AI Driven Design of Semiconductor Alloys with Tuned Effective Masses

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YOUNG SCHOLARS PROGRAM

Data Driven Renewables Research

Northeastern University College of Engineering

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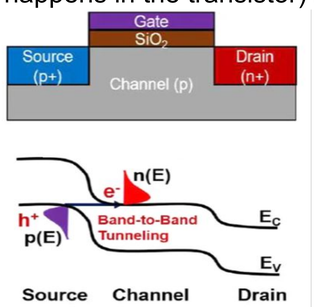
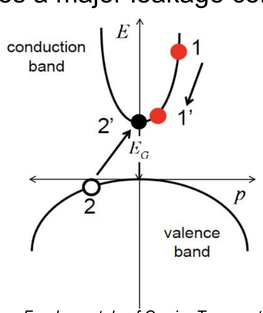
Abstract

Impact ionization affects how semiconductor devices perform under high electric fields. Machine learning (ML) can predict materials properties more efficiently than experimental measurements and first-principles calculations, which are difficult, time-consuming, and expensive. Our goal is to combine physics knowledge with computational data, as well as implementing ML methods to predict properties of semiconductor materials. We scraped roughly 3,000 electron and hole effective mass data points from the Computational 2D Materials Database (C2DB), featurized material compositions using Magpie descriptors, and trained random forest and neural network models to predict effective mass from these features. We demonstrate that our models can be utilized to design a 2D semiconductor alloy ($MoS_2/MoSe_2$ system) with tuned electronic properties, suitability for high-power and high-speed electronic applications.

Background

- ***Impact ionization***: an energetic electron/hole pair transfers energy to create an additional electron–hole pair, driving carrier multiplication
- Determines breakdown behavior in semiconductor devices
- Strongly tied to **effective mass** - lighter carriers gain energy faster, triggering ionization more easily
- Effective mass and impact ionization are expensive and difficult to measure experimentally or compute from first principles, with data available for only a few materials
- Minimizing impact ionization favors: large band gap + heavy effective mass
- But high carrier mobility (needed for fast transistors) favors light effective mass
- At nanometer scales, quantum tunneling (impact ionization happens in the transistor) becomes a major leakage concern



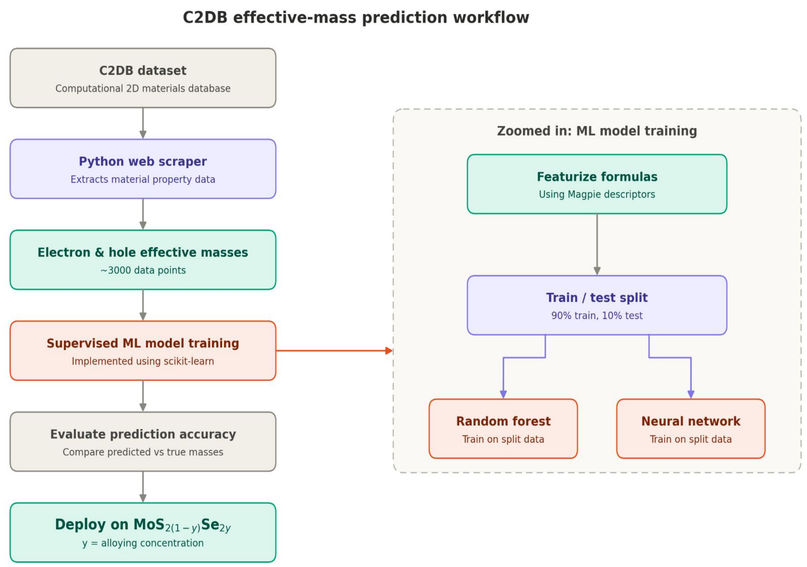


Kanungo *et al.* (2022), *npj 2D Mater Appl* 6, 83. Lundstrom, *Fundamentals of Carrier Transport*, 2nd ed. (2000)

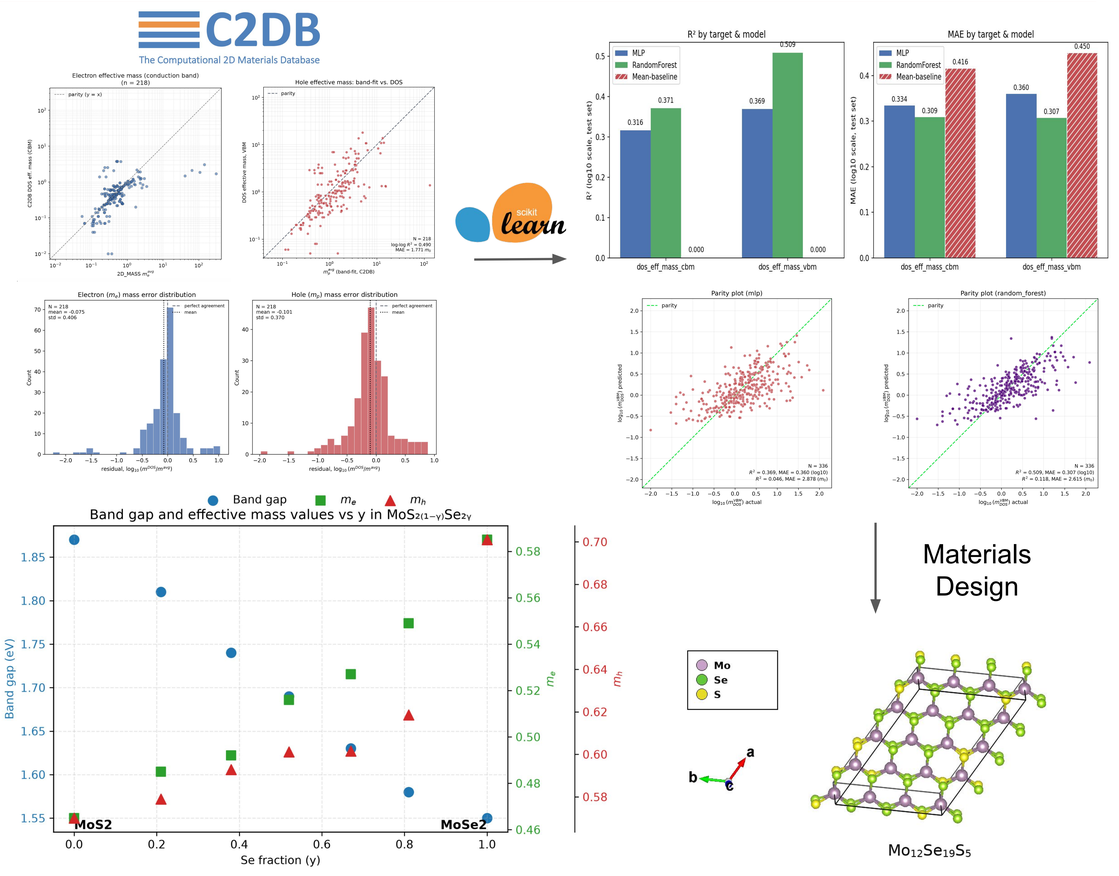
Computational Methods

Software Used:

VSCode, Github, Claude, Python, VESTA, ML, C2DB — The Computational 2D Materials Database



Results



Conclusion and Future Steps

- ML successfully trained on semiconductor alloy effective masses scraped from the C2DB
- Performance of trained ML models is mediocre but capture enough of the correlation to aid materials design (relative changes in the property)
- AI can speed up semiconductor discovery by reducing reliance on expensive quantum mechanical calculations
- Applications include: high-power electronics, faster transistors, and energy-efficient semiconductors

Future Work:

- Expand the training dataset
- Utilize full crystal structures during featurization (rather than compositions)

References

F. Ricci et al. An ab initio electronic transport database for inorganic materials, Scientific data 4 (1) (2017) 1–13.

R. Woods-Robinson et al. Designing transparent conductors using forbidden optical transitions, Matter 6 (9) (2023) 3021–3039.

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