



AI meets battery materials design: status and outlook

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Himalayan Electrochemical Innovation Summit, Chail, India

2 Jun 2026

Acknowledgments



Keith Butler
(UCL)



Reshma



Achintha

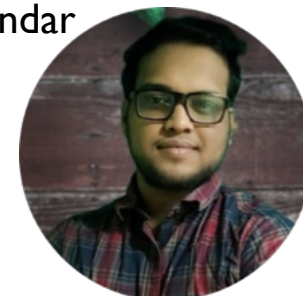


Dereje



Avaneesh

Debsundar



Dec 2025



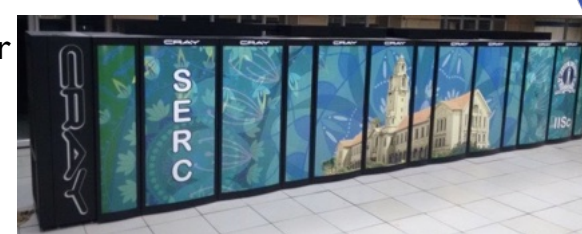
AI meets battery materials design

Param
Utkarsh
(CDAC)



HELIOS 2026 | Sai Gautam Gopalakrishnan

Archer
(UK)

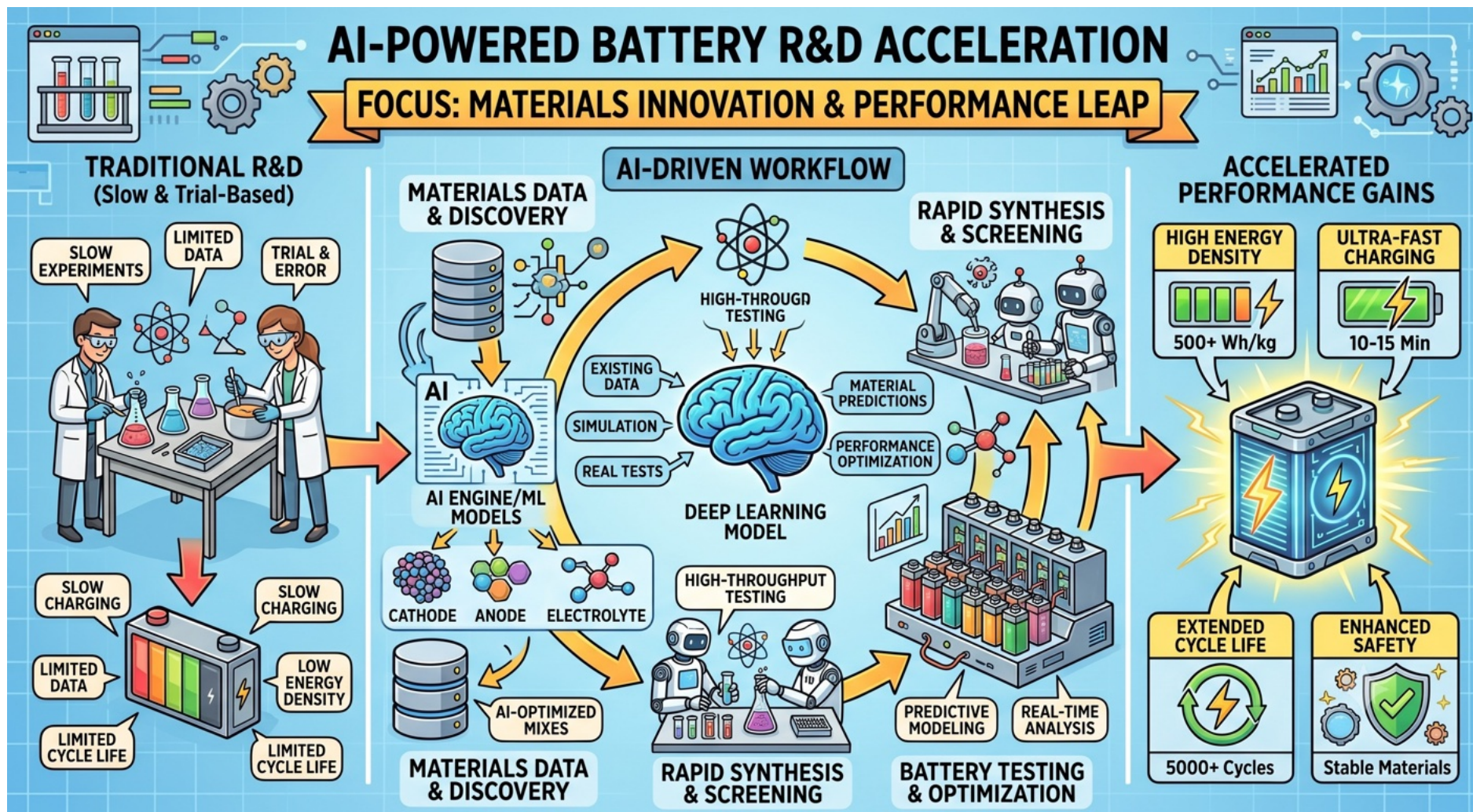


SERC (IISc)





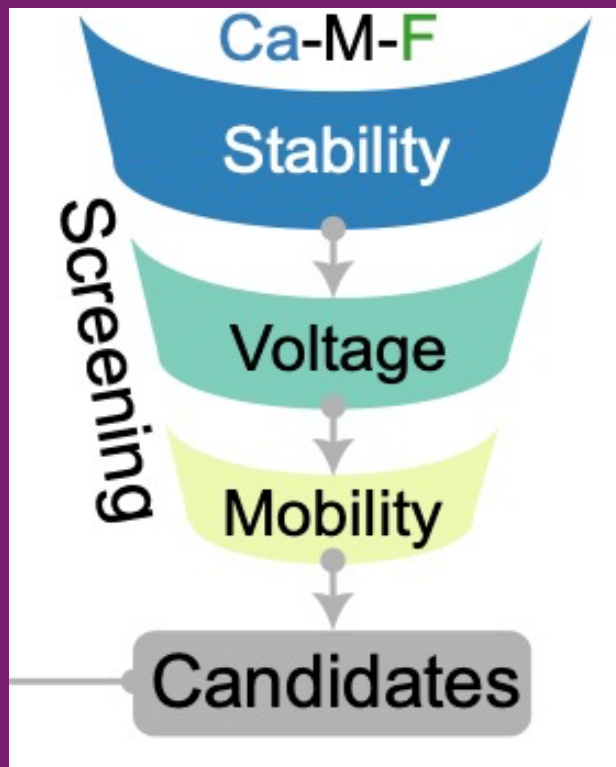
AI can accelerate battery materials design



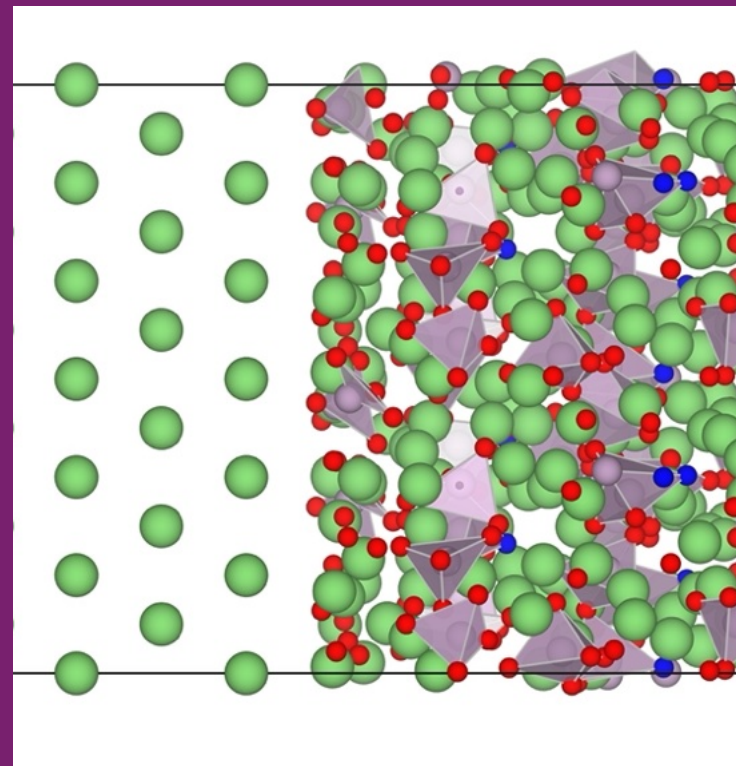
But how?

+ Autonomous experiments?
+ Agents?

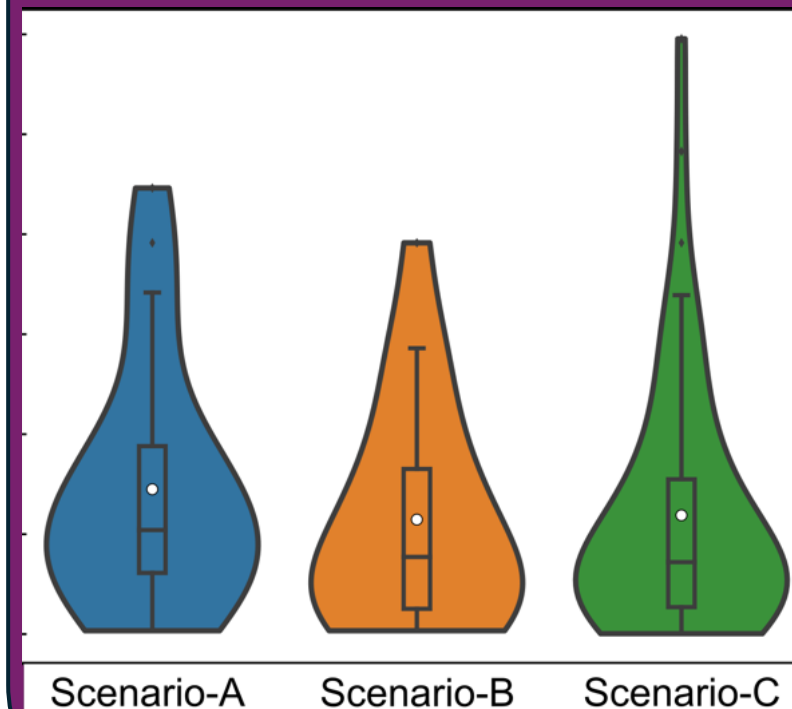
High-throughput screening



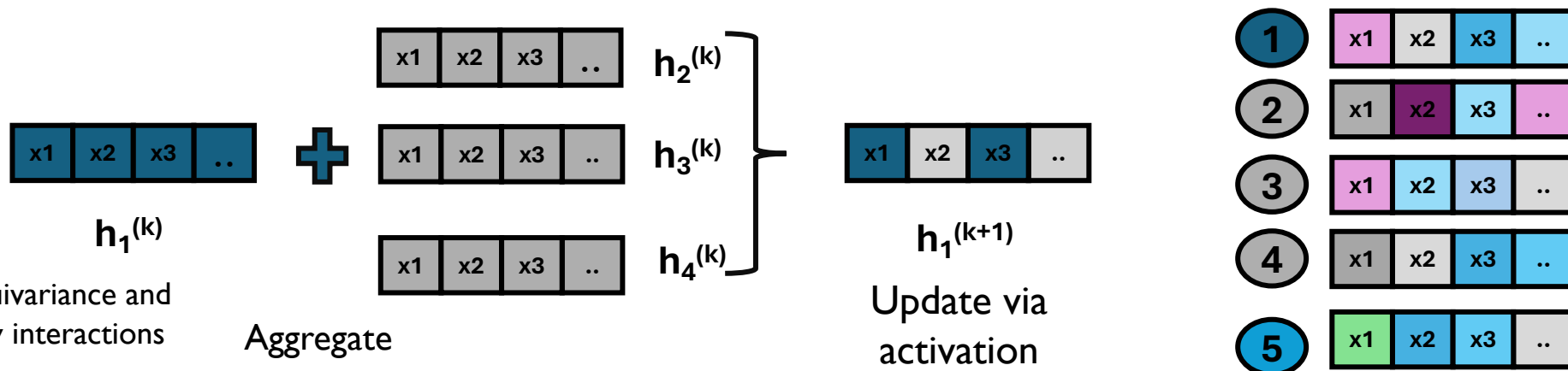
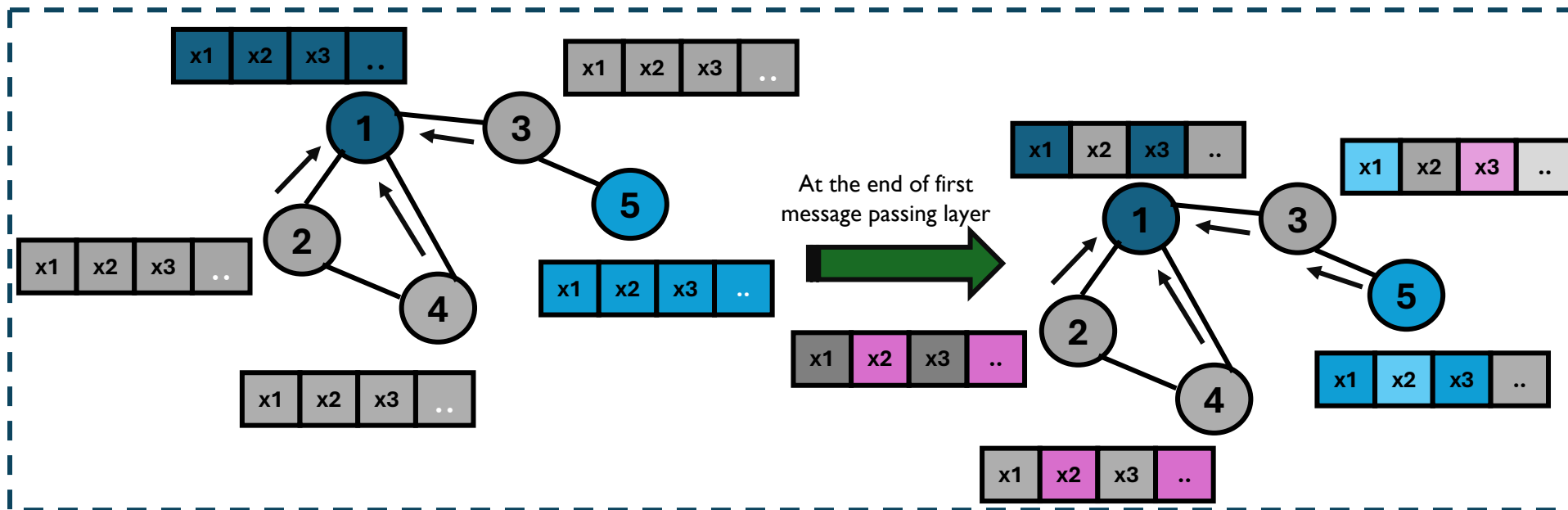
Modelling complex systems



Swift property predictions



Base model architecture: graph neural networks



Add in equivariance and many-body interactions

Aggregate

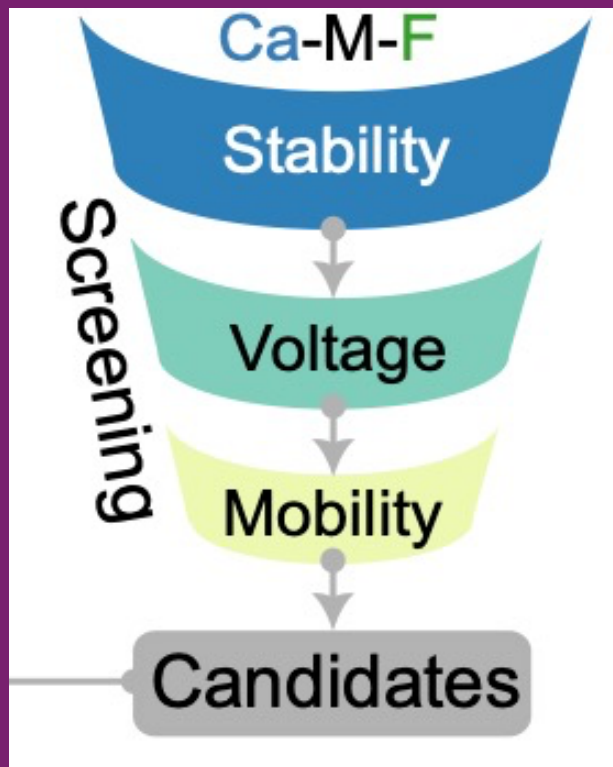
Update via activation

After multiple message passing layers

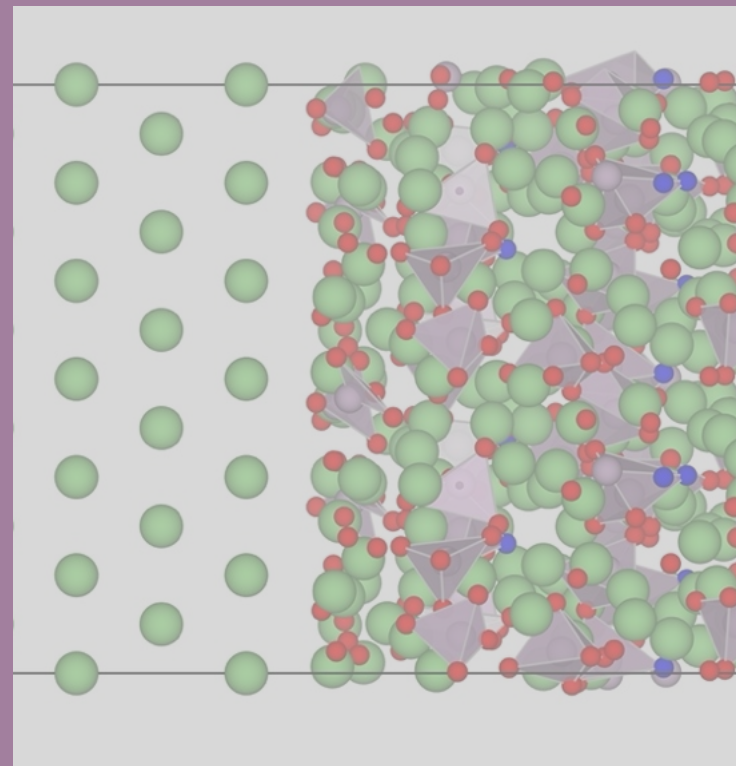
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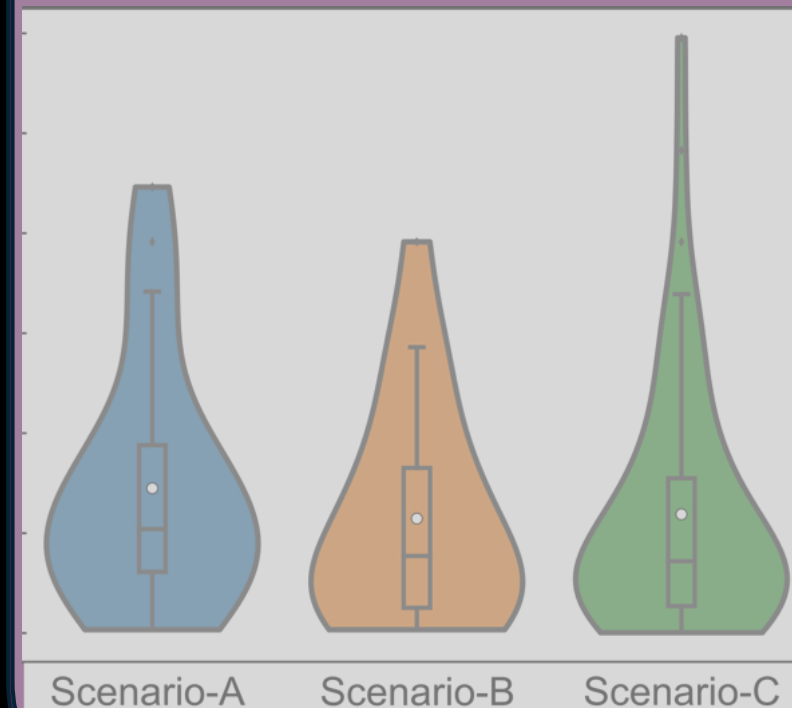
High-throughput screening



Modelling complex systems

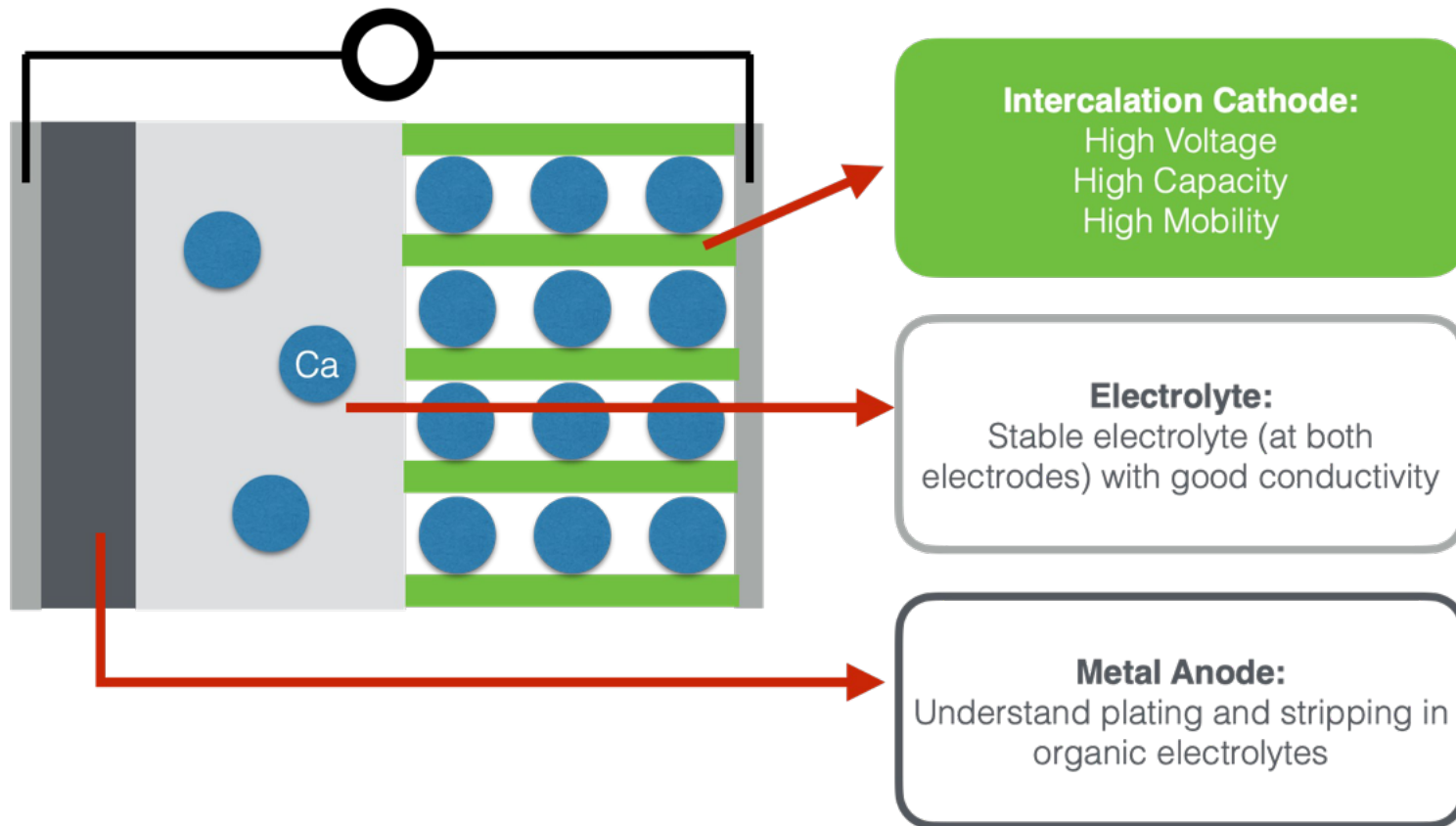


Swift property predictions

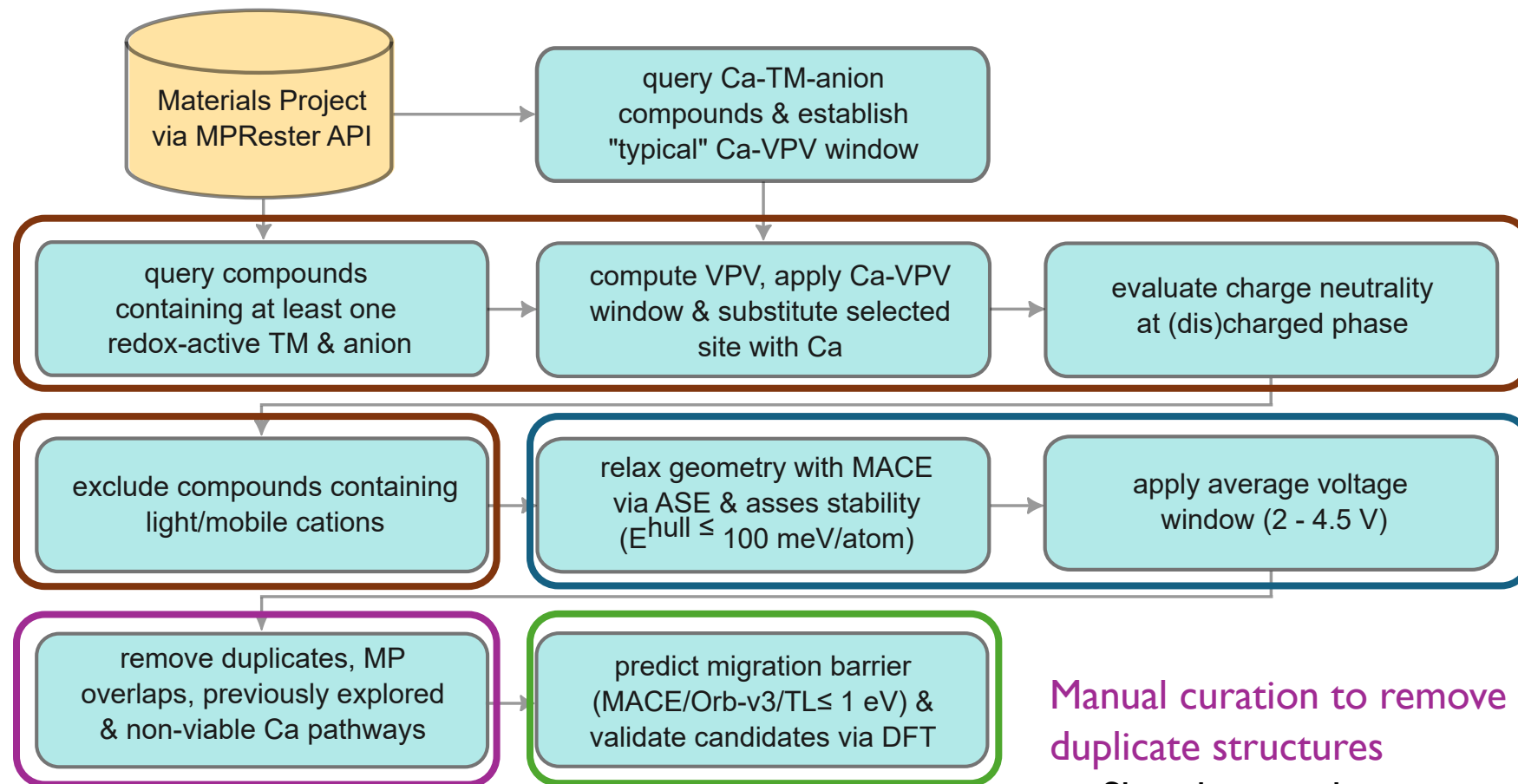


Ca batteries need cathodes: ideal for screening

- Higher volumetric capacity (~ 2077 Ah/l) for Ca vs. Li in graphite (~ 800 Ah/l)
- Less constrained geopolitically; similar standard redox potential to Li
- Need thermodynamically (meta)stable cathodes with high **voltage** and high *mobility*



Workflow: (human) innovation + (AI) speed



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

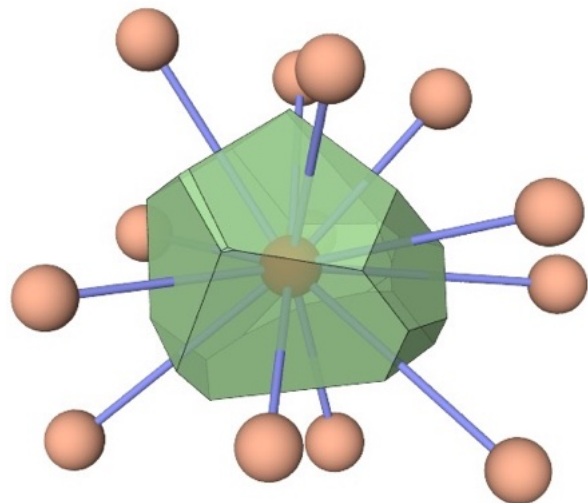
- Slow, but can be automated

AI-filtered candidates, DFT validation

- Validation is computationally heavy

Objective: find cathodes that don't contain Ca *a priori*

- Structures that contain Ca: examined as potential cathodes already
- Need structure to have suitable cation sites or interstitial/void sites to host Ca
 - Check geometric compatibility via Voronoi polyhedral volume (VPV)



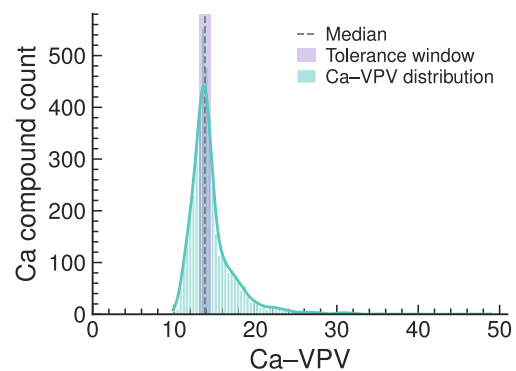
Polyhedral volume that is 'similar' across different coordination environments

- Possibly more robust than using ionic or atomic radius

Define an 'ideal' VPV for Ca

- Based on known/explored (at least ternary) structures in MP that contain Ca

Apply VPV on 52,945 structures: 5,946 filtered

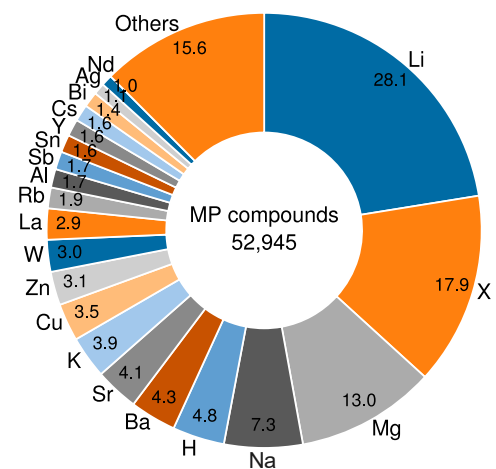
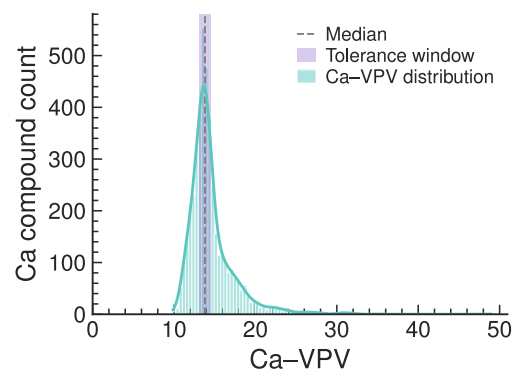


Median: 13.86 Å³

Window: 13.17-14.56 Å³

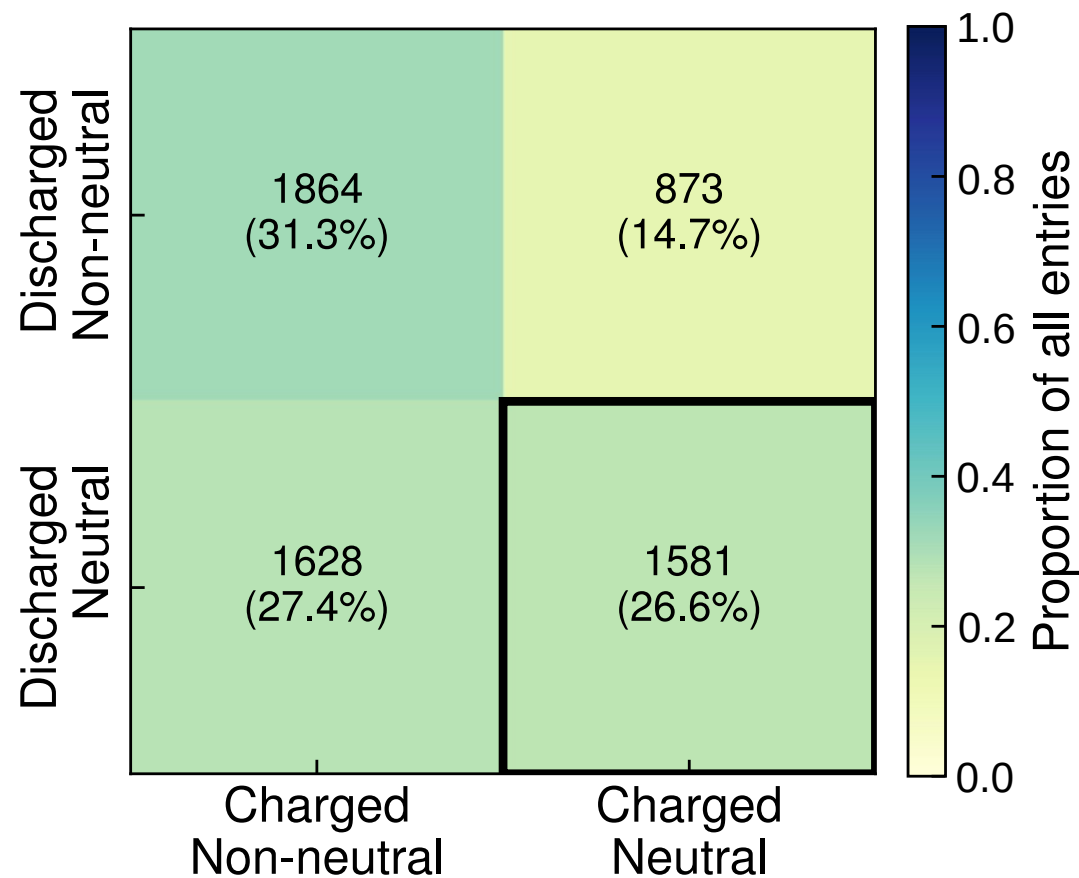
Median VPV: obtained from 4,350 Ca-containing structures in MP

Apply VPV on 52,945 structures: 5,946 filtered



52,945: at least one redox-active transition metal and at least one anion

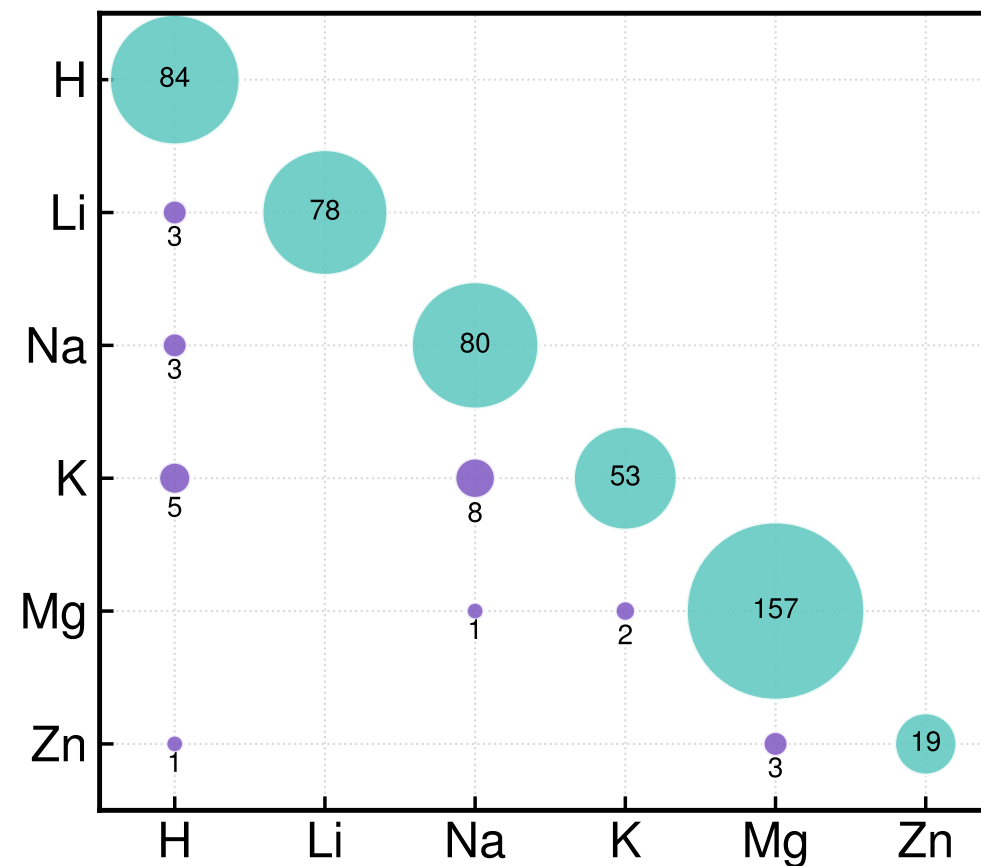
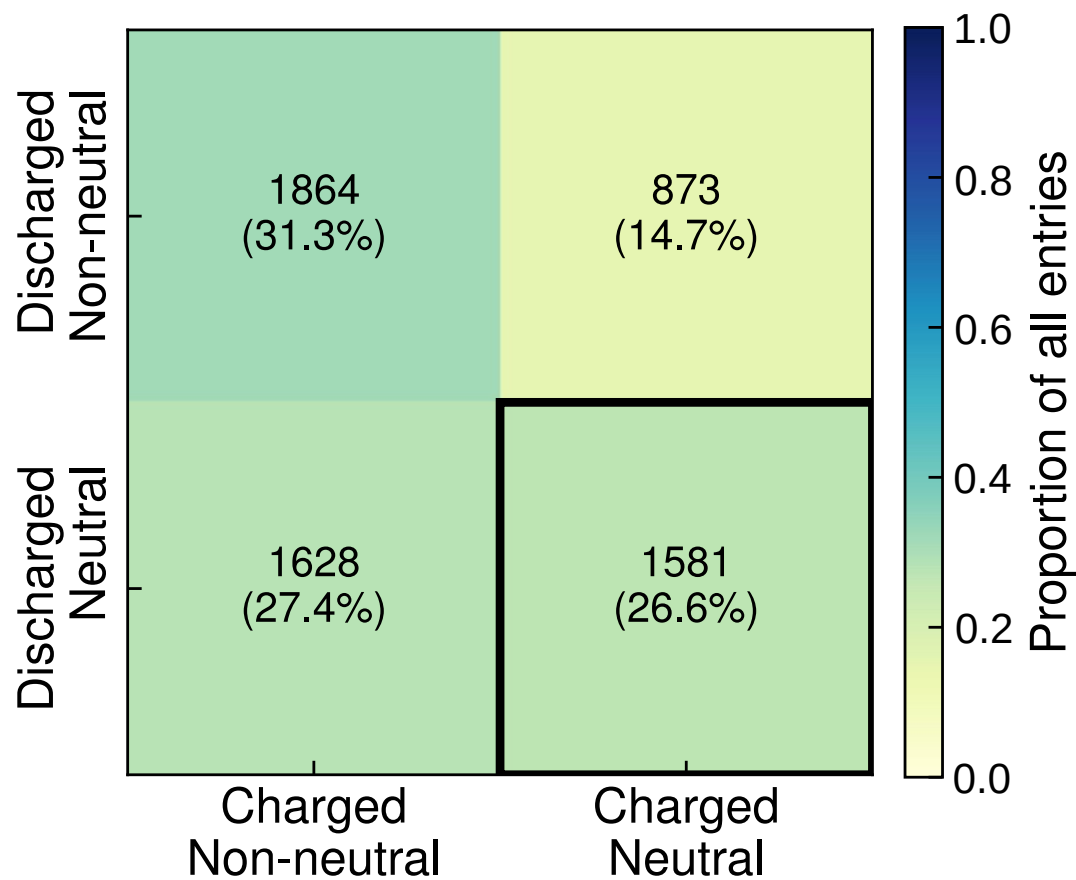
Charge neutrality and non-Ca mobile cation filters: 1,136



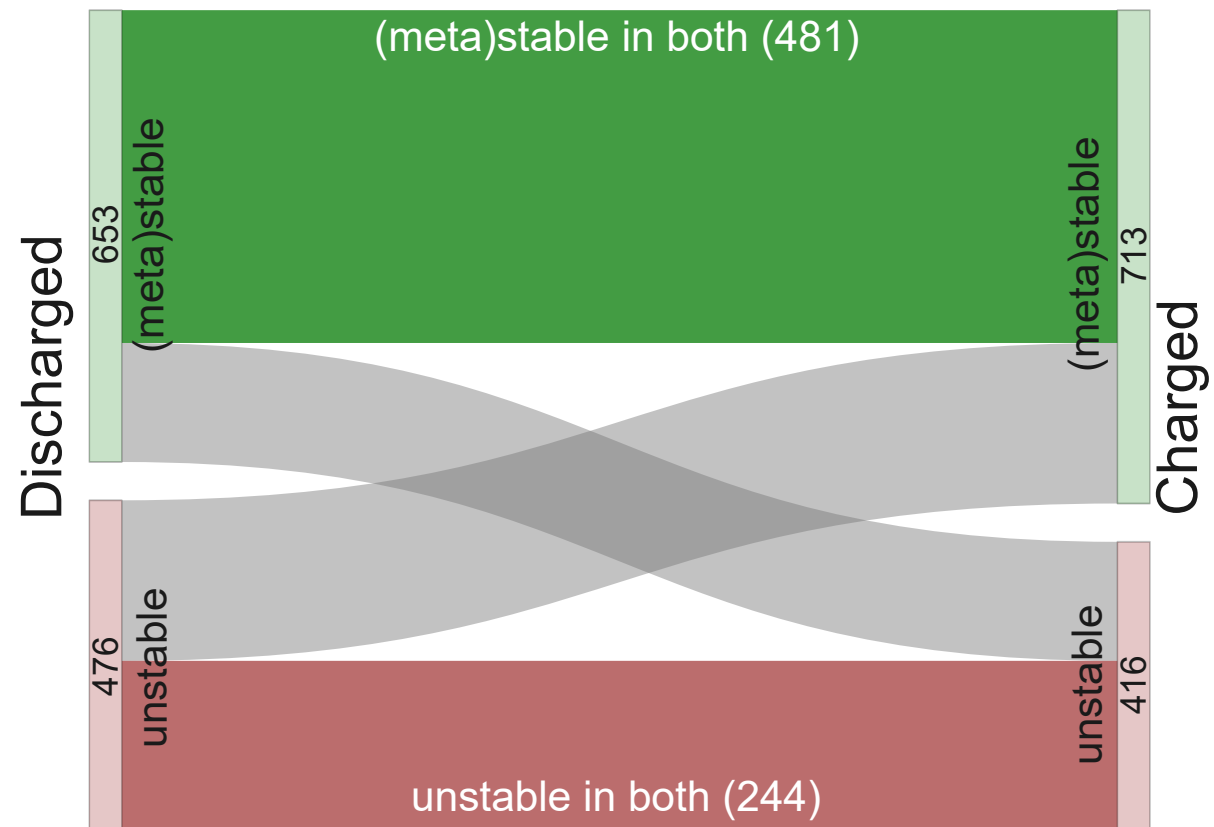
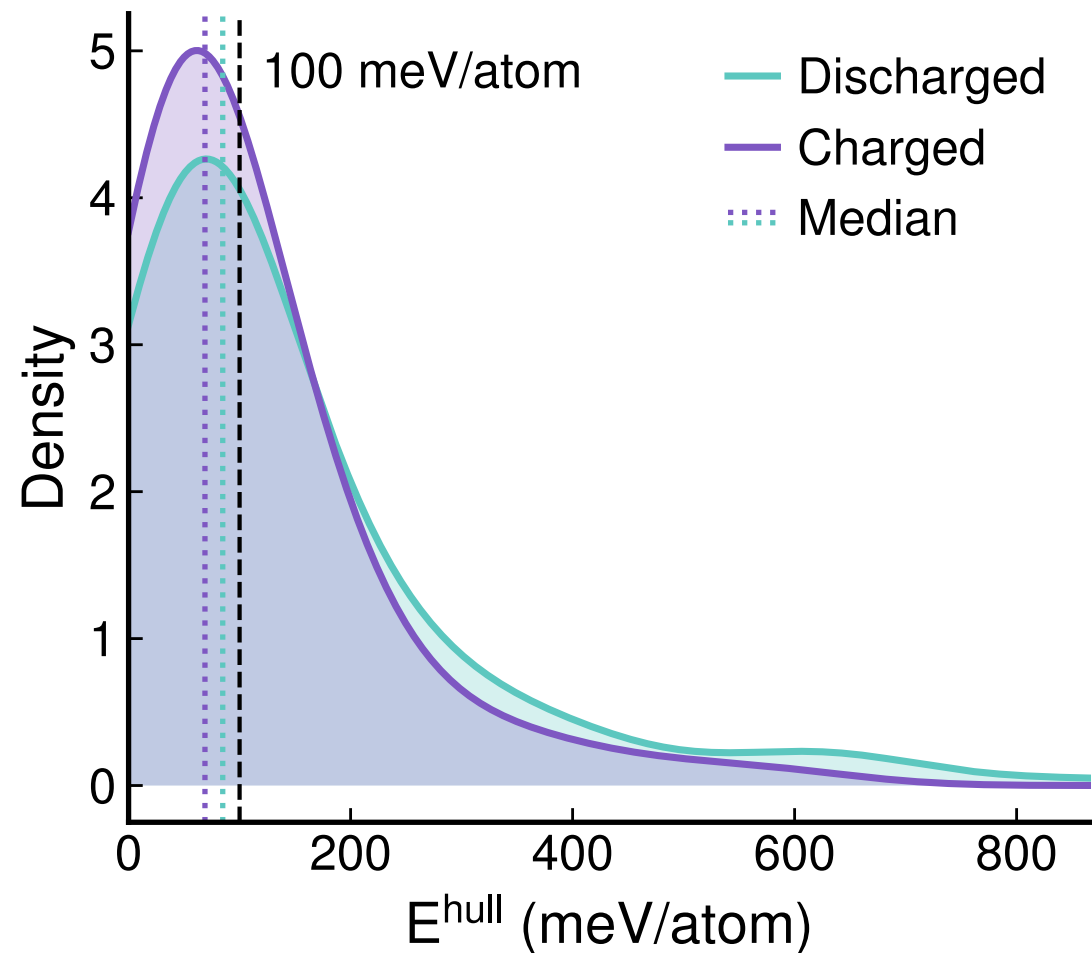
Assign oxidation states per chemical rules to determine charge neutrality

- Redox-active transition metals allowed any fractional oxidation state between +2 to +4, except V (+2 to +5)

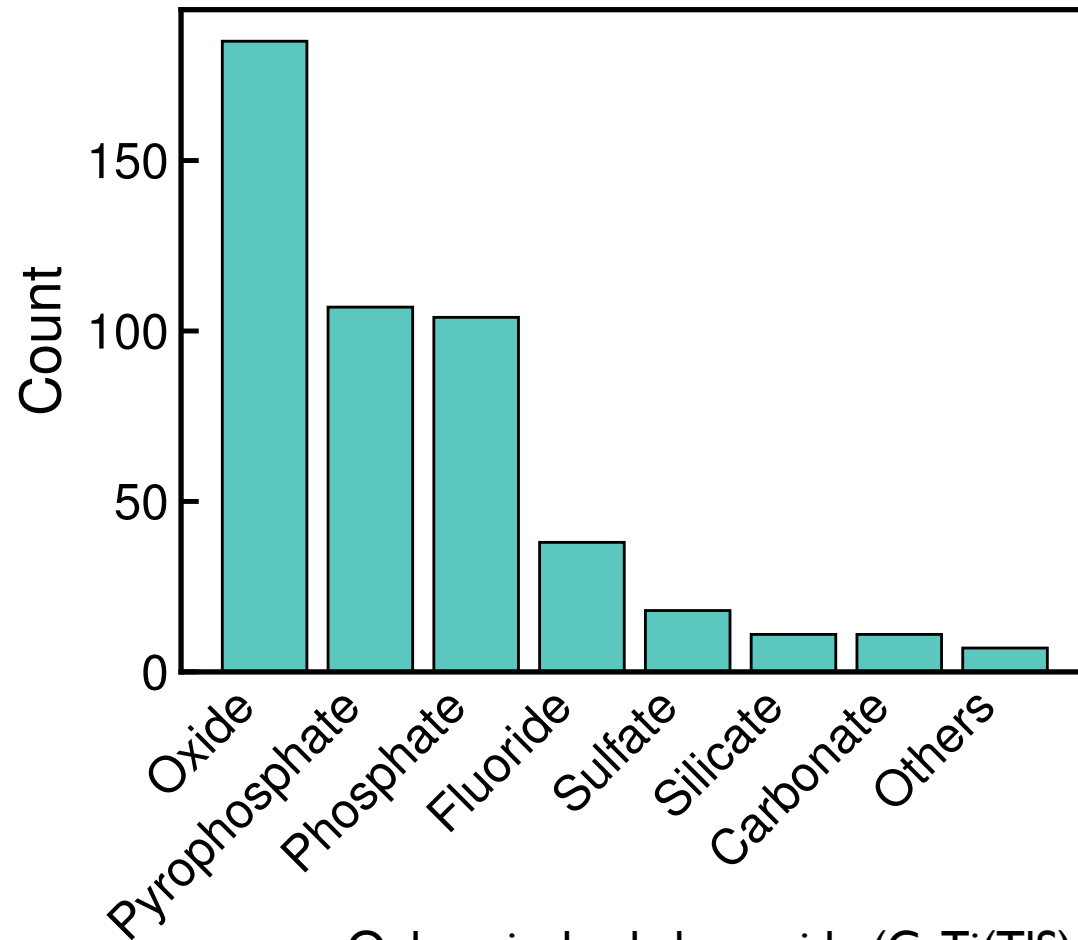
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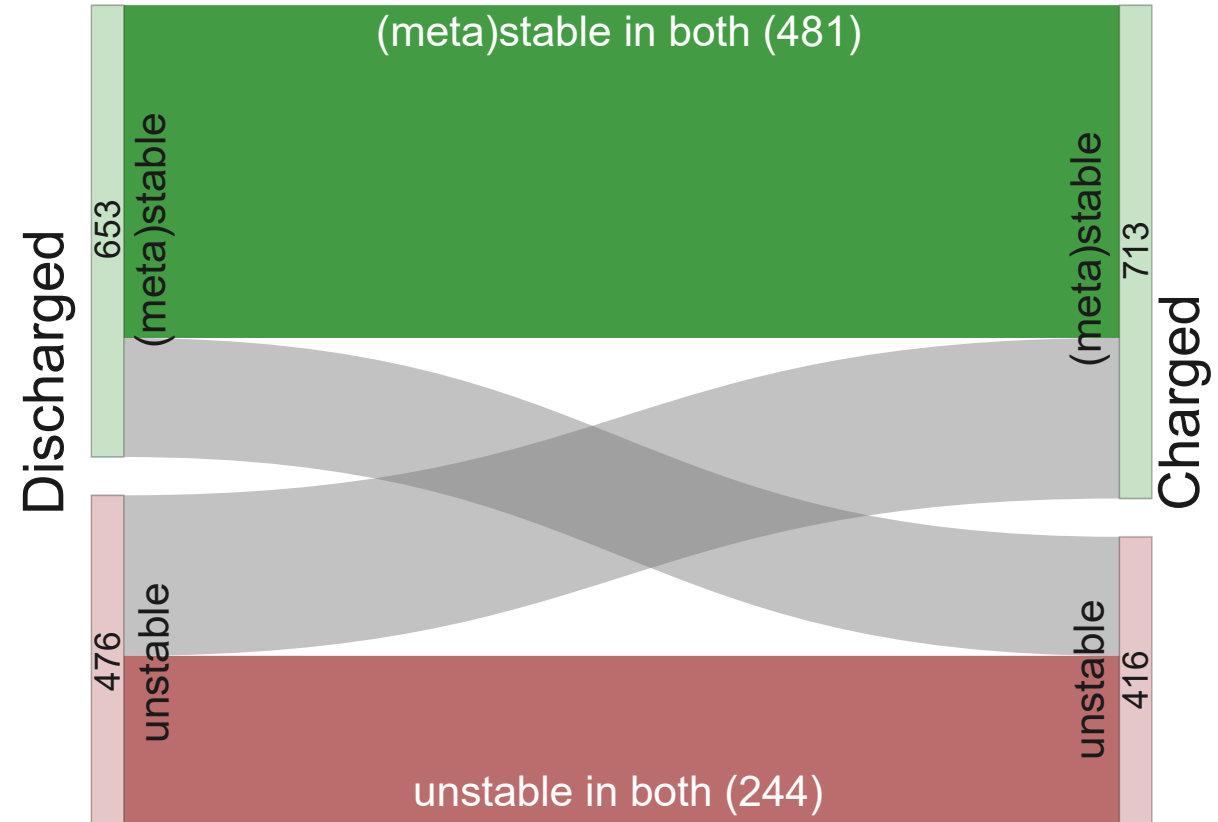
(Meta)stability and voltage: 433



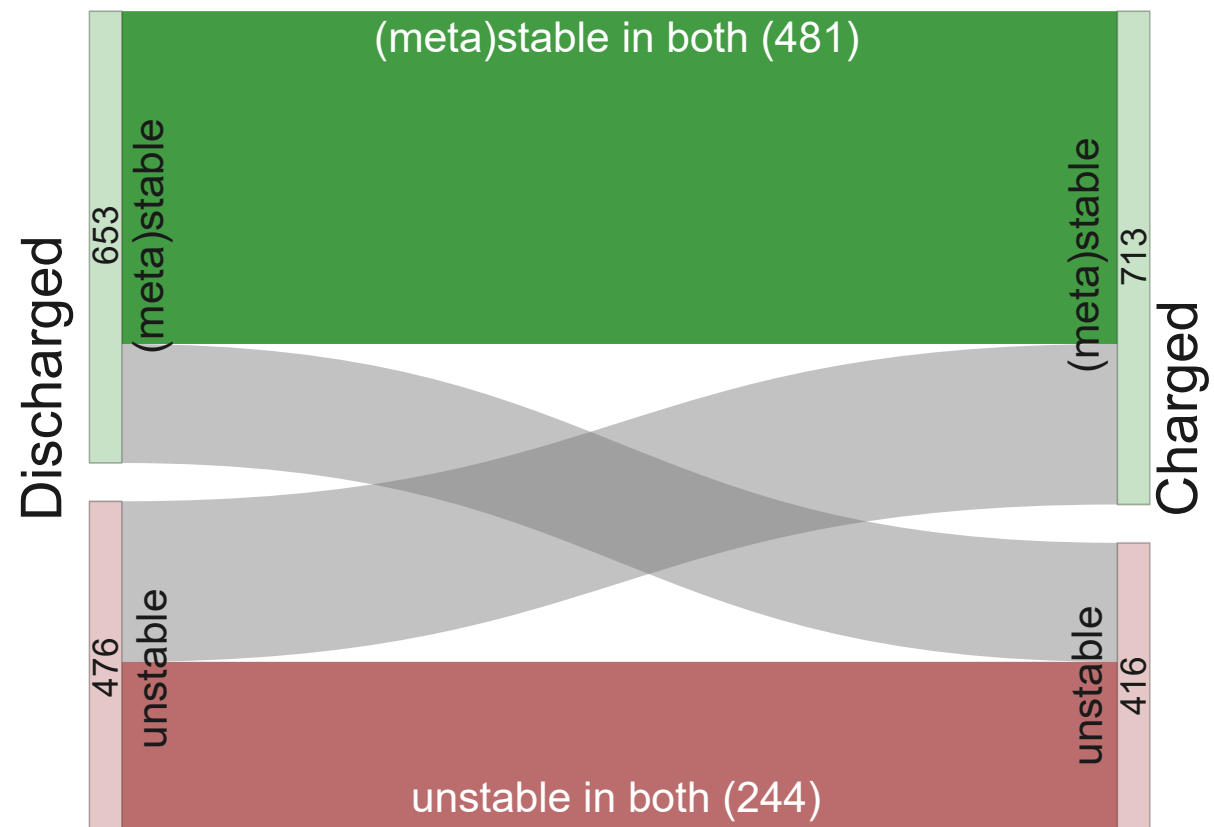
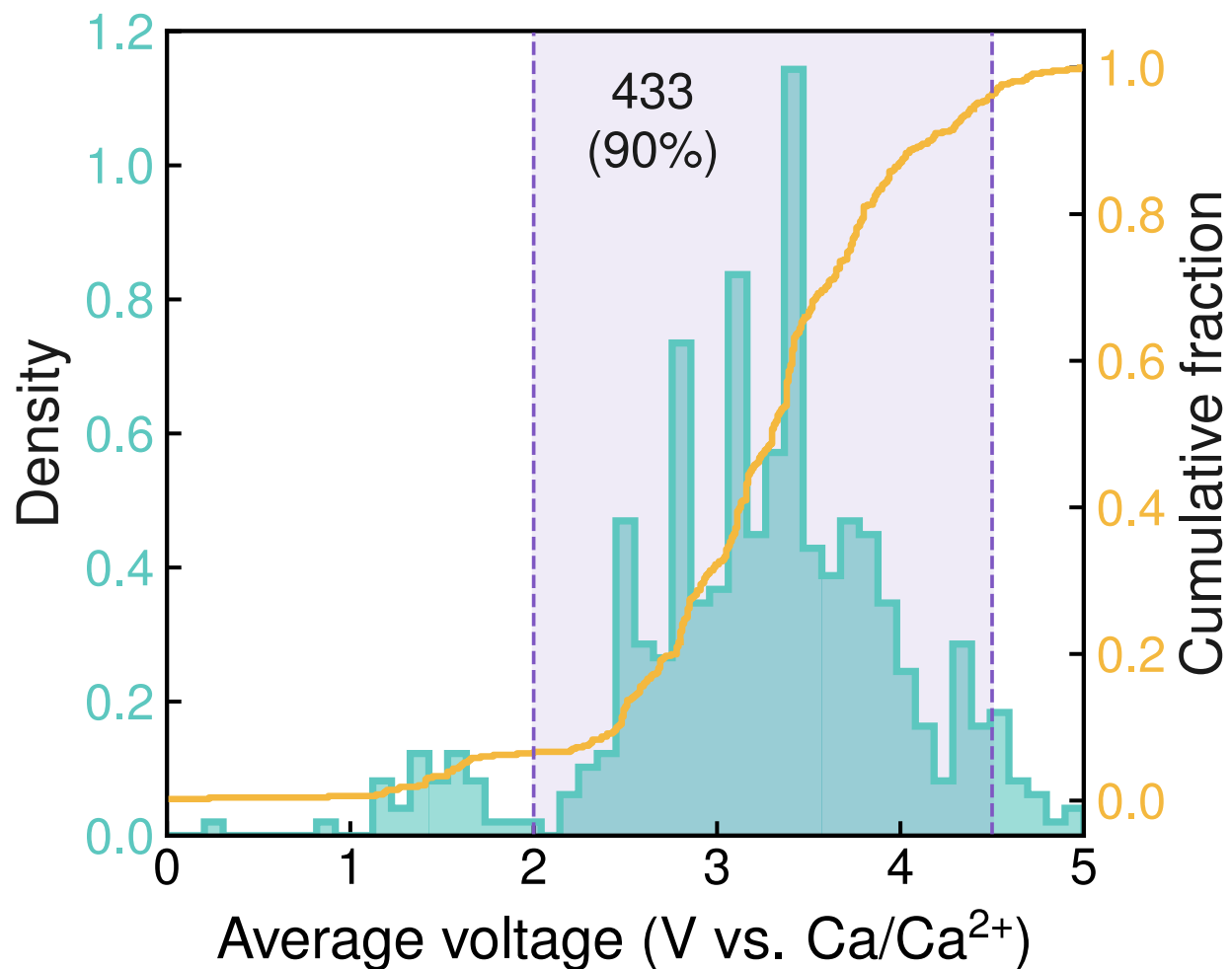
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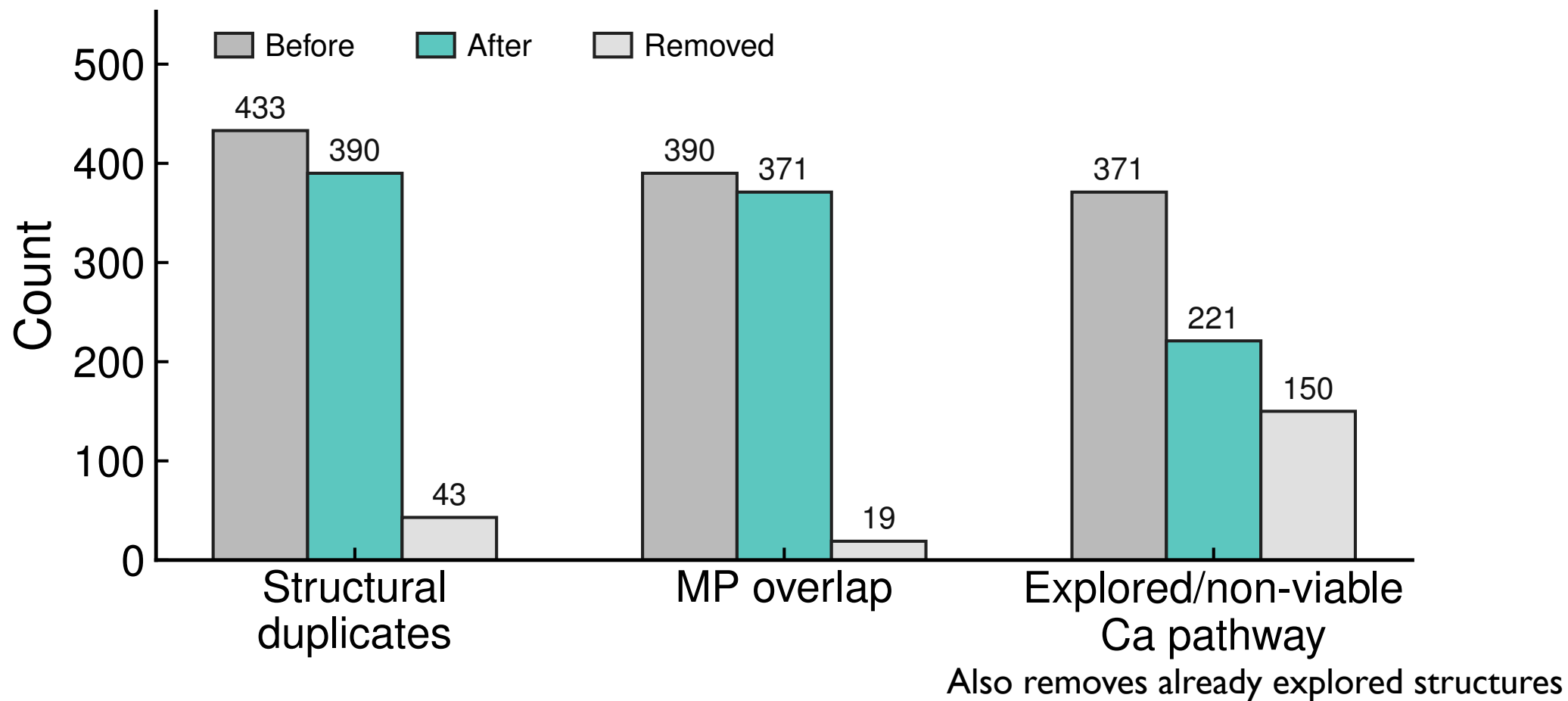
Only a single chalcogenide ($\text{CaTi}(\text{TIS})_4$)!



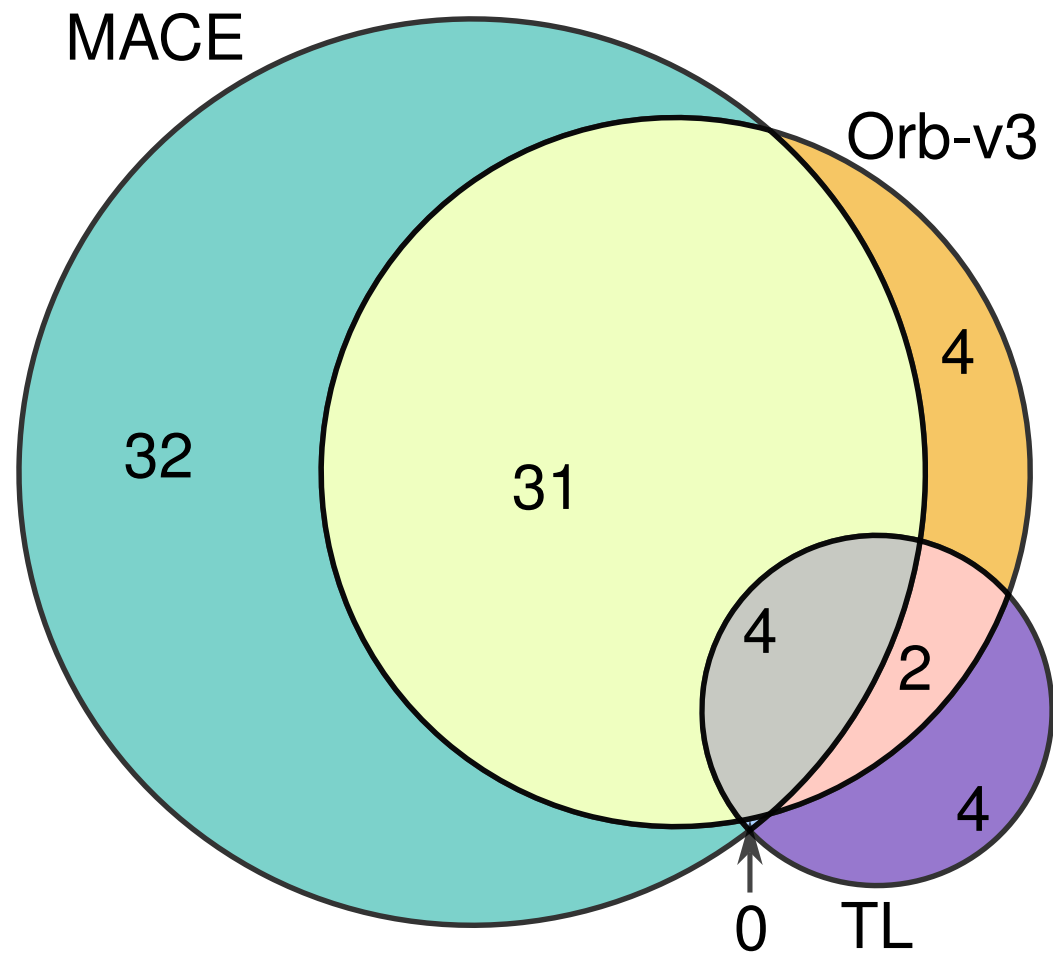
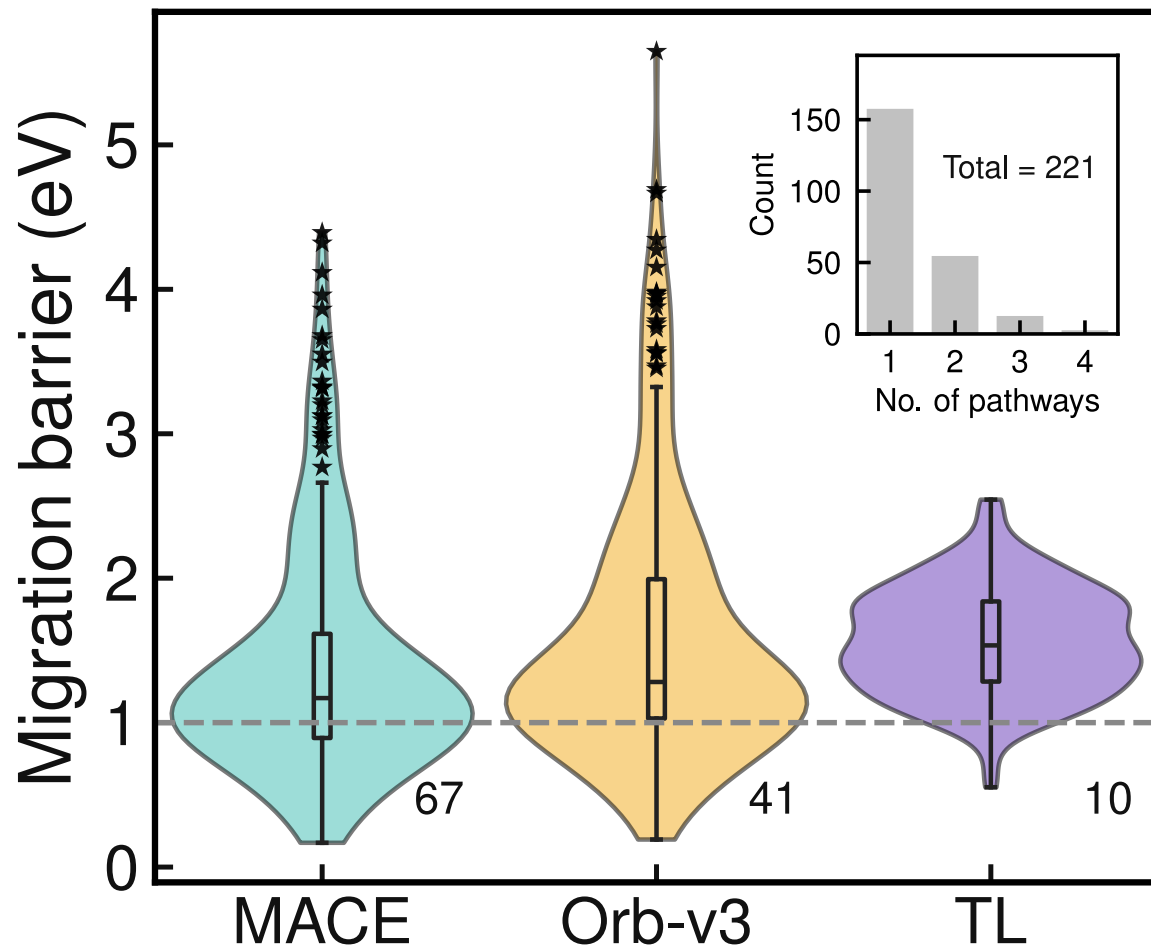
(Meta)stability and voltage: 433



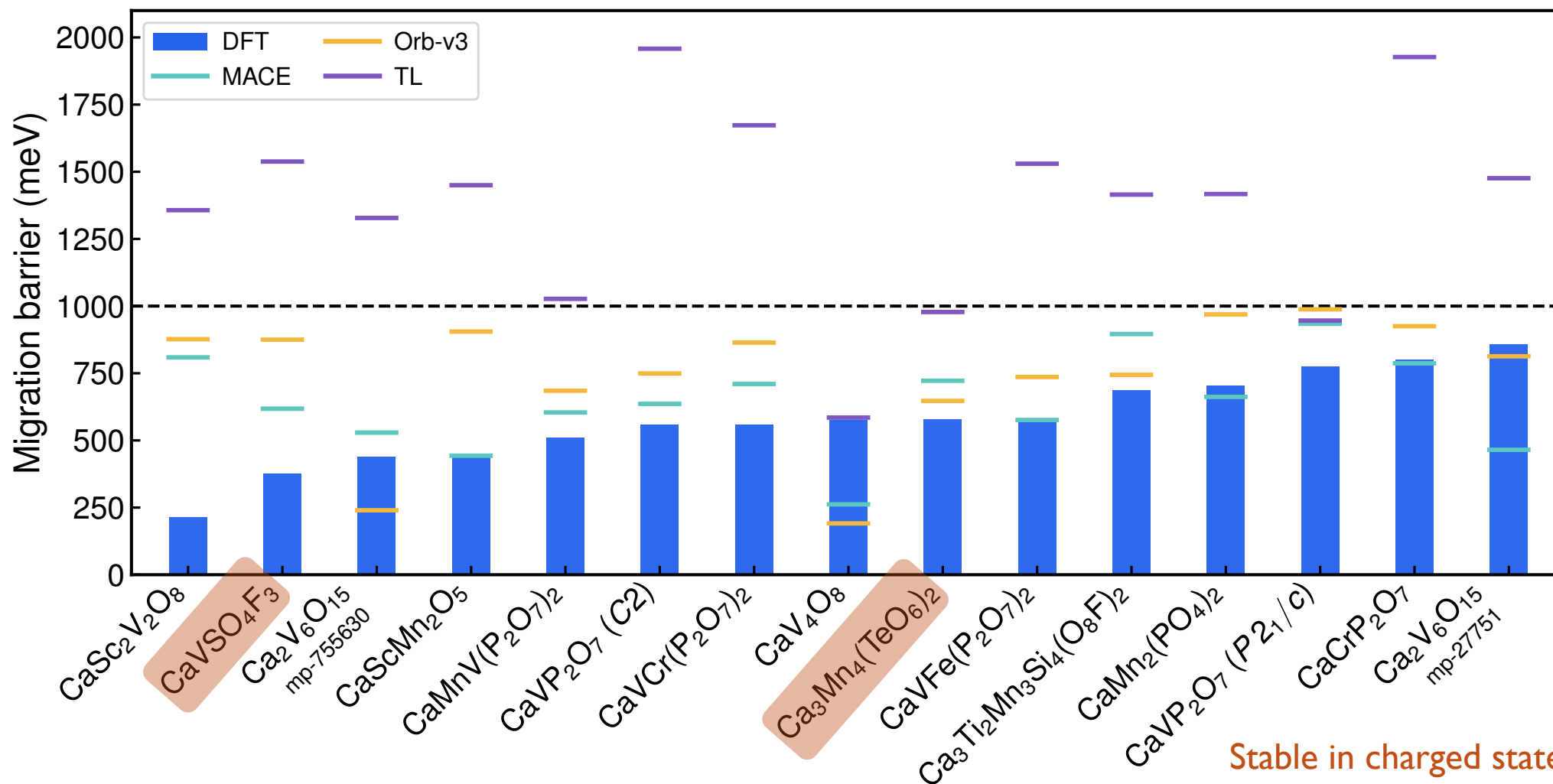
Data curation: remove duplicates, remove overlap with MP, remove non-viable pathways



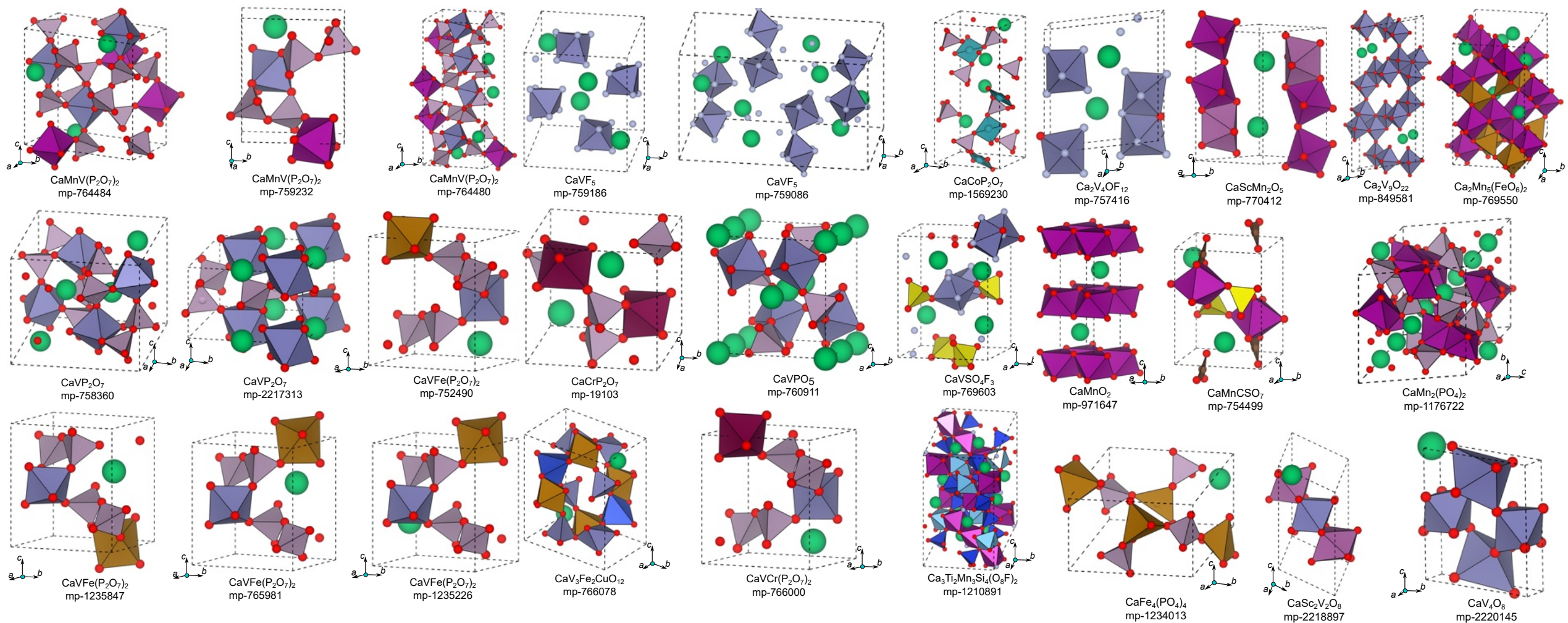
'Ensemble' predictions of Ca mobility: 37 candidates



DFT validation: confirms predictions



Candidates



Take-aways

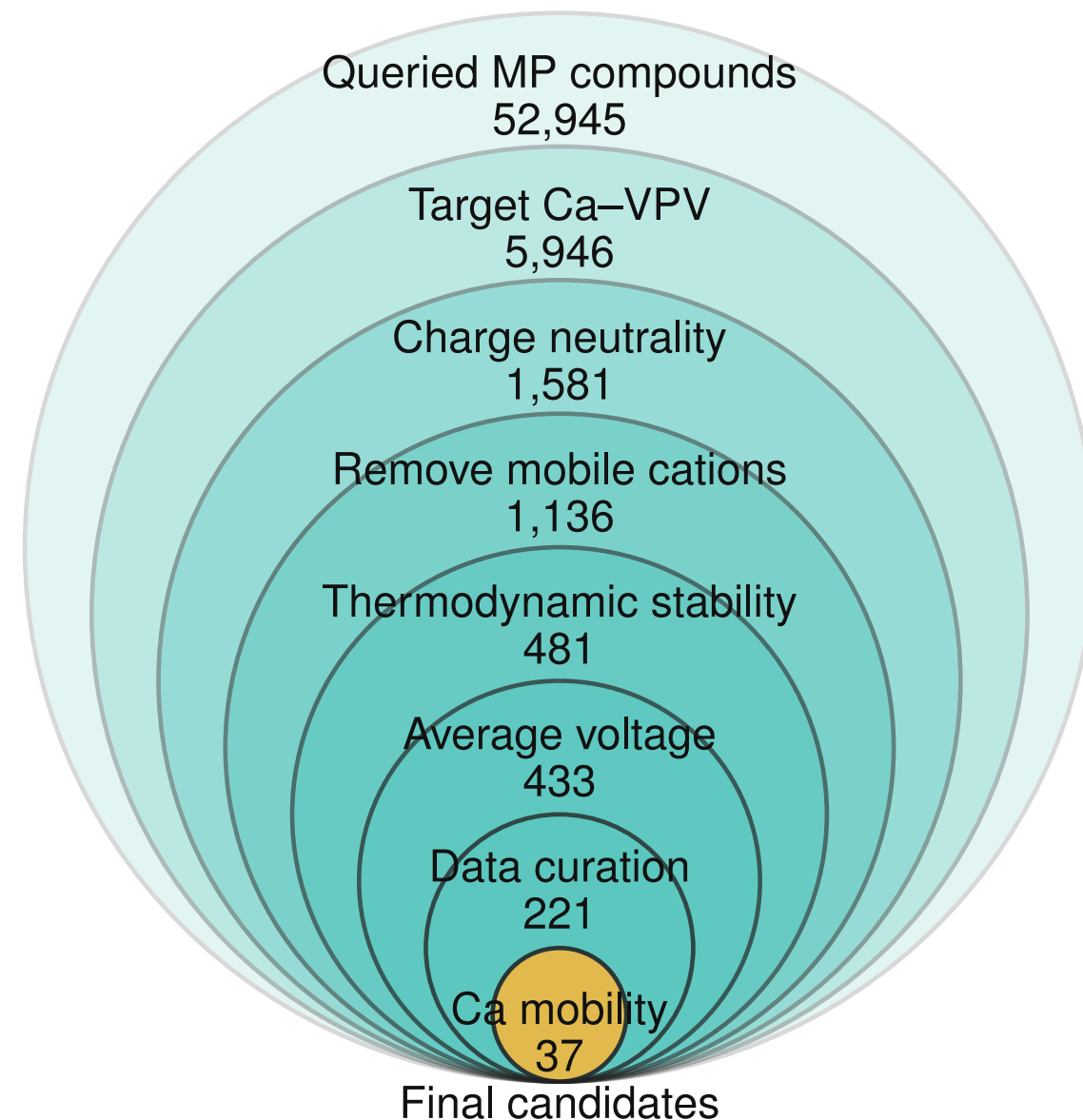
Geometric + Chemical descriptors + filters on (meta)stability, voltage, and mobility – 37 non-Ca containing candidate structures

Foundational MLIPs can accelerate material screening

- Execution < 1 year (possibly faster now)

Ensemble predictions improve reliability

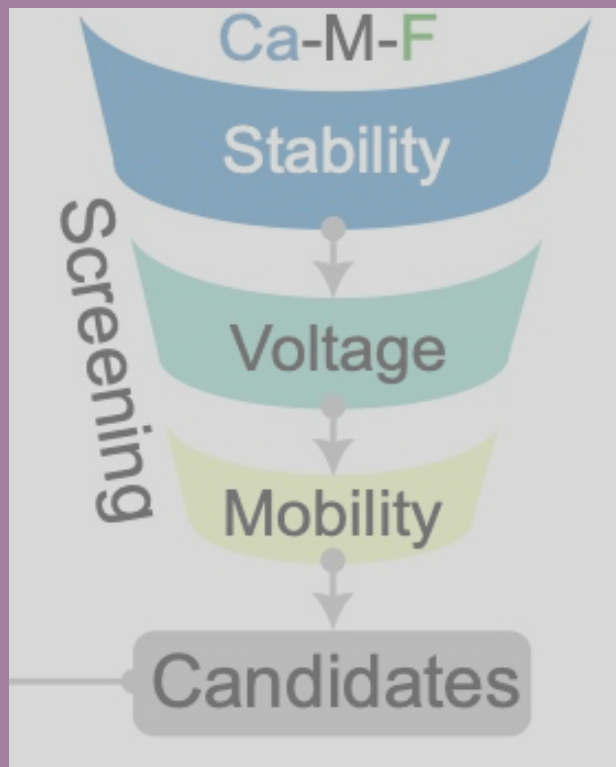
- (Meta)stable candidates with high Ca mobility!



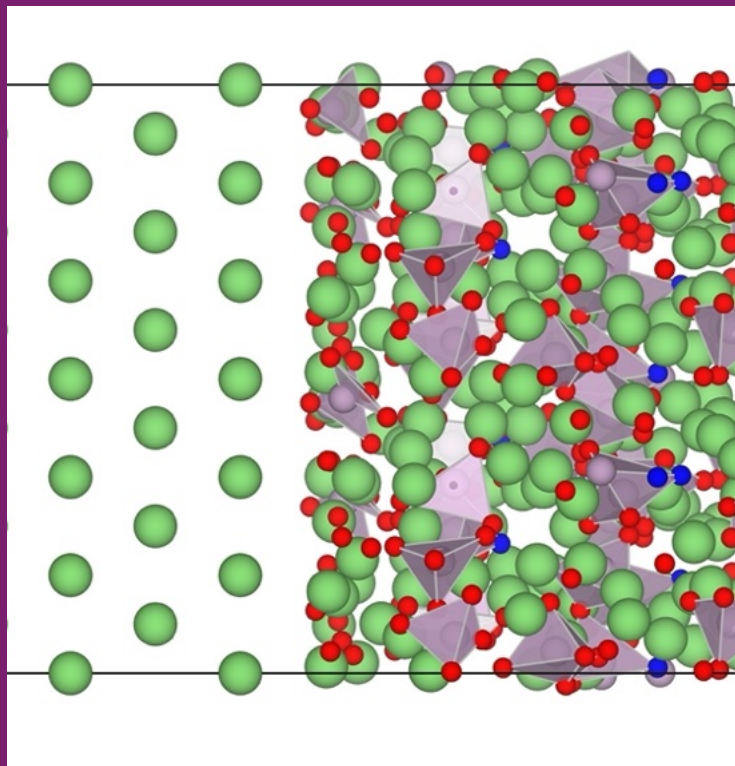
Examples

+Autonomous experiments?
+ Agents?

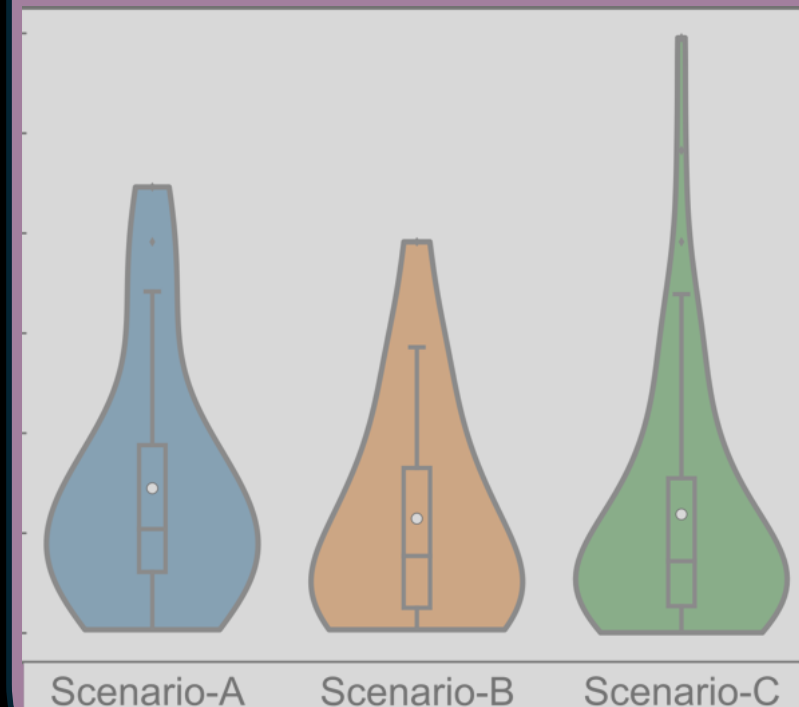
High-throughput screening



Modelling complex systems



Swift property predictions

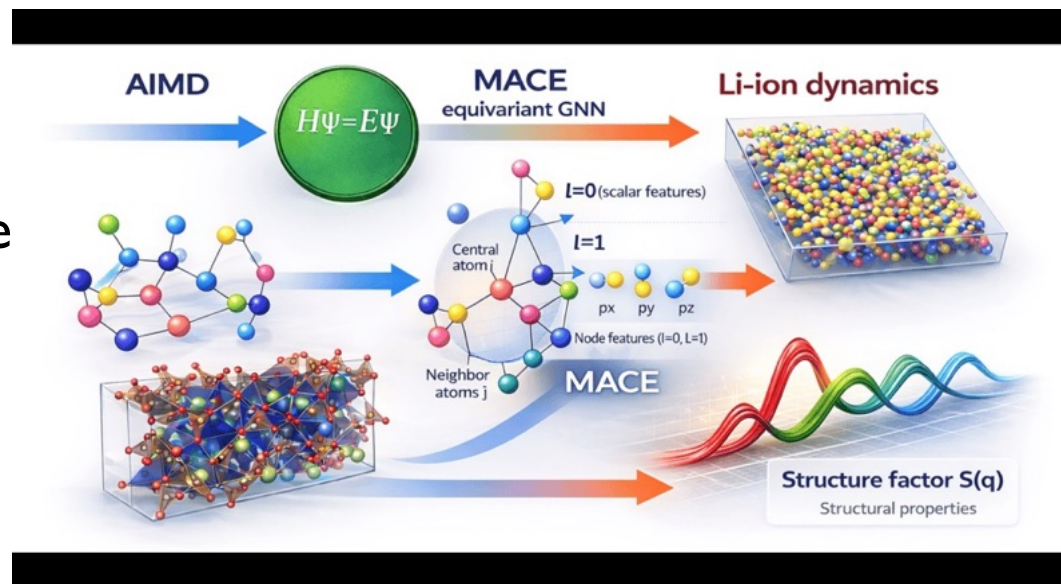


Li₂CO₃: Important component in fuel cells and batteries

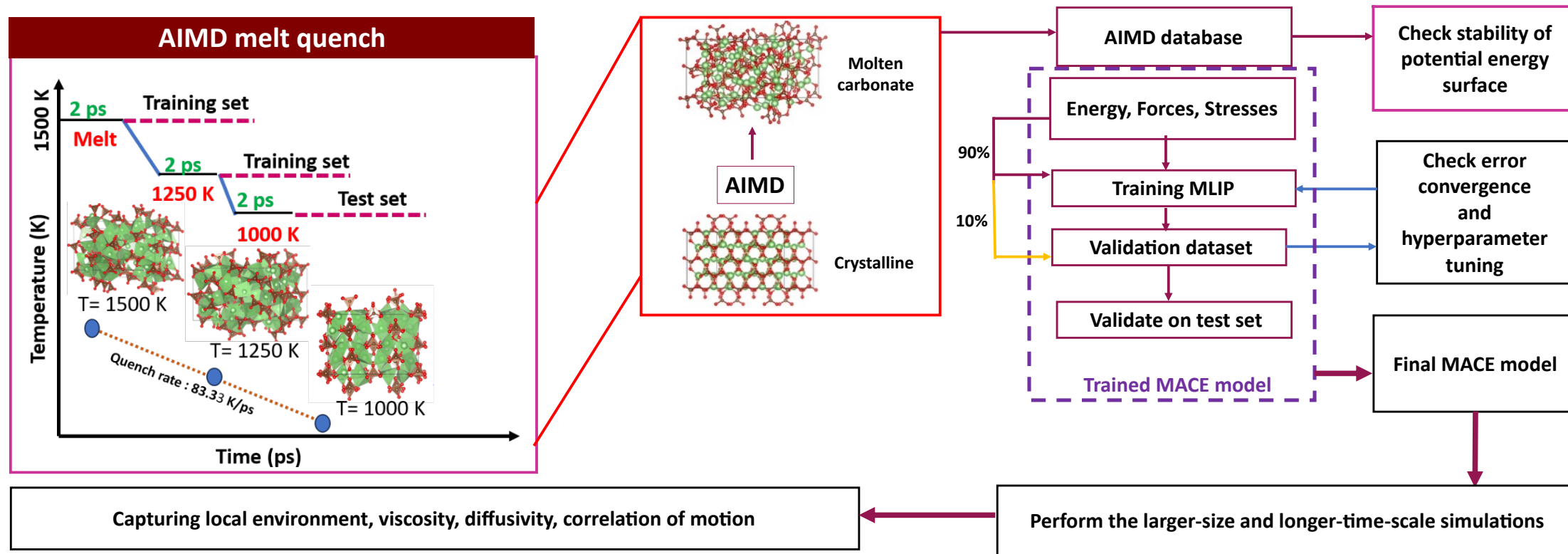
- Molten form in molten carbonate fuel cells; solution/amorphous form in Li-ion batteries
- Atomic structure and ion dynamics in liquid: to be understood
 - Including mechanism of transport

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

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



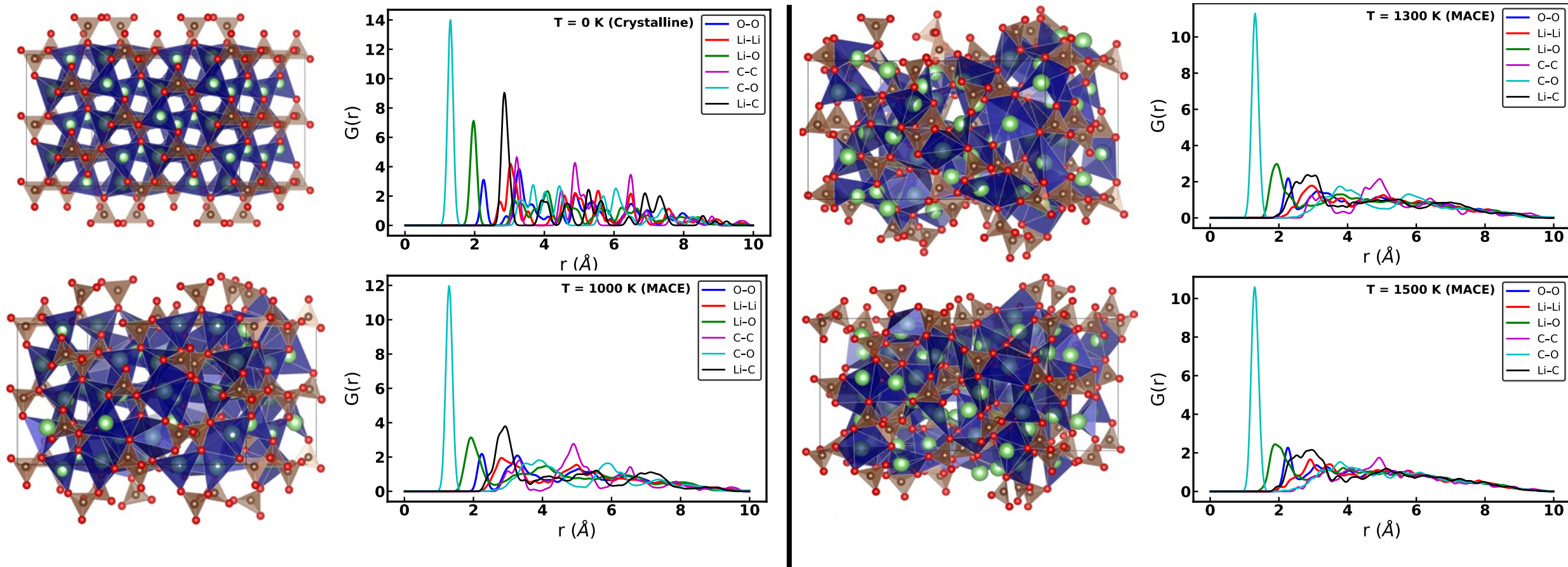
Workflow: use short-term DFT data to train MLIP



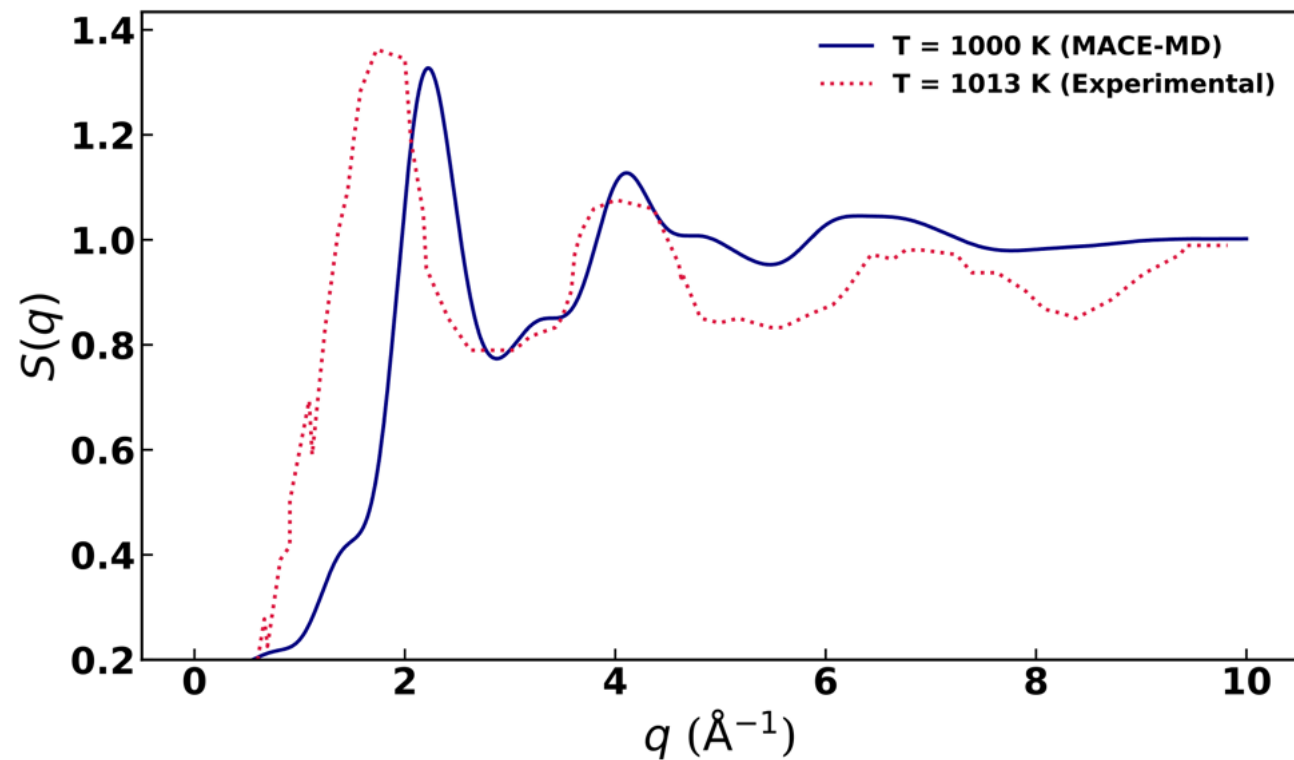
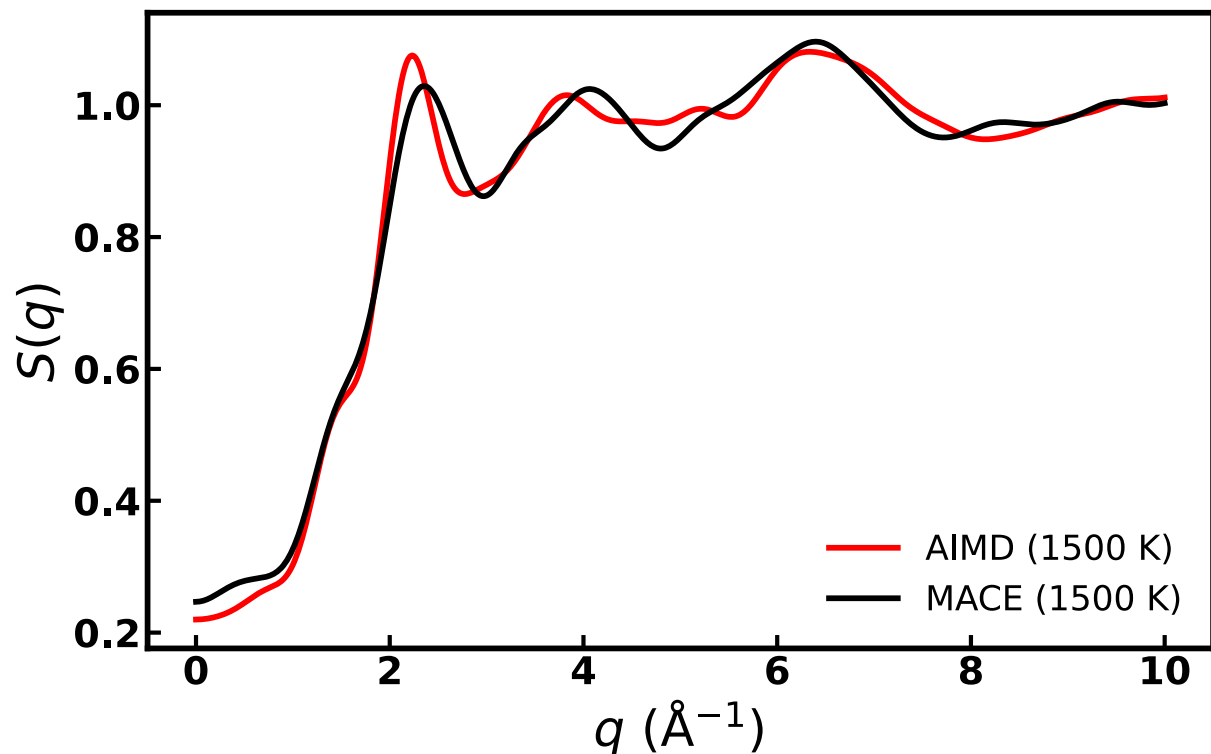
Training set: ~5600 configurations at 1500 K and 1250 K

Test set: configurations at 1000 K; strained structures

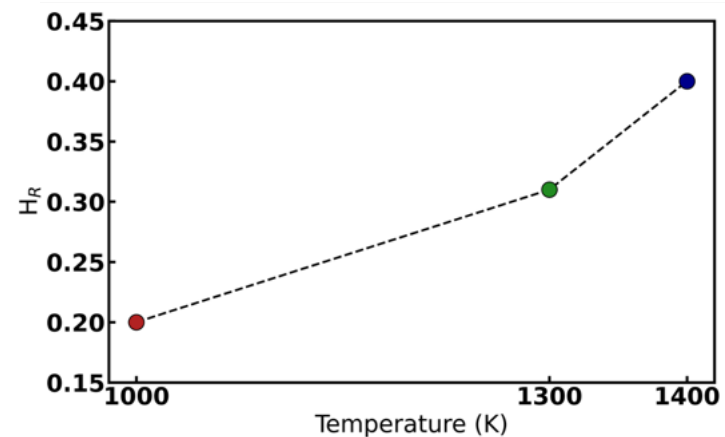
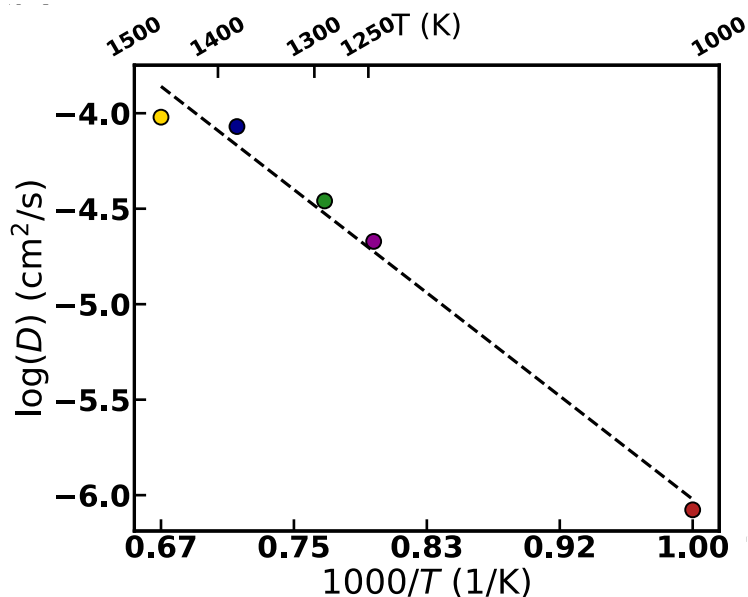
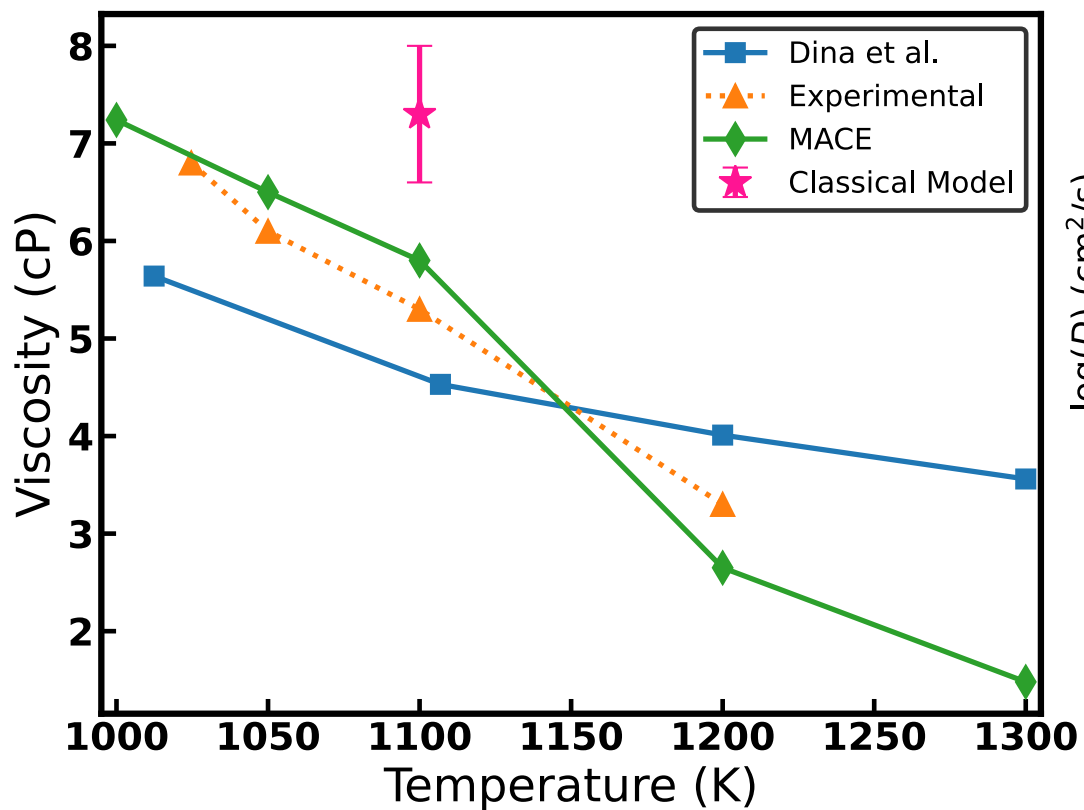
Structure from MLIP: molten with no long range order beyond 1000 K



MLIP-calculated structure factor: matches with AIMD and experiments



Viscosity and transport: match with experiments, mechanism change at 1000 K

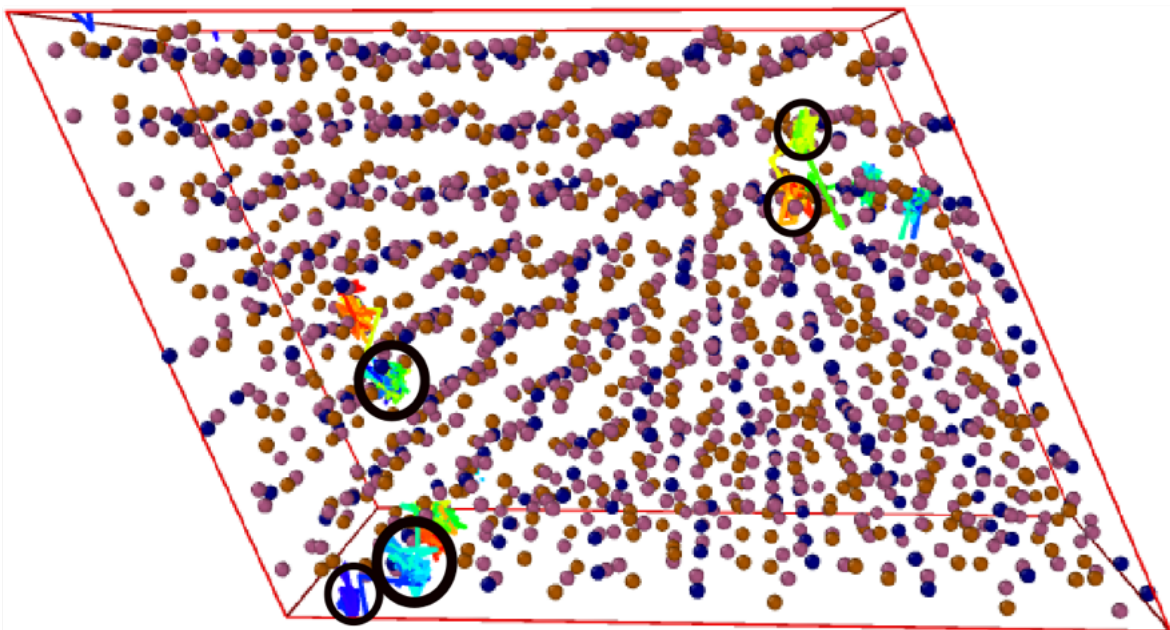


Fairly linear trend in tracer diffusivity (D^*) of Li across temperatures

- Simulations over 0.7 ns, 1536 atoms
- Marked change in Haven's ratio (H_R)
- Indicator of decrease in correlations between Li hops at high temperatures

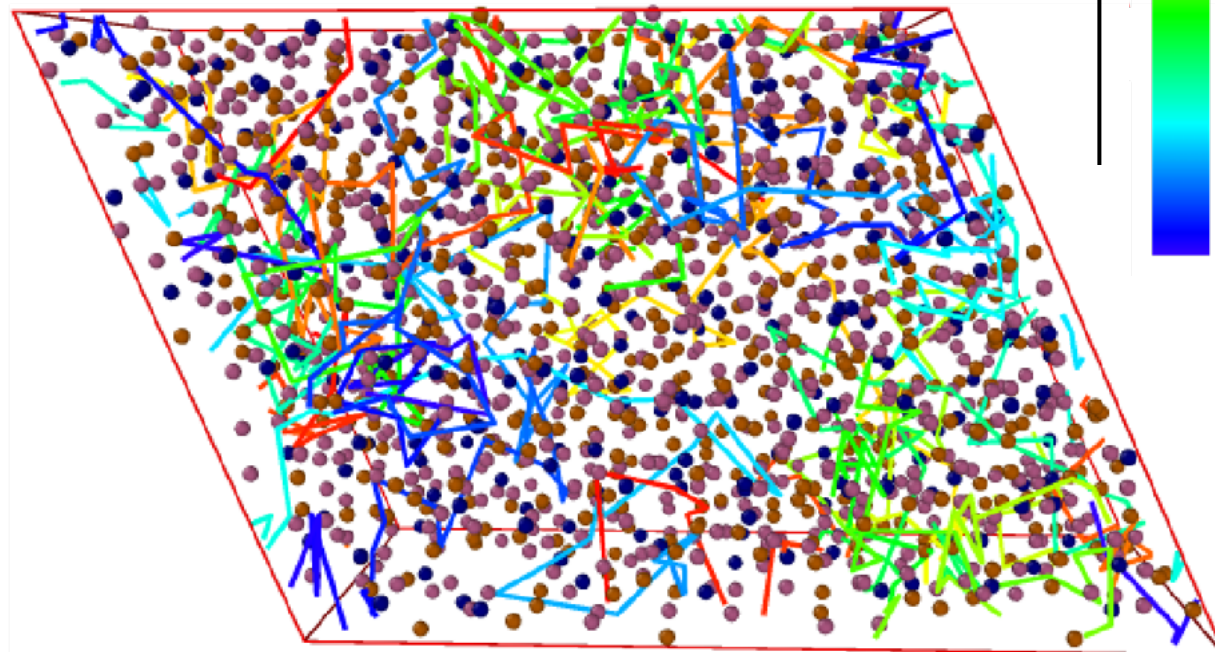
Unwrapped Li trajectories: points at mechanism change

T=1000 K



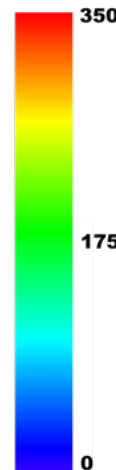
Anisotropic, correlated, transient trapping events

T=1400 K



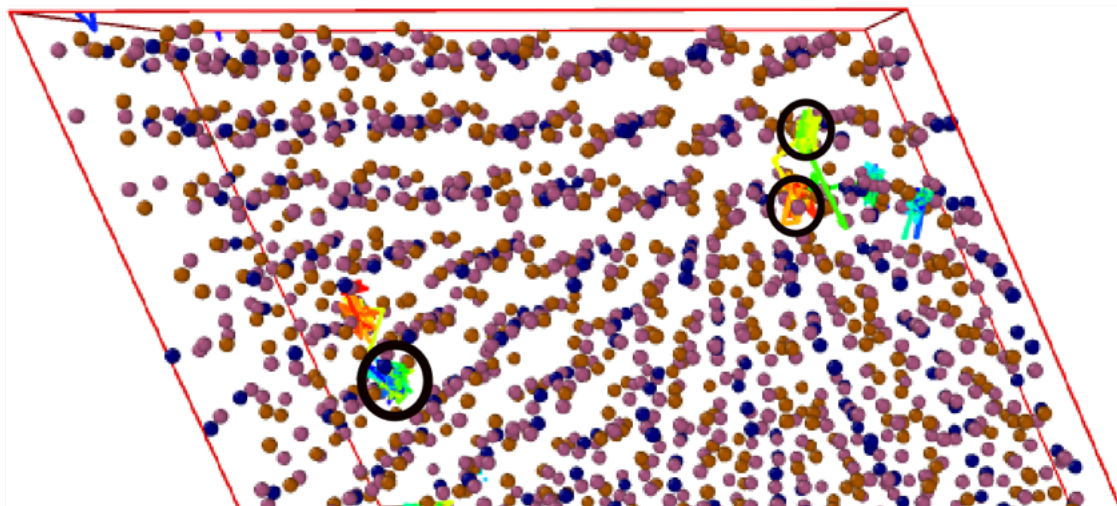
Isotropic, less-correlated, sparse trapping events

time

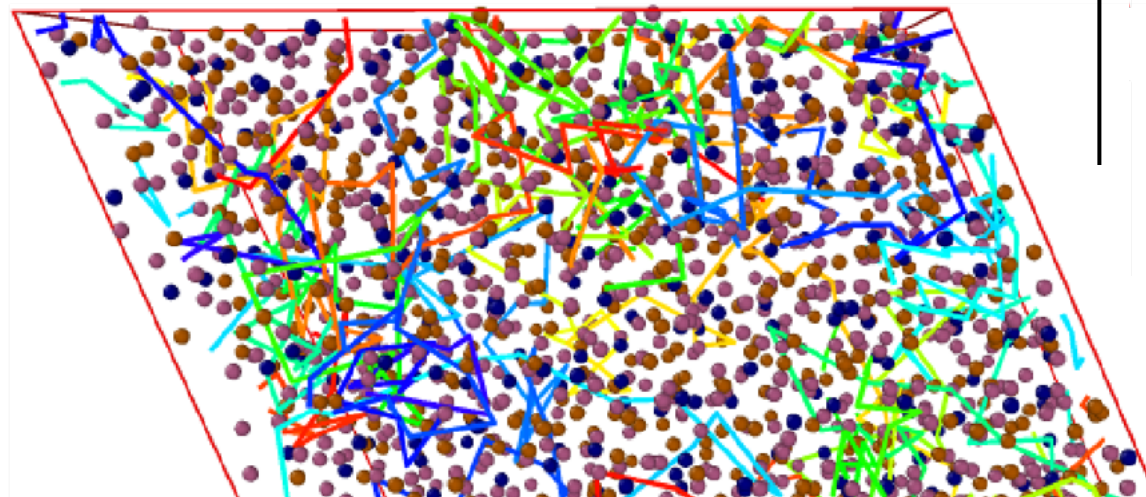


Unwrapped Li trajectories: points at mechanism change

T=1000 K



T=1400 K



time



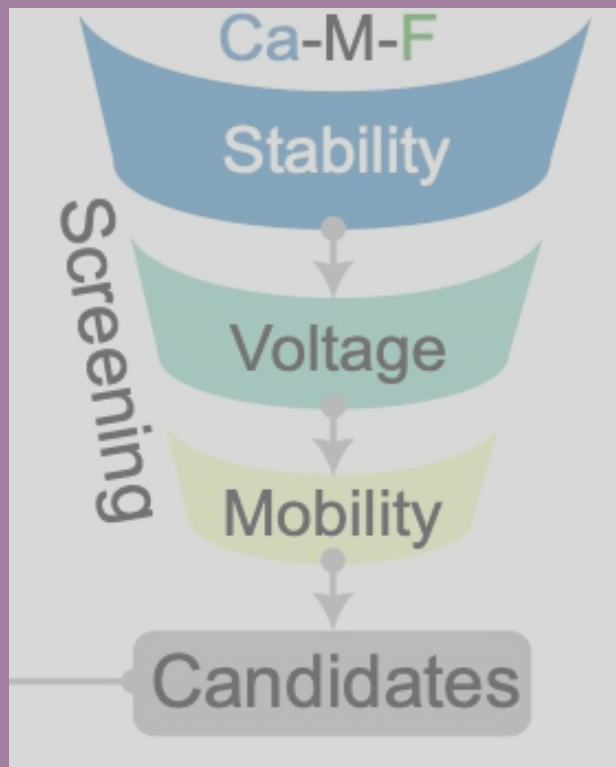
Take-aways:

- Modern MLIP architectures do not require large datasets for training
- Well-trained MLIP can model complex (liquid) systems well, over ns time scales and few 1000 atoms
- Can improve fundamental understanding of transport mechanism in play

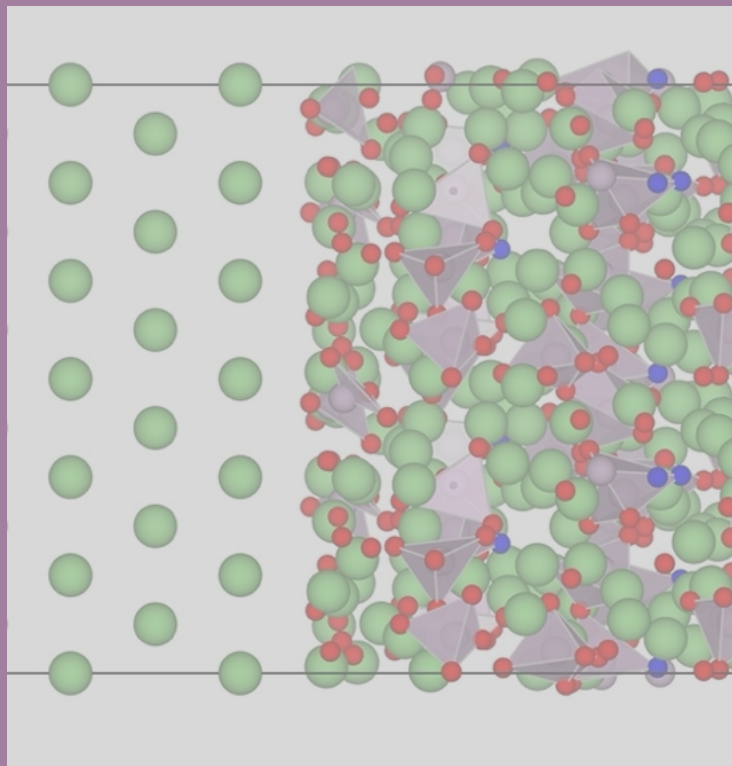
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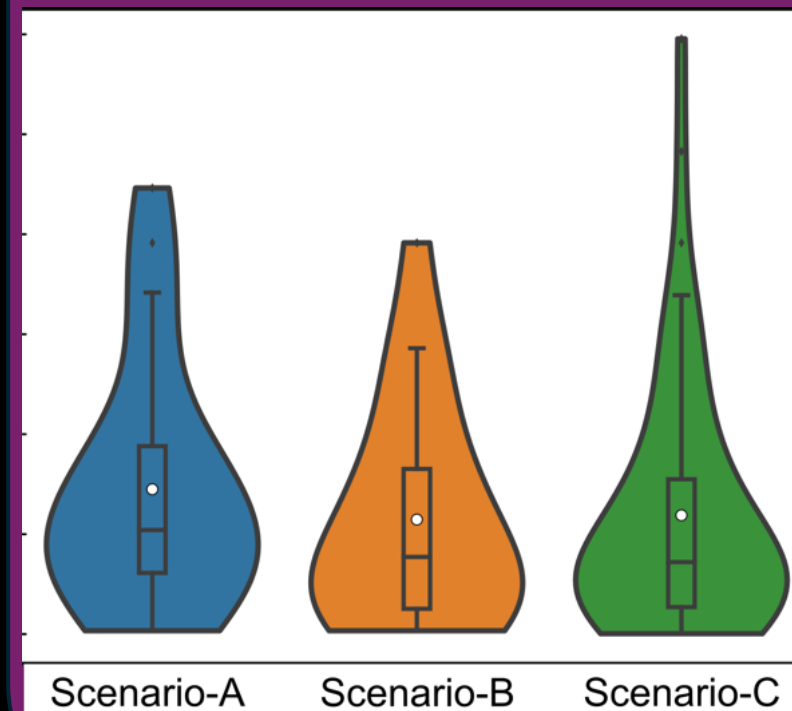
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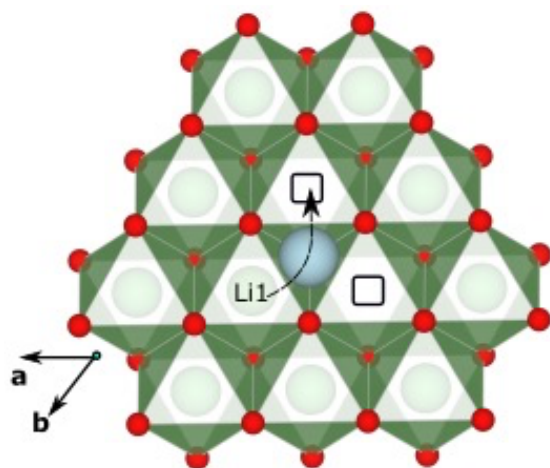
Swift property predictions



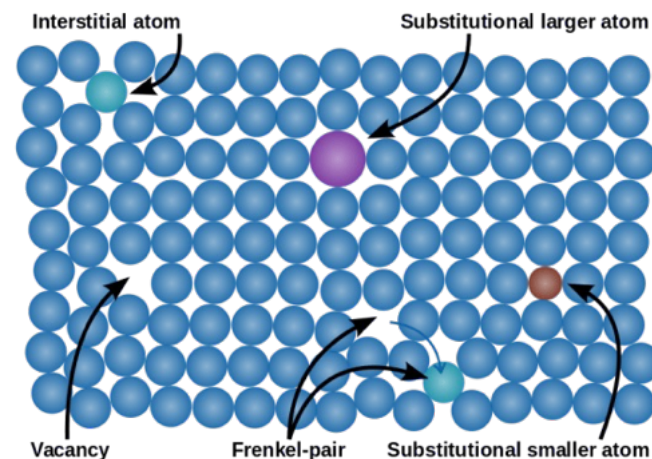
Is transfer learning useful for materials?

Several key material properties that govern performance in applications have limited data

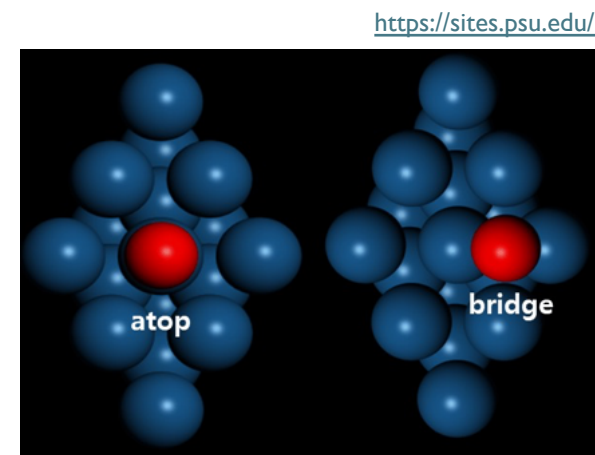
- ‘Small’ datasets ($< 10^4$ datapoints)
 - Ionic mobilities, defect formation energies, adsorption energies,...
- Limits application of deep learning (DL) frameworks



Devi et al., *npj Comput. Mater.* 2022



<https://www.differencebetween.com/difference-between-point-defect-and-line-defect/>



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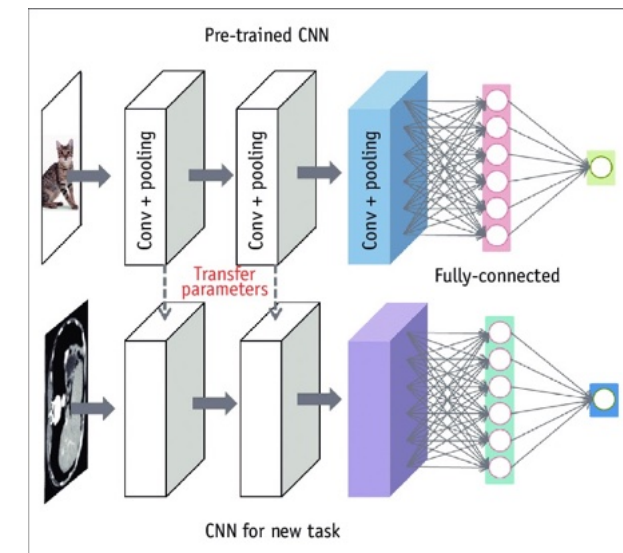
- ‘Small’ datasets ($< 10^4$ datapoints)
 - Ionic mobilities, defect formation energies, adsorption energies,...
- Limits application of deep learning (DL) frameworks

Transfer learning: efficiently use DL frameworks on small datasets

- Pre-train (**PT**) on ‘large’ dataset, fine-tune (**FT**) on ‘small’ dataset

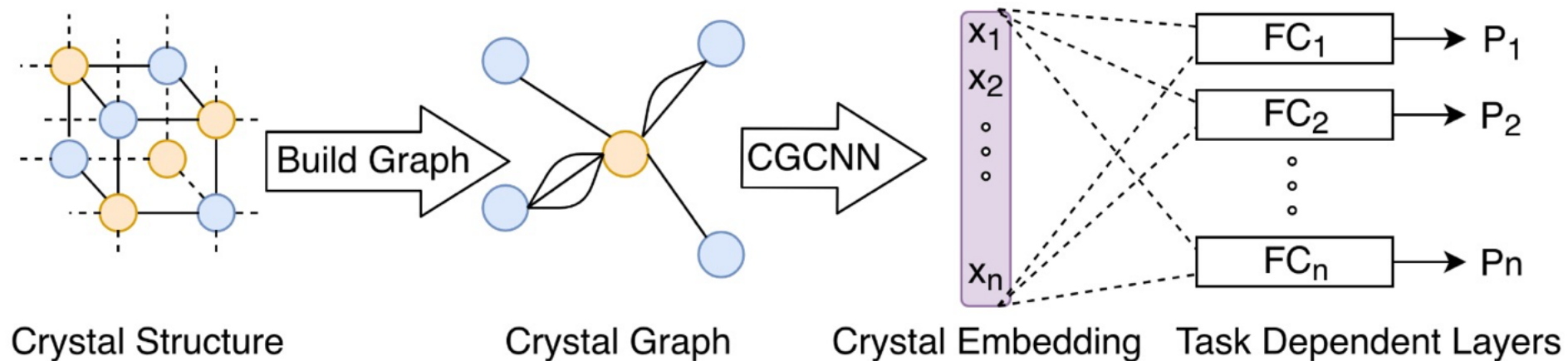
How useful is transfer learning in materials science?

- Ways to generate ‘generalizable’ models?
- Predict a hard-to-estimate quantity?



MPT: (Beta) Generalizable models

Inspiration from literature: multi-task crystal graph convolutional neural network



Multi-property pre-trained (MPT) models can generalize dependence of several properties on the structure

MPT: (Beta) Generalizable models

Band gap of 2D materials (1,103 datapoints) from JARVIS-DFT¹

Model	Test R ²	Test MAE
Scratch	0.635	0.148
MPT (all seven datasets)	0.671	0.125
FE (100K)	0.670	0.127
BG (50K)	0.617	0.138
PH (1256)	0.628	0.145
GV (10,987)	0.626	0.143
EBG (2,481)	0.619	0.143

On average, MPT is 6% and 10% better on R² and MAE than PT-FT

Closest performer to MPT is FE: largest dataset within MPT

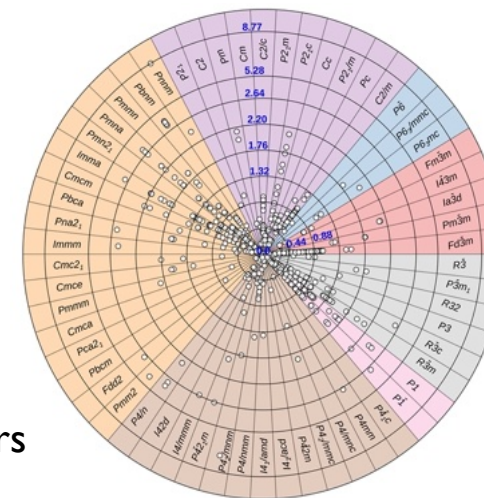
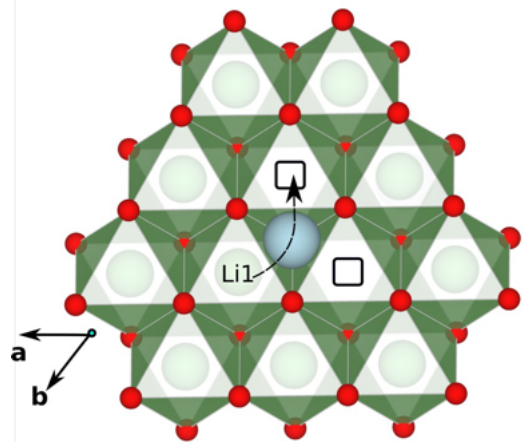
MPT models: may generalize quite well with more properties

FE: Formation energy; BG: Band gap; GV: Shear modulus;
EBG: Experimental band gap

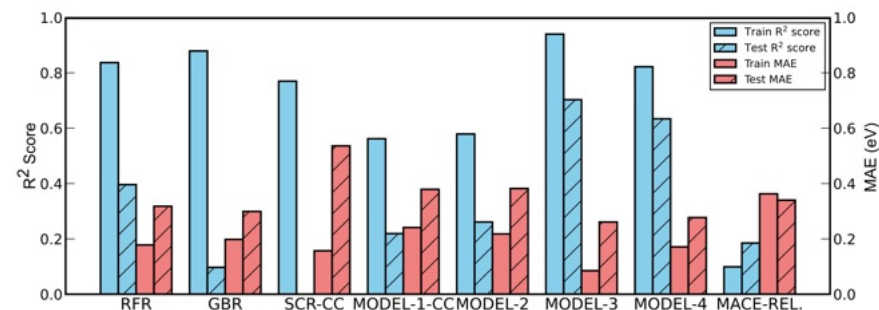
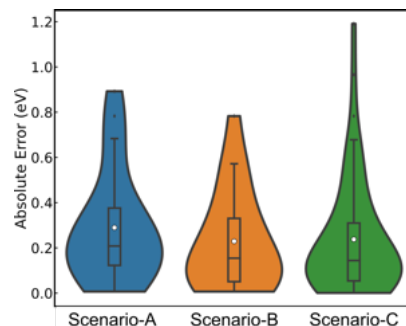
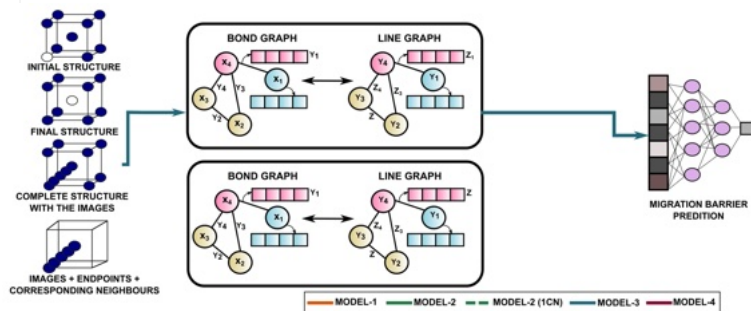
Transfer learning for predicting battery rate performance

Migration barriers → determine rate performance in batteries

Exponential control on diffusivity



Compile a dataset on calculated barriers

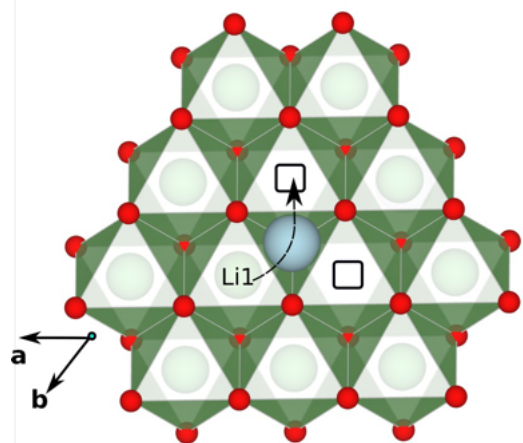


Build a model (graph based architecture)

MODEL-3 (transfer learned) is the best!

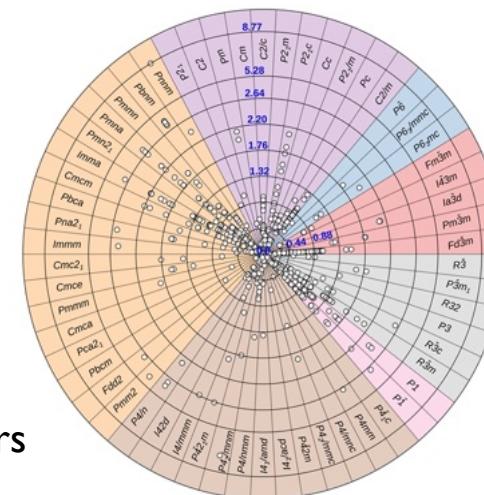
Excellent generalization and classification abilities

Transfer learning for predicting battery rate performance

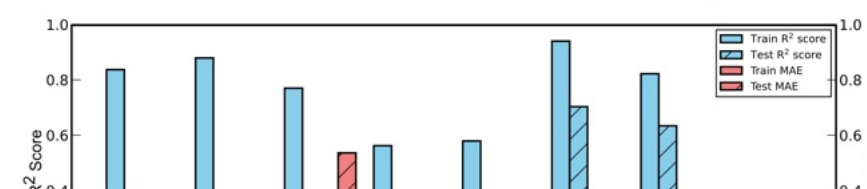
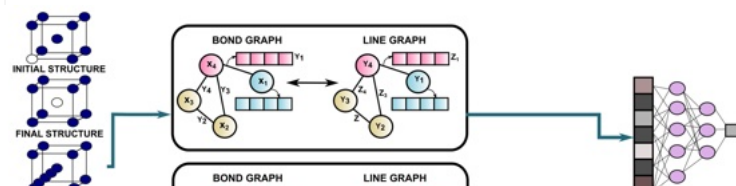


Migration barriers \rightarrow determine rate performance in batteries

Exponential control on diffusivity



Compile a dataset on calculated barriers



Take-away:

- Transfer learned graph architectures can predict difficult-to-estimate structural properties swiftly and accurately



Conclusions

- AI can accelerate battery materials design, in conjunction with robust workflows and sufficient training/validation
- Use of graph models is a common theme in materials science
- Examples of impact on high-throughput screening of Ca-cathodes, modelling molten Li_2CO_3 , and predicting ionic migration barriers swiftly and accurately in inorganic solids

“Geometry-based Discovery of Calcium Battery Cathodes Accelerated by Foundational Machine-Learned Models”, D.B. Tekliye, A.K. Bheemaguli, and G. Sai Gautam, *under review* [[arXiv 2605.29029](https://arxiv.org/abs/2605.29029) (2026)].

“Probing correlated ionic transport and structural anisotropy in molten lithium carbonate”, D. Dey, A. Patra, A.N. Krishnamoorthy, G. Sai Gautam, *under review* [[arXiv](https://arxiv.org/abs/2605.29029) (2026)].

“A literature-derived dataset of migration barriers for quantifying ionic transport in battery materials”, R. Devi, A. Balasubramanian, K.T. Butler, and G. Sai Gautam, *Scientific Data* 12, 1922 (2025).

“Leveraging transfer learning for accurate estimation of ionic migration barriers in battery materials”, R. Devi, K.T. Butler, and G. Sai Gautam, *npj Comput. Mater.* 12, 88 (2026).

saigautamg@iisc.ac.in; <https://sai-mat-group.github.io>; <https://github.com/sai-mat-group>