Hybrid-AI Modeling for Biorealistic Neuromorphic Computing

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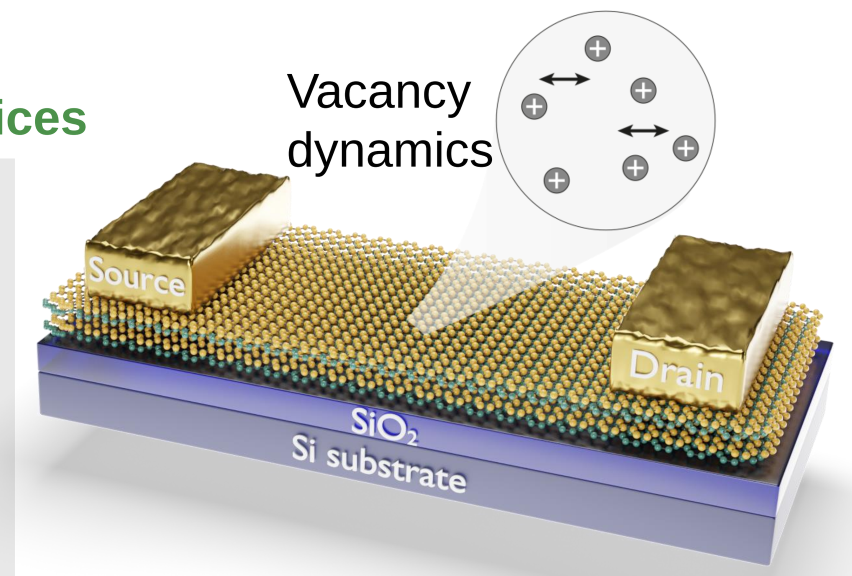
Motivation – Green Electronics

- **Emerging neuromorphic systems** as a solution for energy-efficient artificial intelligence (AI) hardware accelerators
- Ideal neuromorphic system: **high interconnection** and **adaptability** like neurons in the human brain to **accelerate any matrix operation** including **biorealistic learning**

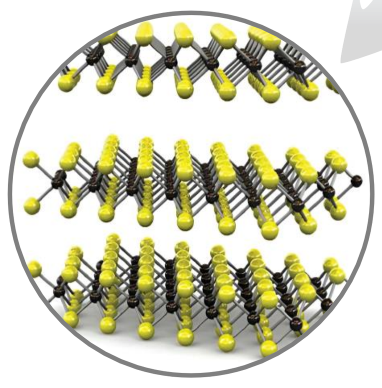
Memtransistors – Bioinspired Electronic Devices

- Memristor + transistor + many contacts [1]
- Biorealistic, general purpose computing [2,3]:
  a) Electrically tunable via gate electrodes
  b) High interconnectivity by many contacts
- Benefits from novel 2D functional materials
- Largely unexplored material and device space [5]



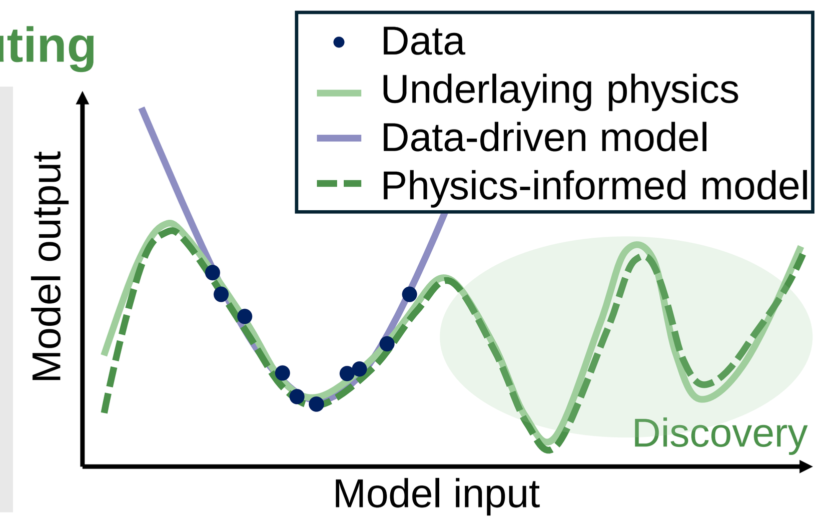
2D Materials – Functional Electronic Materials

- Transition metal dichalcogenides (TMDCs)
- Promising for next-gen. microelectronics [4]
  a) Ultimate scalability
  b) Well-defined electronics properties
  c) Large range of electronics properties
- Memristive mechanisms largely unexplored



Hybrid-AI Modeling – Energy Efficient Computing

- Integrating physical computational models, AI, and empirical data
- Much less data needed than "classical" AI
- Materials and system discovery [6]
- Potential to highly accelerate research and overcome "Edisonian" trial and error approach [7]



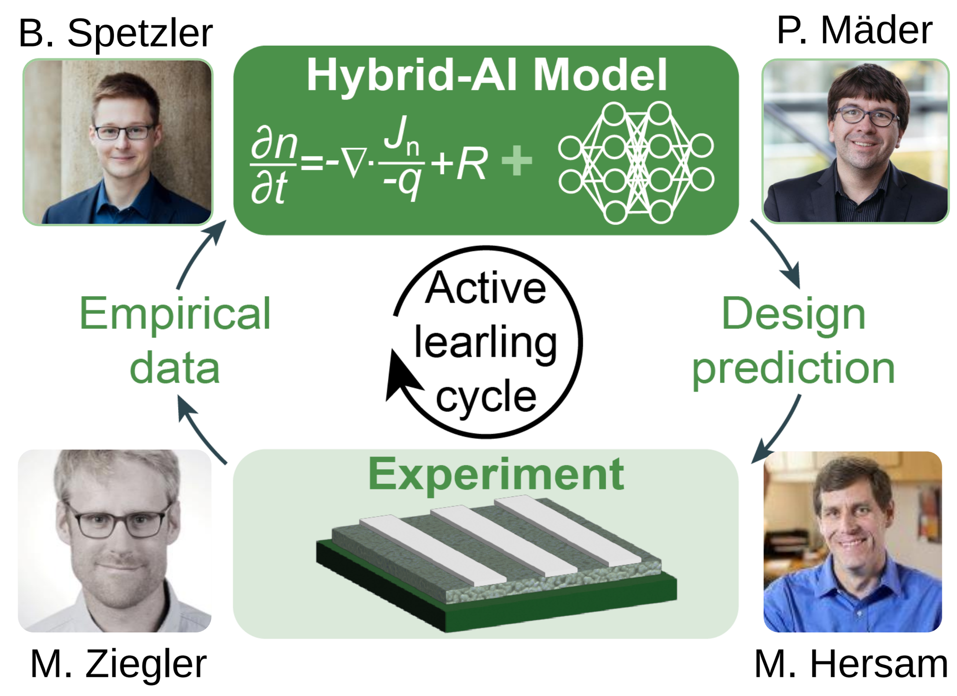
Objectives

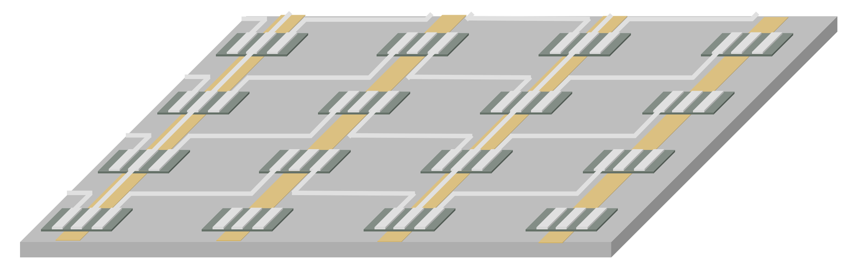
This project aims to investigate a novel hybrid-AI method to tailor general-purpose neuromorphic hardware based on 2D MoS_2 memtransistors.

Main objectives:

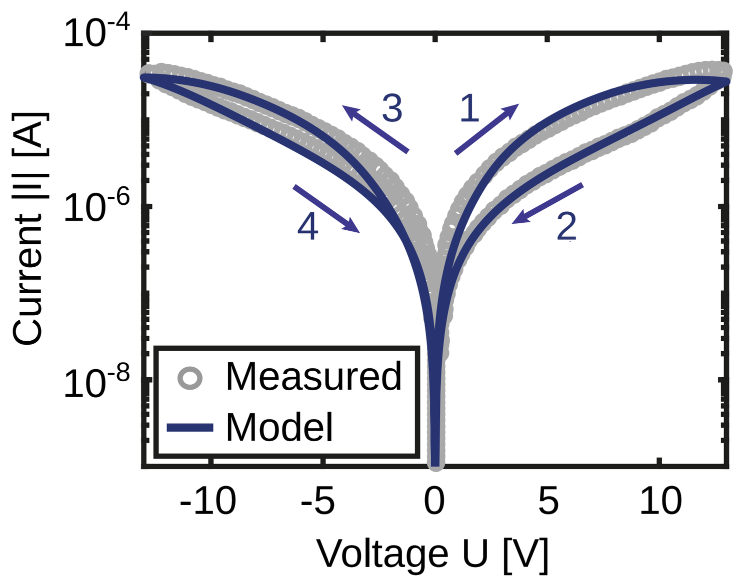
1) Identify switching and tunability mechanism of MoS_2 memtransistors
2) Provide a well-validated and efficient modeling framework for memtransistors
3) Identify and realize system configurations for general-purpose AI accelerators that…

a) …are electrically tunable
b) …permit biorealistic learning
c) …are energy efficient
d) …outperform current systems





Preliminary Work

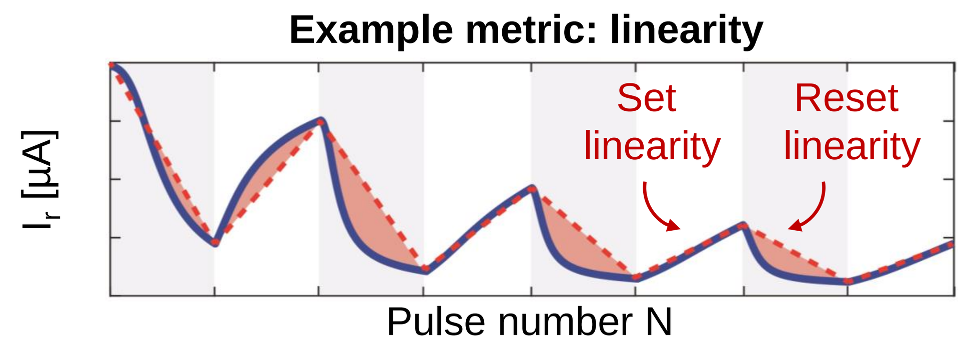


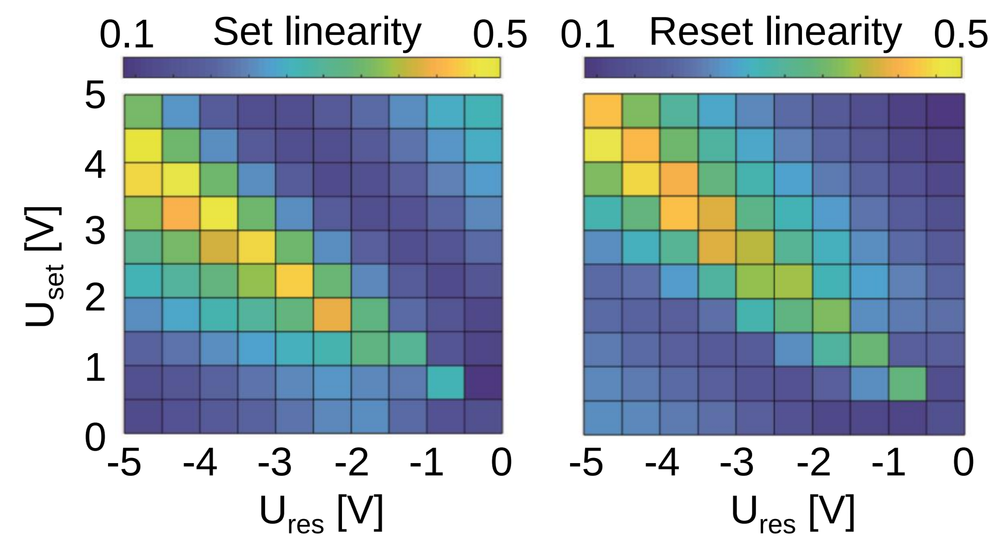
Charge-transport model [6]

- Based on finite volume discretization
- Nonlinear drift-diffusion equations of electrons, holes, vacancies, Poisson's equation and various other effects
- Explains hysteresis in two-terminal devices via vacancy depletion zone
- Validated with measurements on MoS_2

High-throughput simulations

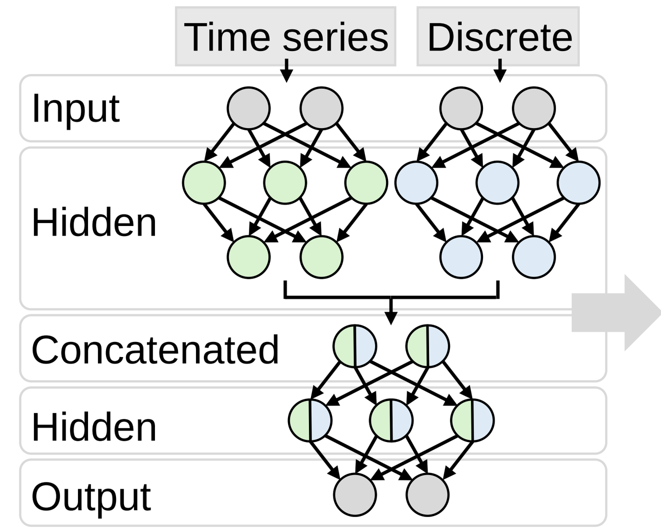
- Screening parameter space as input for data-driven surrogate model
- Here, at the example of one metric (linearity of set/reset)

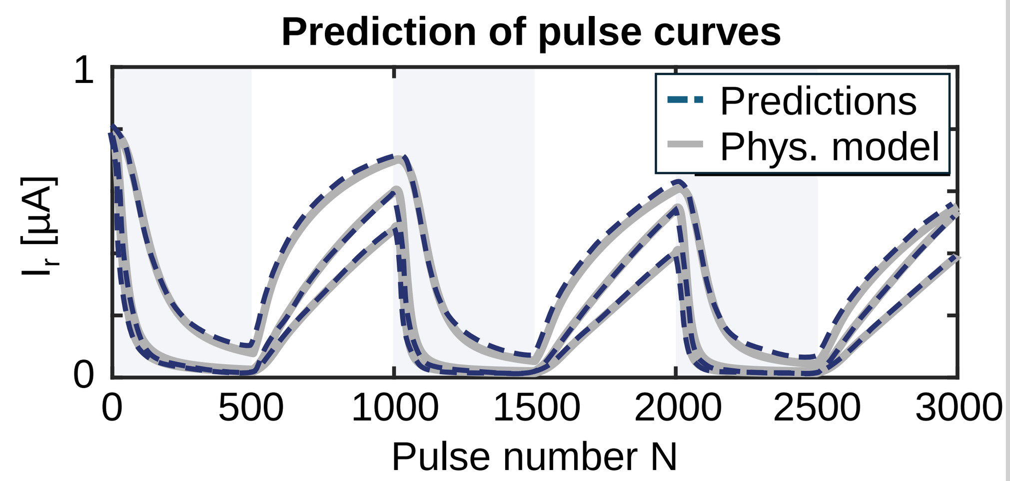




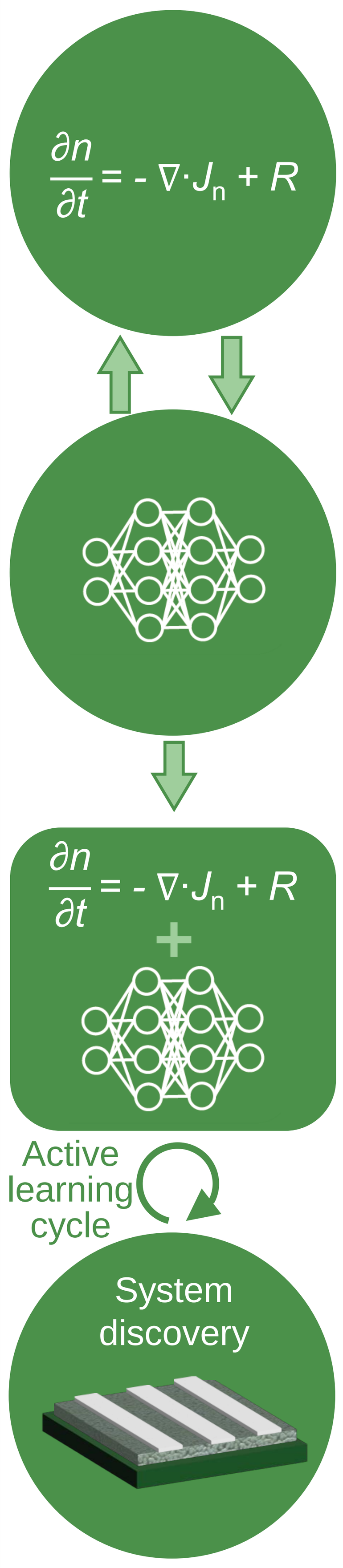
Data-driven surrogate model

- Hybrid LSTM network to predict current-voltage and pulse characteristics
- Accurate and efficient for multi-objective optimization





Work Program & Schedule



WP1 – Charge transport model & switching mechanism (Spetzler)

Objectives: Extend and validate the charge transport model to identify the relevant memristive and electronic mechanisms

- Extend finite volume (FV) charge transport model from preliminary work [8] by new physical mechanisms (with Dr. Patricio Farrell)
- Validation with experimental data (Prof. Mark Hersam/MNES) using the surrogate model from **WP2** for automized optimization

WP2 – Data-driven surrogate mode (Mäder/Spetzler)

Objectives: Investigate data-driven surrogates of the charge transport model for multi-objective optimization tasks

- High-throughput simulations to sample parameter space
- Train data-driven surrogate model to automize validation in **WP1**

WP3 – Hybrid-AI modeling framework (Mäder)

Objectives: Investigate physics-informed methods to set up an energy and data efficient hybrid-AI modeling framework

- Deep operator networks (DeepOnets) for individual equations
- Deep multiphysics and multiscale networks (DeepM&Mnets) [9]
- Benchmark against classical model (**WP1**) and surrogate (**WP2**)

WP4 – Neuromorphic System Discovery (Mäder/Spetzler)

Objective: Set up active learning cycle to discover and realize neuromorphic systems for complex biorealistic learning

- Define suitable metrics for neuromorphic systems - parametrizing
- Continuous feedback and discrepancy modeling with experiments
- Discover and realize of individual devices and entire systems

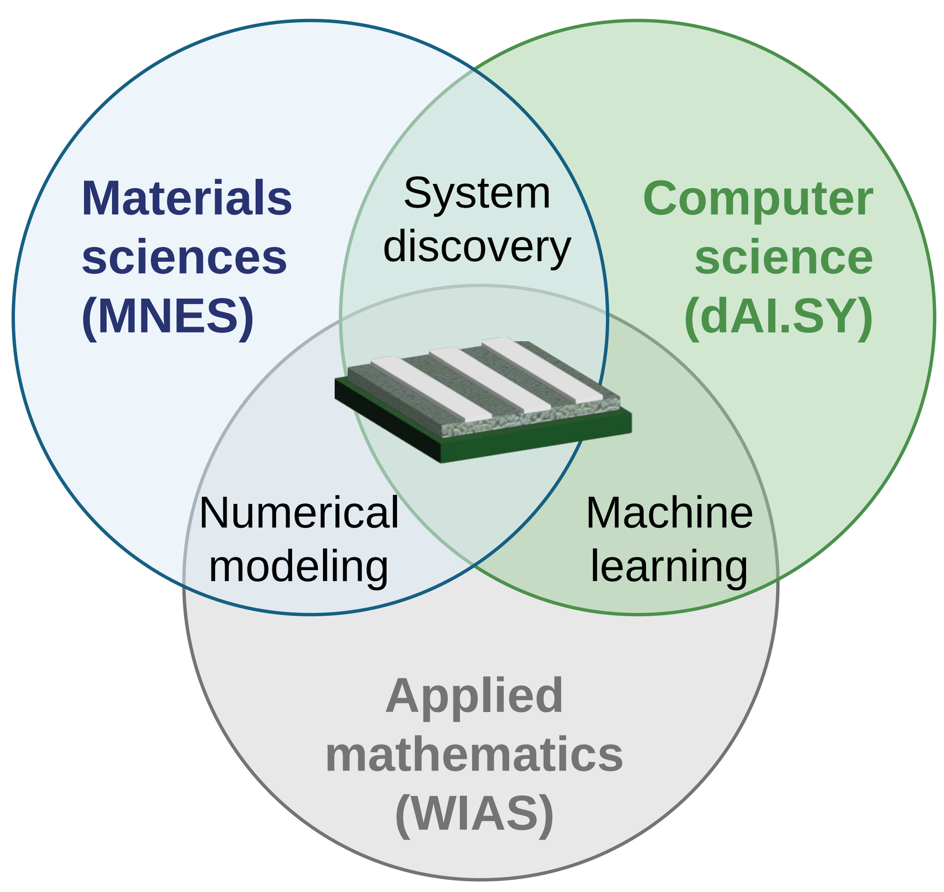
	Mäder (dAI.SY)	2025				2026				2027				2028			
	Spetzler (MNES)	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
WP1	Charge transport model																
WP2	Data-driven surrogate																
WP3	Hybrid-AI framework																
WP4	System discovery																

Prospects

- Establishes hybrid-AI modeling at TU Ilmenau
- New benchmarks for energy-efficient computing
- Provides training in…
  …device technology
  …computational physics
  …machine learning

Highly relevant beyond memtransistors [4]

Emerging paradigm in physical sciences [6]



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[2] Bergeron, H.; … ; **Hersam, M.** *Adv. Funct. Mater.* **2020**, *30*, 2003683.
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[6] Raabe, D.; et al., *Nat. Comput. Sci.* 2023, *3*, 198–209.
[7] Karniadakis, G. E; et al. *Nat Rev Phys* 2021, *3*, 422–440.
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[9] Cai, S.; et al., *Journal of Computational Physics* **2021**, *436*, 110296.

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