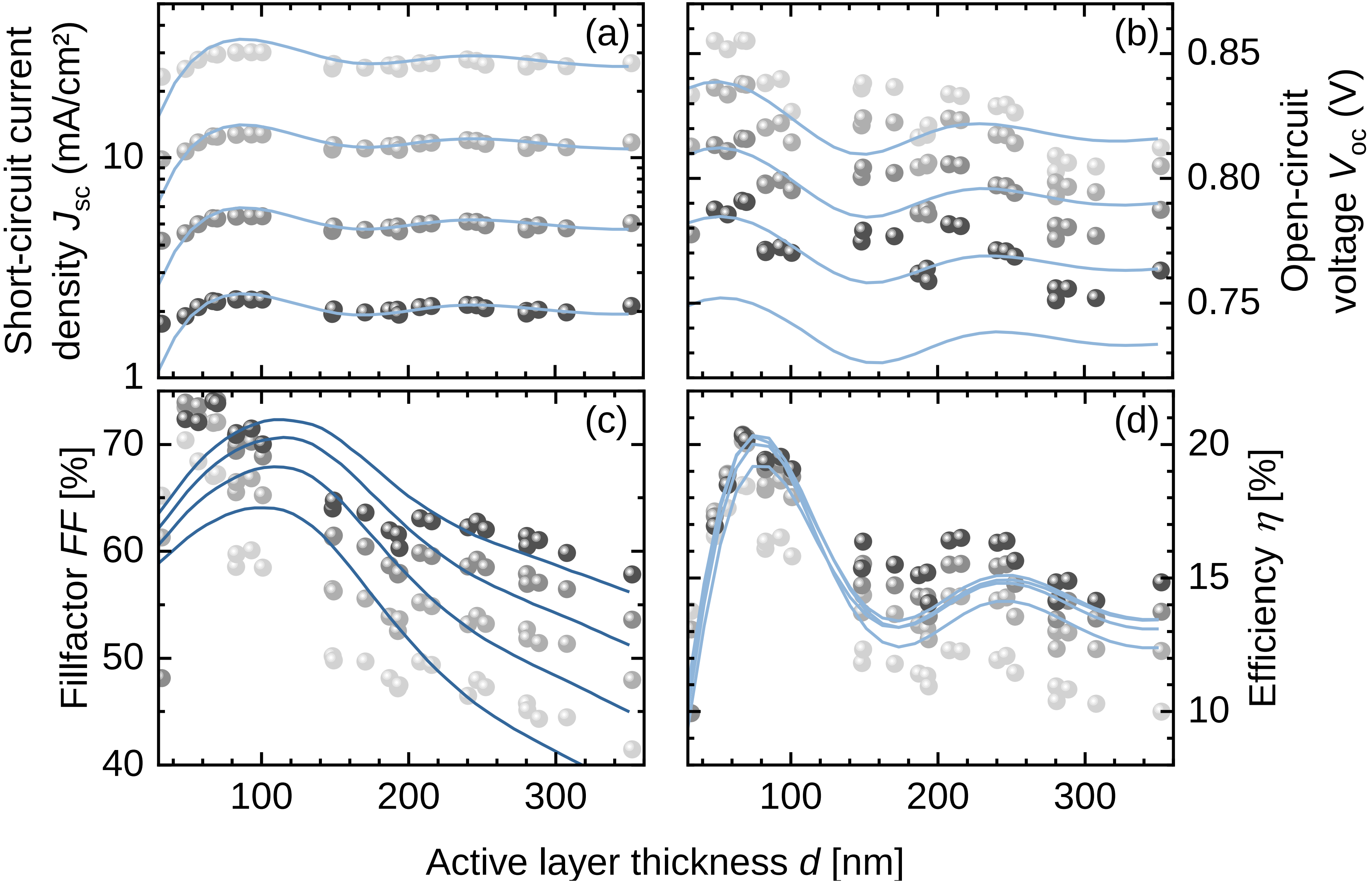


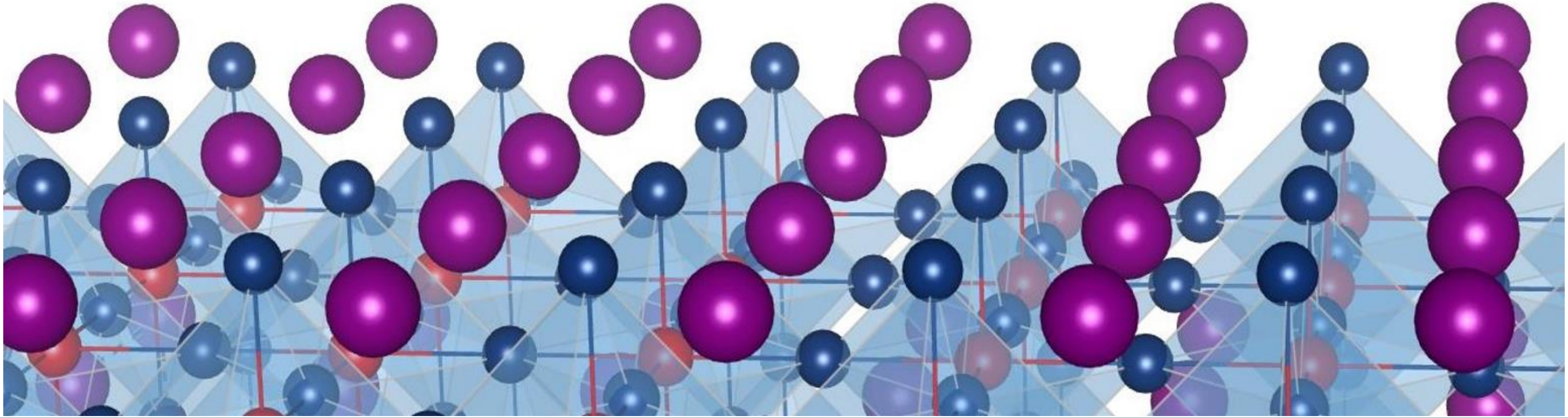
$$\Delta J_{\mathrm{rec}}(V,\Phi) = J_{\mathrm{illu}}(V,\Phi) - J_{sc}(\Phi)$$

Cornerplots



Trends with Thickness

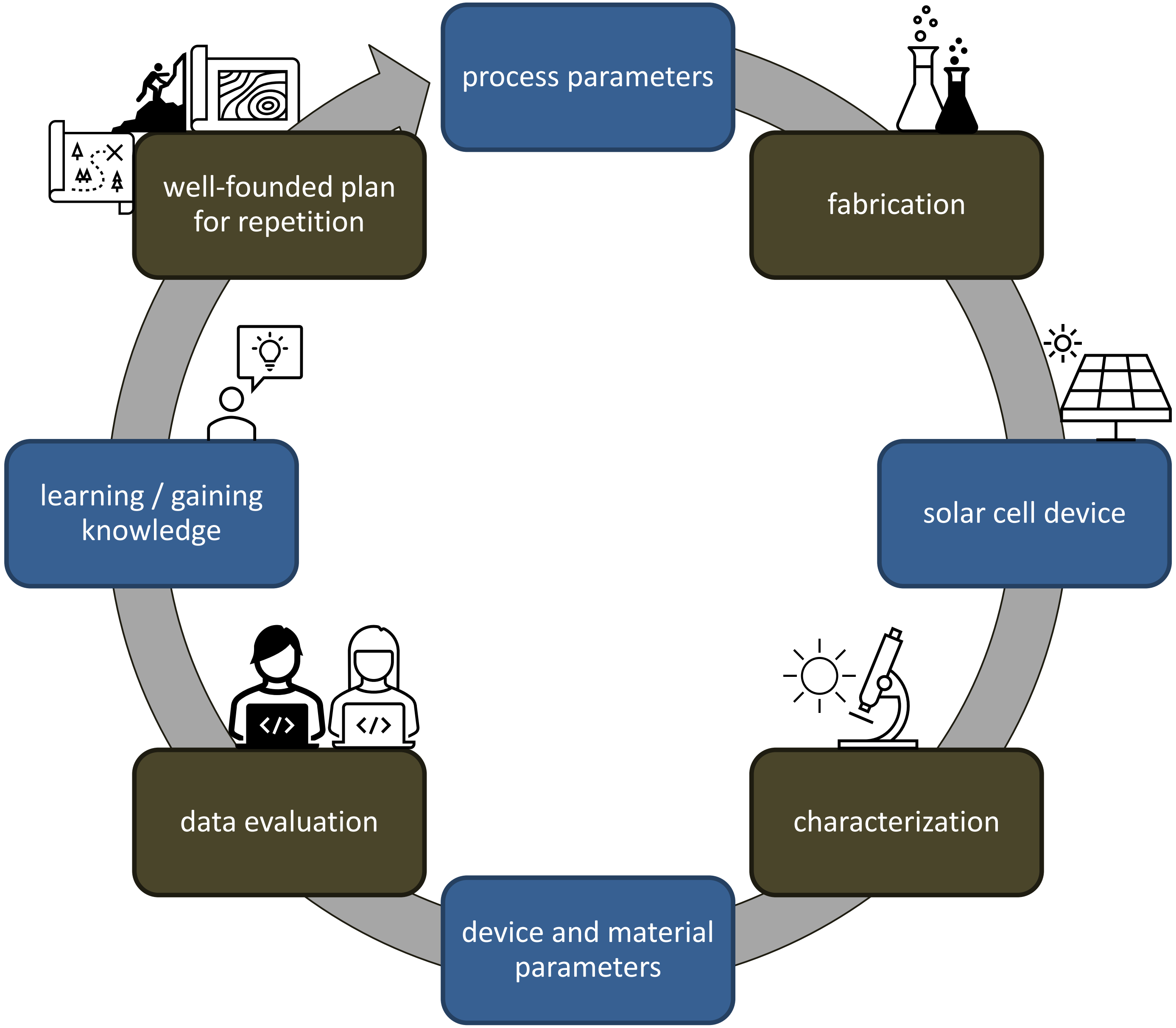




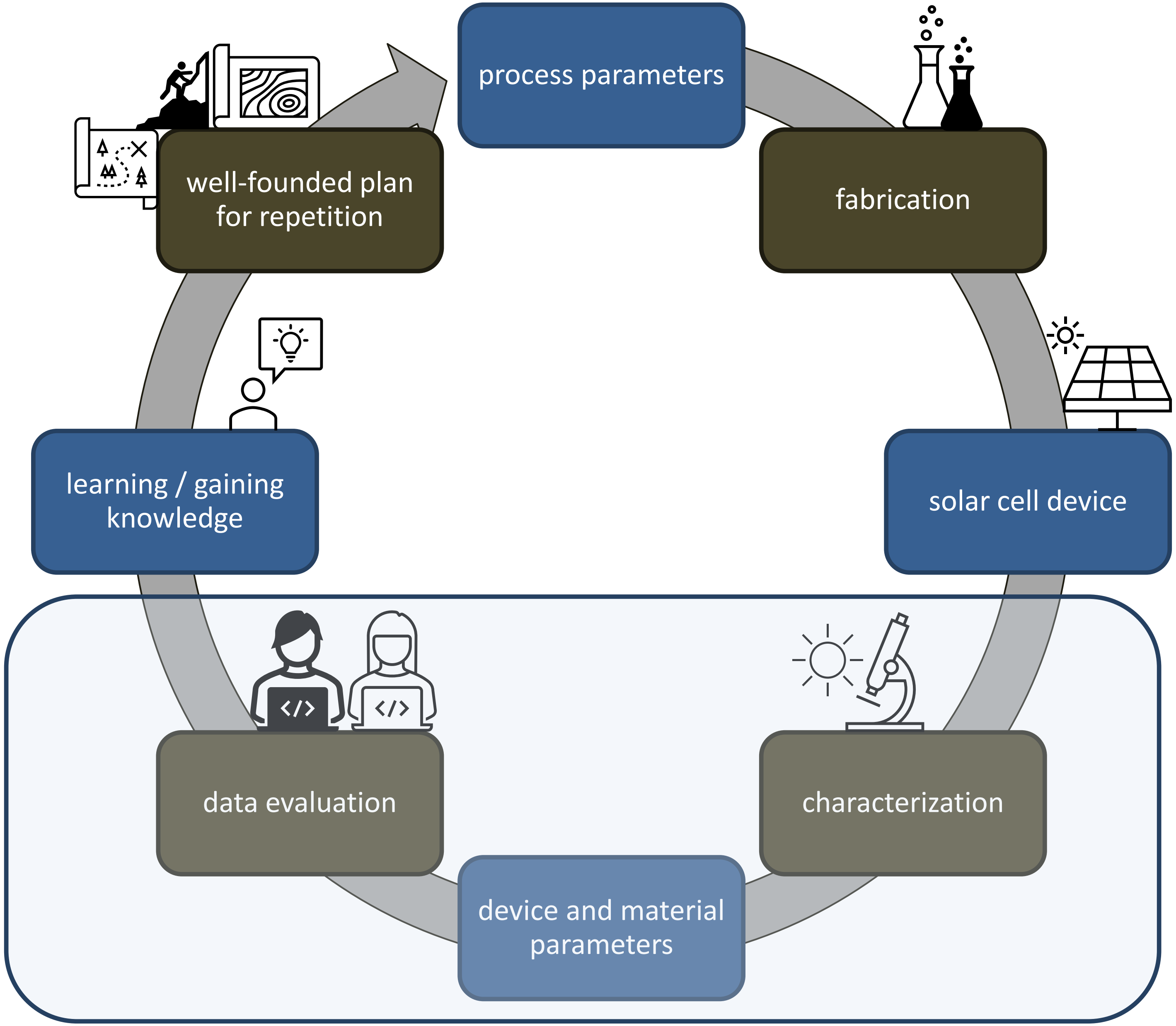
Part 2: The Value of Device Characterization

For the Purpose of Device Optimization

How we imagine scientific progress in the field

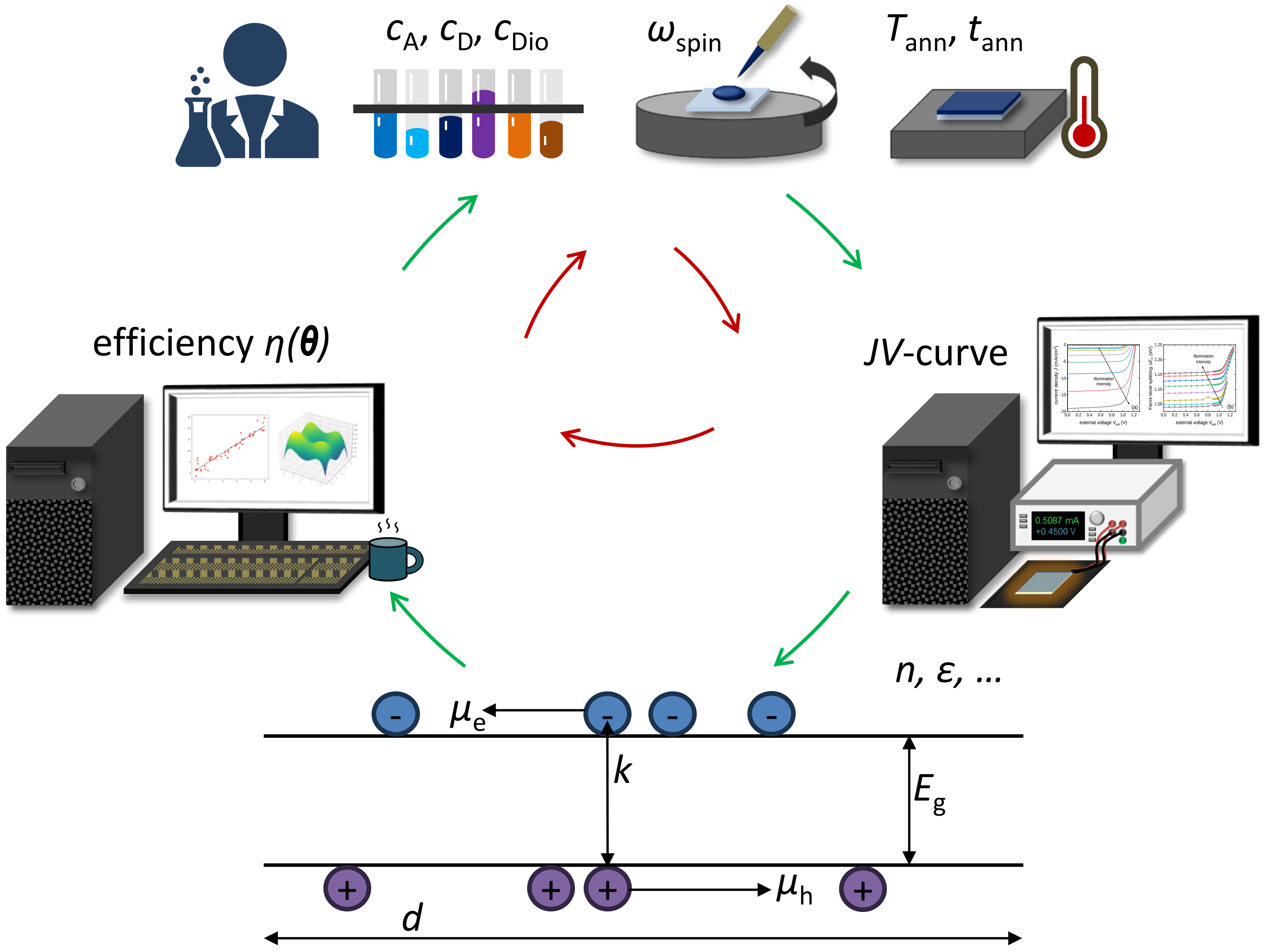


How we imagine scientific progress in the field



Is this important for papers and our understanding or for device optimization itself?

Idea: Test 2 Options in Virtual Laboratory

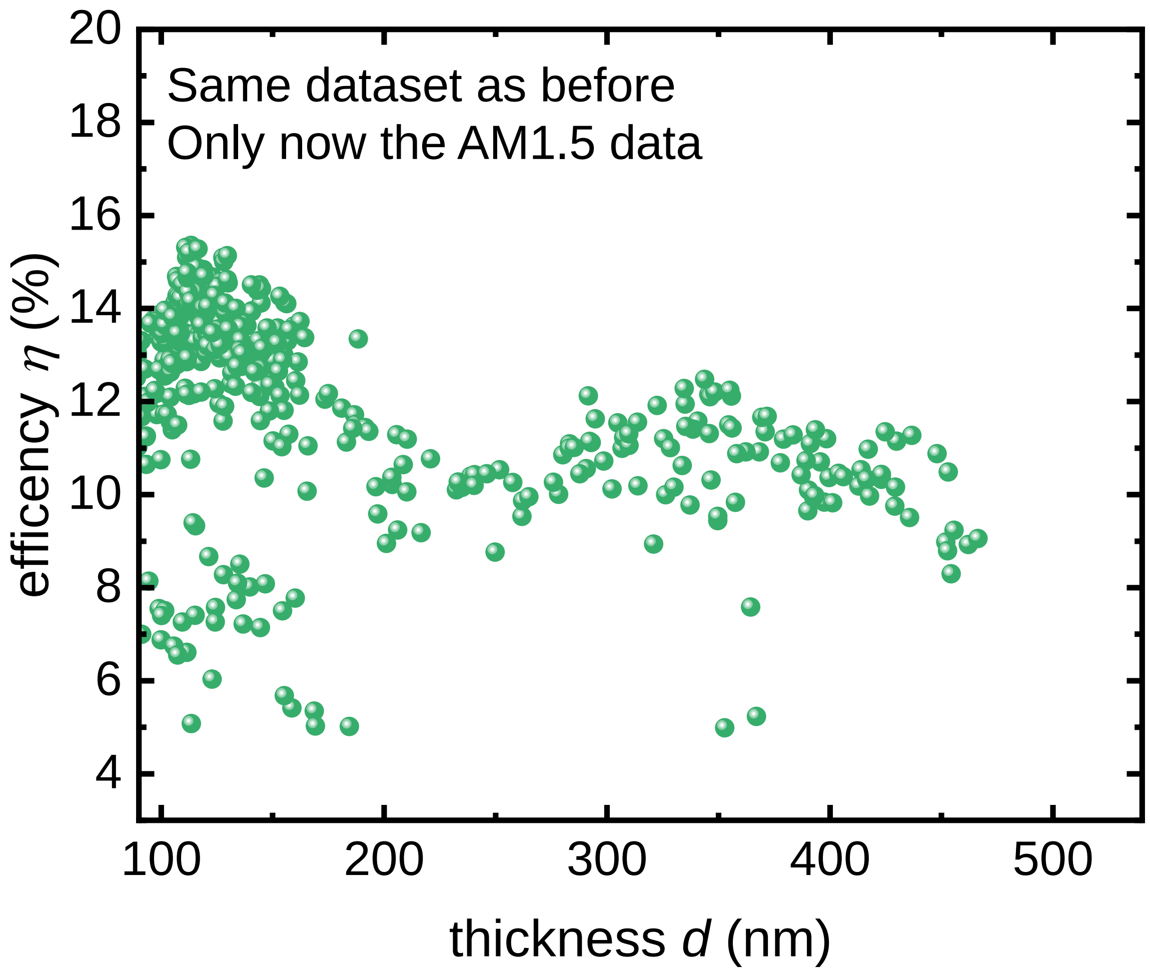


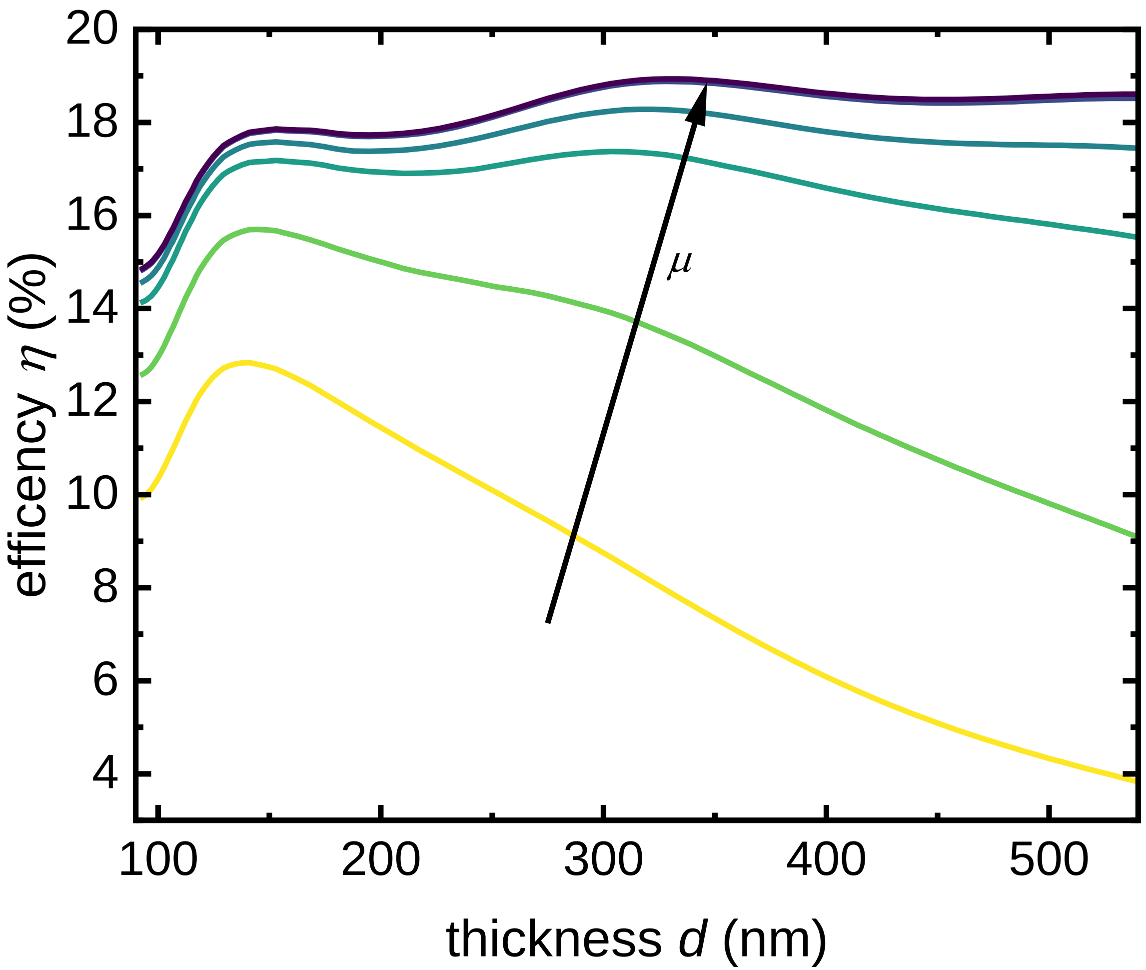
Option 1:
- Process parameters → JV curve
- JV curve → efficiency
- Efficiency → new process parameters

Option 2:
- Process parameters → JV curve
- JV curve → mobility, recombination coefficient, etc…
- Mobility, rec... → efficiency
- Efficiency → new process parameters

Experimental Basis

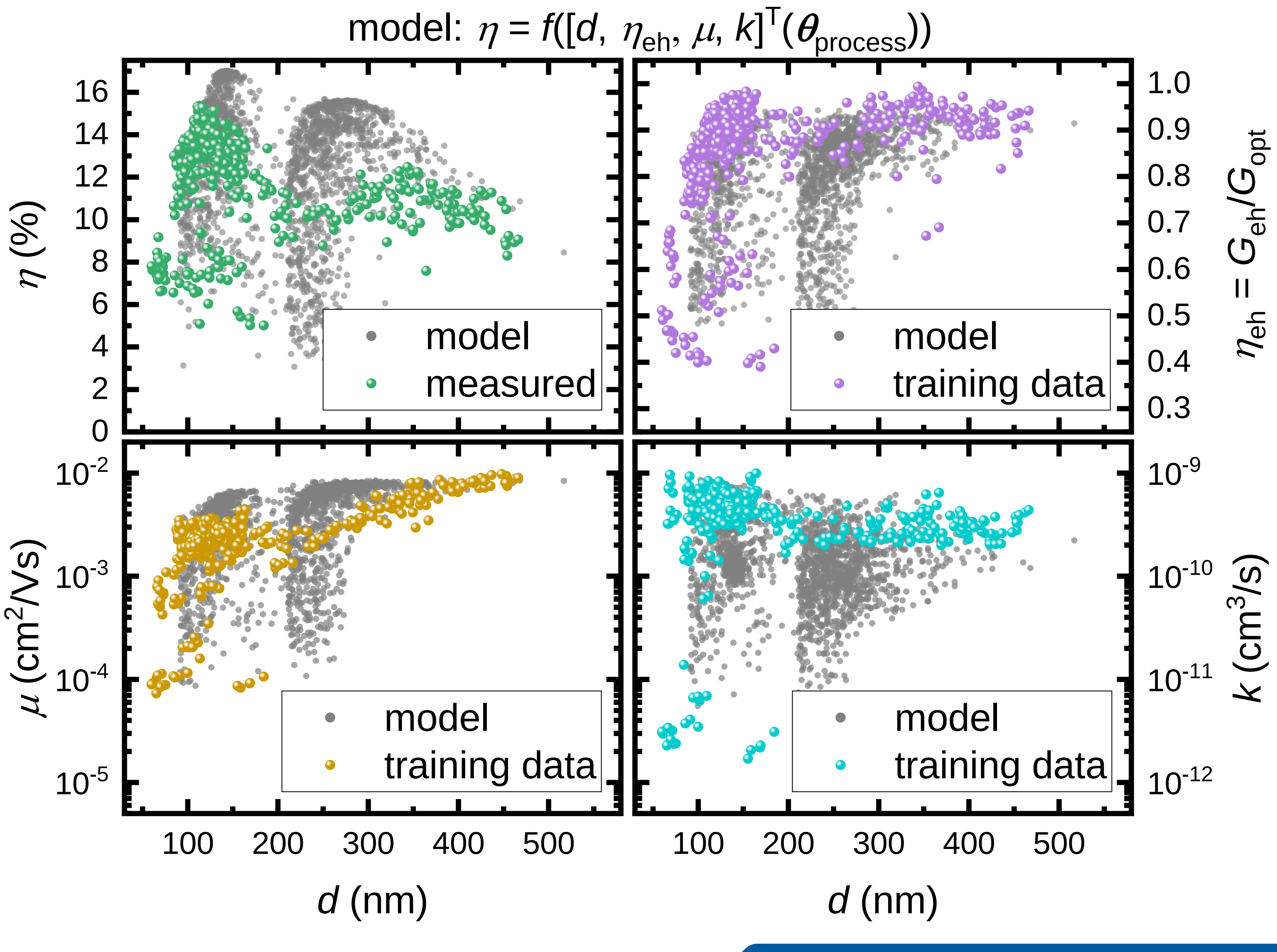
To feed the virtual laboratory



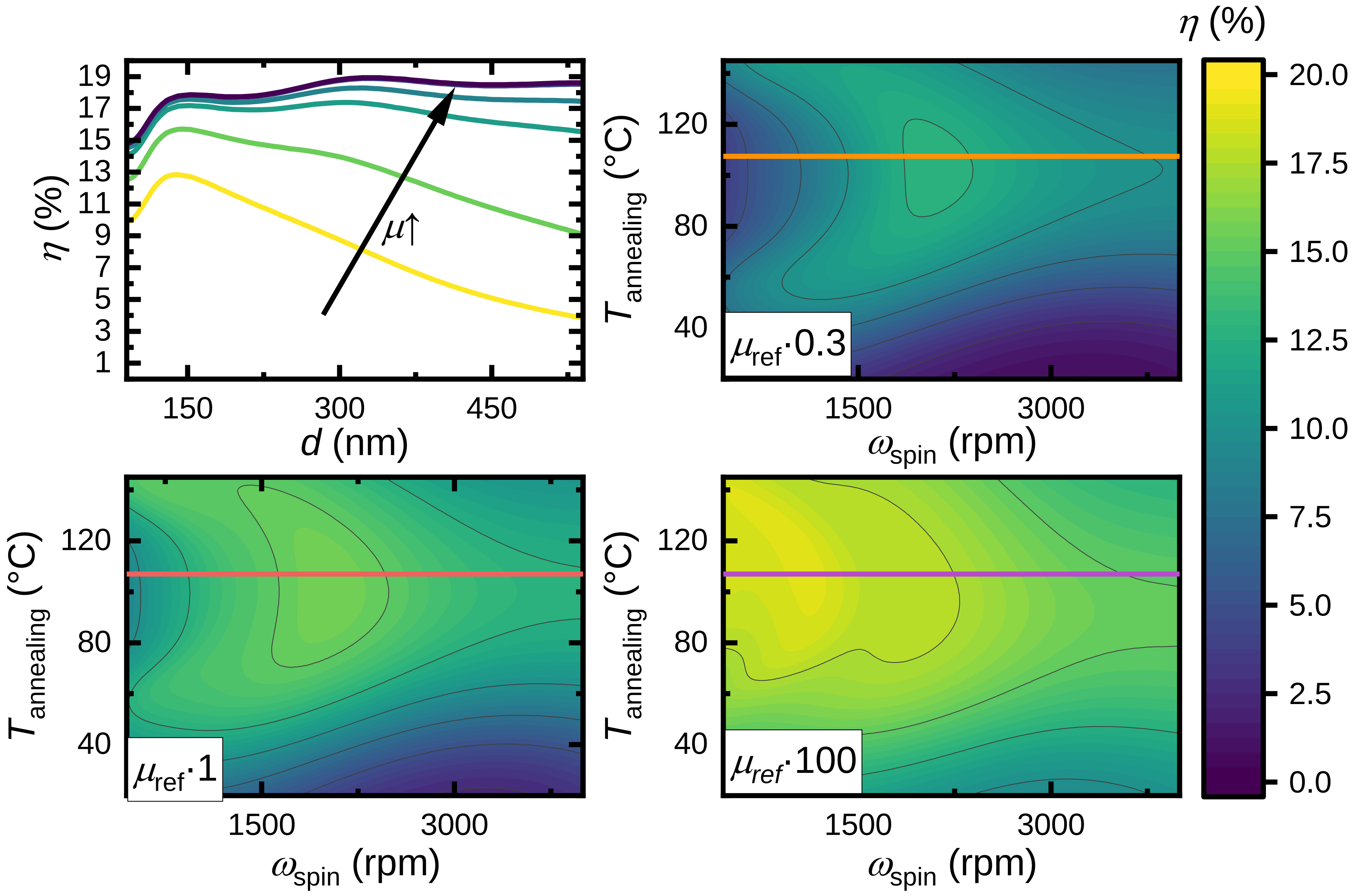


Linking Process with Material Parameters

1. Fit simple model to experimental *JV* data
2. Infer material parameters
3. Plot them vs. process parameters
4. Create a multidimensional function aproximation for material vs. process parameters using a SVR
5. Use this as the „truth“ for the virtual laboratory

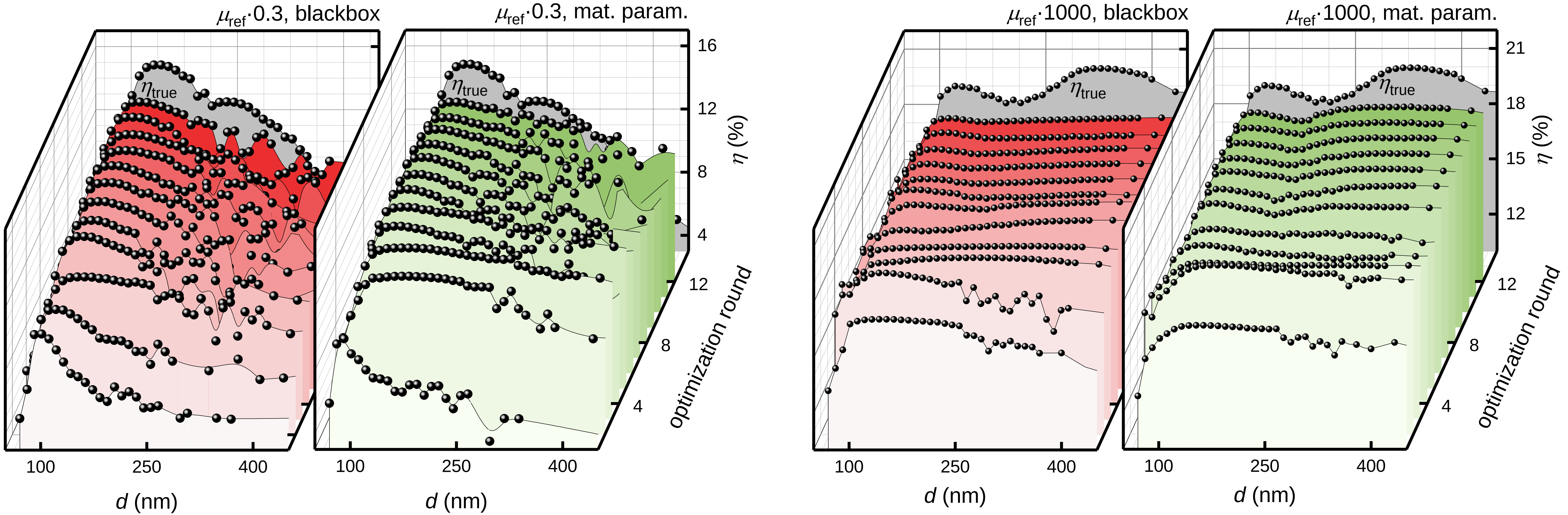


Example slices through the SVR model



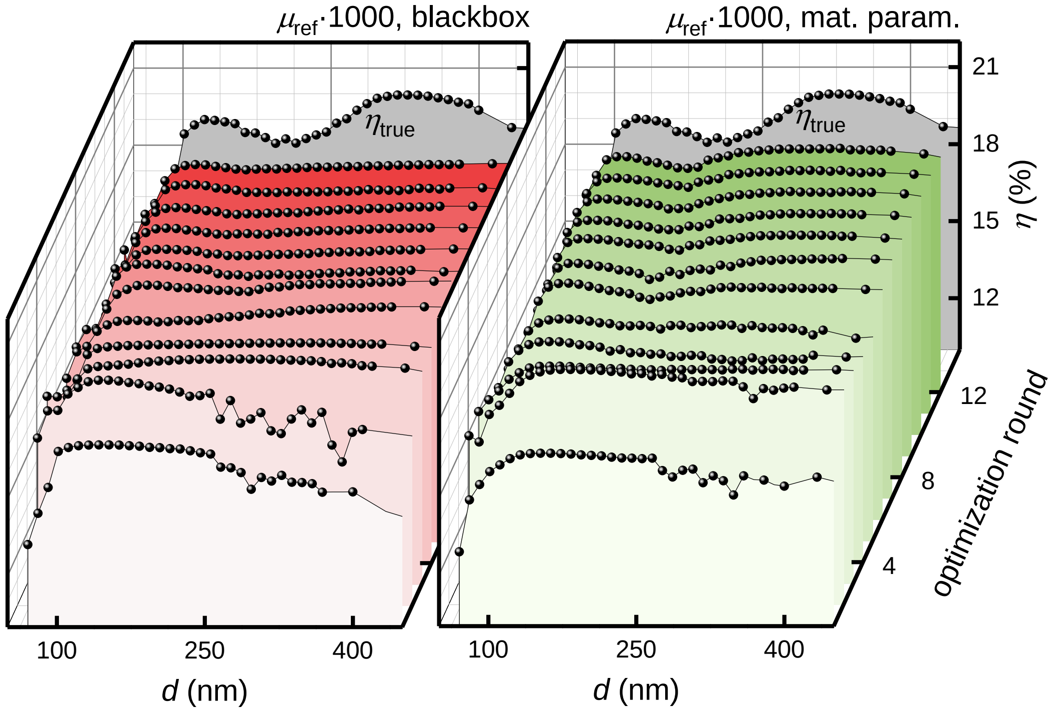
Comparison blackbox optimization

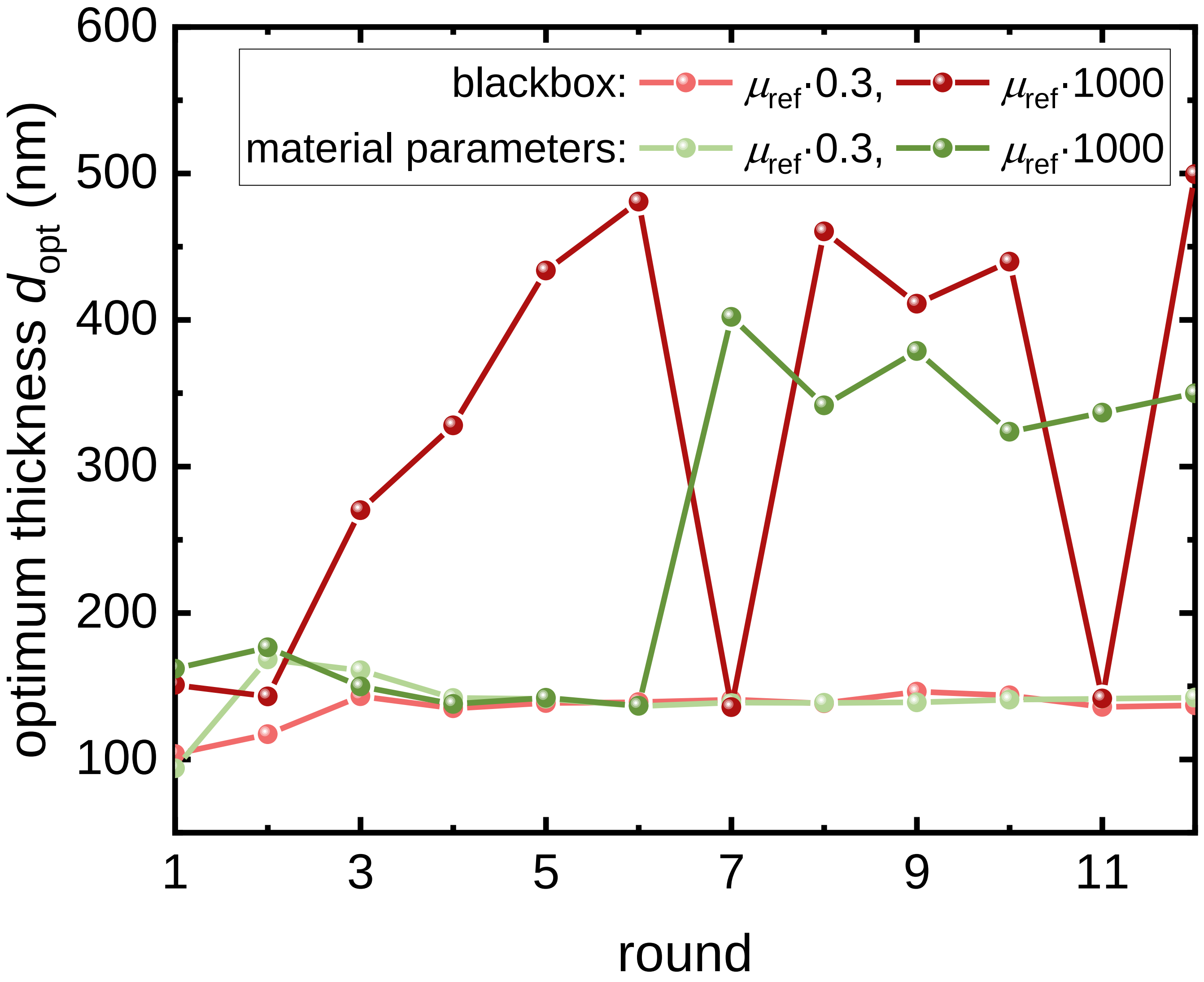
Vs. material-parameter-based optimization



Low mobility High mobility

Does the optimization find the 2nd interference maximum?

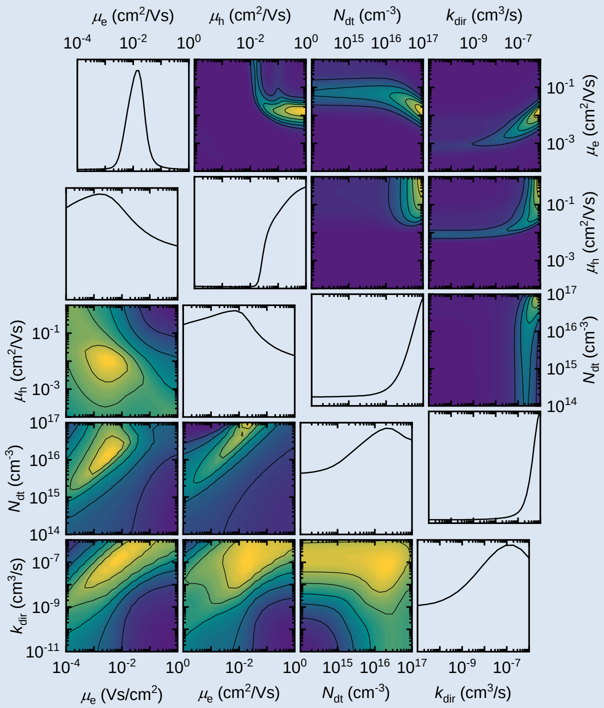




Conclusions

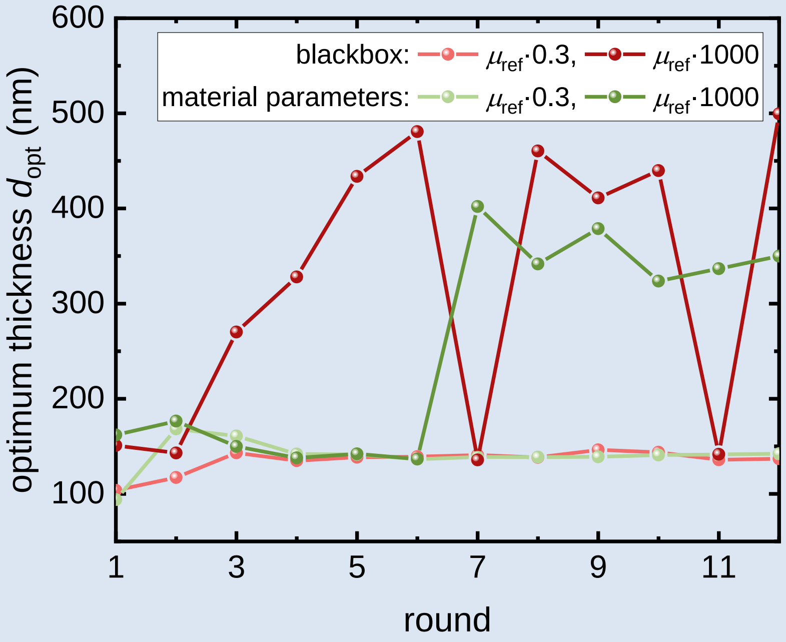
1) Inferring Parameters

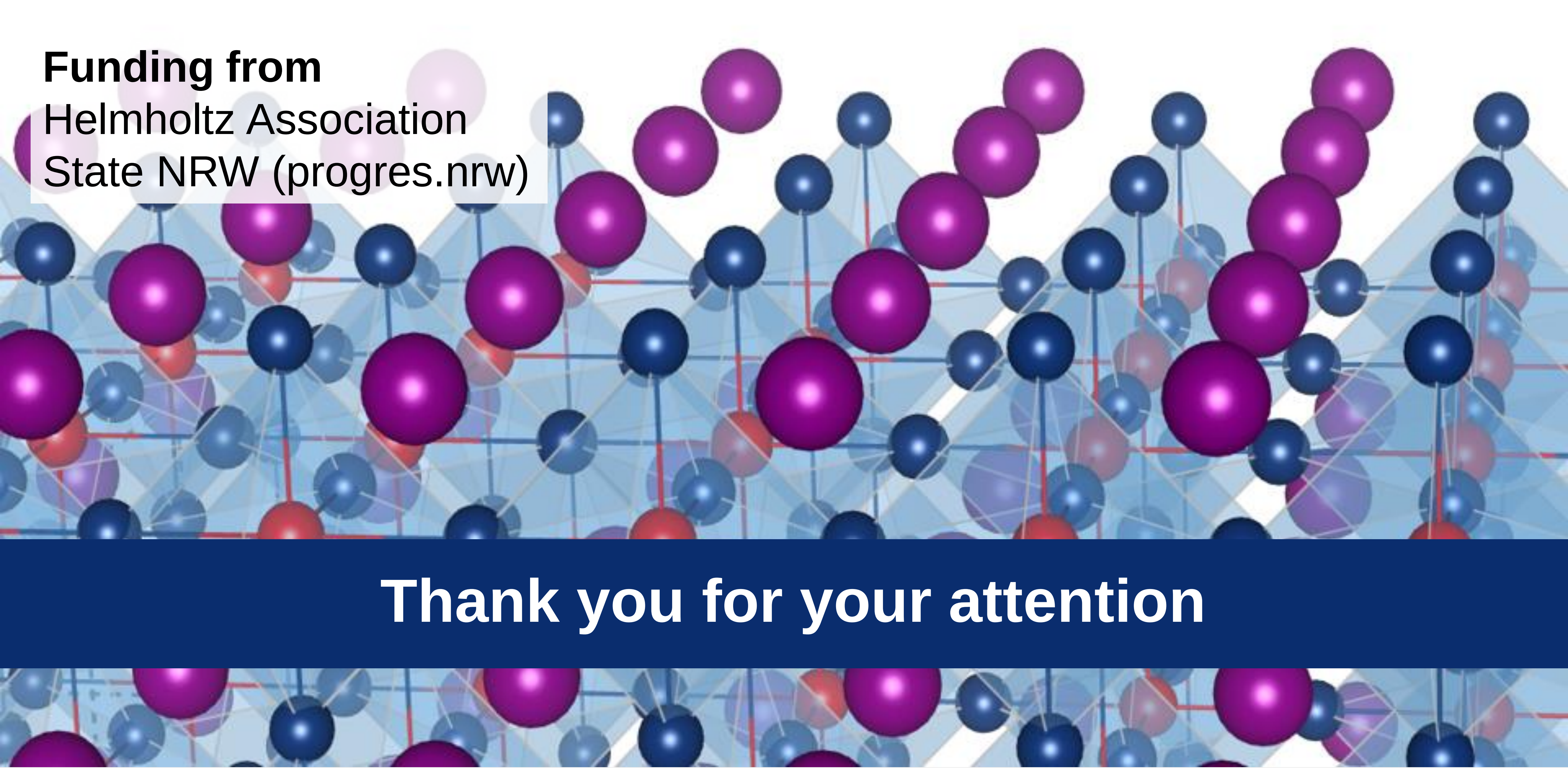
- NNs interpolate well and look up well
- Trained NNs can therefore accelerate simulations by a factor ~10^4 for *JV* curves
- Allows finding likely material parameters



2) Inferring Parameters

- Models+Characterization might help to find optima in complex η(process parameter) situations.





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Thank you for your attention

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

JÜLICH Forschungszentrum