AI for Materials: Accelerating simulations

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National Research Roadmap for Accelerated Materials Design, International Centre for Theoretical Sciences, Bengaluru, India
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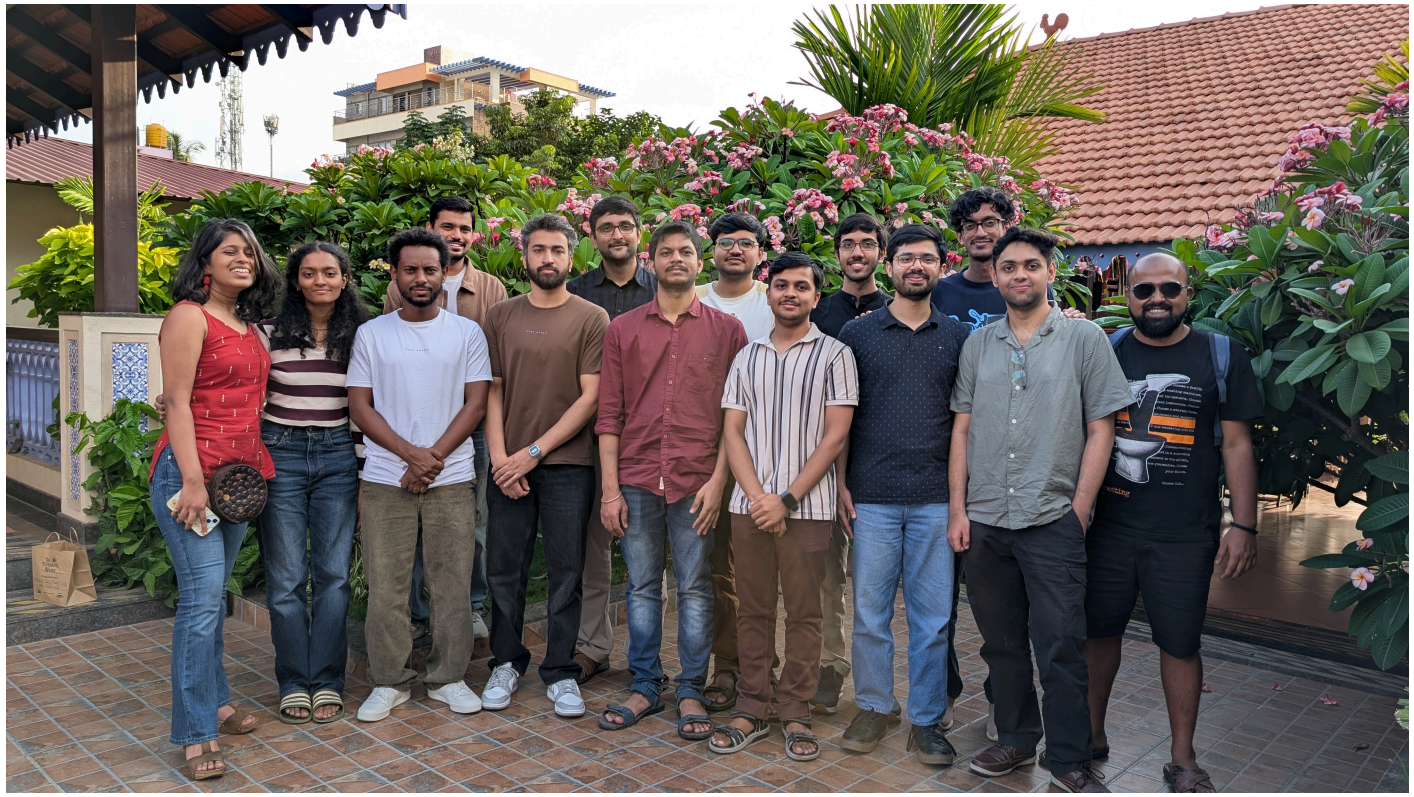
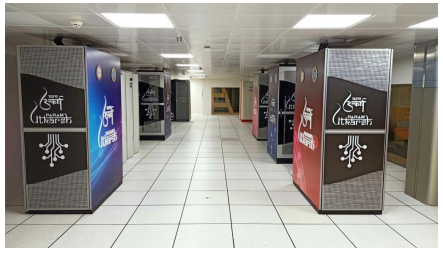
Acknowledgments



Jun 2026

SERC (IISc)

Fugaku (Japan)

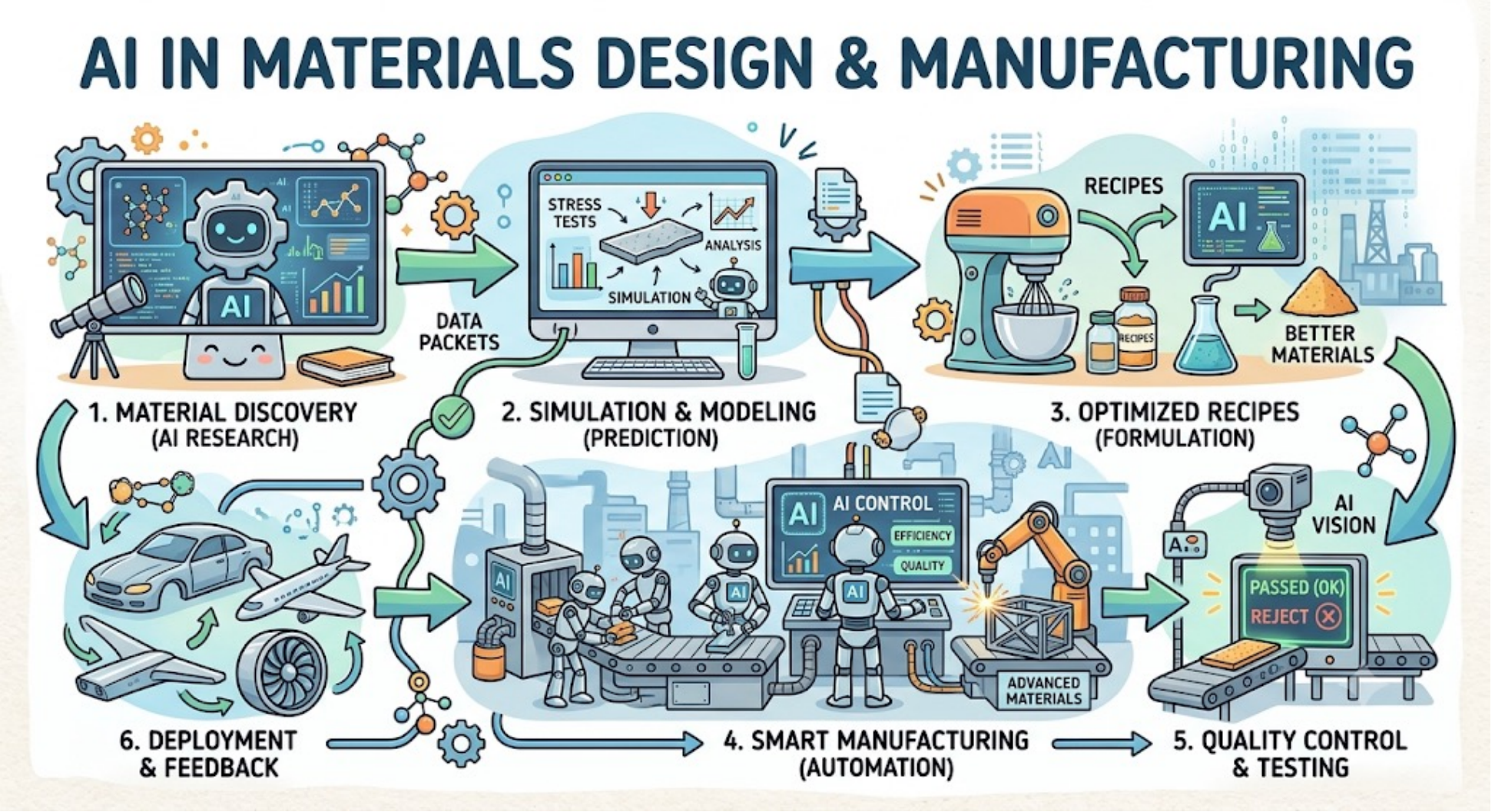


Param Utkarsh (CDAC)

Archer (UK)

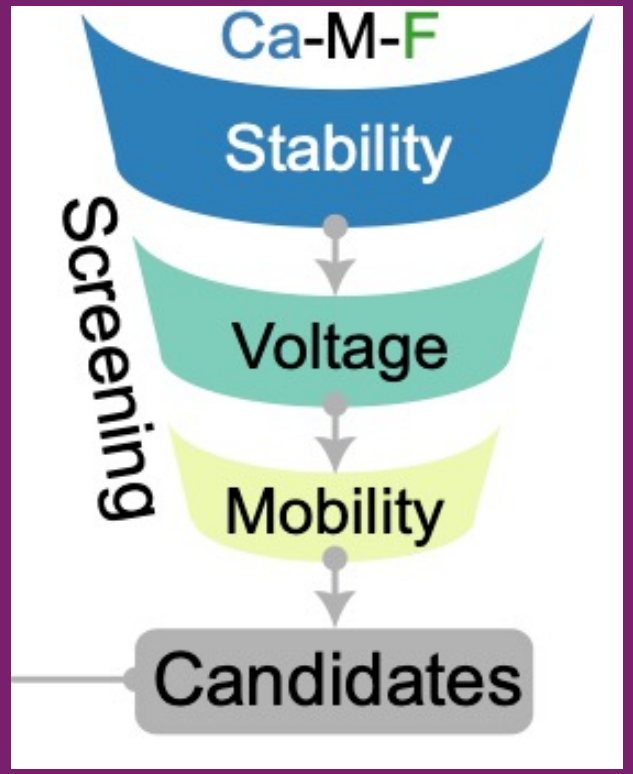
Jureca (Germany)

How AI thinks it can improve materials?

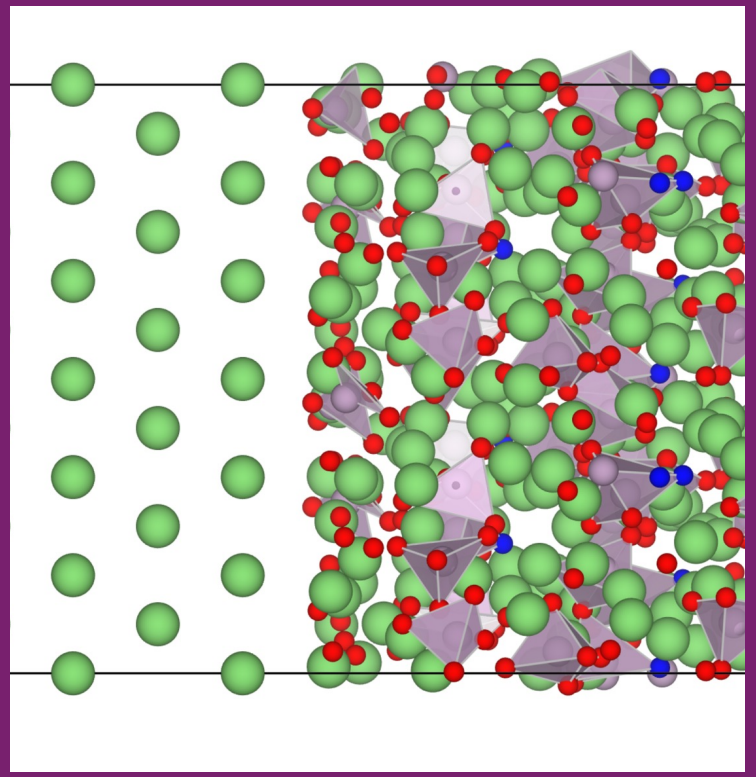


Examples in materials discovery and design

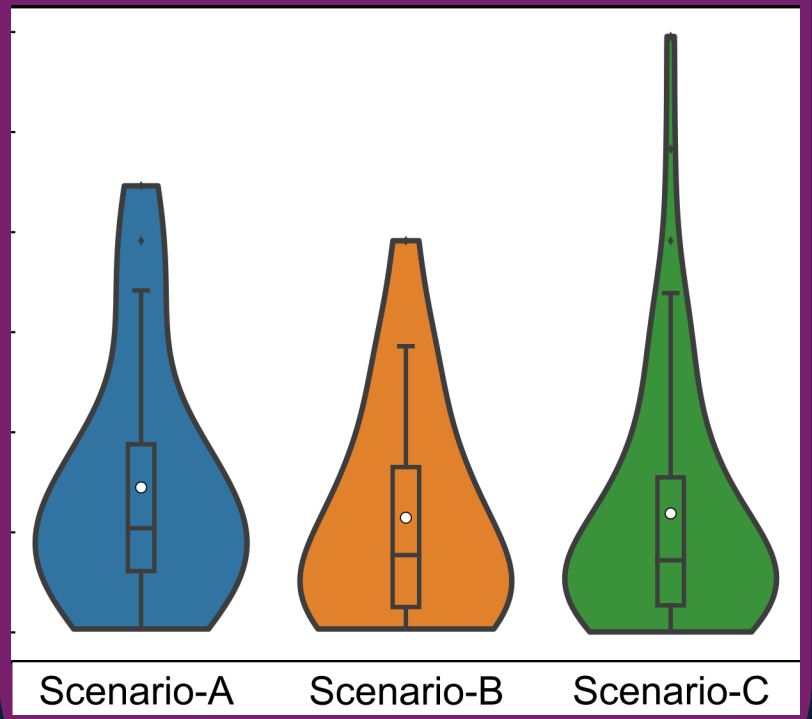
High-throughput screening



Modelling complex systems

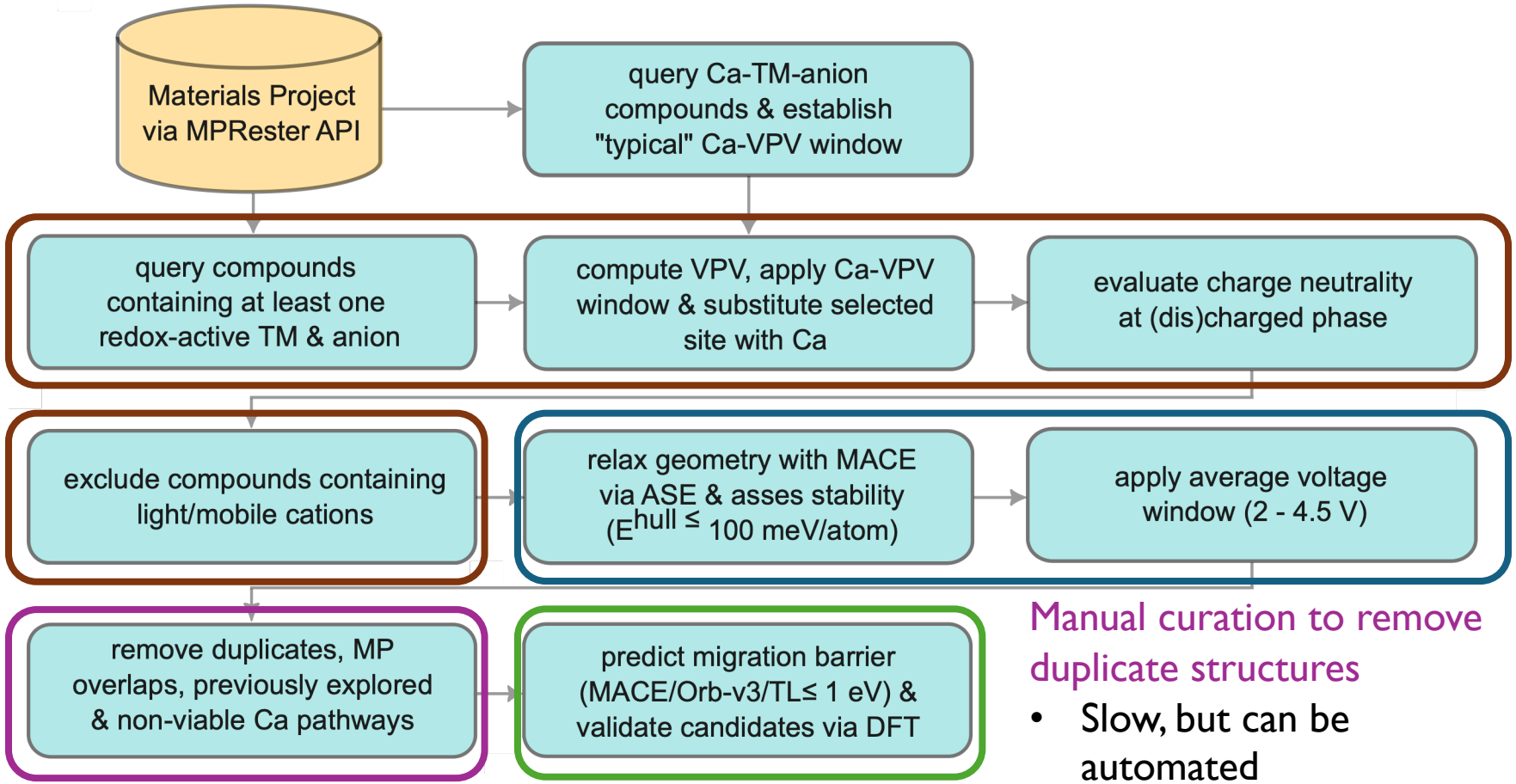


Swift property predictions



Materials discovery: AI-driven high-throughput screening

Objective: find cathode materials for Ca-batteries (beyond Li-ion)



Geometric and chemical criteria: human inputs

- Removes 'unphysical' and 'non-realistic' candidates

AI inputs: improves speed

- Typically done with high-throughput density functional theory (DFT)
- Foundational machine learned interatomic potentials (MLIPs) used

Manual curation to remove duplicate structures

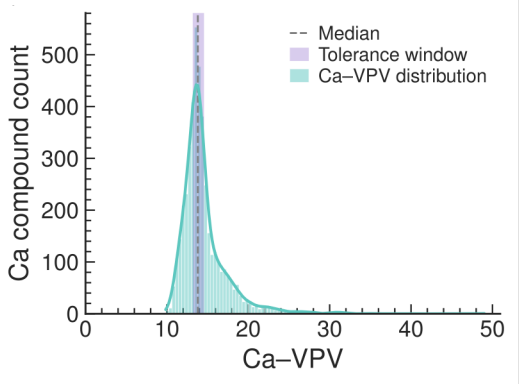
- Slow, but can be automated

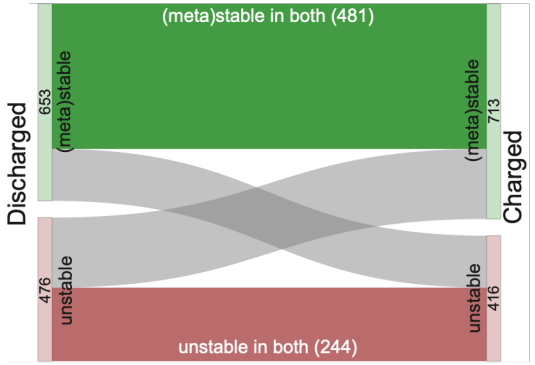
AI-filtered candidates, DFT validation

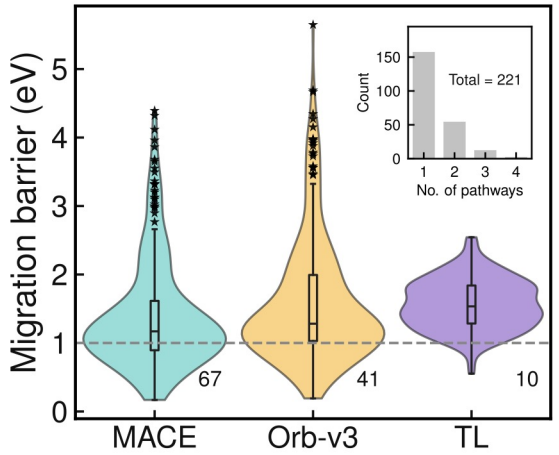
- Validation is computationally heavy

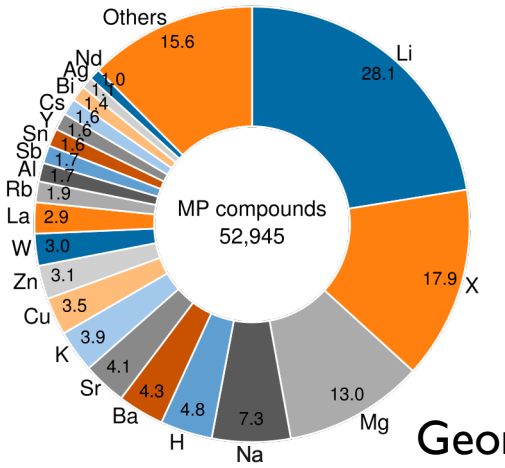
Materials discovery: AI-driven high-throughput screening

AI-driven workflow generates 37 promising candidates!

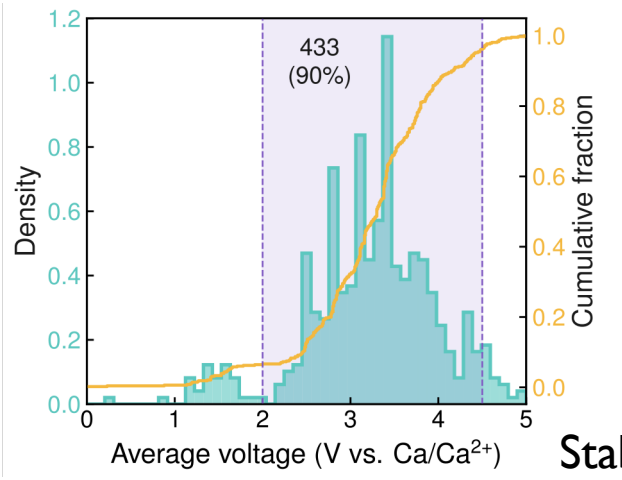




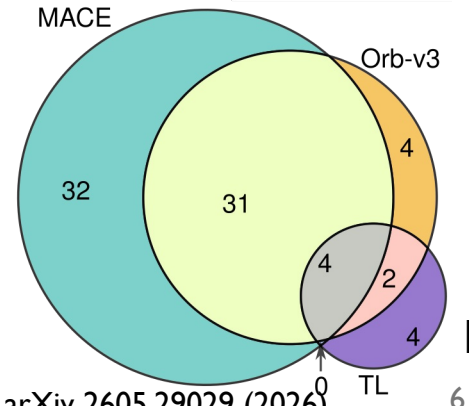




Geometry



Stability+Voltage



Mobility

Tekliye et al., arXiv 2605.29029 (2026)

Materials discovery: AI-driven high-throughput screening

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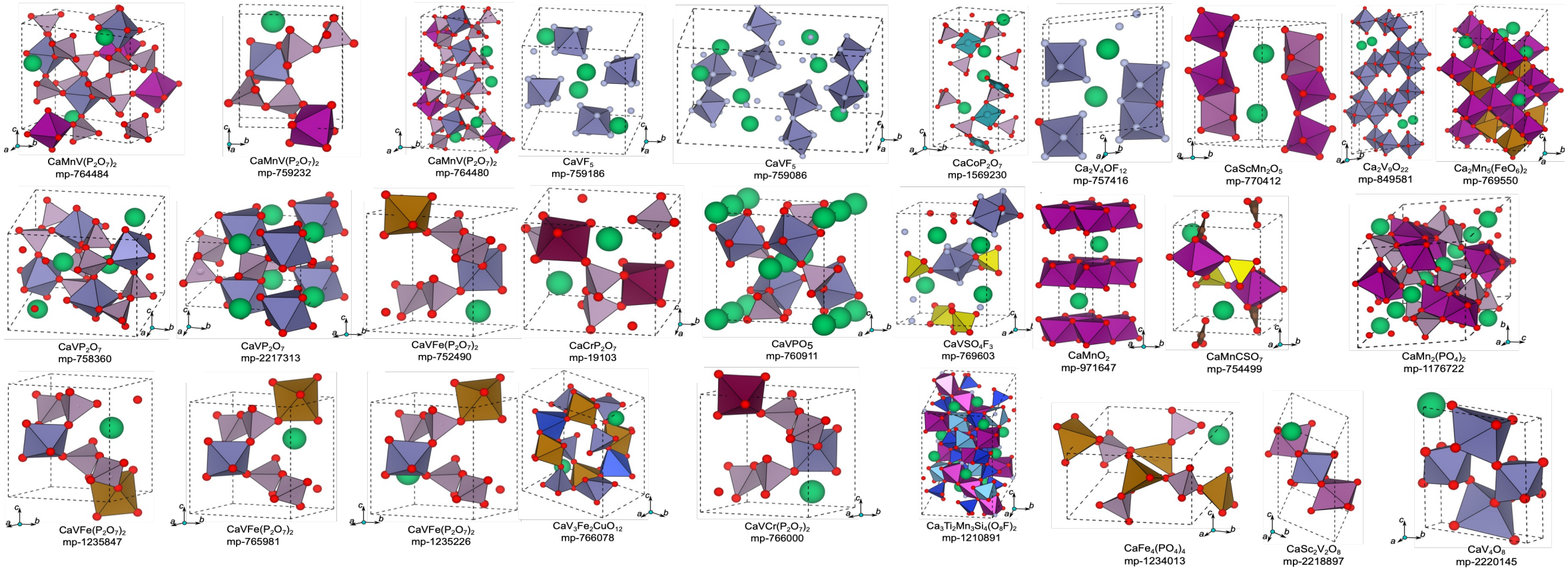
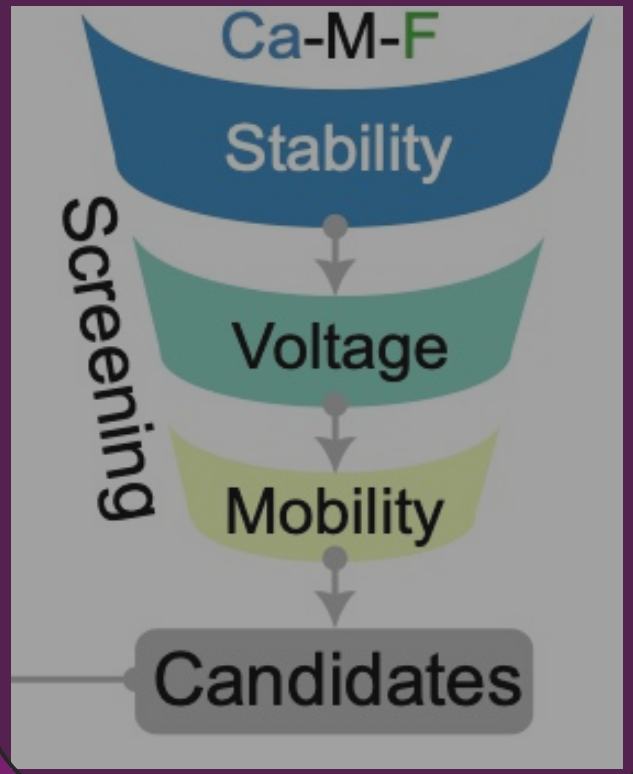
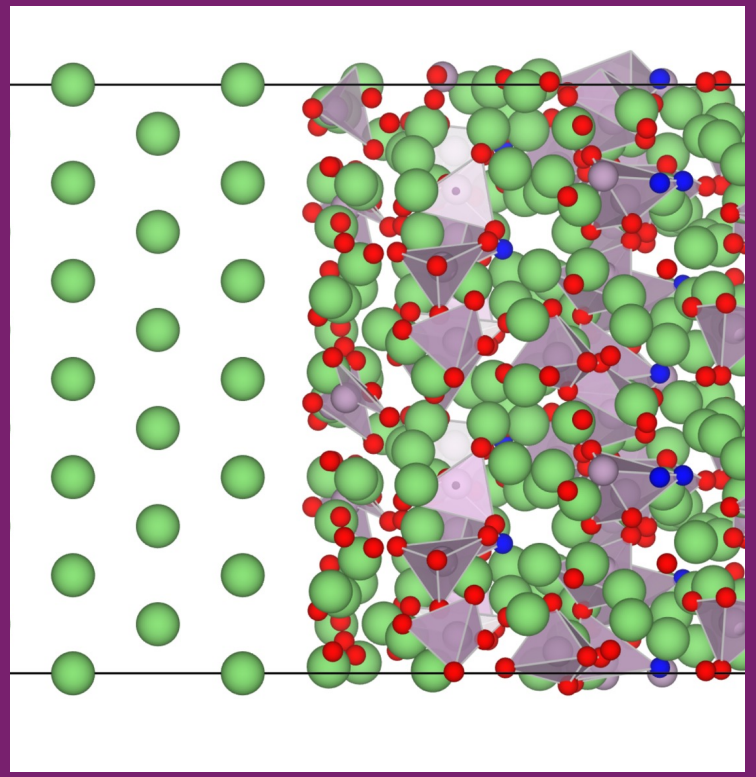


Examples in materials discovery and design

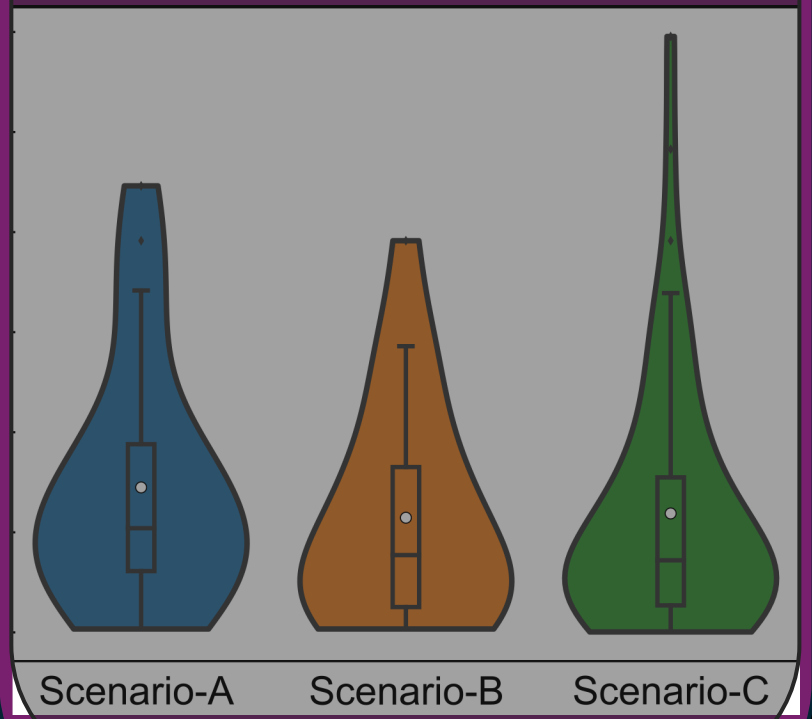
High-throughput screening



Modelling complex systems

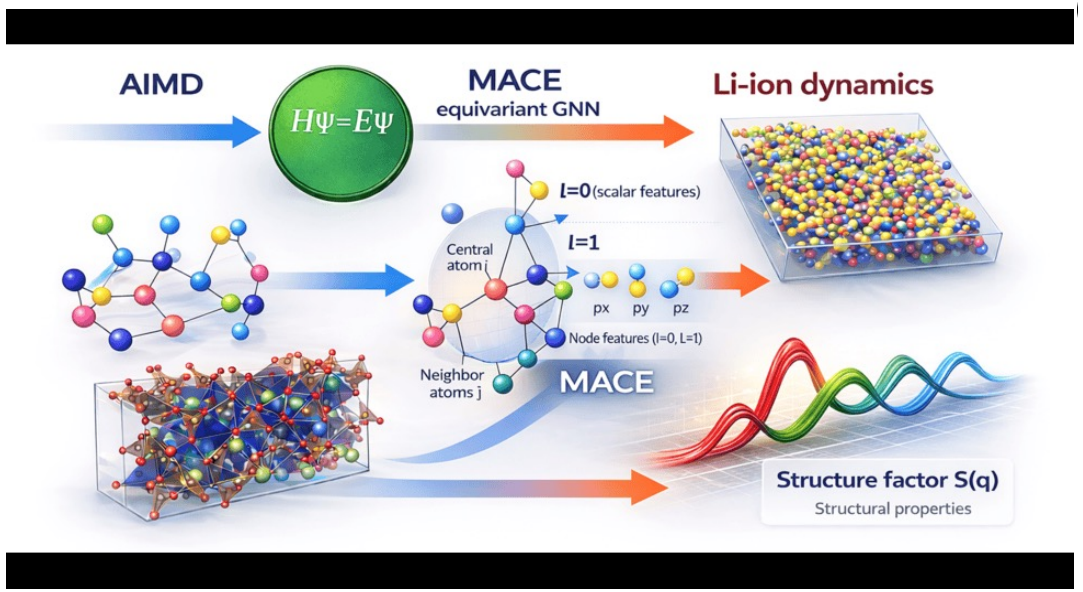


Swift property predictions



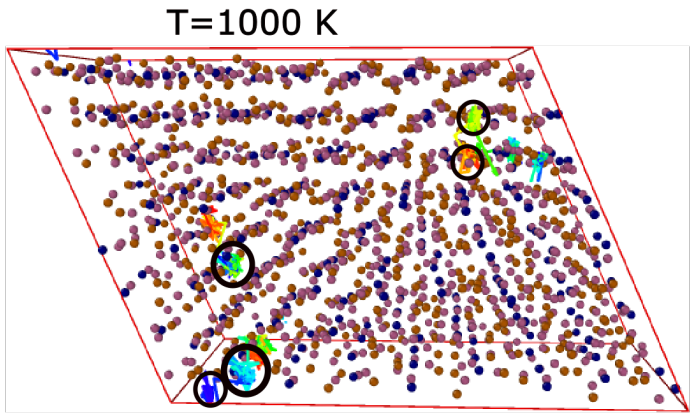
Materials design: AI for modelling complex systems

Molten Li_2CO_3: important ingredient for molten salt fuel cells and carbon capture → structural and ionic transport not known fully

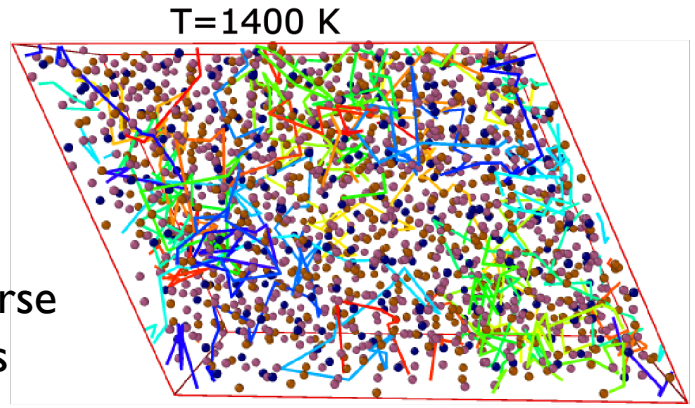


Classical DFT: can't model large scale/long time

- Use trained (specific) MLIPs
- MLIP choice: MACE/NequIP



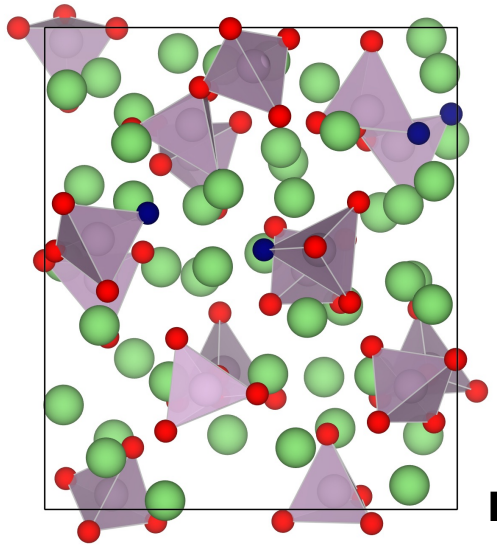
Anisotropic, correlated, transient trapping events



Unveil complex transport processes!

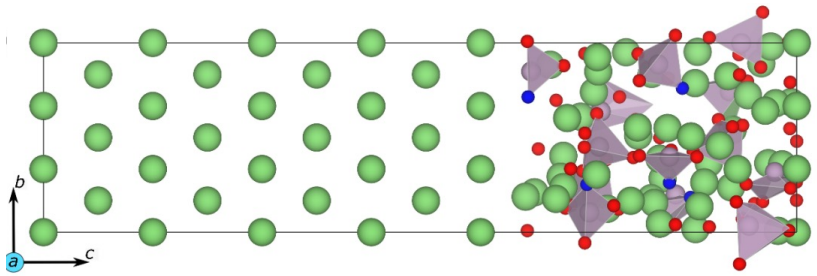
Isotropic, less-correlated, sparse trapping events

Materials design: Modelling amorphous electrolytes and electrodes



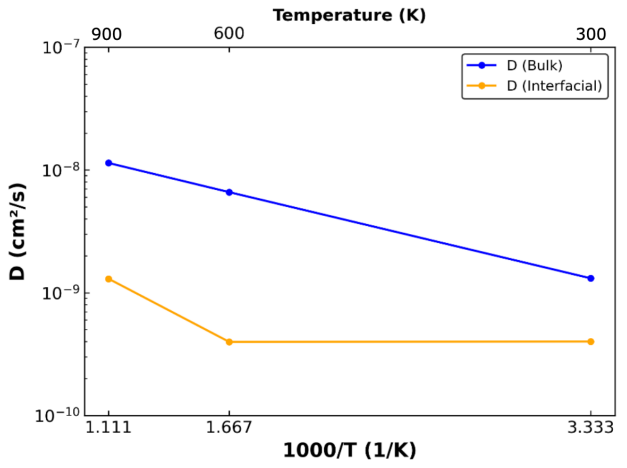
Amorphous solid electrolytes
- Reasonable Li-conductivity, hinder dendrite growth
- Case of LiPON

Modelling amorphous structures
- Non-trivial with classical *ab initio*
- Employ machine learned interatomic potentials (MLIPs)

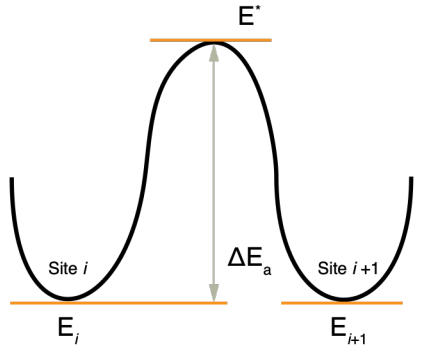


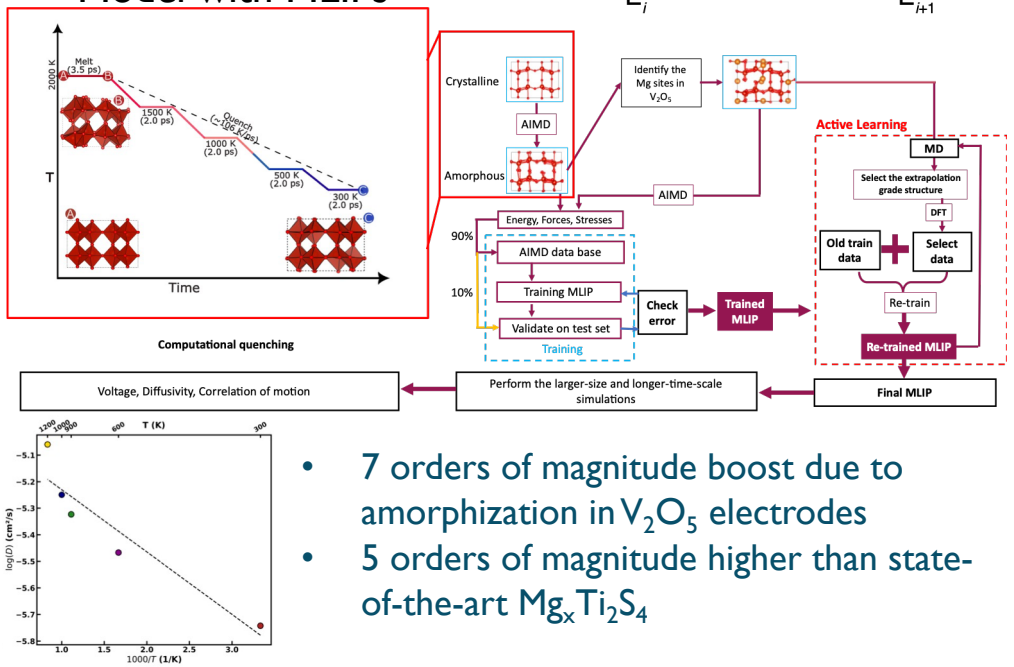
Similar diffusivities in bulk and across the interface: possible kinetic limitation for dendrite growth

A. Seth, R.P. Kulkarni, and G.Sai Gautam, **ACS Mater. Au 2025,** 5, 458-468



Amorphous materials can flatten potential energy landscapes and improve ionic mobility in multivalent (Mg) systems
- Can be electrode materials
- Model with MLIPs





- 7 orders of magnitude boost due to amorphization in V_2O_5 electrodes
- 5 orders of magnitude higher than state-of-the-art $Mg_xTi_2S_4$

V. Choyal, D. Dey, and G.Sai Gautam, **Small 2025,** 21, e05851

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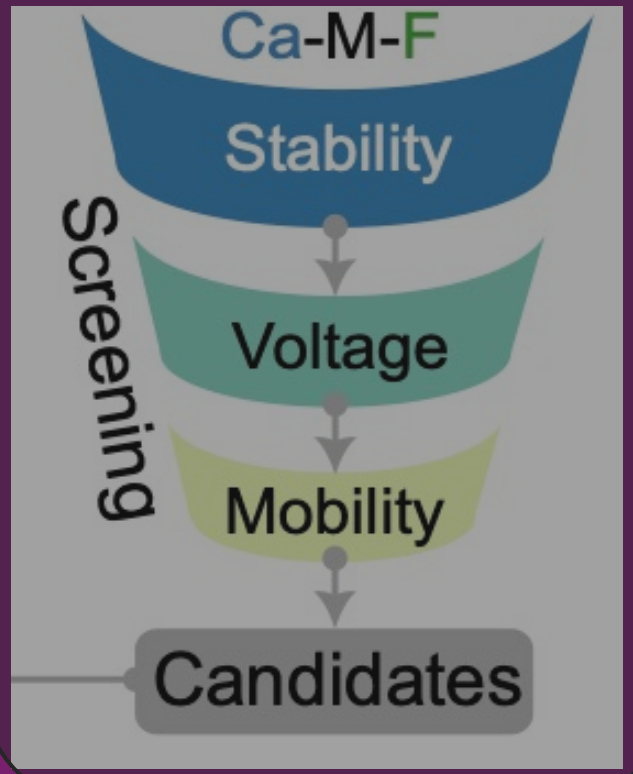
High-throughput screening



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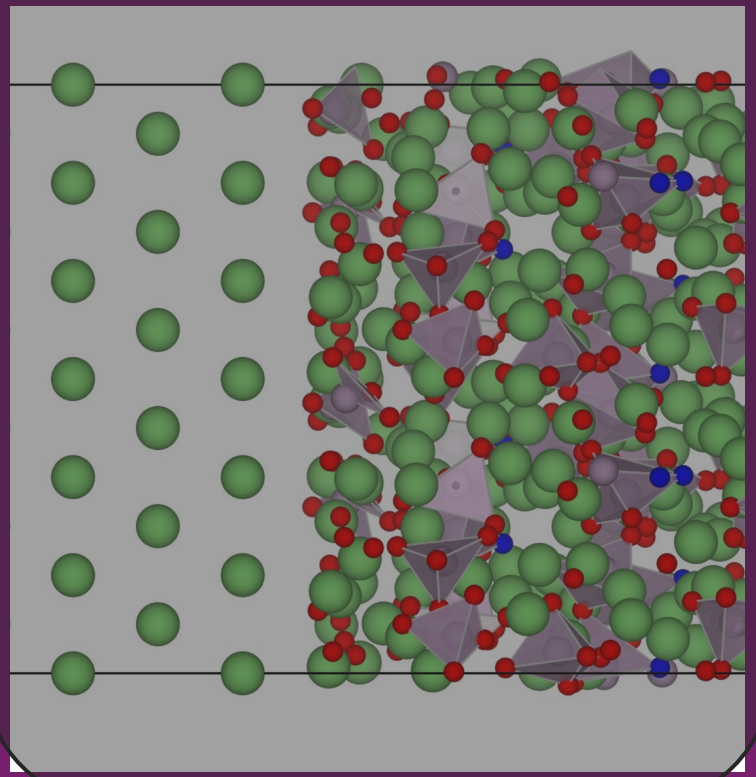
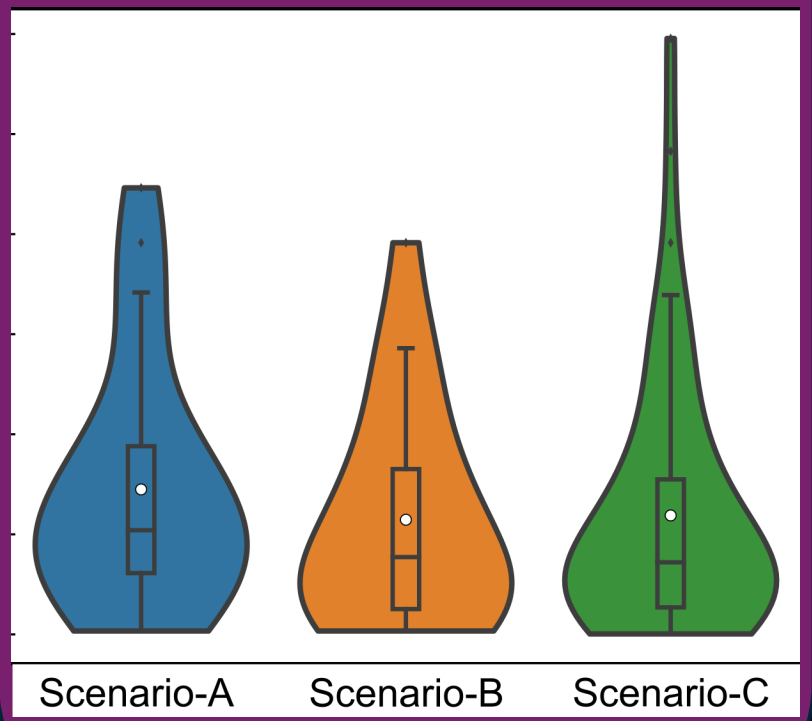
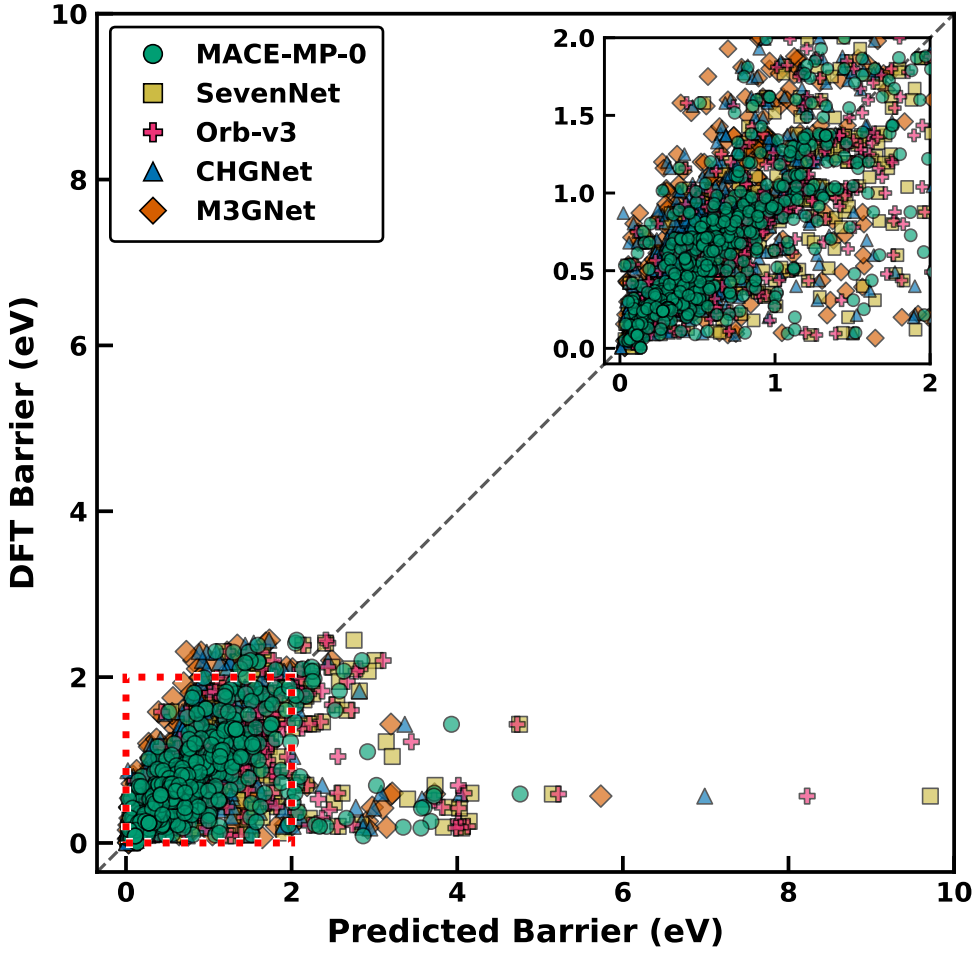


Swift property predictions



Property predictions: generalized AI has shortcomings



MACE-MP-0

MACE-MP-0 is best with an MAE of 0.310 eV

- M3GNet: highest MAE of 0.349 eV

SevenNet

Removal of 35 outliers (>1 eV error), out of 574 datapoi
reduces MAE of MACE-MP-0 to 0.202 eV

Orb-v3

- Orb-v3 best with 37 outliers removed, MAE of 0.198
- uMLIPs also exhibit convergence difficulties in NEBs

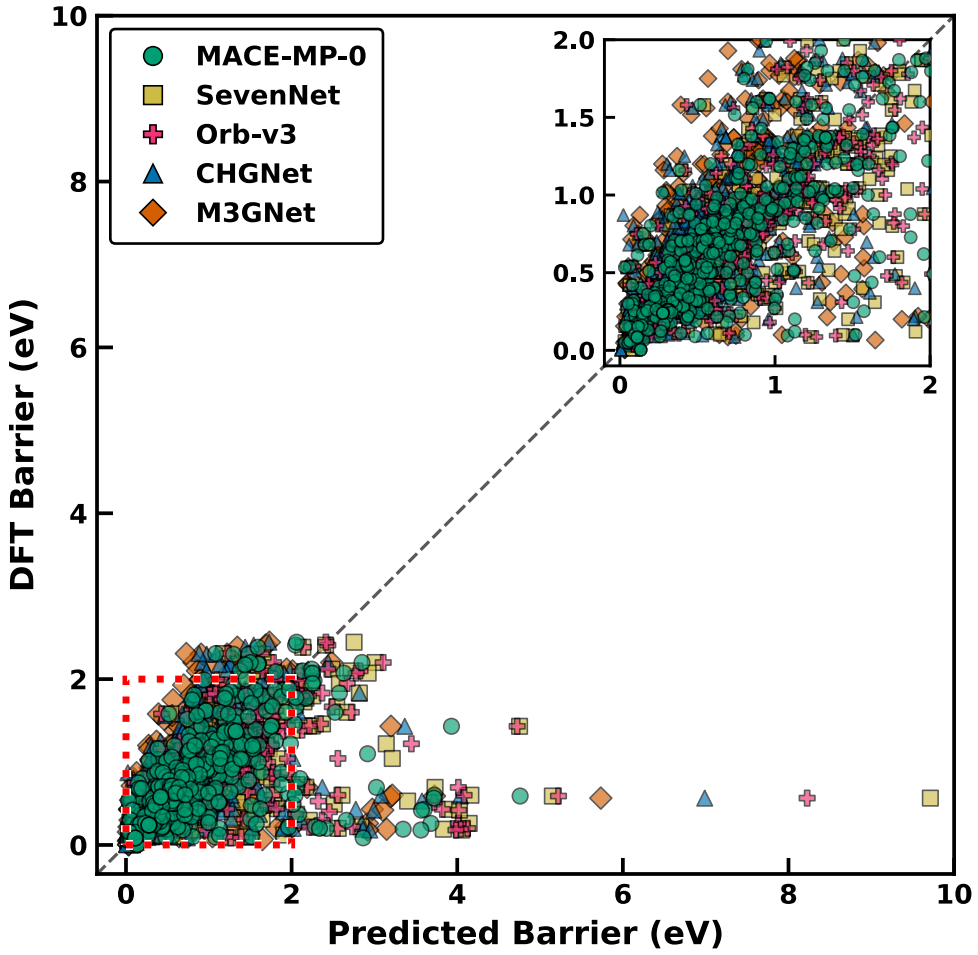
CHGNet

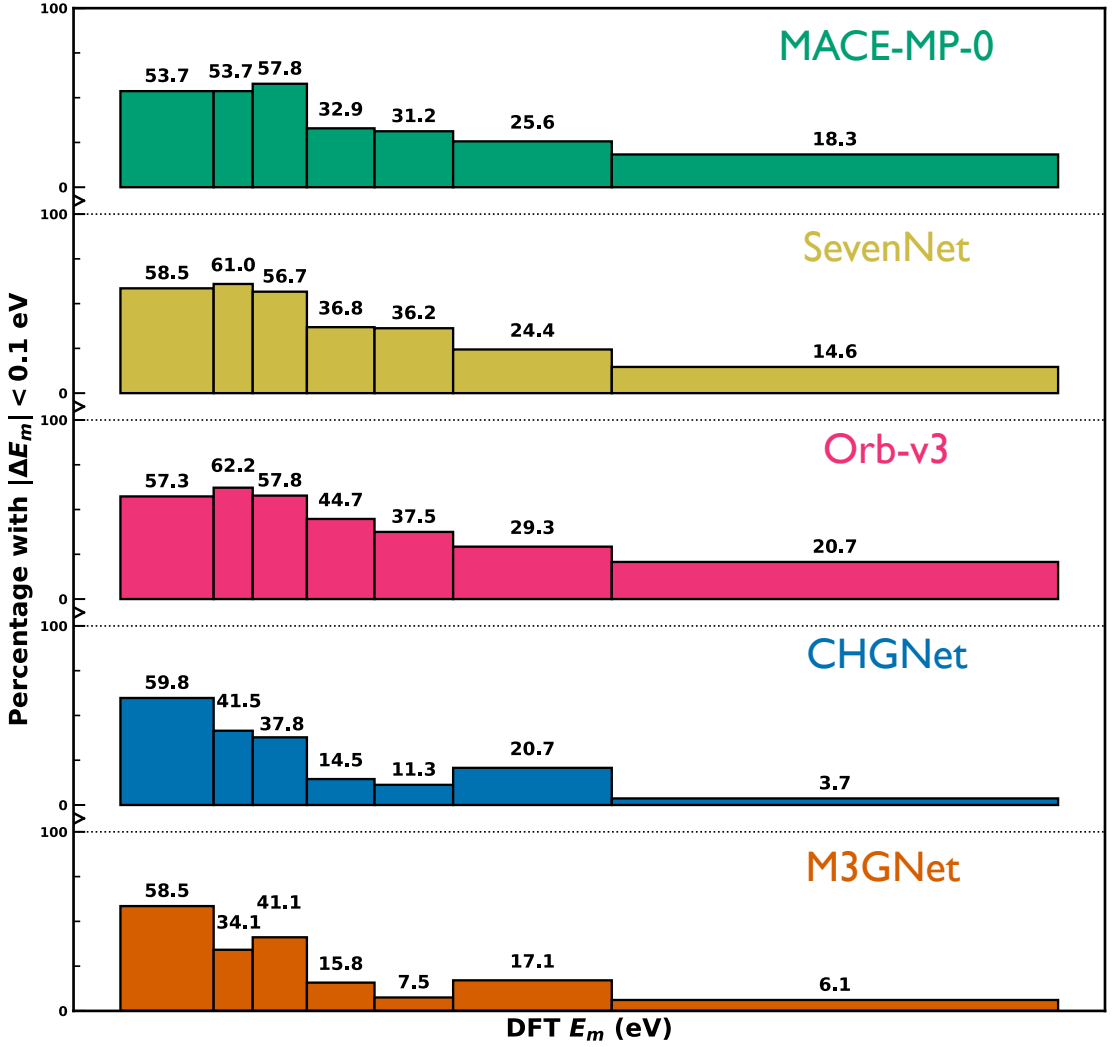
M3GNet and CHGNet have systematically under-estimat

M3GNet

*Out of 621 datapoints, 37 removed due to convergence difficul

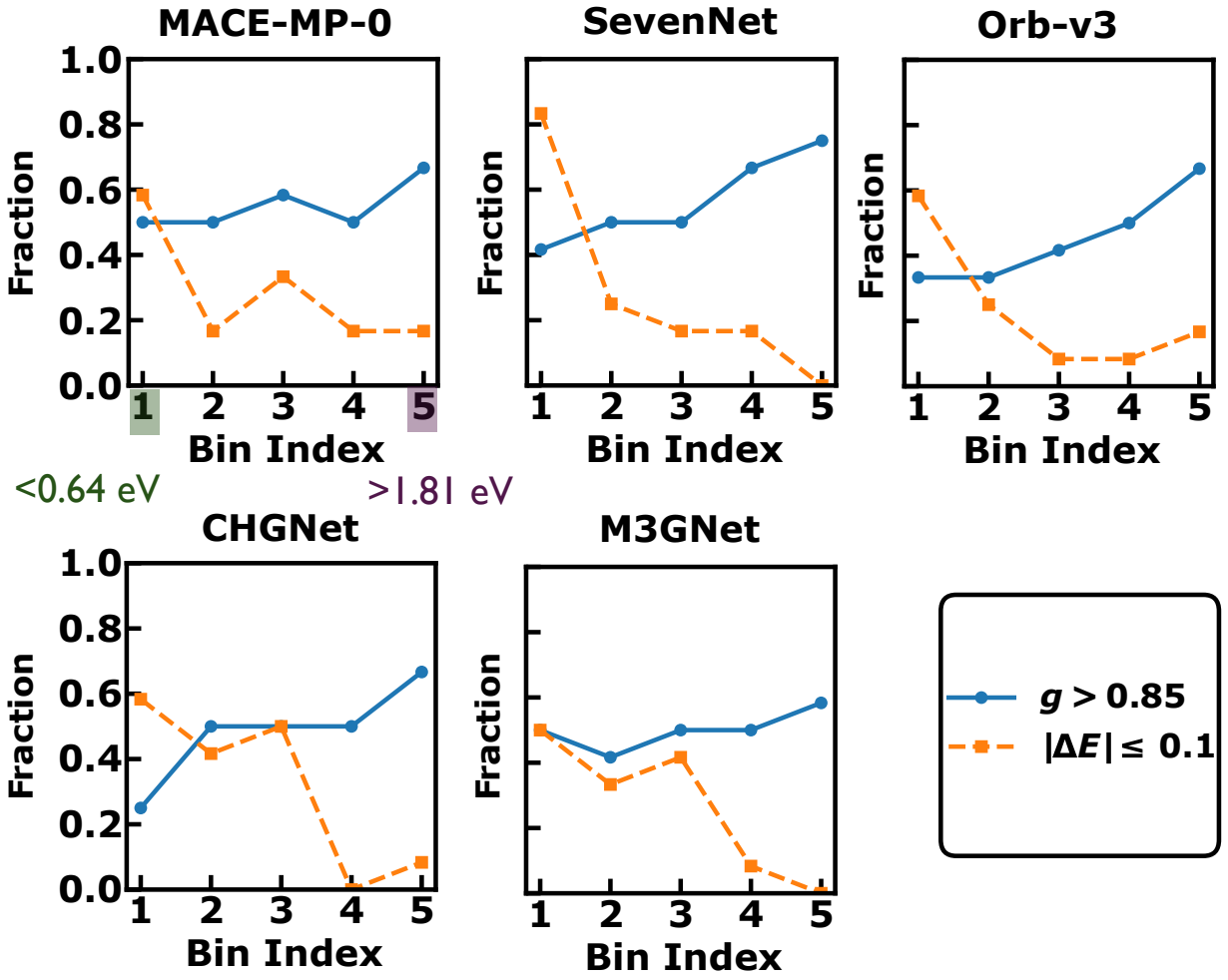
Property predictions: generalized AI has shortcomings





Bheemaguli et al., **Digital Discovery 2026,** 5, 1809-1819

Property predictions: right answer (E_m) for wrong reasons (geometry)



Geometry predictions become better as E_m increases

- So does error on E_m!

Better predictions of low E_m values don't correlate with better geometry predictions

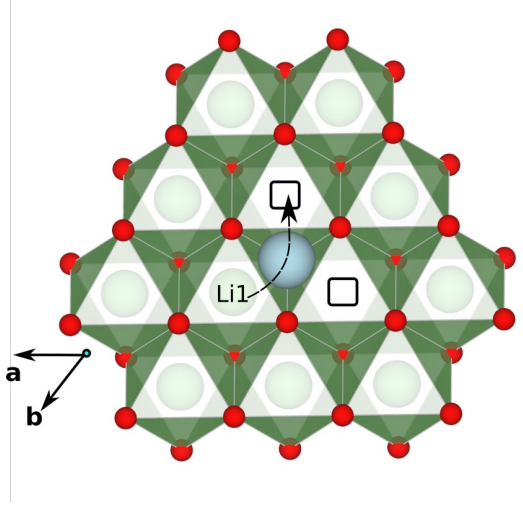
- 'Flatter' energy surfaces: possibly lower geometry influence

MACE-MP-0 and Orb-v3 provide most robust geometry predictions

- Can increase speed of DFT-NEB by up to 60% reduction in electronic steps
- But highly varying

Bheemaguli et al., **Digital Discovery 2026,** 5, 1809-1819

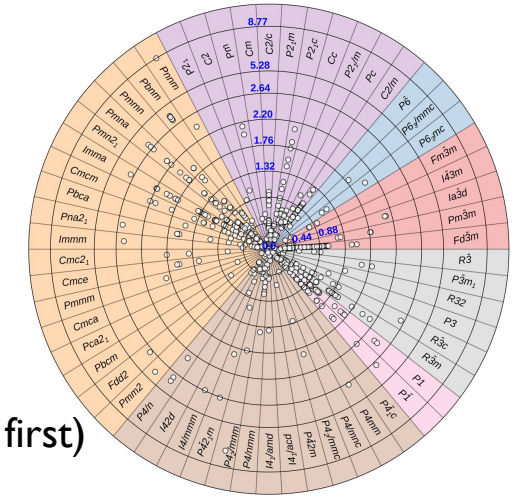
Property predictions: AI for predicting ionic transport in solids



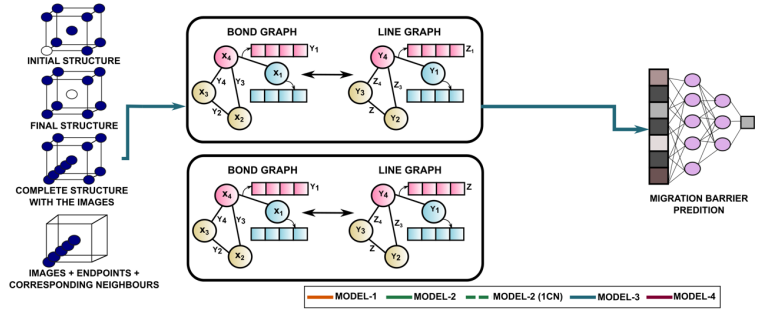
Migration barriers (E_m) → determine rate performance in electrochemical devices

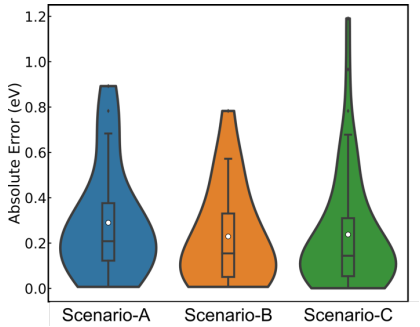
Exponential control on diffusivity

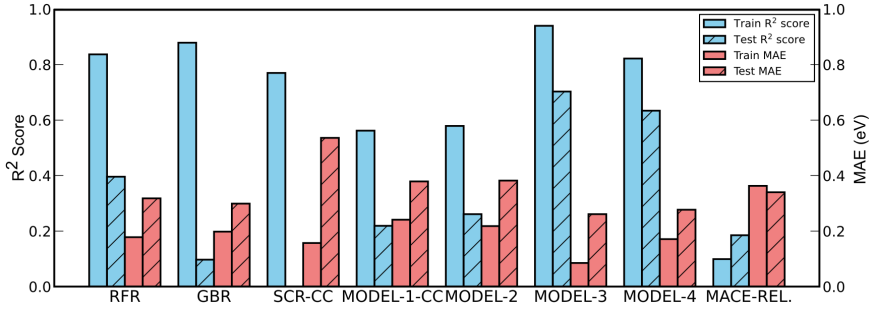
Difficult to computationally predict or experimentally measure → Can AI help?



Compile a dataset on calculated barriers (need data first)







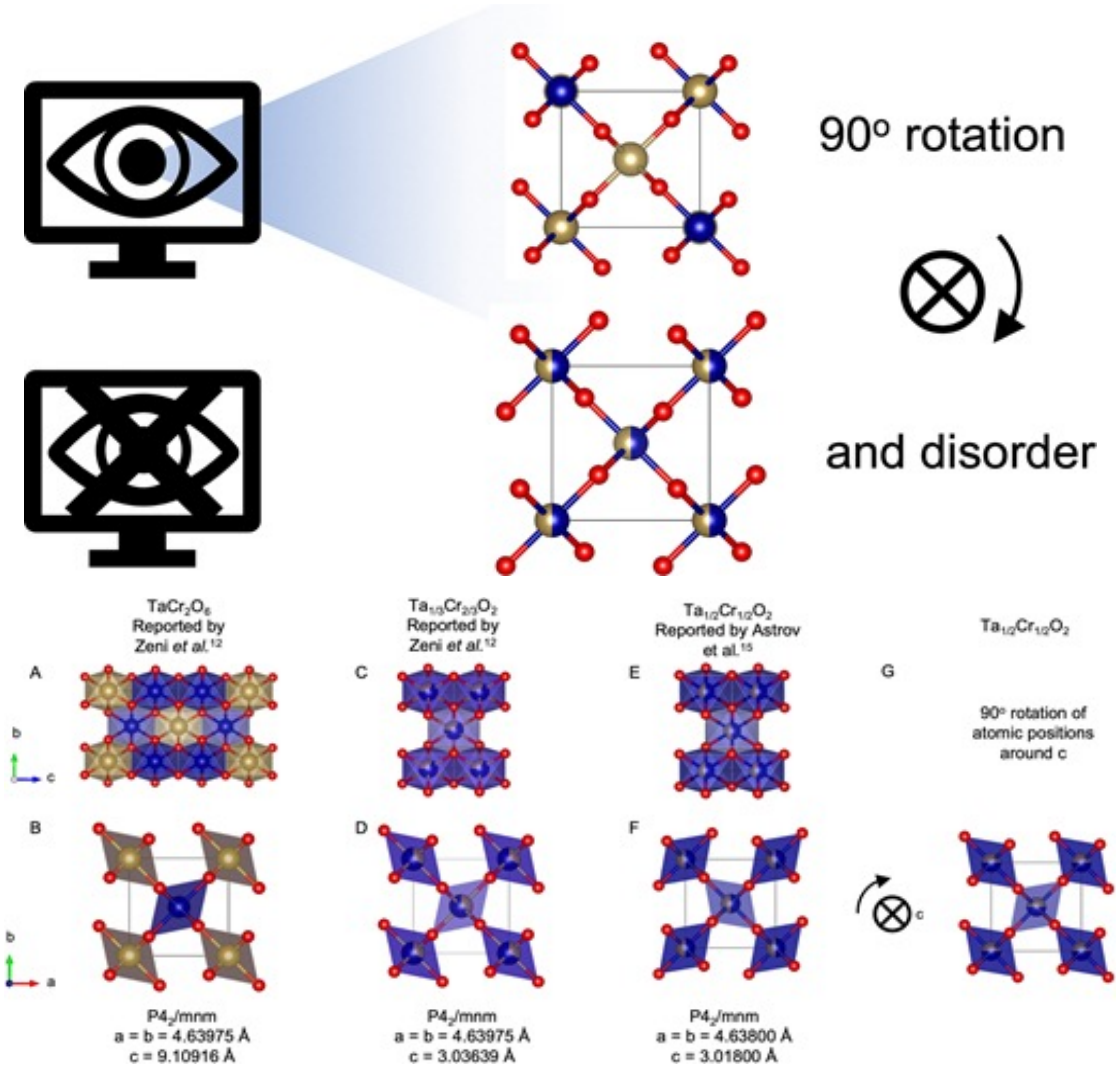
Build a model (graph based architecture)

MODEL-3 (transfer learned) is the best!

Excellent generalization and classification abilities for MODEL-3

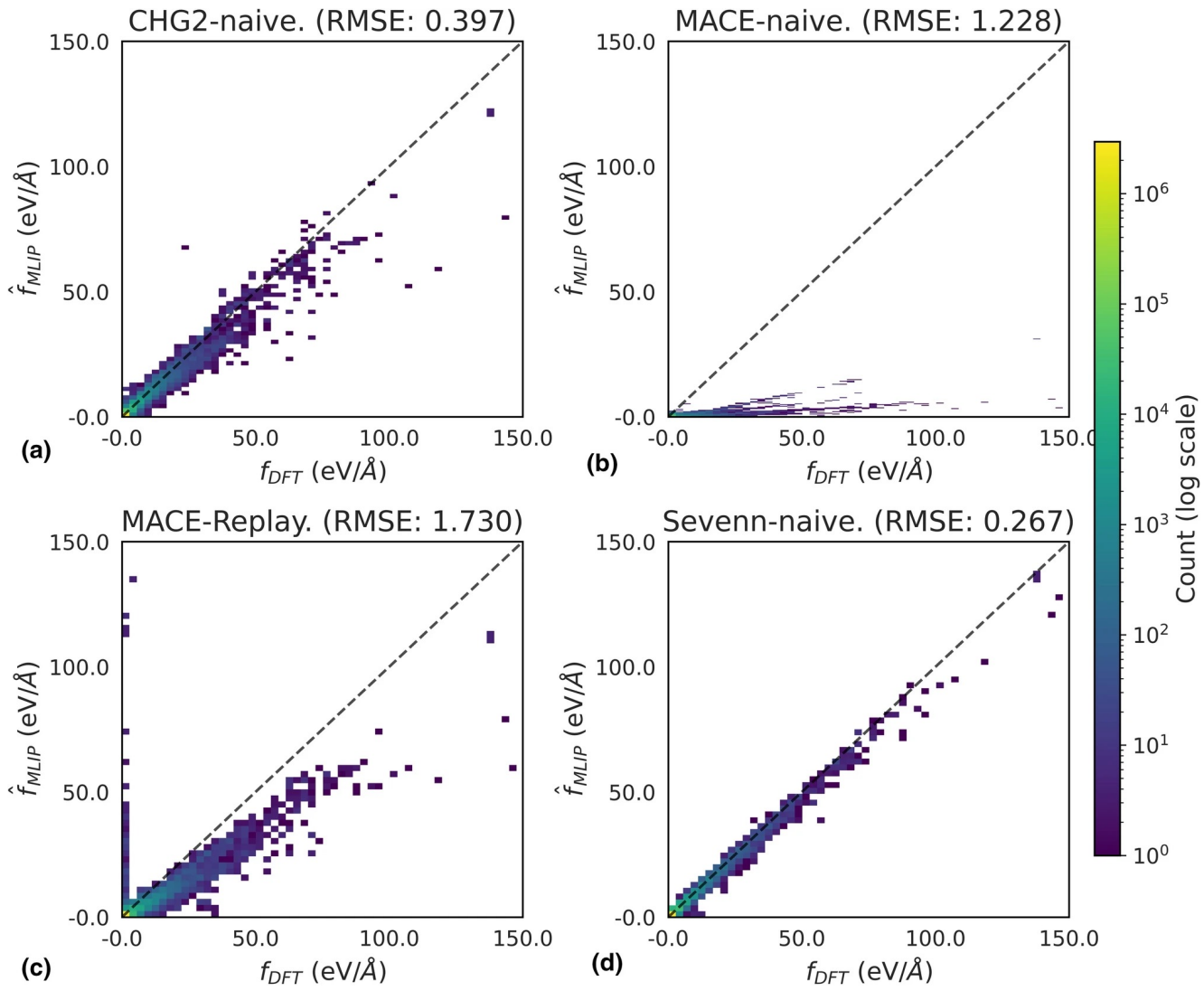
Work to be done

- Generative models



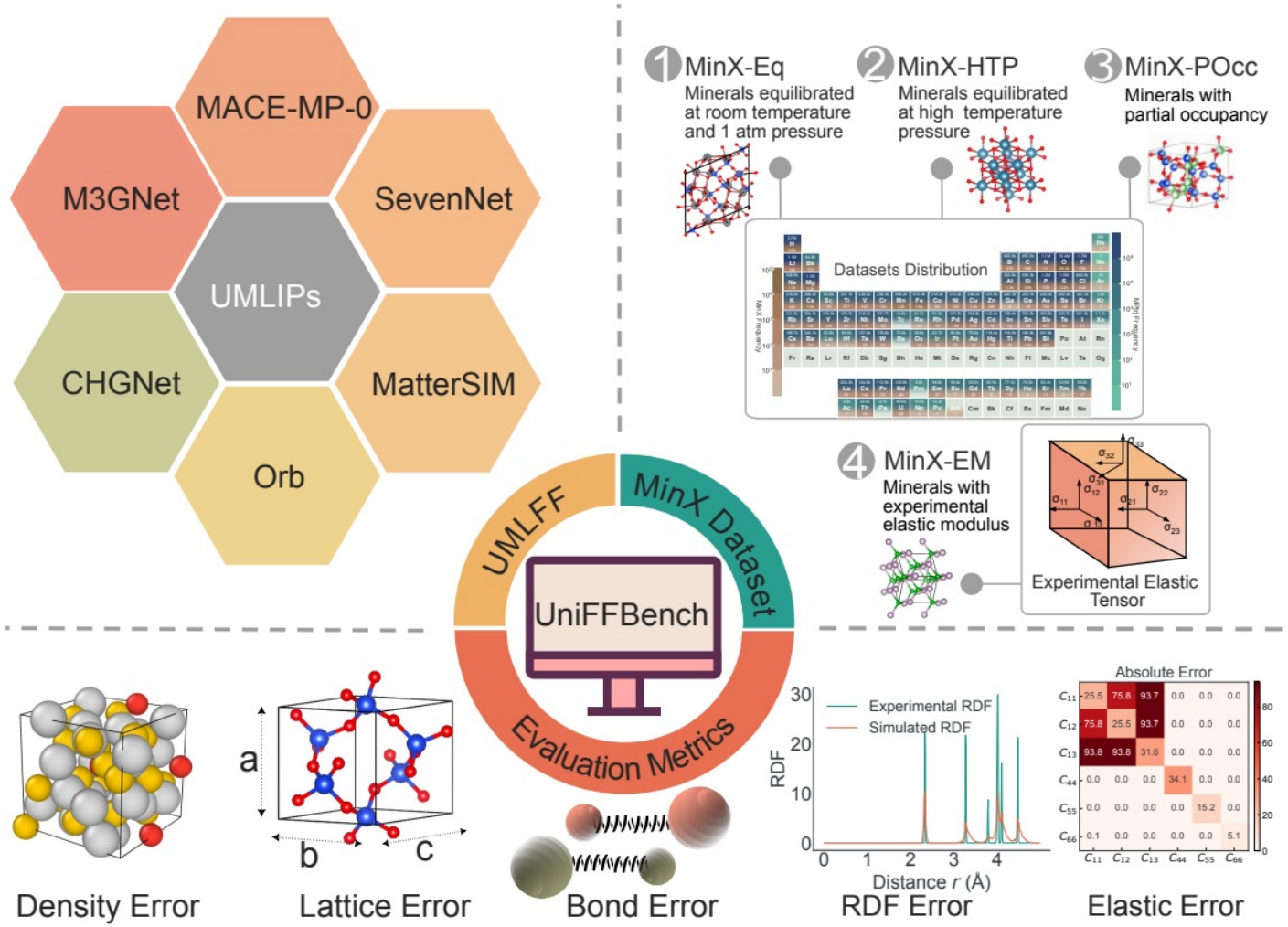
Work to be done

- Generative models
- Fine-tuning potentials



Work to be done

- Generative models
- Fine-tuning potentials
- Property predictors



Outlook: what's next and what's needed?

- Computational tasks are getting easier, faster, and more accurate
  - Large chunk of DFT calculations, coding tasks can now be accelerated
  - Beyond-DFT: also on the verge of improving throughput
  - Indian context: steer away from transformers?

- Agentic workflows for simulations: boon or bane?
  - AI agents (mostly language models) interacting with specific models and deciding on next 'experiments' (or simulations) to do
  - Workflow automation is easier to implement than agentic workflows?
  - Validation is going to remain a bottleneck always: suite of specific models?
  - General purpose or specific agents?
  - Identify blind spots for human experts? Or, Reduces human creativity in the long run?

- What do experimentalists like theorists to build?

- More funding for model building than specific domains/products?
  - My opinion: most funding calls (scope vs. money given), review processes (random meetings), and outcomes are disappointing (forget transparency, etc.)