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Physics-Informed Graph Neural Network for Circuit Compact Model Development

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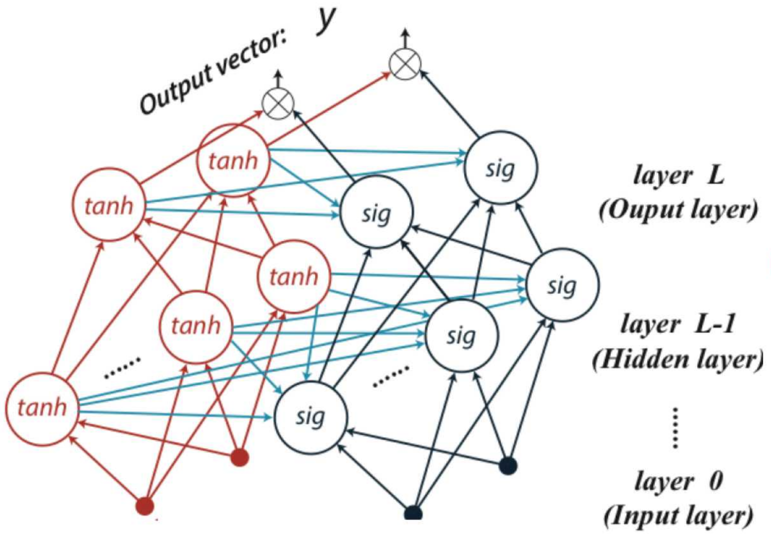
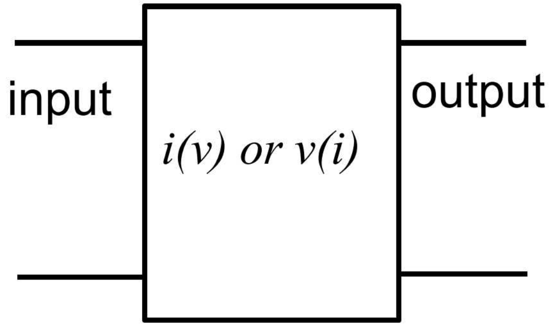
Machine Learning for Compact Model Development

- Traditional compact model development (CMD) takes multi-years and multi-institutional efforts.
- Data-driven machine learning (ML) is being actively explored for fast CMD [1-2].





✓ Fast CMD (a functional black box)

❌ Physics-agnostic, may lead to unphysical predictions

❌ Ignore high-fidelity physics from TCAD simulation

New opportunity: combine TCAD physics and data-driven ML for rapid and physics-based circuit compact model development

[1] M. Li, O. İrsoy, C. Cardie and H. G. Xing, IEEE J. Explor. Solid-State Computat. vol. 2, pp. 44-49, Dec. 2016.

[2] K. Aadithya, P. Kuberry et al., arXiv:2001.01699, 2020.

pigNN-CMD Methodology

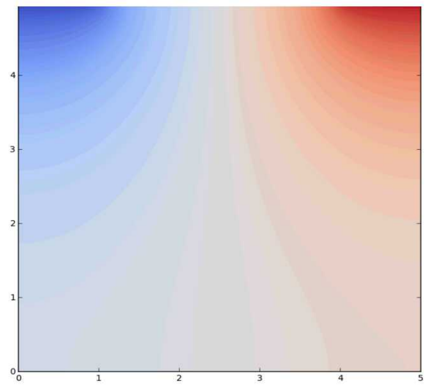
We propose the physics-informed graph neural network (pigNN) methodology for circuit CMD

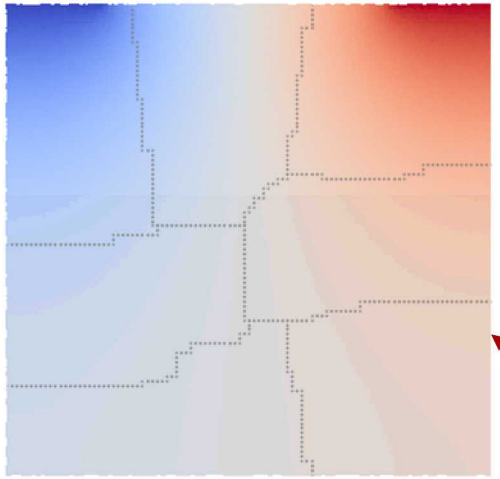
Physics Priming (PP)
(Perfunctory TCAD)

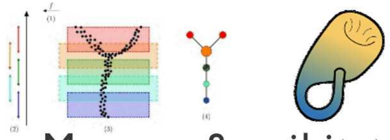
Region Recognition (RR)
(ML + TDA)

Topology Tailoring (TT)
(TCAD-informed ML)

Interaction Identification (II)
(seeded w/ established CMs)







Mapper & scikit-tda

Loosely calibrated TCAD simulations

- Use machine learning (ML) classification and topological data analysis (TDA) methods to process TCAD physical fields
- Determine physically important regions as they evolve through a sweep of bias/time conditions.

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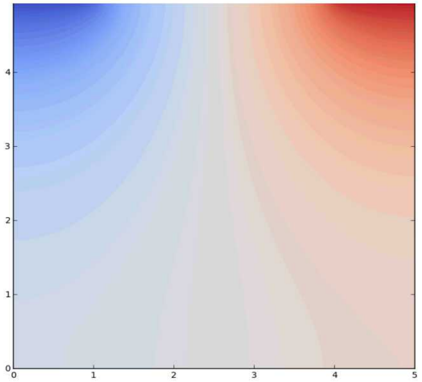

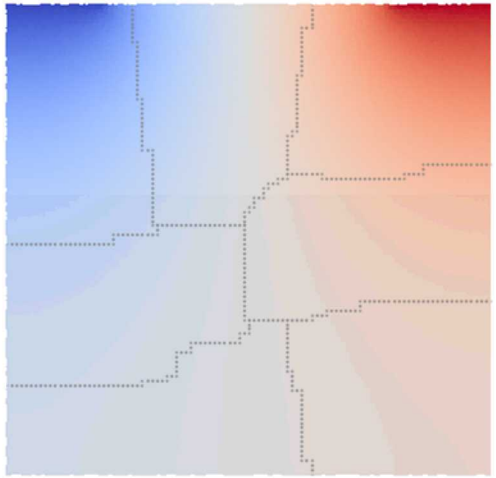

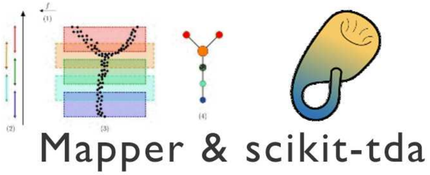

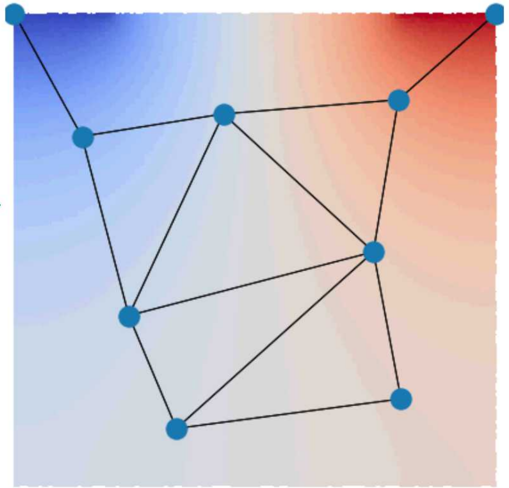

Determine the intrinsic device topology using TCAD-informed ML

Loosely calibrated TCAD simulations

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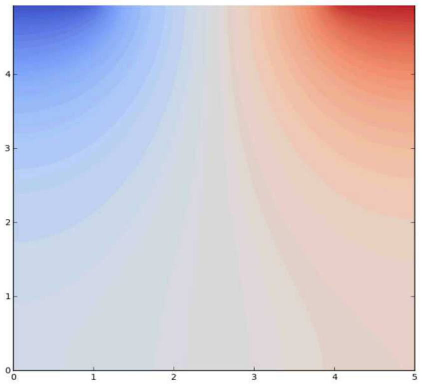
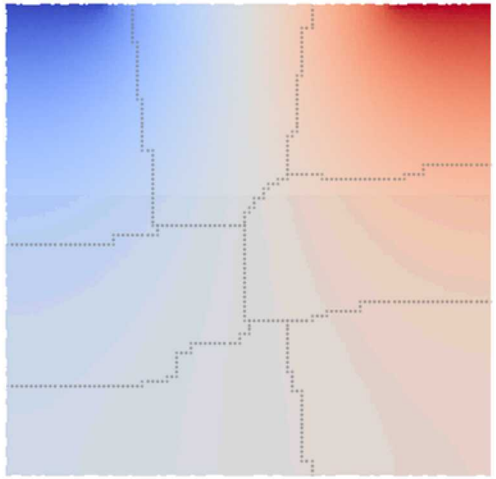
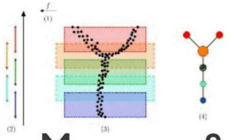
(Perfunctory TCAD)



Loosely calibrated TCAD simulations

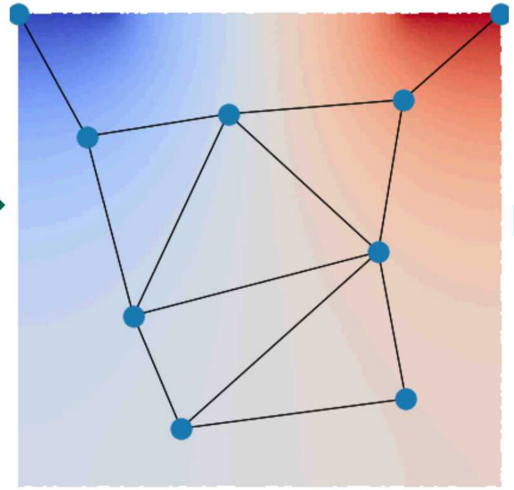
Region Recognition (RR)
(ML + TDA)



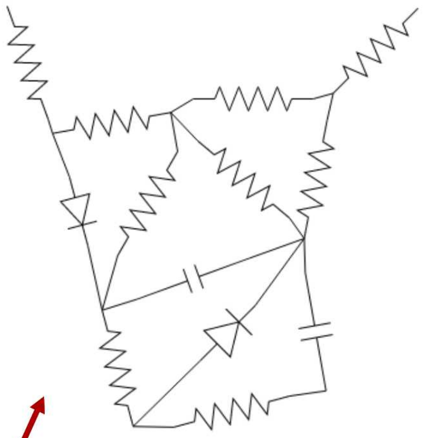


Mapper & scikit-tda

Topology Tailoring (TT)
(TCAD-informed ML)



Interaction Identification (II)
(seeded w/ established CMs)



- Populate graph edges with components based on local responses from TCAD
- Enforce Kirchhoff's current law at each node during ML learning

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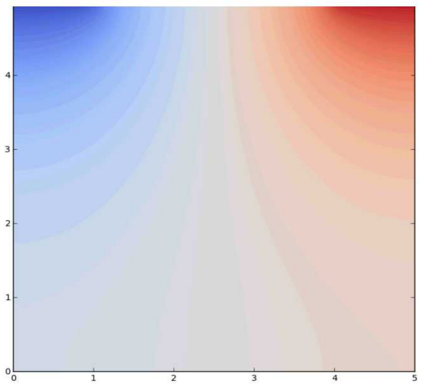
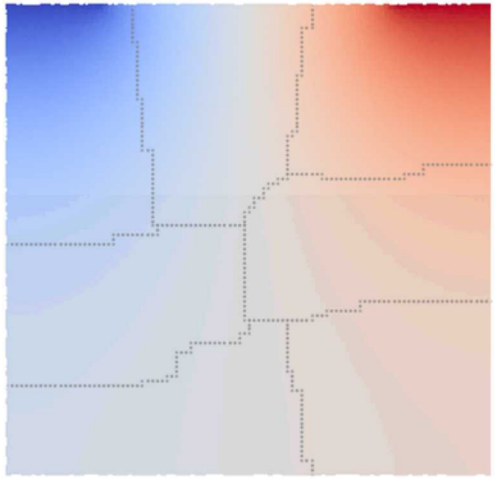


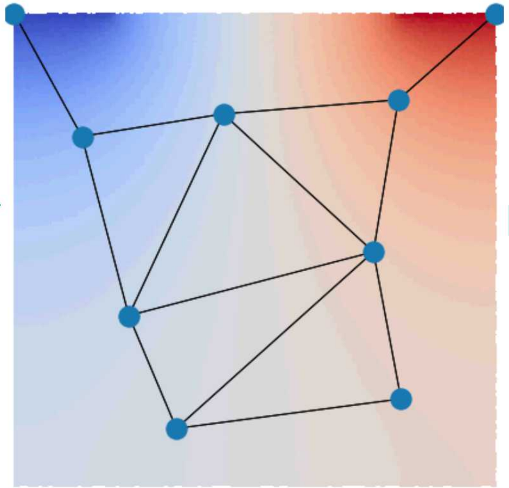
CHARON

Loosely calibrated TCAD simulations

Region Recognition (RR)
(ML + TDA)



Topology Tailoring (TT)
(TCAD-informed ML)



Interaction Identification (II)
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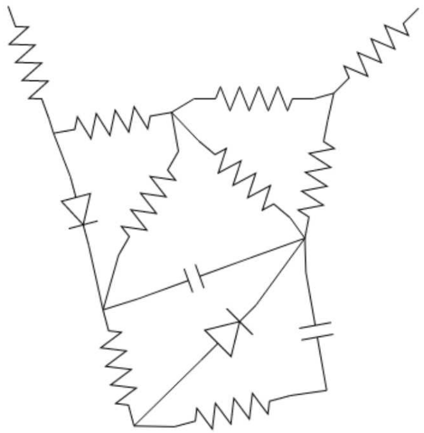

Xyce
PARALLEL ELECTRONIC SIMULATOR

Train and Adapt
(using available experimental data)

Diode Compact Model for a pigNN-Graph Edge

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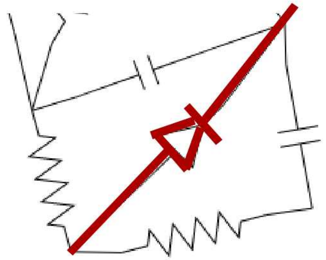
What is a good compact model for a diode located at an edge?

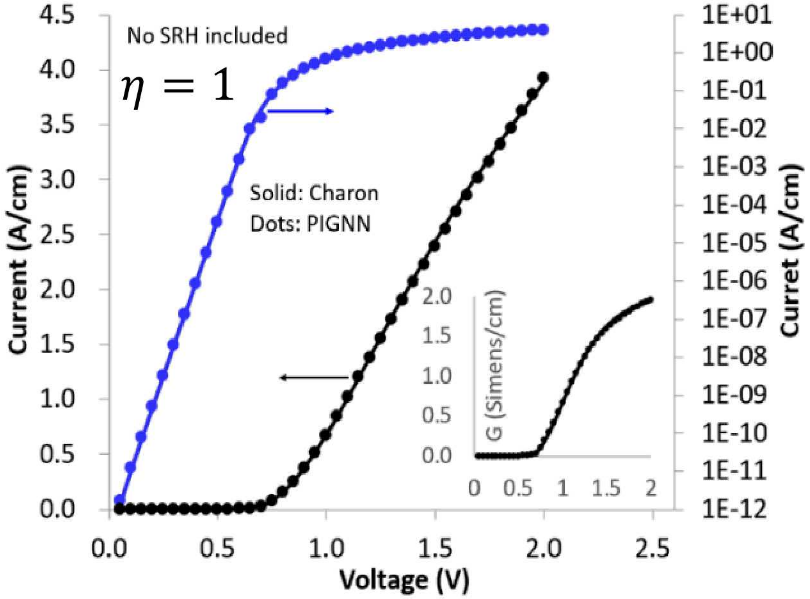


- Apply TDA method with physical fields to isolate a localized diode
- Process TCAD physical fields to obtain response for the diode
- Apply data-driven neural network to develop compact model for the diode

$$I_D = [1 - w(V_D)] I_0 \left(e^{\frac{qV_D}{\eta k_B T}} - 1.0 \right) + V_D G_D(V_D)$$

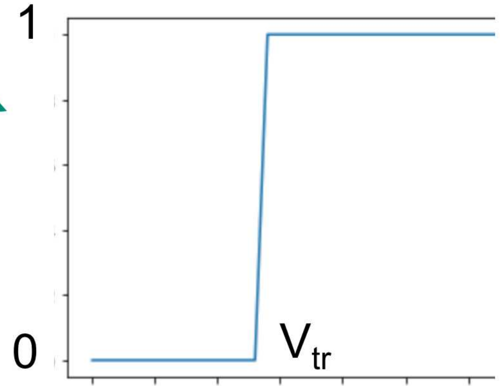
Voltage-dependent conductance learned using neural network

$$G_D(V_D) = w(V_D)\left(1 - \frac{V_{tr}}{V_D}\right) G_0 + w(V_D)\left(1 - \frac{V_{tr}}{V_D}\right) G_{NN}(\mathrm{V_D})$$



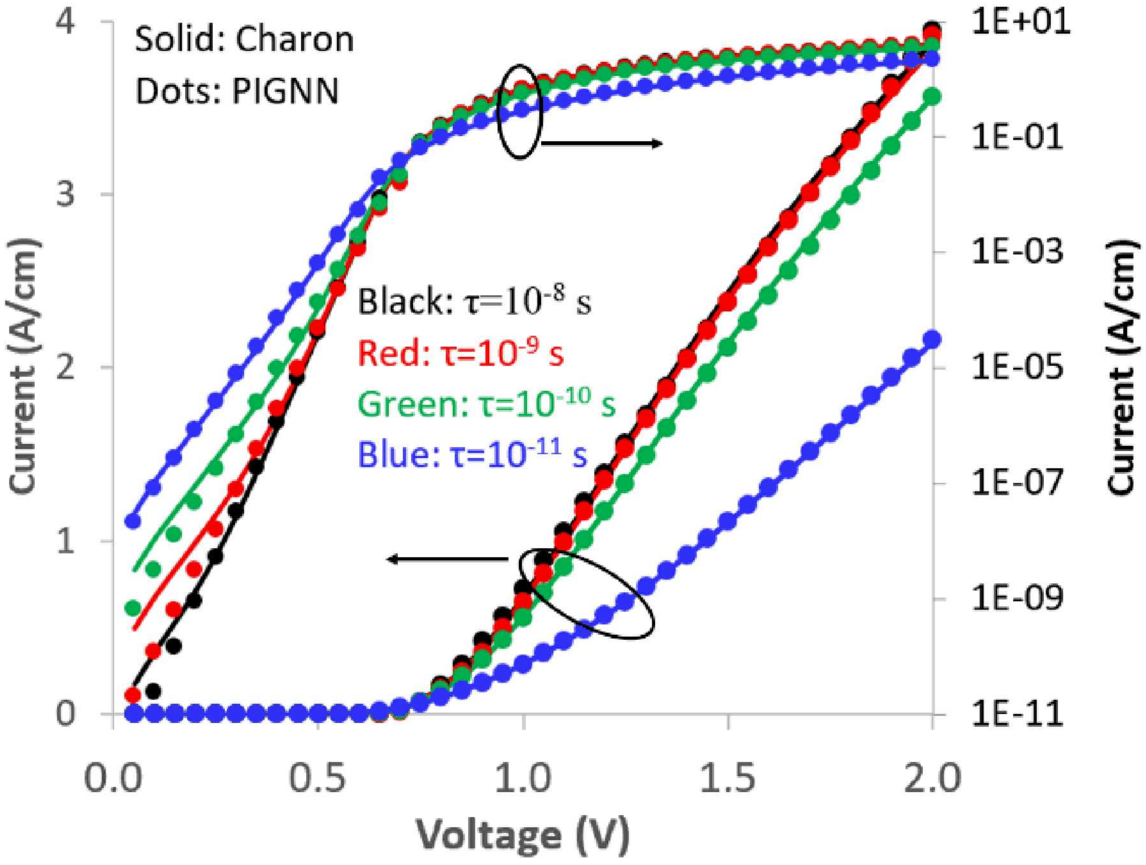
$$w(V_D) = 0.5\left[\tanh\left(10^5 (V_D - V_{tr})\right) + 1.0\right]$$

A differentiable function that transitions the diode response smoothly from an exponential region to a quasi-linear region



Voltage Independent Non-ideality Factor

- Recombination effect increases the diode current in the low forward bias region
- Voltage-independent non-ideality factor partially captures the recombination effect



$$I_D = [1 - w(V_D)]I_0\left(e^{\frac{qV_D}{\eta k_B T}} - 1.0\right) + V_D G_D(V_D)$$

τ (s)	I_0 (A/cm)	η
No SRH	1.71×10^{-13}	1.0
10^{-8}	1.35×10^{-12}	1.13
10^{-9}	5.14×10^{-12}	1.21
10^{-10}	2.37×10^{-10}	1.46
10^{-11}	1.02×10^{-8}	1.75

NN-learned Variables

Voltage independent non-ideality factor cannot accurately model the voltage dependent recombination effect.

NN Loss Function Design for Diode Compact Model

- Recombination effect is inherently voltage dependent
- Need voltage-dependent non-ideality factor to accurately capture the recombination effect

$$I_D = [1 - w(V_D)]I_0\left(e^{\frac{qV_D}{\eta(V_D)k_BT}} - 1.0\right) + V_D G_D(V_D)$$

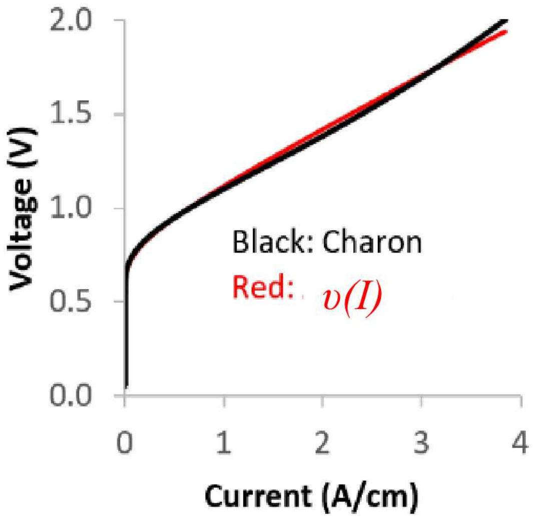
$$\eta(V_D) = 1 + \eta_{NN}(V_D)$$ ⟵ Voltage-dependent non-ideality factor learned using NN

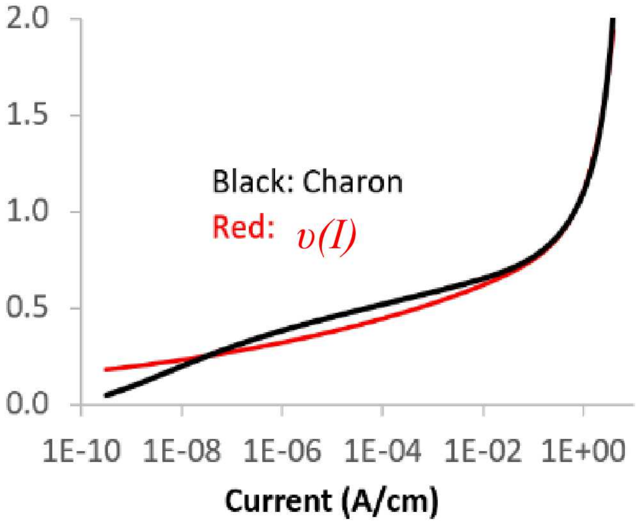
- A good NN loss function is needed to achieve accurate results due to mixture of exponential and quasi-linear current response

Proposed NN loss function: $\boxed{\mathcal{L} = [v(I_{NN}) - v(I_t)]^2/[v(I_t)]^2}$

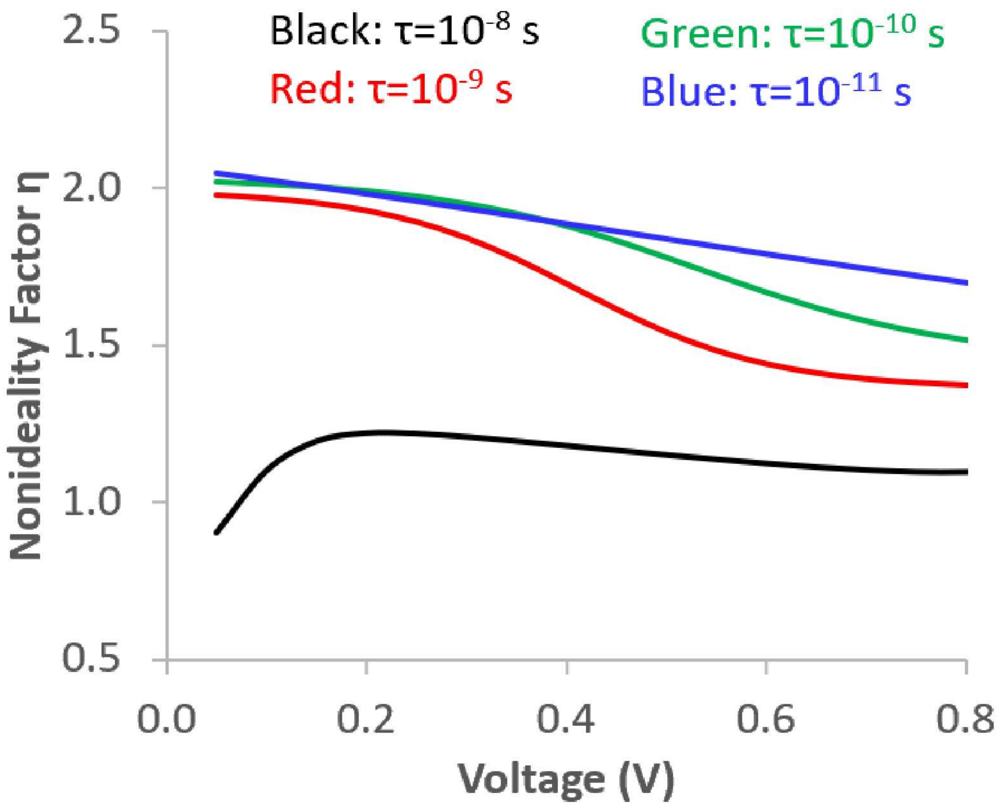
$$v(I) = (aI)^b \times \tanh(dI - e) + fI$$

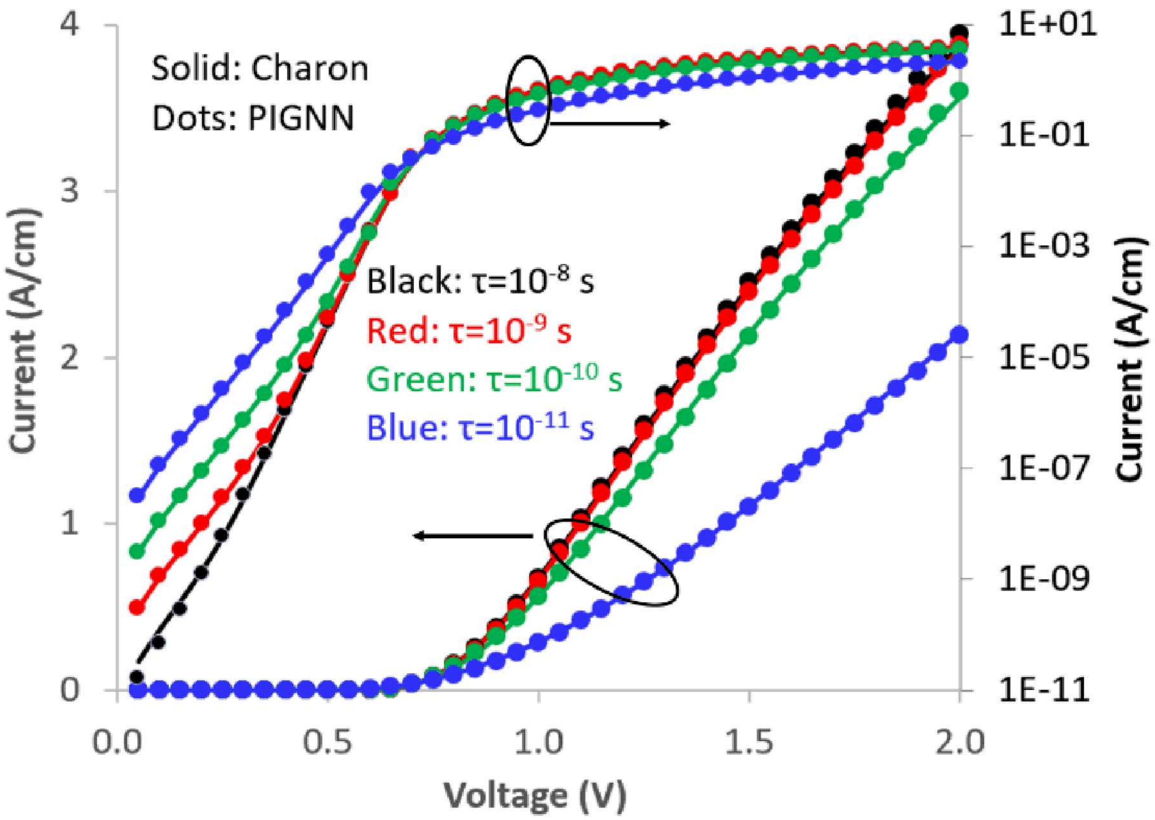
✓ Map the logarithmically separated current range to a linearly separated voltage range
✓ Use regression to determine a, b, d, e, f





Voltage Dependent Non-Ideality Factor



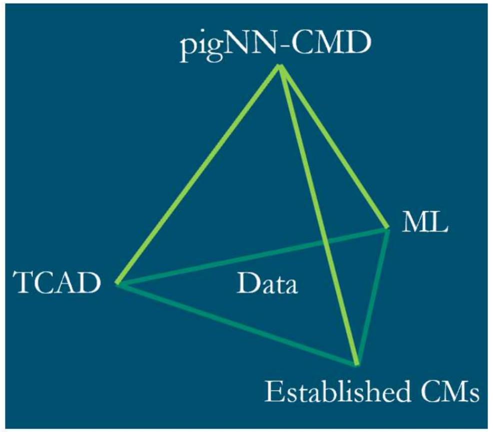


NN-learned non-ideality factor indeed shows a strong voltage dependence.

Voltage-dependent non-ideality factor allows us to accurately model the recombination effect.

Summary

- Presented the pigNN methodology for compact model development that brings together data-driven ML, TCAD, and existing compact models.



- Developed accurate compact model for a non-ideal PN diode that represents a non-linear edge in a pigNN graph

- Applying the pigNN methodology to other semiconductor devices (e.g., bipolar transistor) & other engineering areas (e.g., mechanics, EM).