Machine learning approach for C-V-f fingerprint analysis of recombination in perovskite solar cells

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Perovskites/Intro

- Lead halide perovskites: promising material used for thin film solar cells
- 4% → > 25% efficiency in just 12 years of research
- High absorption coefficient: <1 um thickness
- Defect tolerant material: high efficiency despite simple processing techniques
- To push efficiencies even higher, defects must be identified and minimized

Task = Approximate energy landscape

Problem = Sequences are discrete!
Solution (a) = Dequantization

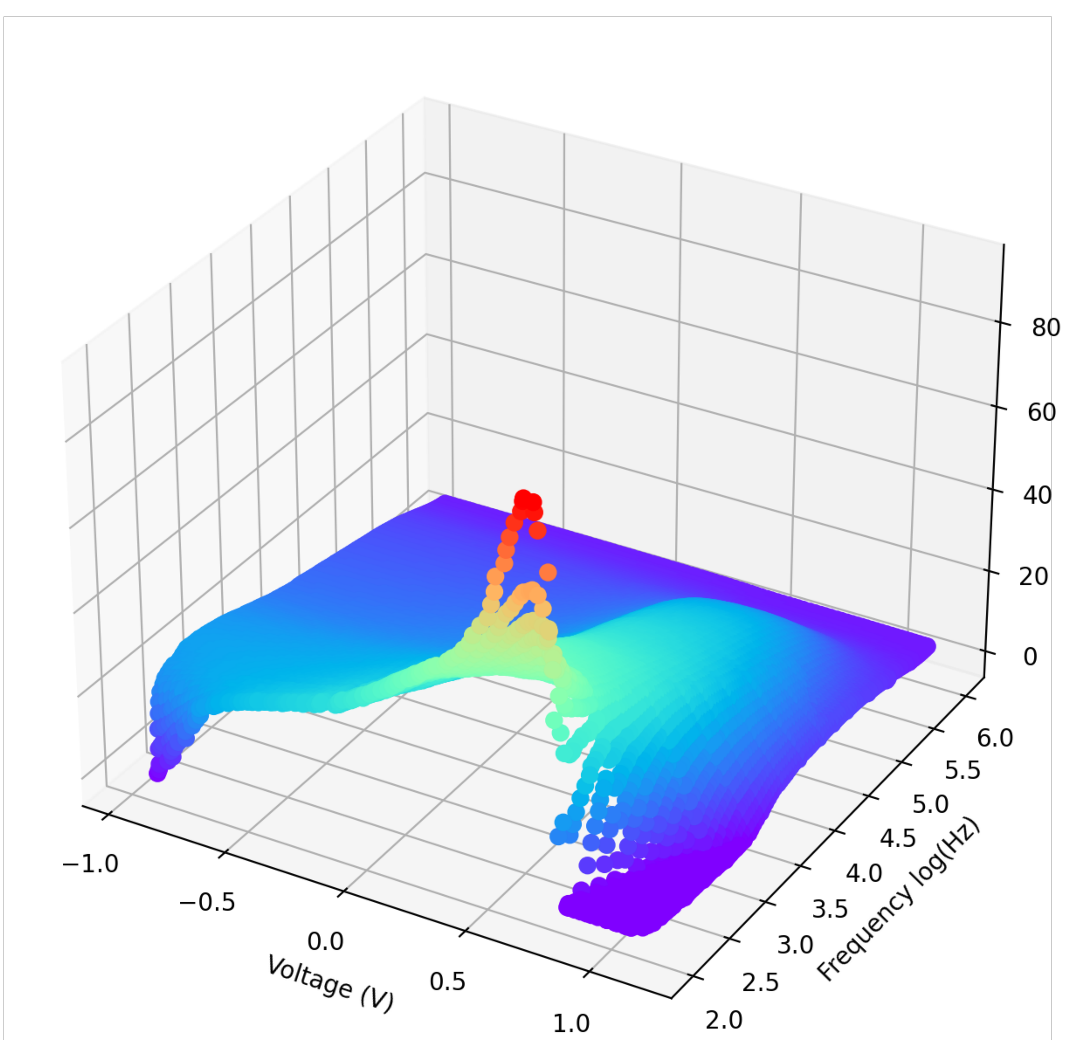
Summary

- Simulation of 9 variables shows bulk and interface defects have largest influence on loss map
- Simulated devices with varied bulk and interface recombination have unique loss maps
- Experimental loss map matches lower range of bulk defect, with contribution from interface defects

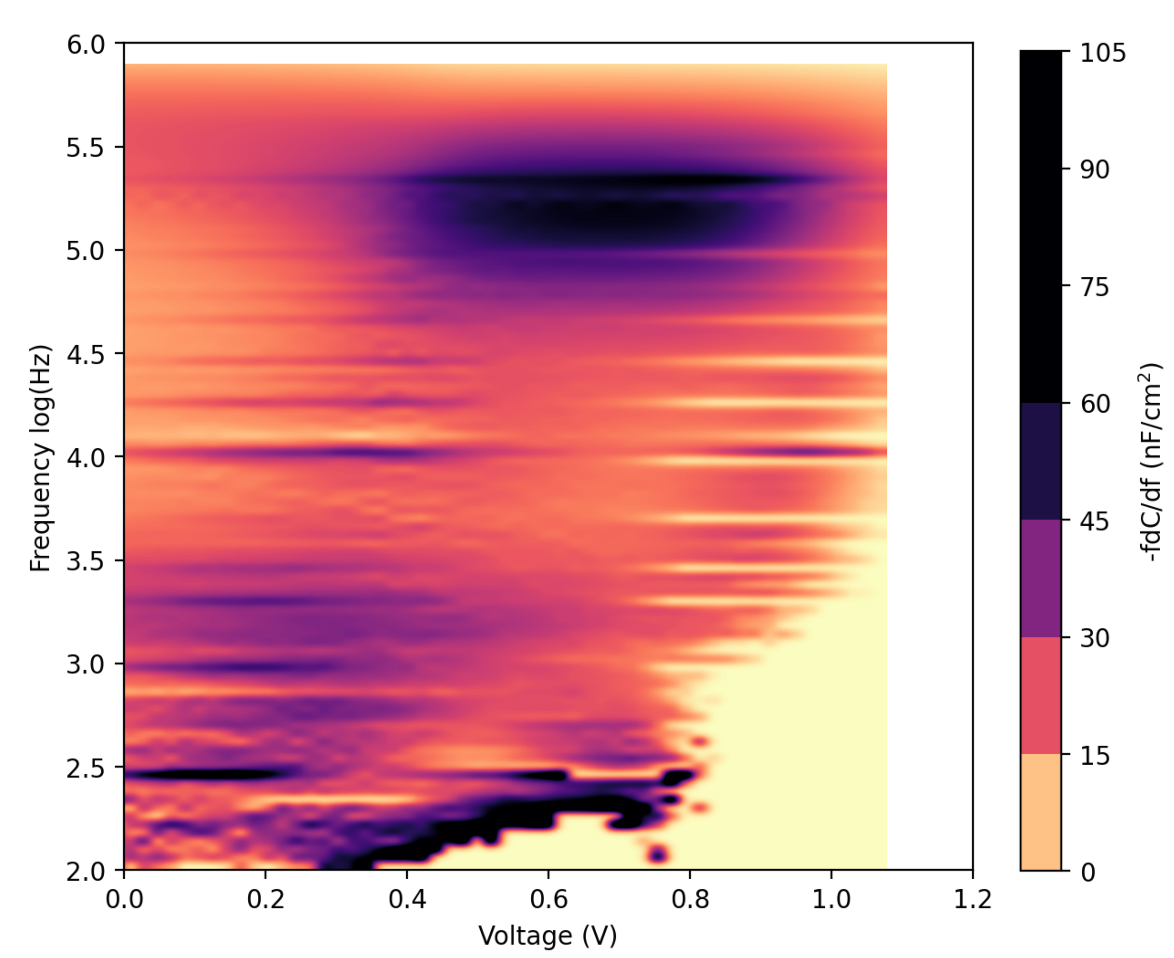
Capacitance measurement techniques are powerful methods for characterizing semiconductor devices. **Voltage dependent admittance spectroscopy (C-V-f)** has recently been used to characterize **electronic loss mechanisms** in CIGS solar cells [1]. Processed C-V-f data yields a **fingerprint** “loss map” that is a convolution of multiple loss mechanisms.

Drift-diffusion modeling can be used to **simulate a large dataset** of C-V-f loss maps with **known defect characteristics.** By training a **machine learning algorithm** with simulated data, dominant loss mechanisms can be identified in solar cell samples.

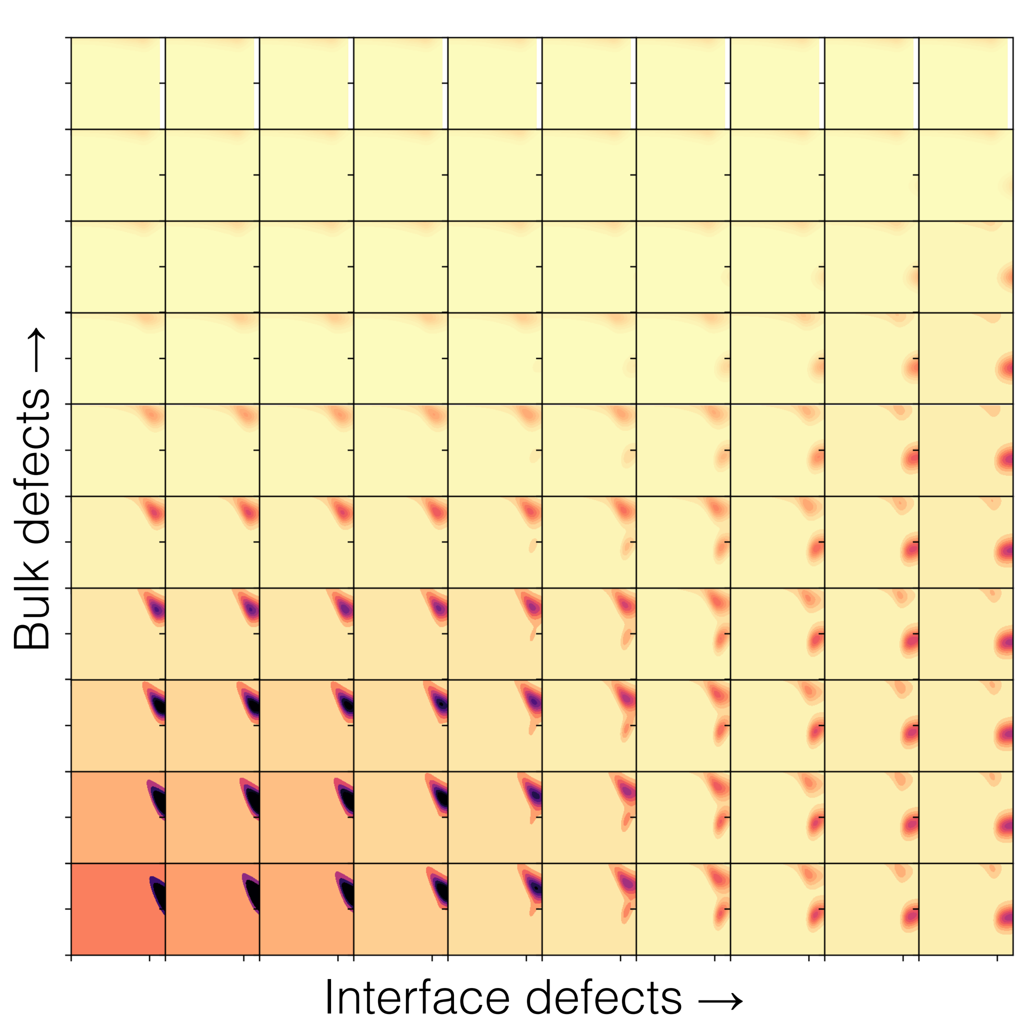
C-V-f data



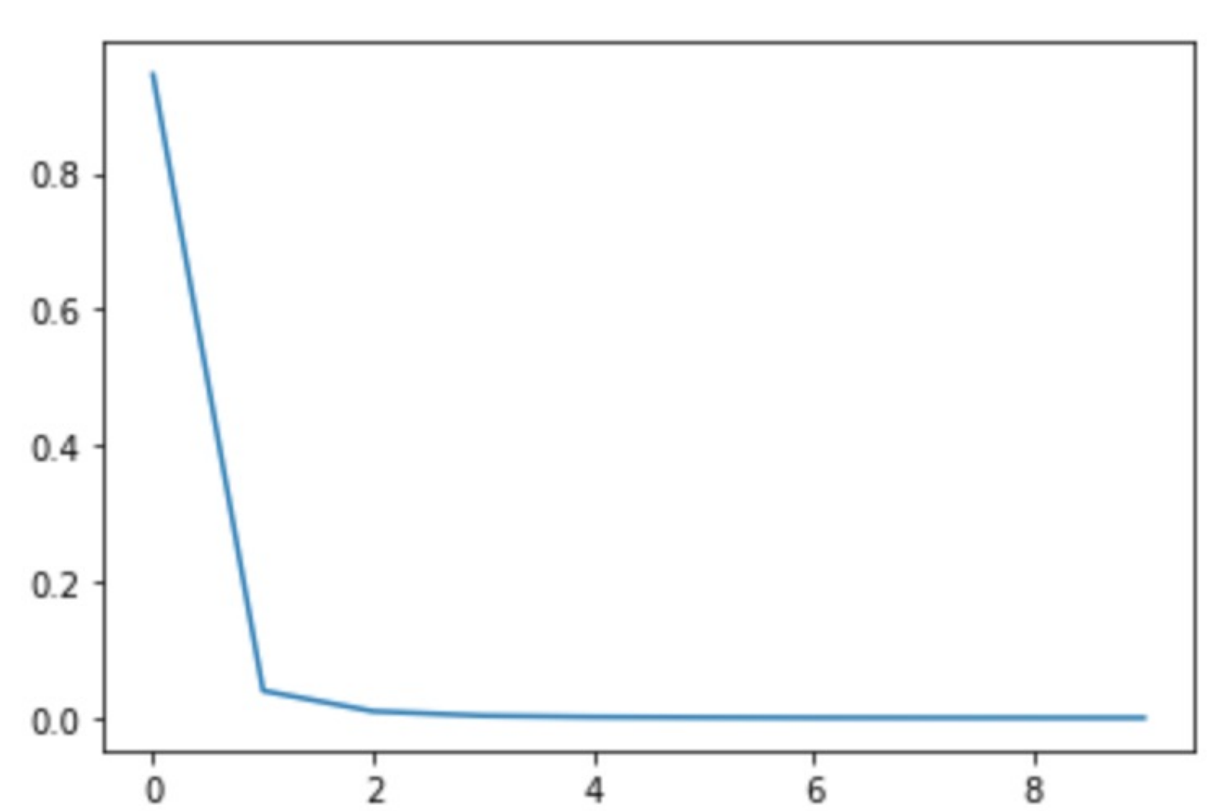
Fingerprint loss map



Large simulated dataset

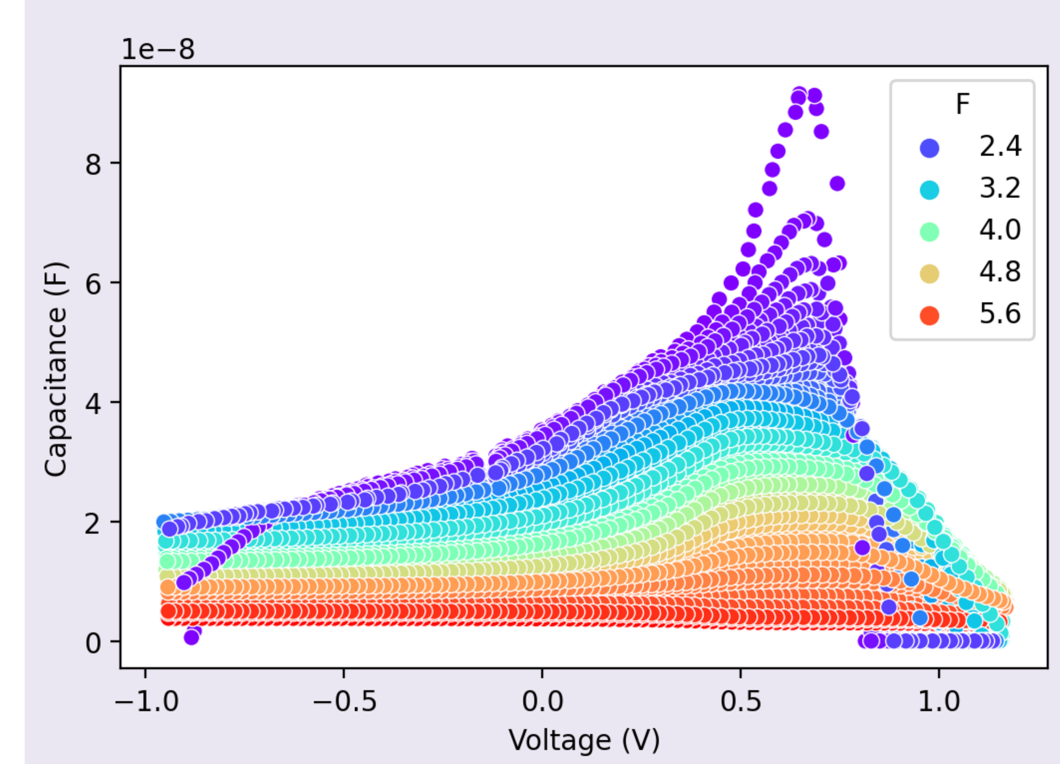


PCA

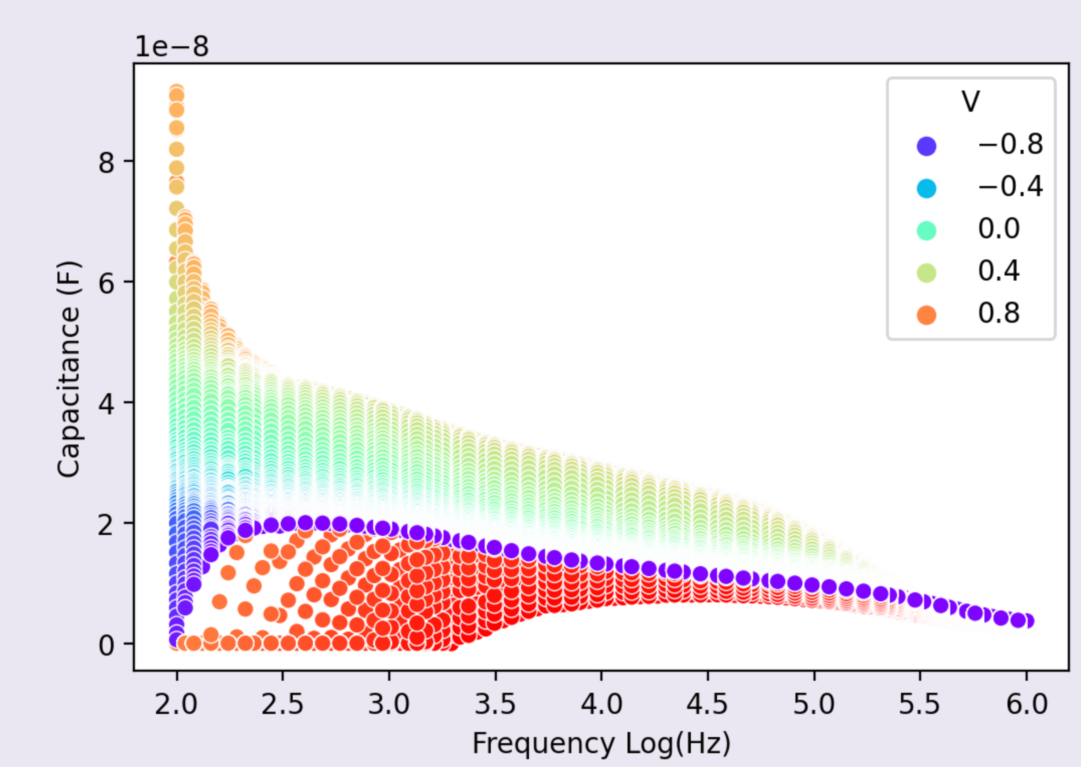


Capacitance measurements

Shape of capacitance curves varies with voltage and frequency



Probe broad band of voltage and frequency



[1] Hopf et al. “Mutation effects predicted from sequence co-variation.” (2017)
[2] Riesselman et al. “Deep generative models of genetic variation capture the effects of mutations.” (2018)
[3] Riesselman et al. “Accelerating protein design using autoregressive generative models.” (2019)
[4] Frank Noe et al. “Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning.” (2019)