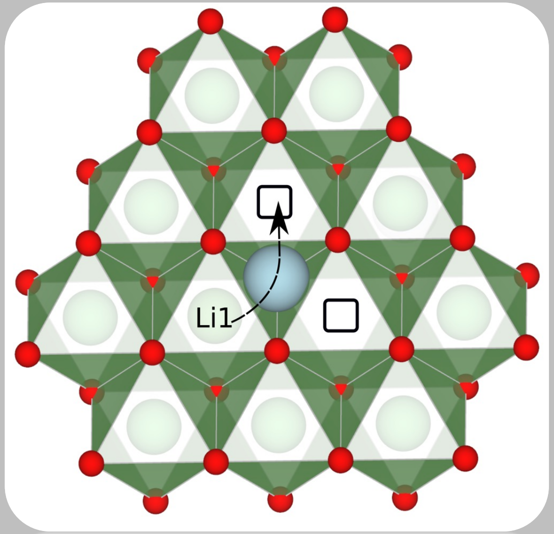
Elucidation and prediction of ion transport in battery materials: A first-principles and machine learning study



Ph. D. Thesis Defence

Presenter
Reshma Devi P (Sr. No.18599)
5th Year Ph.D. student

Under the Guidance of
Dr. Sai Gautam Gopalakrishnan
Associate Professor

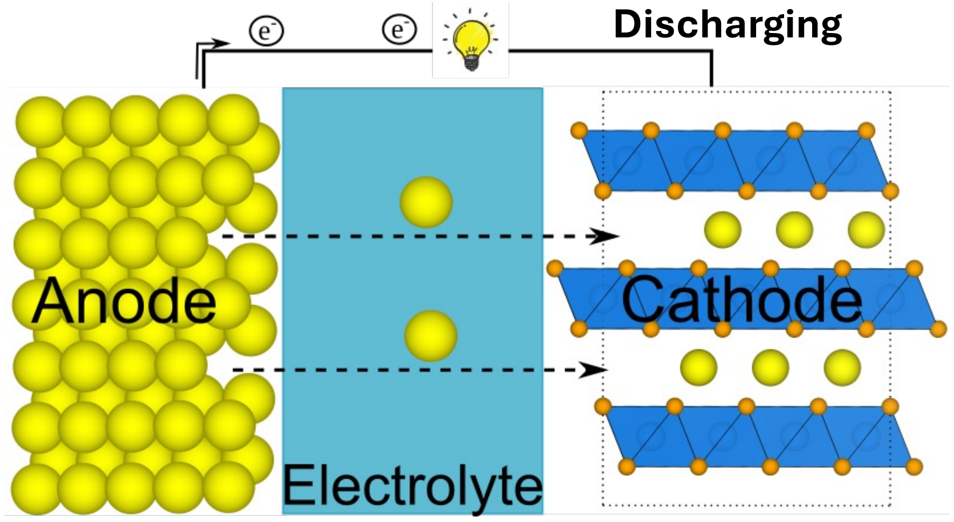
Department of Materials Engineering
Indian Institute of Science

Date: 17th November 2025

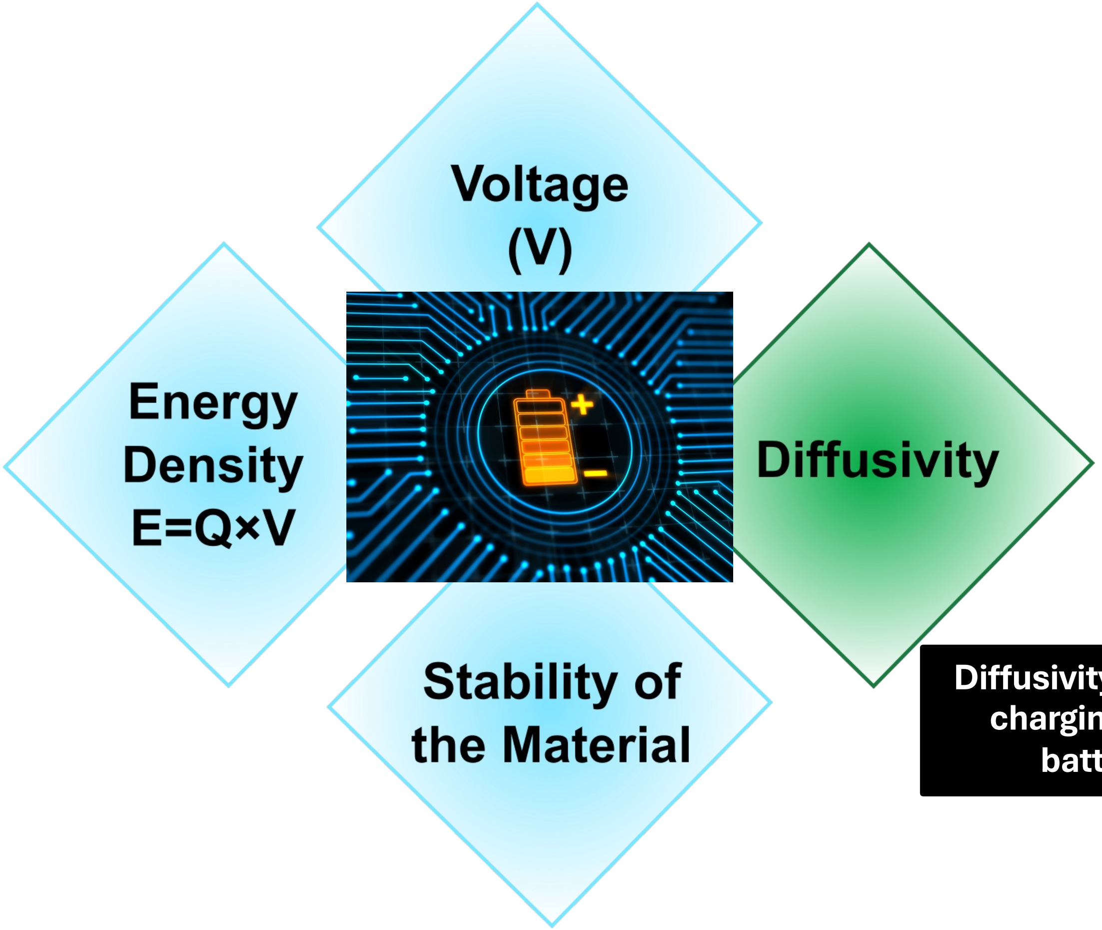
Email: reshmadevi@iisc.ac.in

Migration Barriers: A bottleneck in Battery Design

- Rechargeable Alkali-ion batteries: Essential energy storage solution



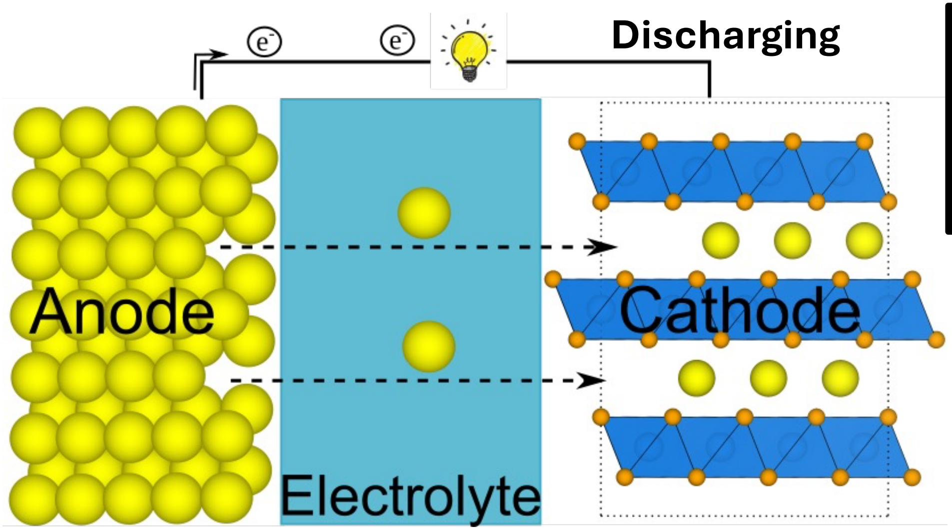
Usage of better Materials ==> Better Performance



Diffusivity determines the charging rates of your battery system

Migration Barriers: A bottleneck in Battery Design

- Rechargeable Alkali-ion batteries: Essential energy storage solution
- Next generation electric devices benefit from high energy density materials with better charging/discharge rates

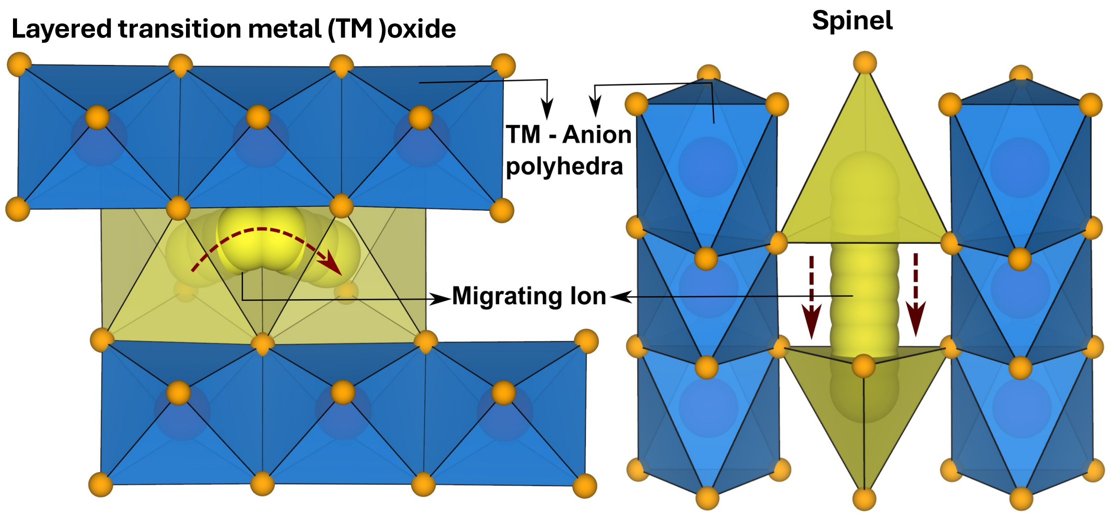


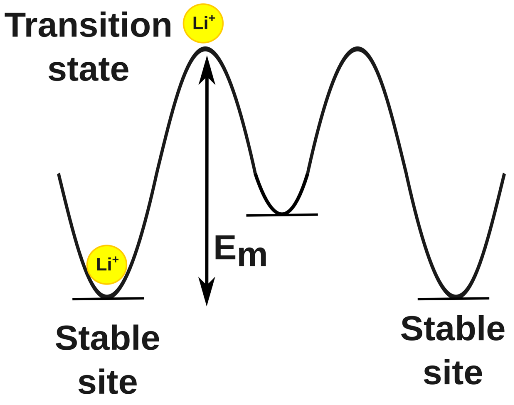
Estimating ionic diffusivity is highly important for novel material discovery

- In intercalation electrodes and electrolytes ionic diffusivity within the bulk influence the rate performance

$$D = D_0 \exp\left(\frac{-E_m}{K_B T}\right)$$

D : Ionic diffusivity
D_0 : Diffusivity pre-factor
E_m : Migration barrier
K_B : Boltzmann constant
T : Temperature

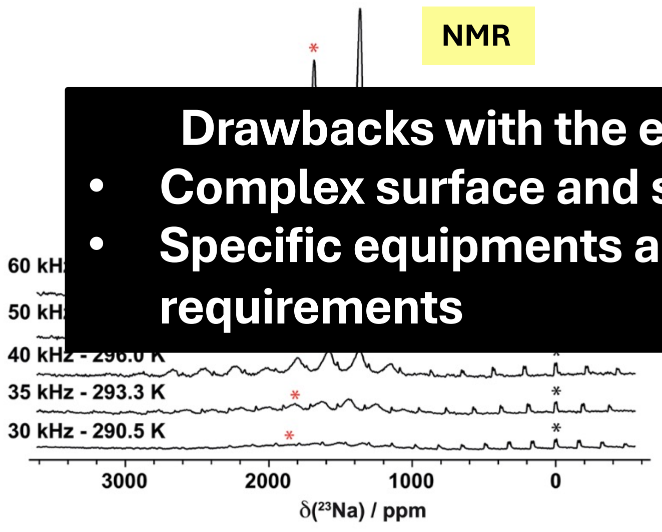


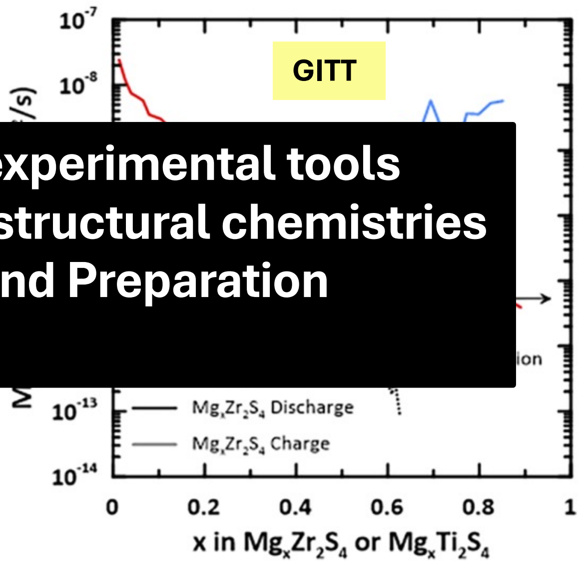


Minimum energy path (MEP)

Estimation of E_m is highly tricky

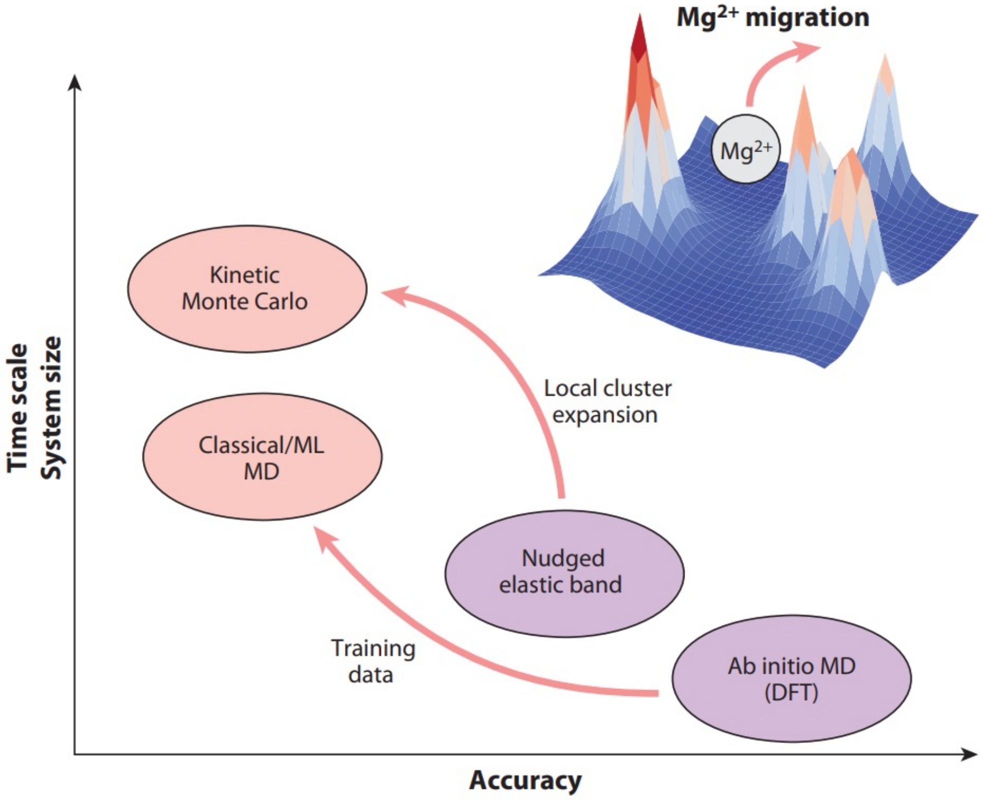
- Experimentally E_m is estimated using techniques like Galvanostatic intermittent titration technique (GITT)[1], electrochemical impedance spectroscopy (EIS), and nuclear magnetic resonance (NMR)[2]





Drawbacks with the experimental tools

- **Complex surface and structural chemistries**
- **Specific equipments and Preparation requirements**



- Computationally E_m is estimated using ab initio molecular dynamics (MD) and **nudged elastic band (NEB)** techniques

Drawbacks with the computational tools

- **Small simulation cell size**
- **Shorter time and length scales**
- **Significant computational time**

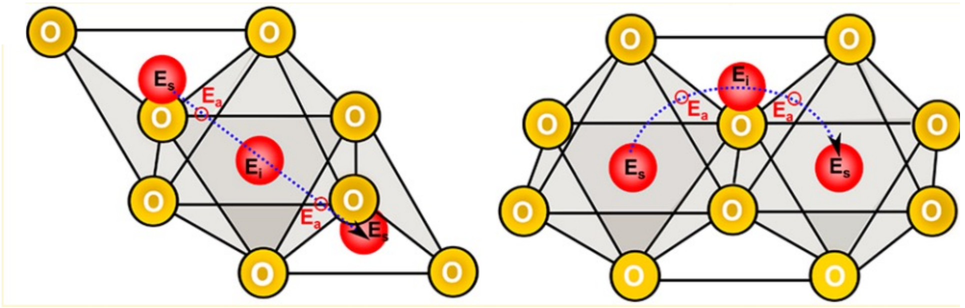
How can we estimate E_m faster with reliable accuracy?

1. Bonnick et al., Chem. Mater. , 30(14), (2014)
2. R. J. Clement et al., Annu. J. Mater. Chem. A, 5, 4129 (2017)
3. Gao et al., Annu. Rev. Mater. Res. 52:6.1-6.30(2022)

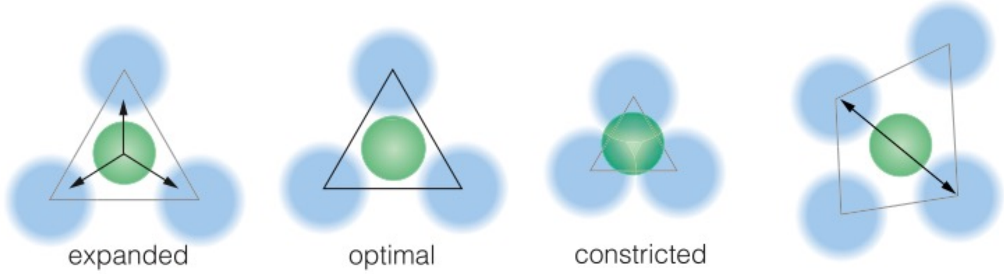
Insights so far from the literature - Design principles and Models

Materials design rules for multivalent ion mobility in intercalation structures [1]

- Avoid preferred coordination environment
- Reduce changes in the coordination numbers during migration



Searching ternary oxides and chalcogenides as positive electrodes for calcium batteries [2]



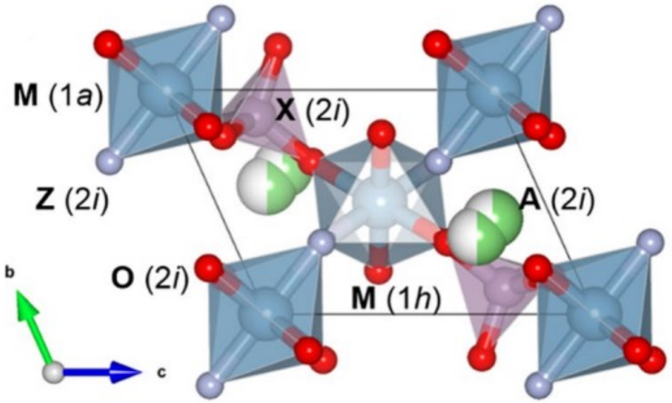
- Select structures with optimal diagonal/area/volume fraction of migrating cation
- Reduce changes in the volume fraction during migration

Models to estimate E_m directly

- Jalem et al., utilized descriptor-based machine learning (ML) or Neural Network(NN) models to predict E_m in 72 Olivines($AMXO_4$)[3] and 317 Tavorites ($AMXO_4Z$)[4]

  A: Li/Na; M: Main group element; X: Group 14,15,16; Z: F/Cl/Br/I

- Reported R^2 score: 0.978 and root mean squared error (RMSE):0.0619



1. Rong et al., Chem. Mater. 27, 6016-6021 (2015)
2.Lu et al., Chem. Mater. 33, 5809-5821 (2021)
3. Jalem et al., Sci Rep, 8,5845 (2018)
4. Jalem et al., J. Mater. Chem. A, 2, 720-734 (2014)

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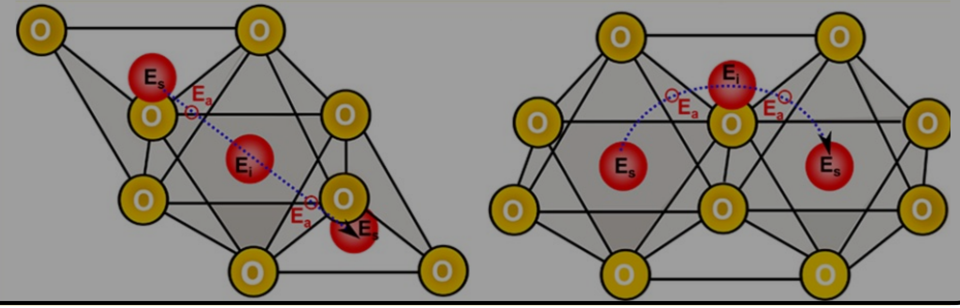
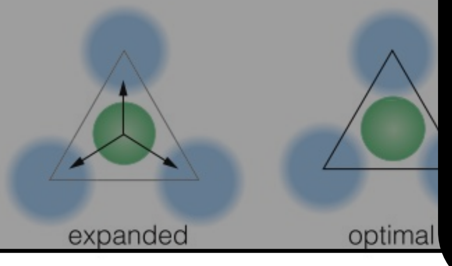


Searching ternary oxides



al/area/volume

migration

Significant Limitations

- Poor generalizability across different chemistries or structures
- Trained on specific chemistries or structures
- Less Predictive accuracy outside the scope of training dataset

Models to estimate E_m directly

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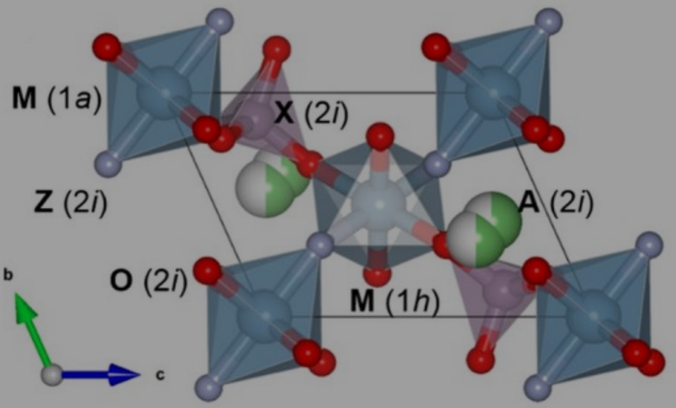

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3. Jalem et al., Sci Rep, 8,5845 (2018)
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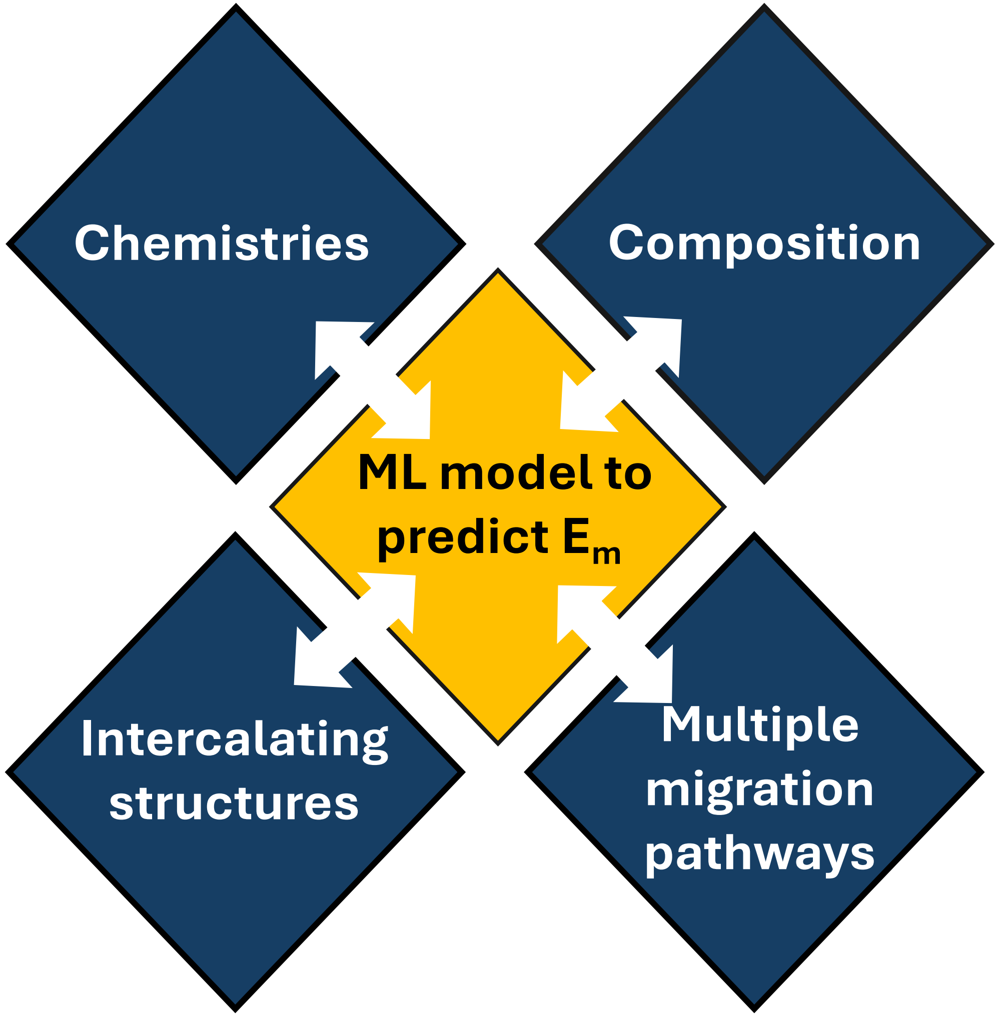
Faster and accurate estimation of E_m is important

What do we propose?



1. How accurately can the current state of the art techniques estimate E_m?

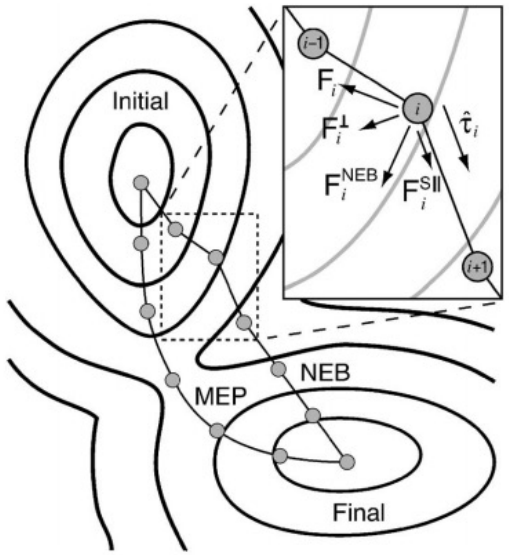
2. Do we have a reliable database with different chemistries, composition and structures to construct an ML model to predict E_m?

3. Constructing a generalizable ML model

   A. How do we solve the data-inadequacy issue?

   B. How do we construct a generalizable model with all the insights gained so far?

3 handles and 9 distinct systems considered



- **NEB**[1] calculations directly evaluate E_m
- Estimates the saddle point by optimising the perpendicular component of the force
- In climbing image **(CI)**, spring forces on the image with highest energy is removed

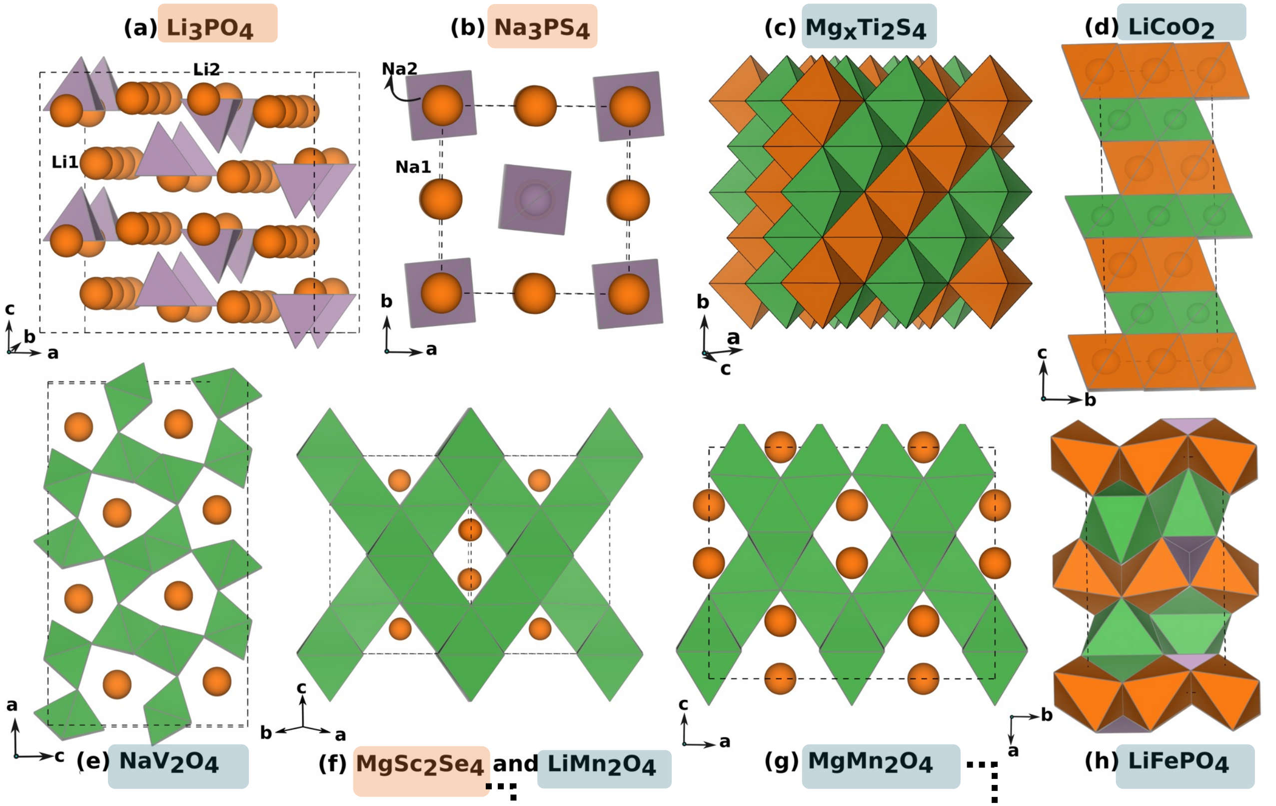
NEB used in conjunction with Density Functional Theory(DFT)[2,3]

Exchange correlational (XC) functional

1. Strongly constrained and appropriately normed (SCAN) [4]
2. Generalized gradient approximation (GGA) [5]
3. DFT + Hubbard(U) [6]

Addition of uniform background charge (NELECT)

Addition of CI approximation



3 electrolytes

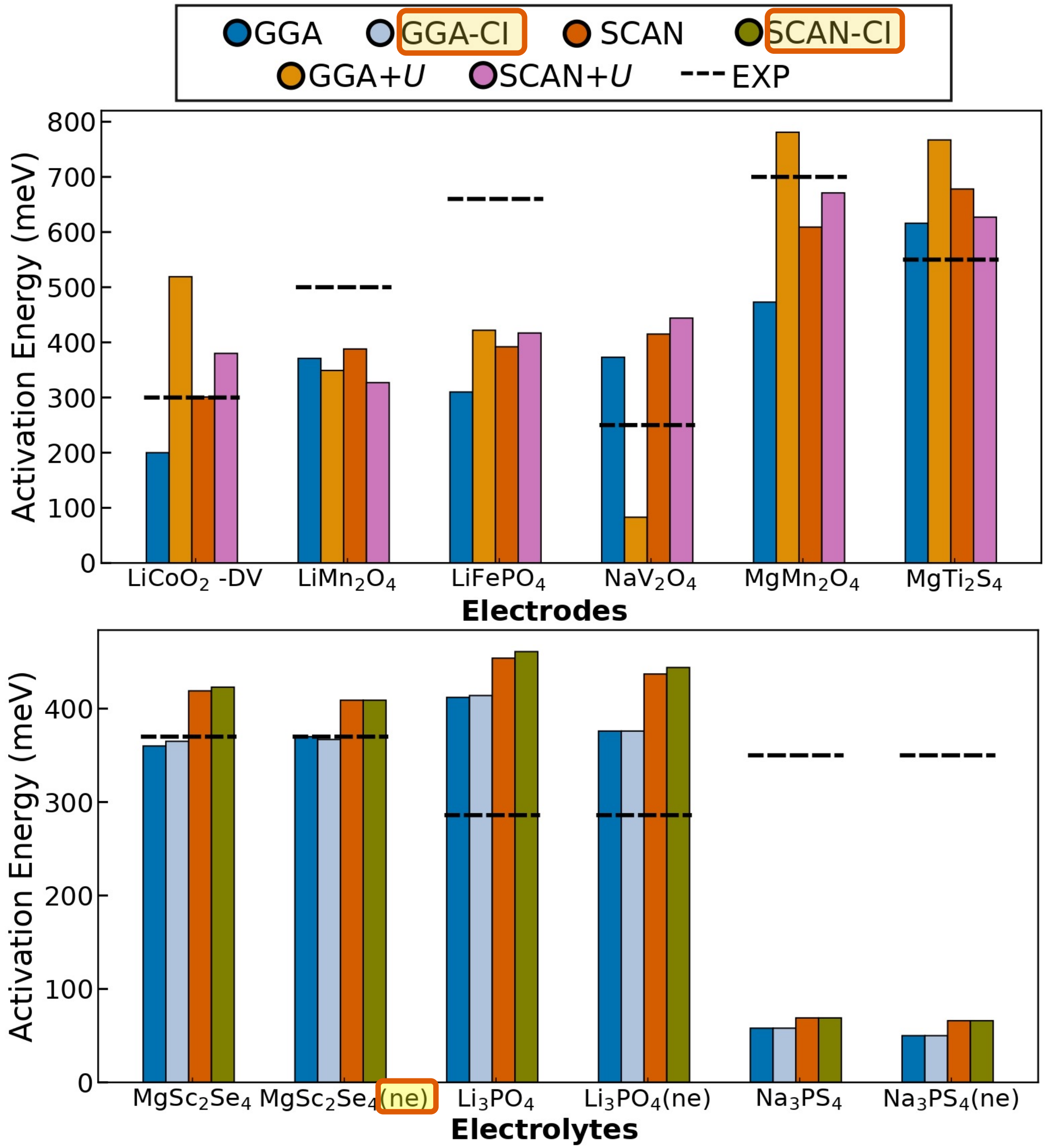
6 electrodes

Why these systems?

- Heterogeneity of intercalation ion
- Diversity of structural frameworks
- Availability of experimental data

1. Sheppard et al., Chem. Phys. 128, 134106 (2008)
2. Kohn & Sham, Phys. Rev. 140, A1133 (1965)
3. Hohenberg et al., Phys. Rev. 136, B864 (1964)
4. Sun et al., Phys. Rev. Lett. 115, 036402 (2015)
5. Perdew et al., Phys. Rev. Lett. 77, 3865 (1996)
6. Anisimov et al., Phys. Rev. B 44, 943 (1991)

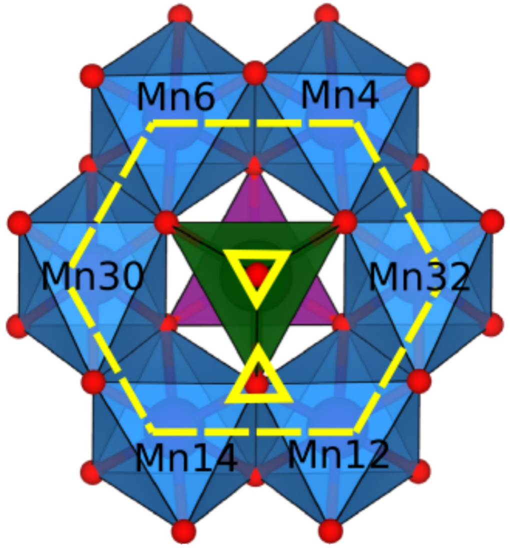
SCAN exhibits better numerical accuracy on average



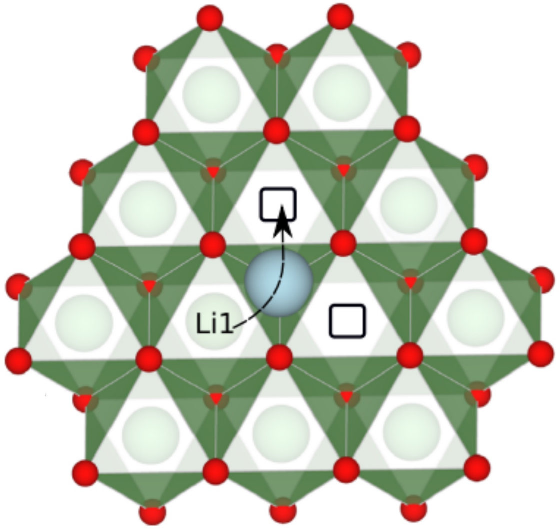
- Addition of NELECT or CI does not affect E_m
- E_m from SCAN > E_m from GGA
- E_m from SCAN+*U* < GGA+*U*

SCAN has lower mean absolute error (MAE = 140 meV) compared to other functionals (>145 meV)

Two Systems to highlight the trends and anomalies

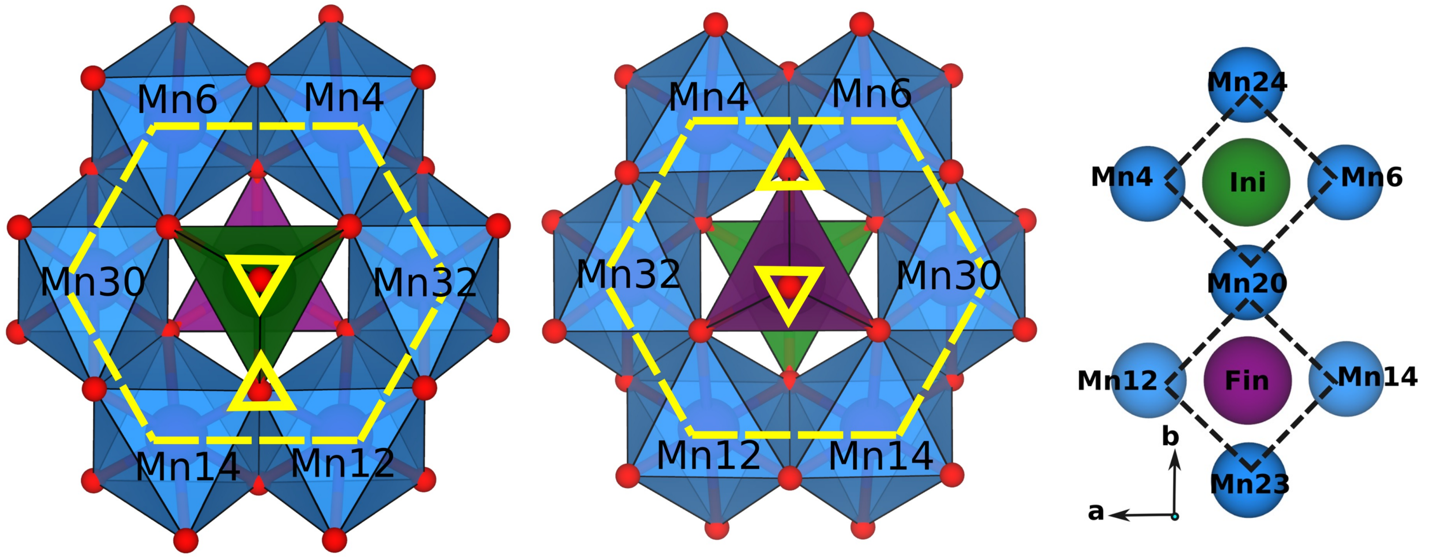


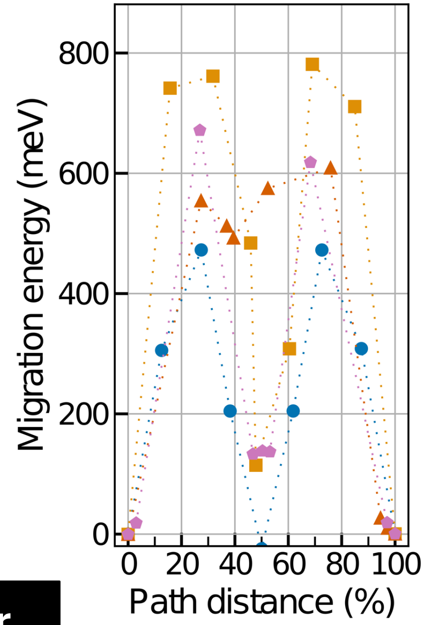
$MgMn_2O_4$

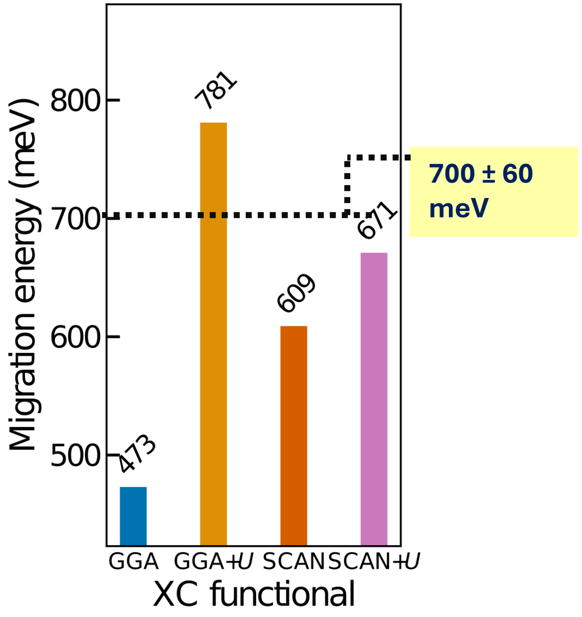


$LiCoO_2$

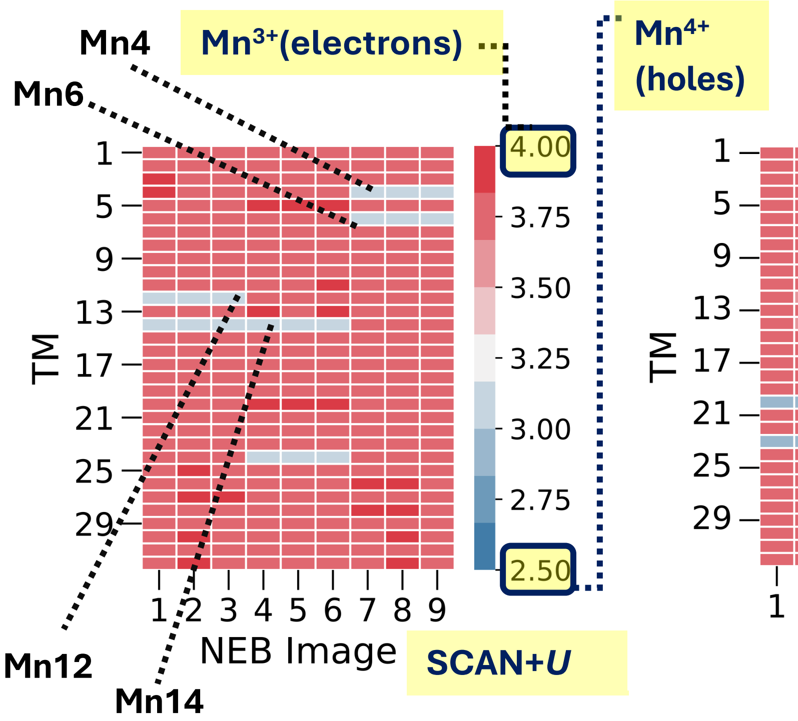
Spinel-$MgMn_2O_4$: GGA underestimates significantly

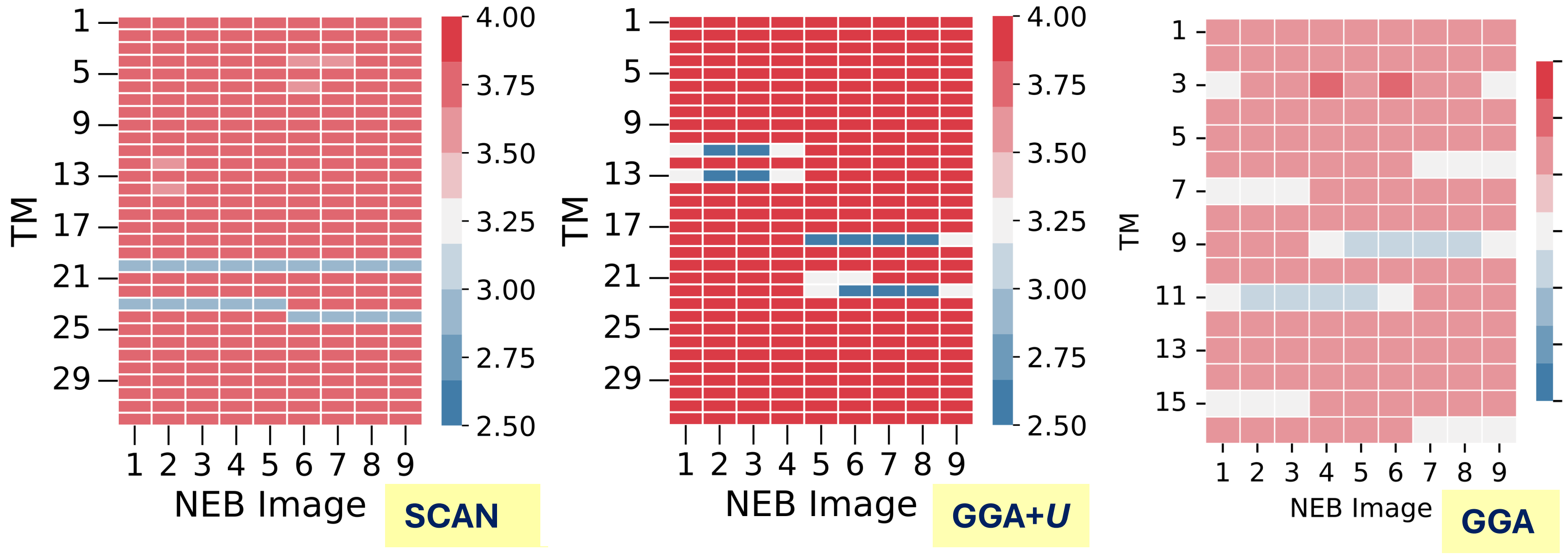




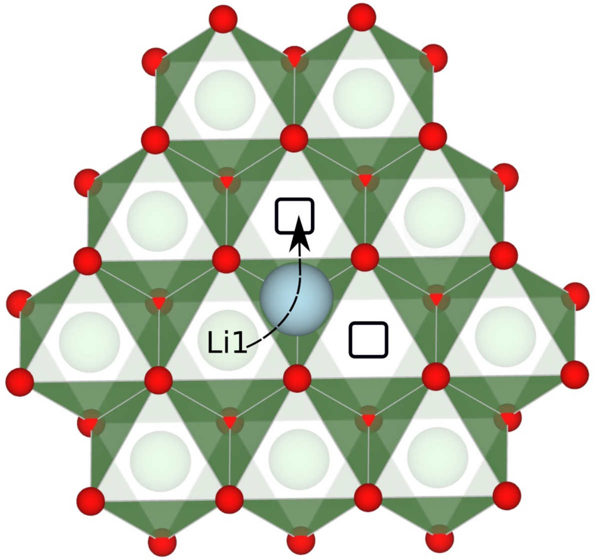


$MgMn_2O_4$ is a semiconductor



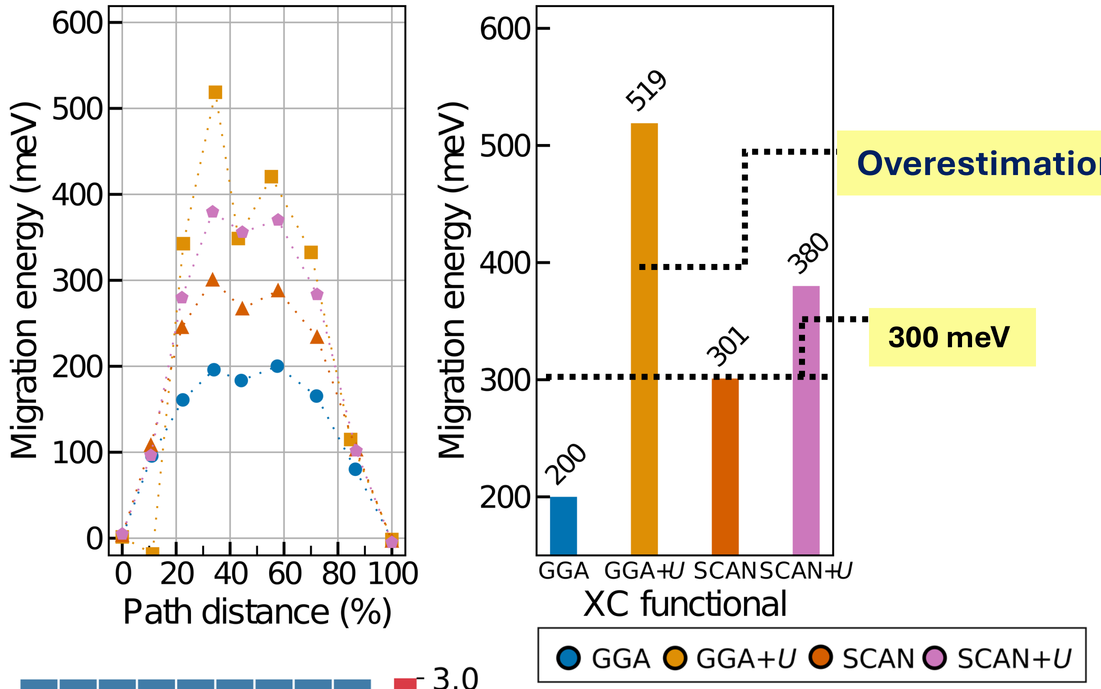


Layered-$LiCoO_2$: GGA+*U* overestimates significantly

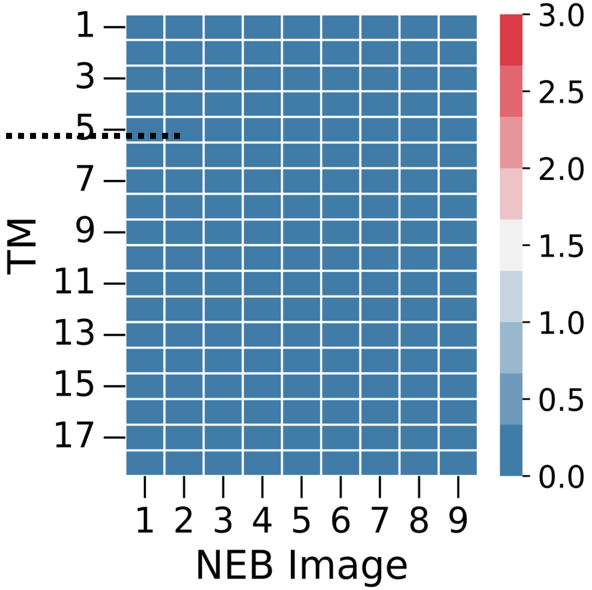


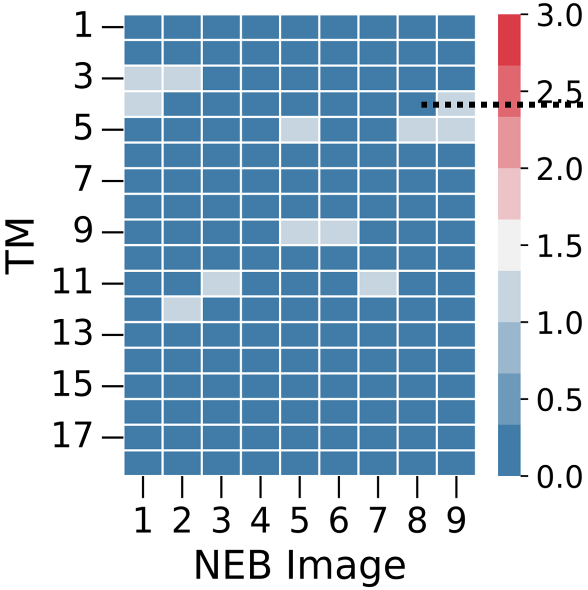
Tetrahedral site hop (TSH)

$LiCoO_2$ is metallic for most of the Li compositions



Overestimation by GGA+*U*





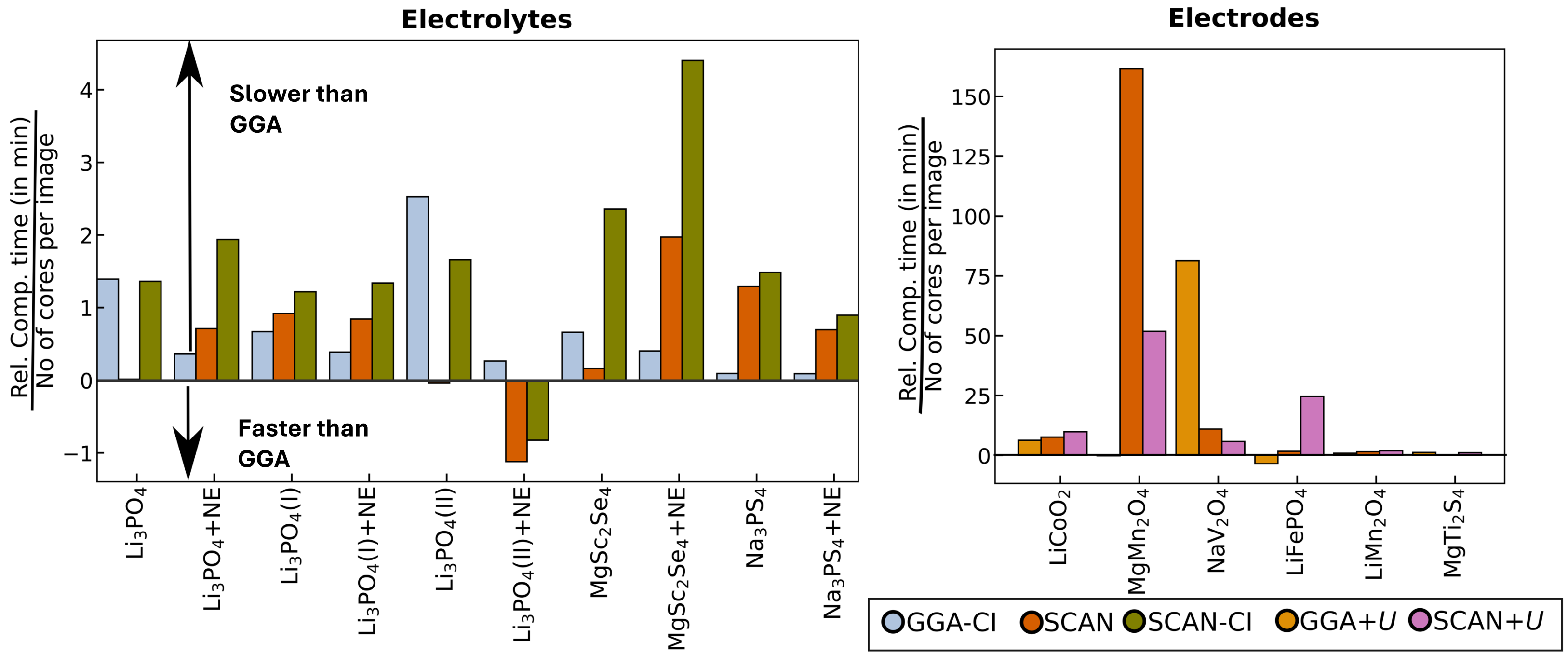
Other functionals

GGA+*U* shows spurious localization of electrons

Computational cost: Is SCAN-NEB worth it?

- SCAN has better numerical accuracy on average when compared to other XC functionals
- SCAN (and SCAN+*U*) captures the underlying electronic structure well

But is SCAN worth pursuing? → **Need to look at the computational time**



- Computational time reduces by 75% in the case of GGA/GGA+*U* vs. SCAN
- SCAN is typically faster than SCAN+*U*
- Convergence difficulties encountered in the case of SCAN/SCAN+*U*

GGA for "quick" estimation

SCAN for "better" accuracy

Q2: Can we obtain a reliable dataset of E_m to construct an ML model?

Title: **A literature-derived dataset of migration barriers for quantifying ionic transport in battery materials**

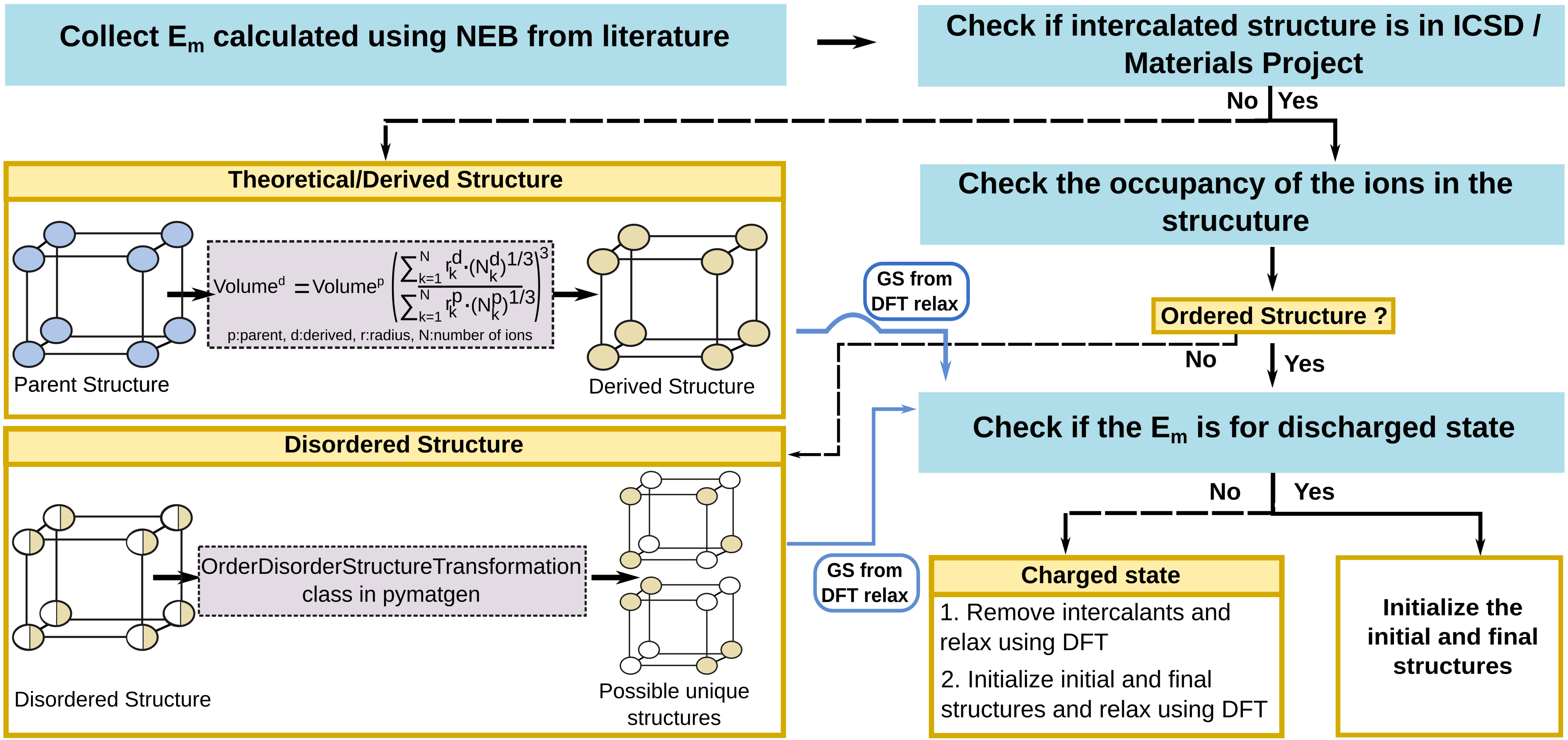
Authors: Reshma Devi, Avaneesh Balasubramanian, Keith T. Butler & Gopalakrishnan Sai Gautam

Journal: **To be submitted to Scientific Data**

Keith T. Butler

Avaneesh Balasubramanian

Structural data generation for each datapoint in the curated database

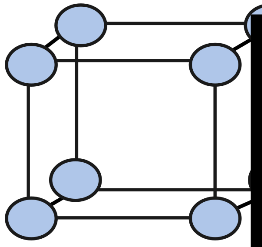


Structural data generation for each datapoint in the curated database

Collect E_m calculated using NEB from literature → Check if intercalated structure is in ICSD / Materials Project

No | Yes

Theoretical/Derived Structure

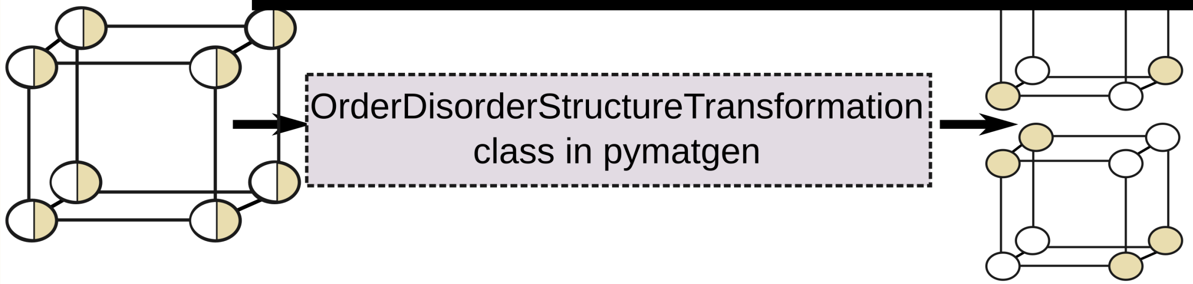


Parent Structure

Check the occupancy of the ions in the strucuture

Ensuring completeness and reliability

- Comprehensive methodology and structural information availability
- Prioritized GGA (or GGA+U) E_m values over other XC functionals
- Well labelled plots/images of E_m/MEP availability



Disordered Structure

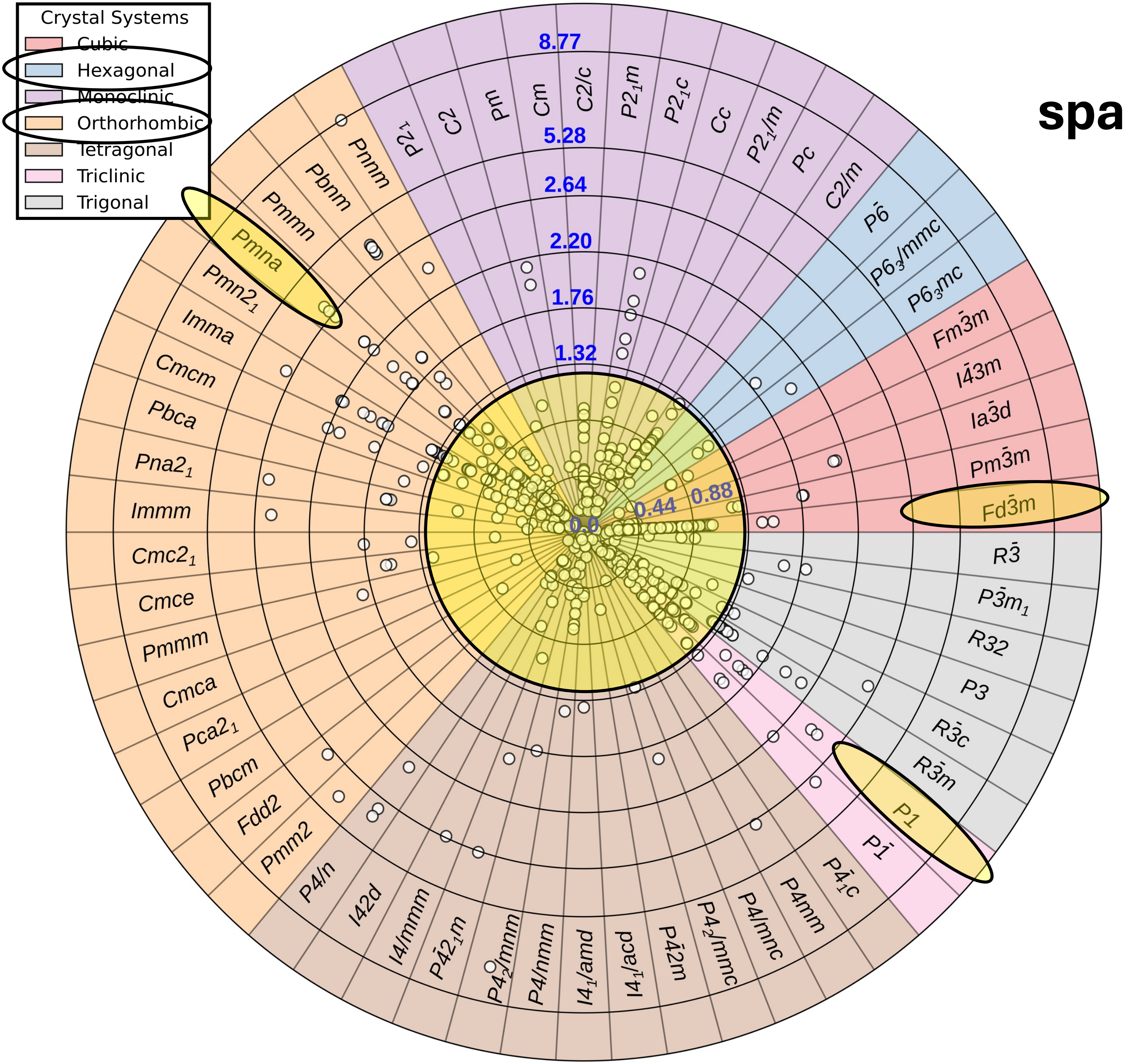
Possible unique structures

GS from DFT relax

Charged state

1. Remove intercalants and relax using DFT
2. Initialize initial and final structures and relax using DFT

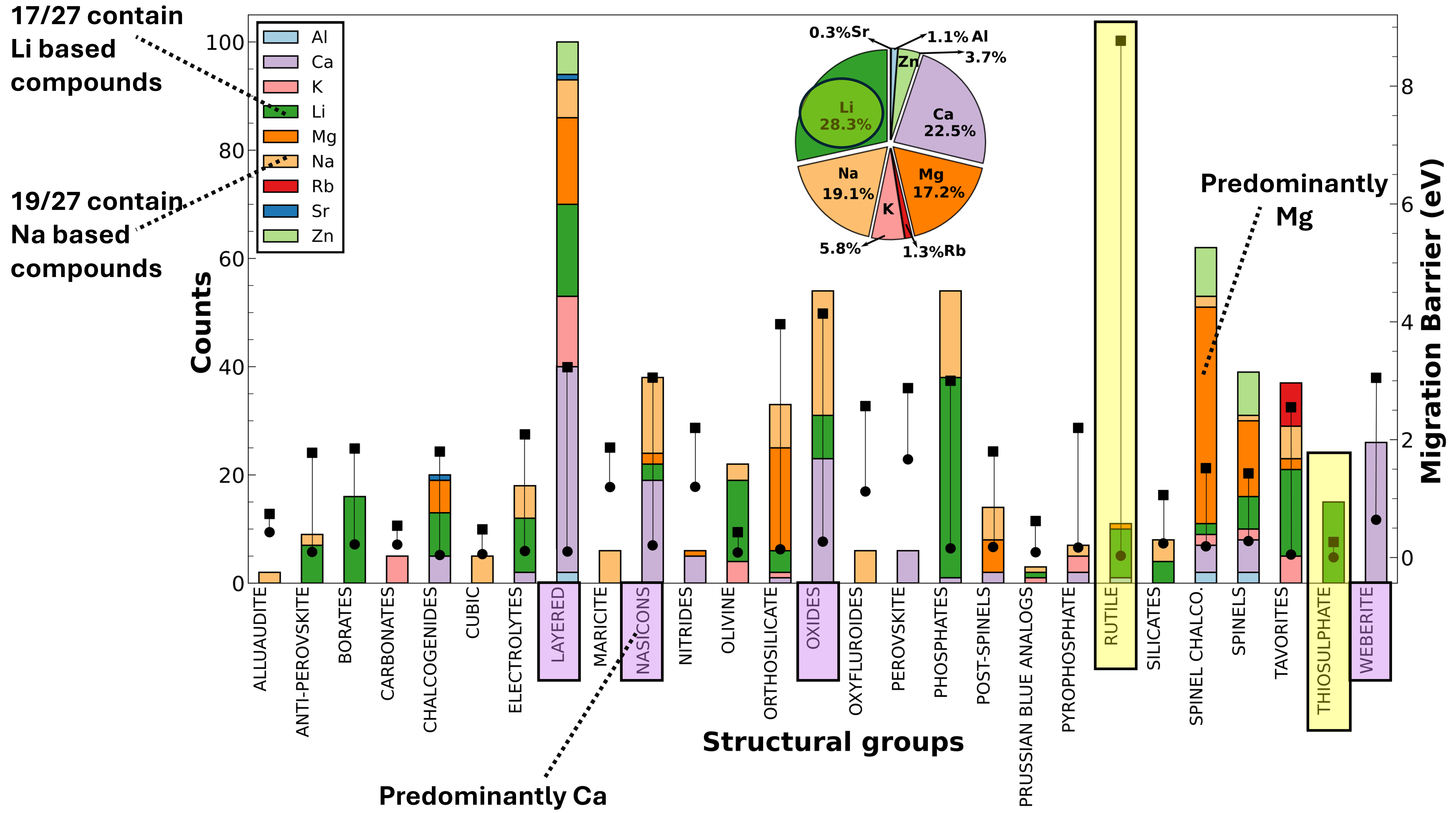
Initialize the initial and final structures



Database of 619 datapoints spanning 58 different space groups across 7 crystal systems

- E_m values range between 0.03 to 8.77 eV
- 528: Electrodes; 91: Electrolytes
- ***Fd$\bar{3}$m*** (Cubic spinels) contribute 94 data entries followed by ***Pnma*** and ***P1*** from orthorhombic and triclinic crystal systems respectively
- Highest: Orthorhombic (206); Lowest: Hexagonal (6)
- Skewed distribution
  - 73.4% of E_m < 1eV
  - 19.4% of E_m between 1-2 eV
  - 7.2% Exceed 2eV

Data distribution across 27 structural groups spanning 9 intercalants



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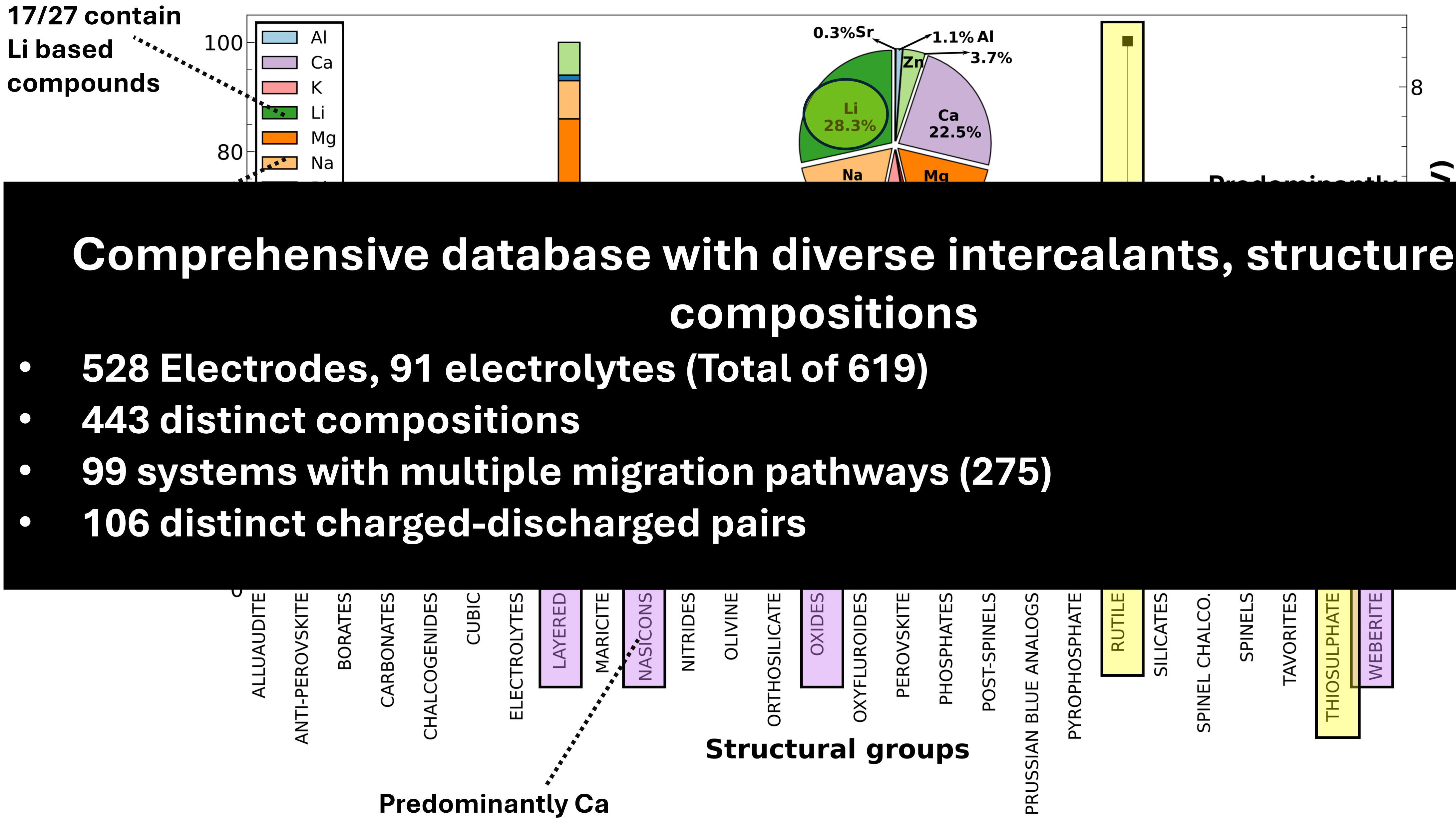


Comprehensive database with diverse intercalants, structures and compositions

- 528 Electrodes, 91 electrolytes (Total of 619)
- 443 distinct compositions
- 99 systems with multiple migration pathways (275)
- 106 distinct charged-discharged pairs

Q3 A: How do we solve the data inadequacy issue in materials science?

Title: **Optimal pre-train/fine-tune strategies for accurate material property predictions**

Authors : Reshma Devi, Keith T. Butler & Gopalakrishnan Sai Gautam

Journal: **npj Computational Materials**

THE ROYAL SOCIETY

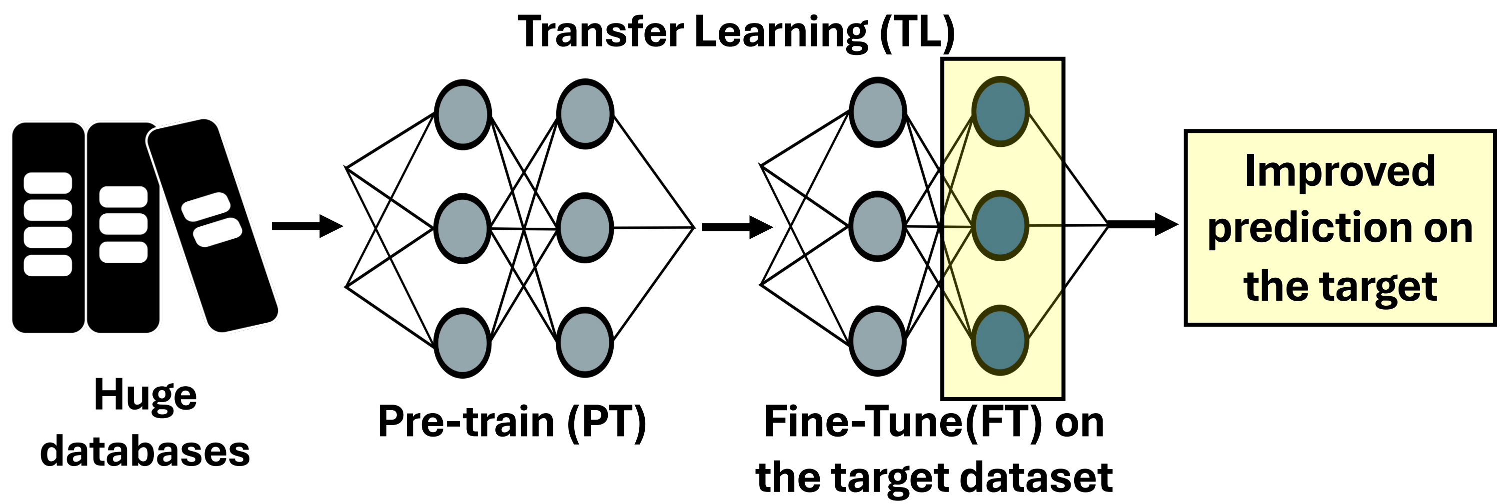
Keith T. Butler

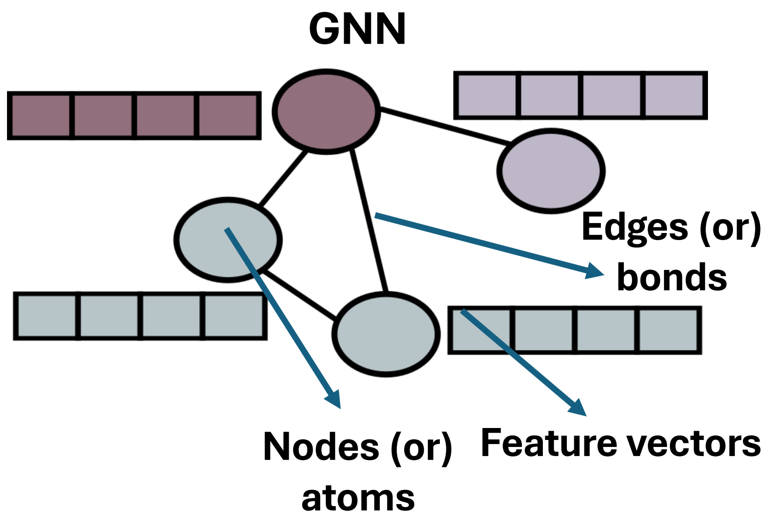
UCL

How to handle data inadequacy in materials science?

- The accuracy of a Machine Learning (ML) model depends on
  - ❑ Quality of data
  - ❑ **Quantity of data** → **Challenging aspect to meet for specific material properties**
  - ❑ Model framework
  - ❑ Training algorithm
- Complex models like Graph Neural Networks (GNNs) perform better at datapoints > 10^4

Construct new models that have less variance when trained on small datasets





Objectives

- What is the best way to do pair-wise TL?
- Is there a strategy to create generalized models that can learn on multiple properties simultaneously?

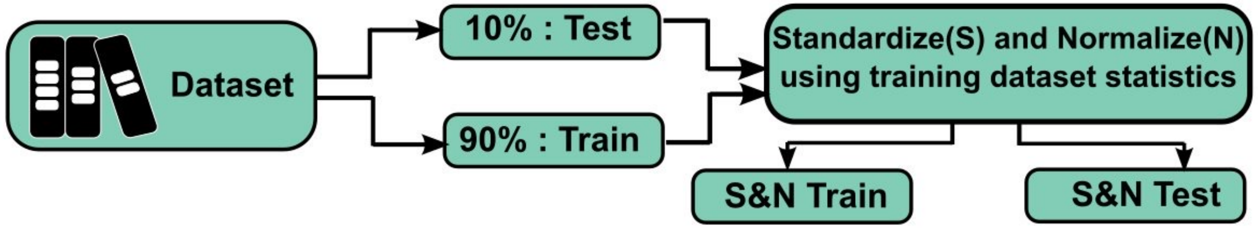
1. Kumar et al. 2024. 2D Mater.

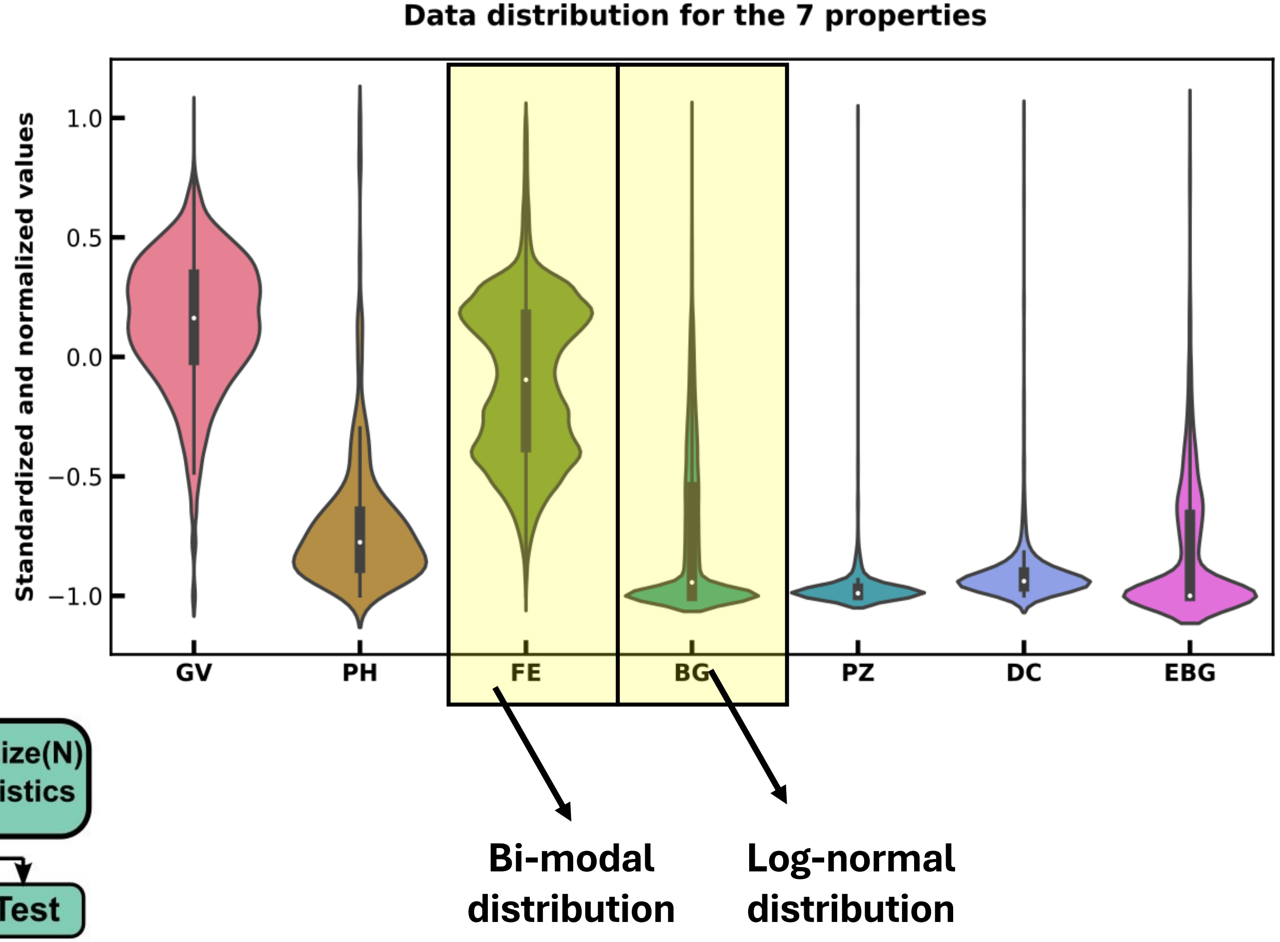
Workflow in obtaining a generalized model

1. Dataset collection and clean-up
2. What parameters to optimize for pair-wise TL?
   - Data sampling
   - Learning rate
   - FT strategy
   - No. of Datapoints
3. Benchmarking the performance of pair-wise models against scratch
4. Construction and benchmarking of generalized models

7 datasets spanning different distribution

Datasets from Matminer[1]	# of Datapoints
Piezoelectric modulus (PZ)	941
Dielectric constant (DC)	1056
Phonons (PH)	1265
Experimental Band gap (EBG)	2481
GVRH (GV)	10987
Band gap (BG)	106113
Formation energy (FE)	132752

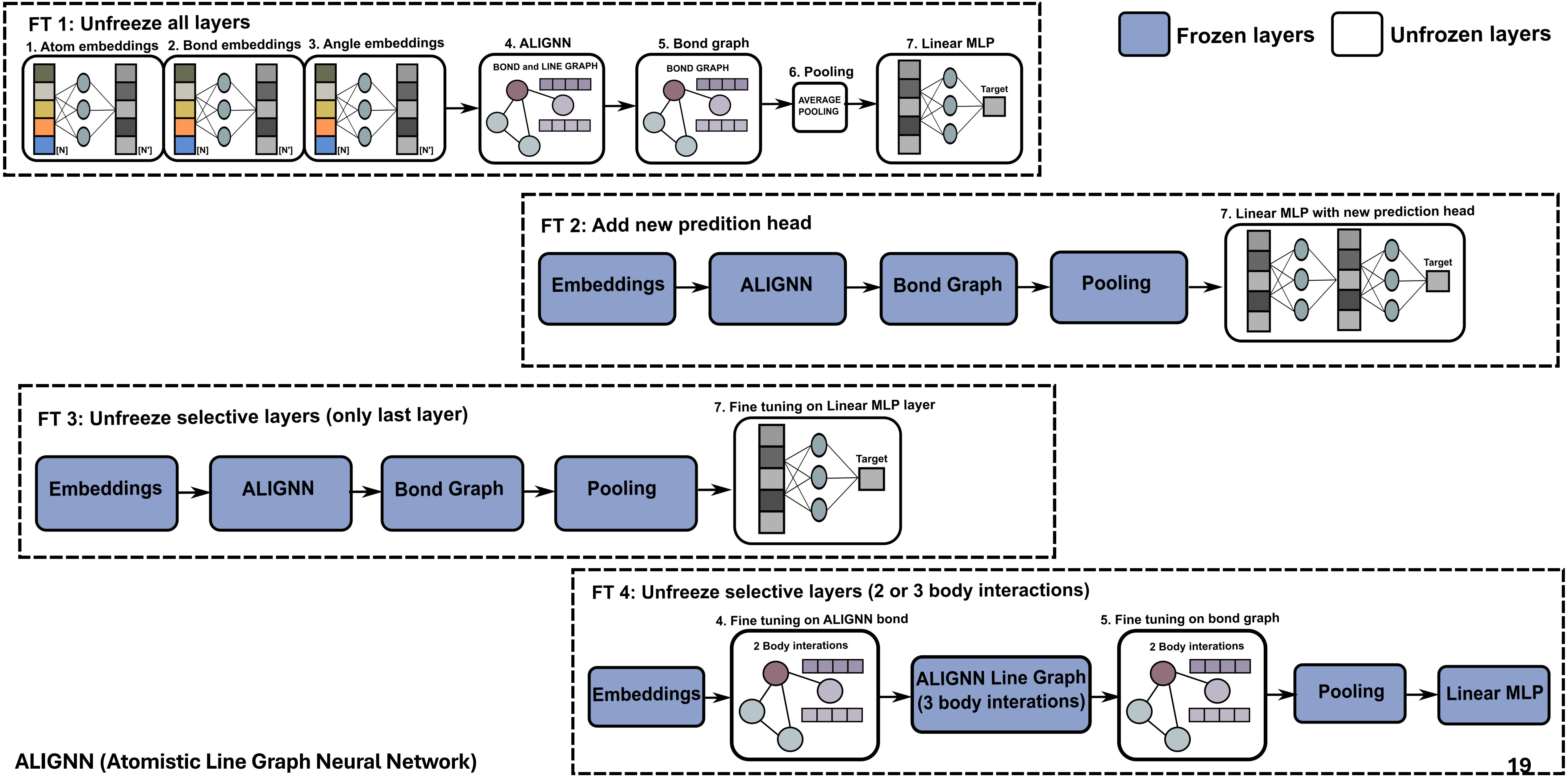




- The test dataset was never used in any of the PT or FT stages
- We report only the test scores in all our results

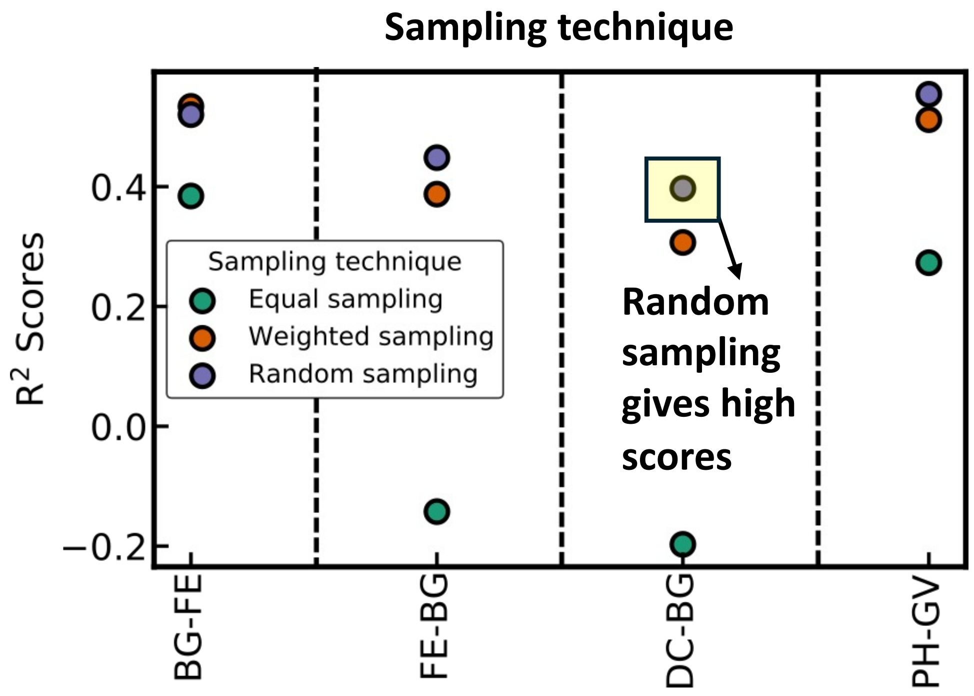
1. Ward et al. 2018. Comput. Mater. Sci.

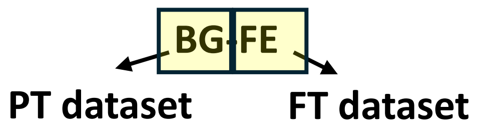
4 Fine-tuning strategies



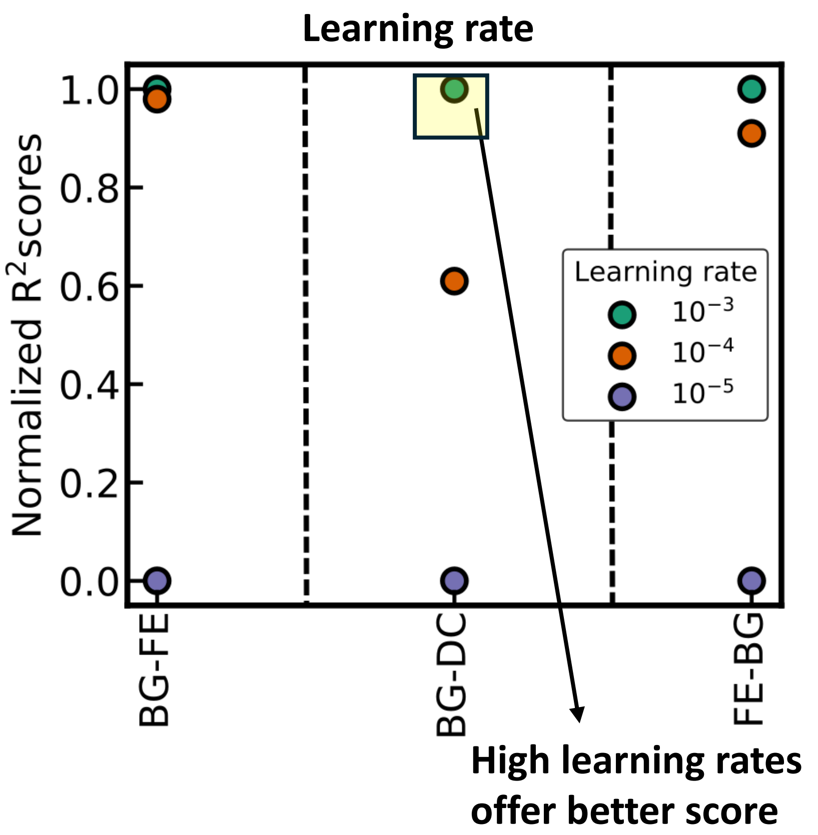
ALIGNN (Atomistic Line Graph Neural Network)

High learning rates and Random sampling for better R^2 scores





Datapoints: 500
Epochs: 500
Batch size: 16
Learning rate: 10^{-4}
(for sampling technique)



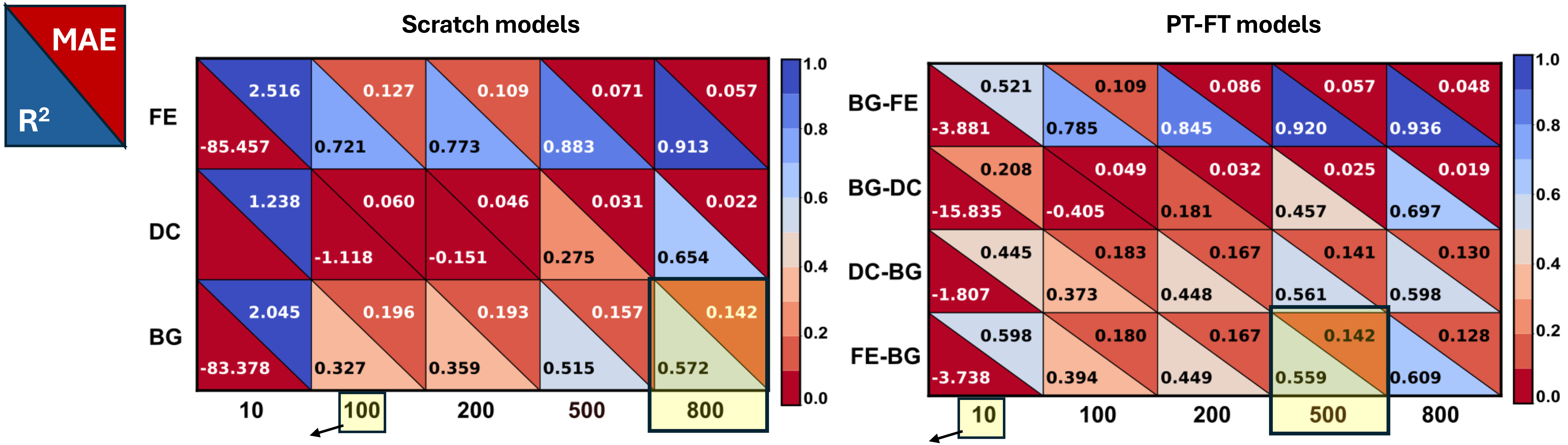
Selective PT-FT pairs were used considering the enormity of the calculation

EBG: Experimental Band gap
GV: GVRH
PZ: Piezoelectric modulus
DC: Dielectric constant

BG: Band gap
PH: Phonons
FE: Formation energy

Random sampling, high learning rates, and high number of datapoints improvise the performance

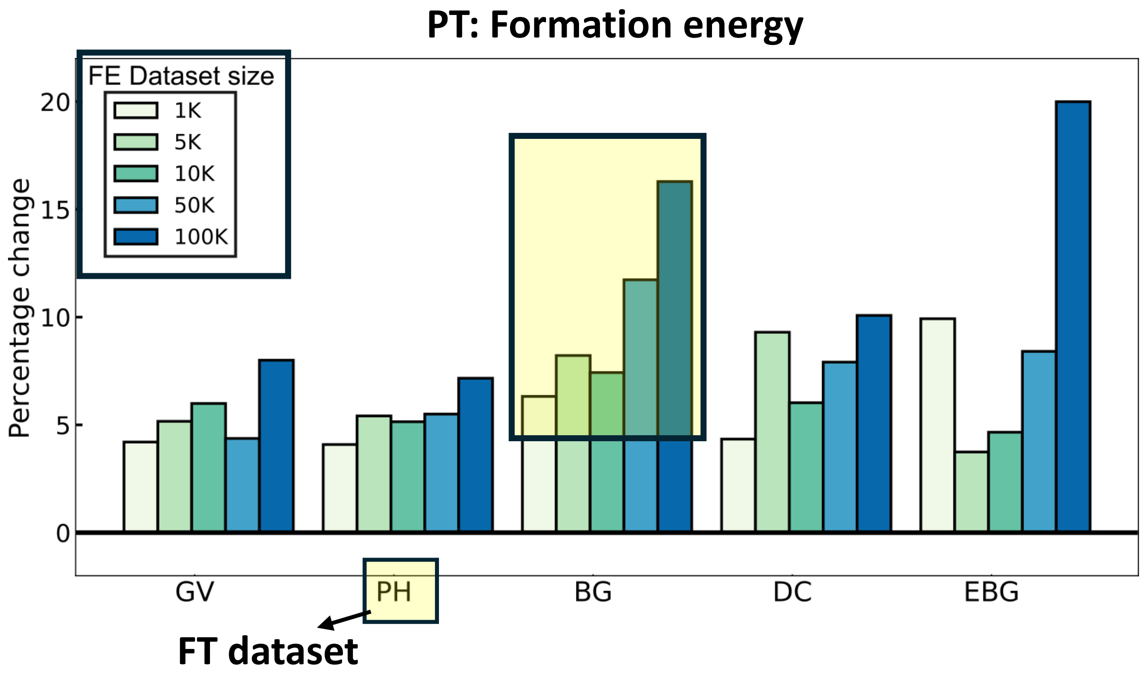
Influence of FT size: R^2 scores increase as FT size increases

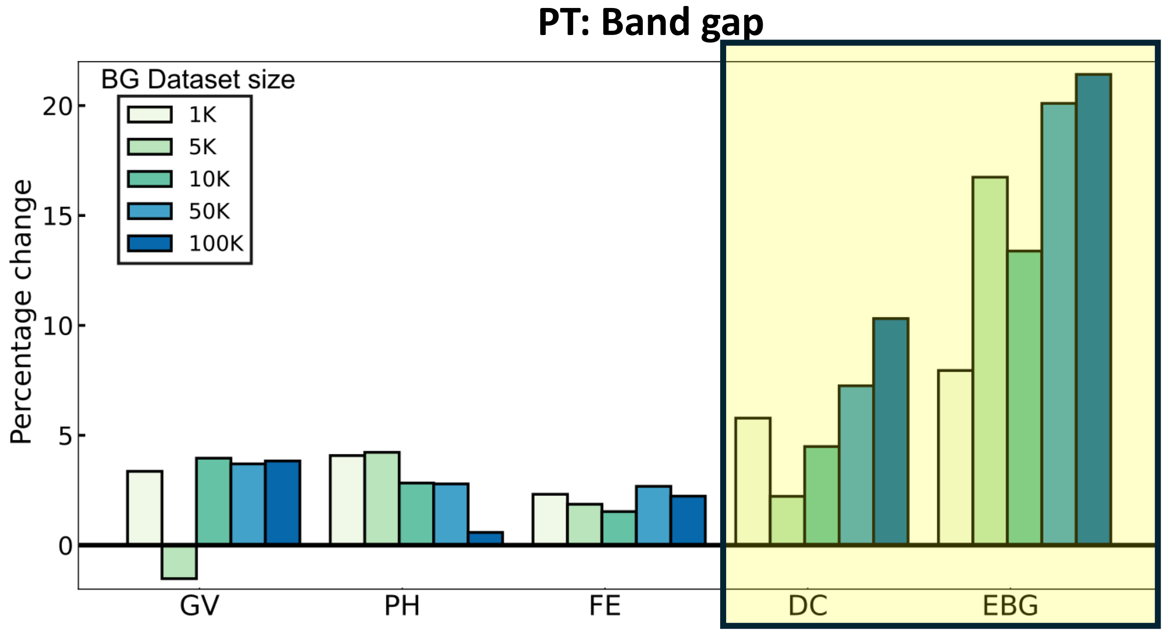


FT size of 800 is identified as optimal and fixed for all following experiments

PT size: 941 (smallest dataset size considered)
FT strategy: Unfreeze all layers
Experiments repeated for 5 different random trials and the mean results are plotted

Influence of PT size: R^2 scores increase as PT size increases





- PT **with FE(100K)** offers the best performance across all FT datasets
- Non-monotonic trend at smaller PT sizes

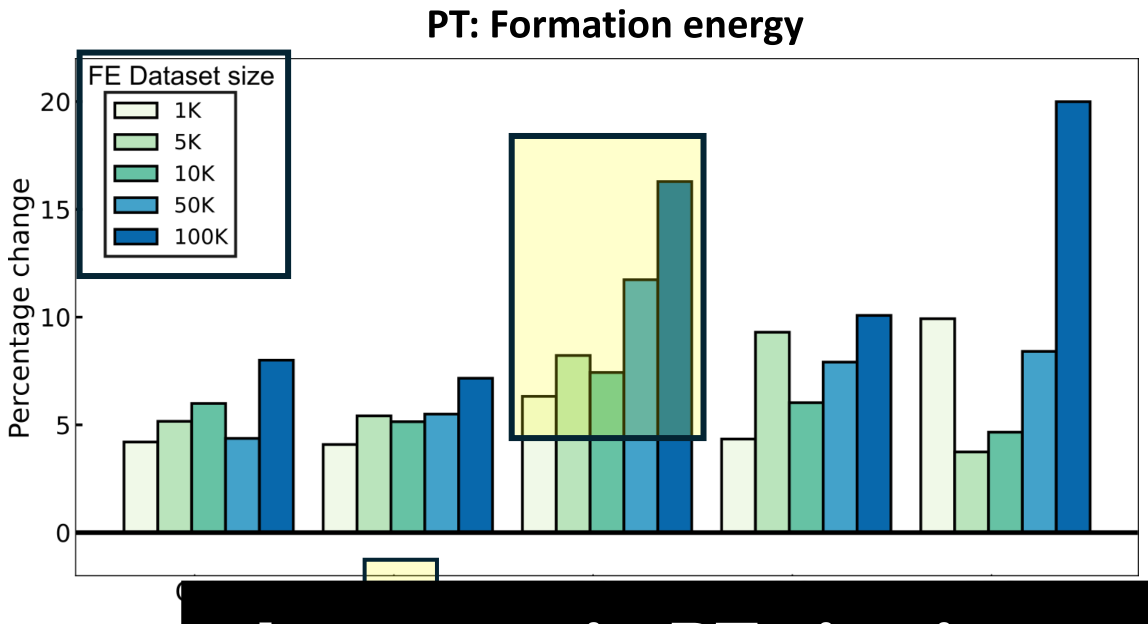
- PT with **BG(50K)** offers the best performance across all FT datasets
- Non-monotonic trend at smaller PT sizes
- BG(100K) Performs specifically better for DC and EBG

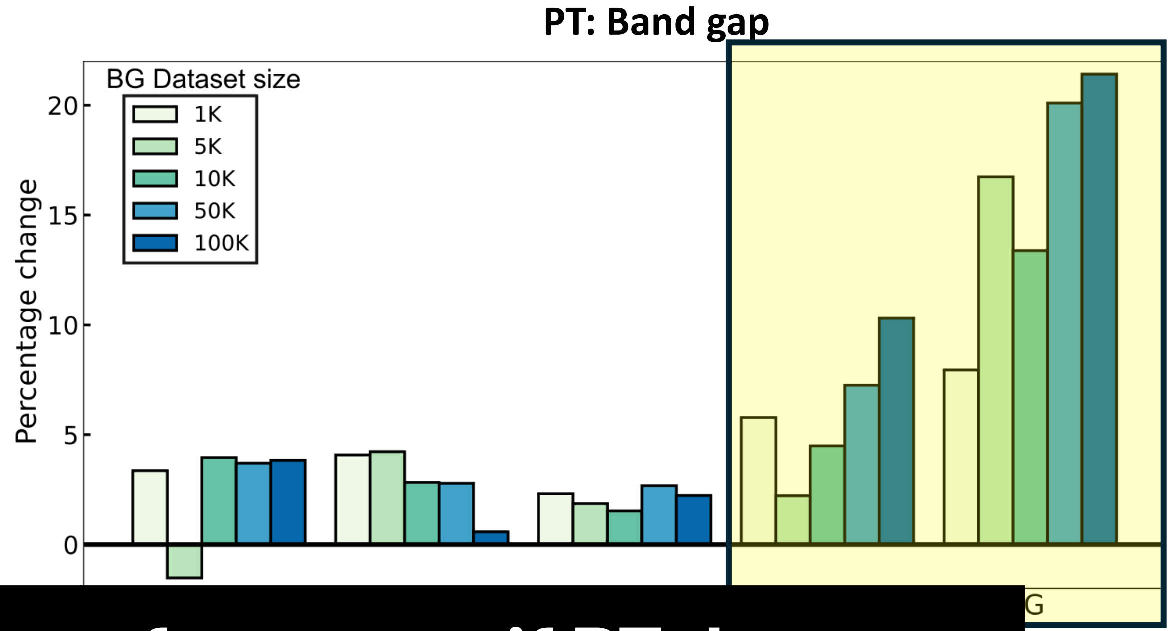
PT size: Largest 2 of the 7 datasets considered – FE and BG
FT strategy: Unfreeze all layers
FT size: 800
Experiments repeated for 5 different random trials and the mean results are plotted

EBG: Experimental Band gap
GV: GVRH
PZ: Piezoelectric modulus
DC: Dielectric constant

BG: Band gap
PH: Phonons
FE: Formation energy

Influence of PT size: R^2 scores increase as PT size increases





Increase in PT size improves performance if PT dataset has normal distribution or if it is correlated with the FT dataset

- PT w … ance … s
  acro …
- Non … or DC
  and EBG

PT size: Largest 2 of the 7 datasets considered – FE and BG
FT strategy: Unfreeze all layers
FT size: 800
Experiments repeated for 5 different random trials and the mean results are plotted

EBG: Experimental Band gap
GV: GVRH
PZ: Piezoelectric modulus
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BG: Band gap
PH: Phonons
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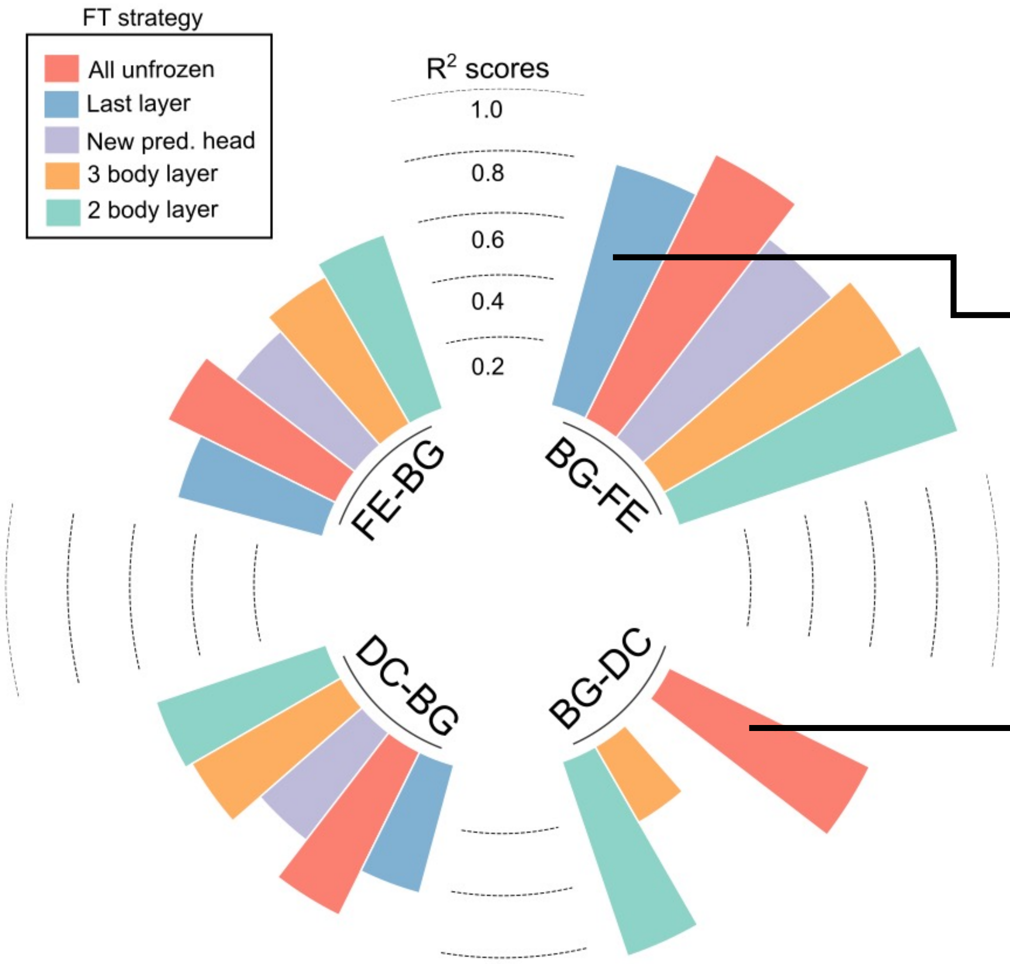
What is the best FT strategy?



PT size: 941
FT size: 800

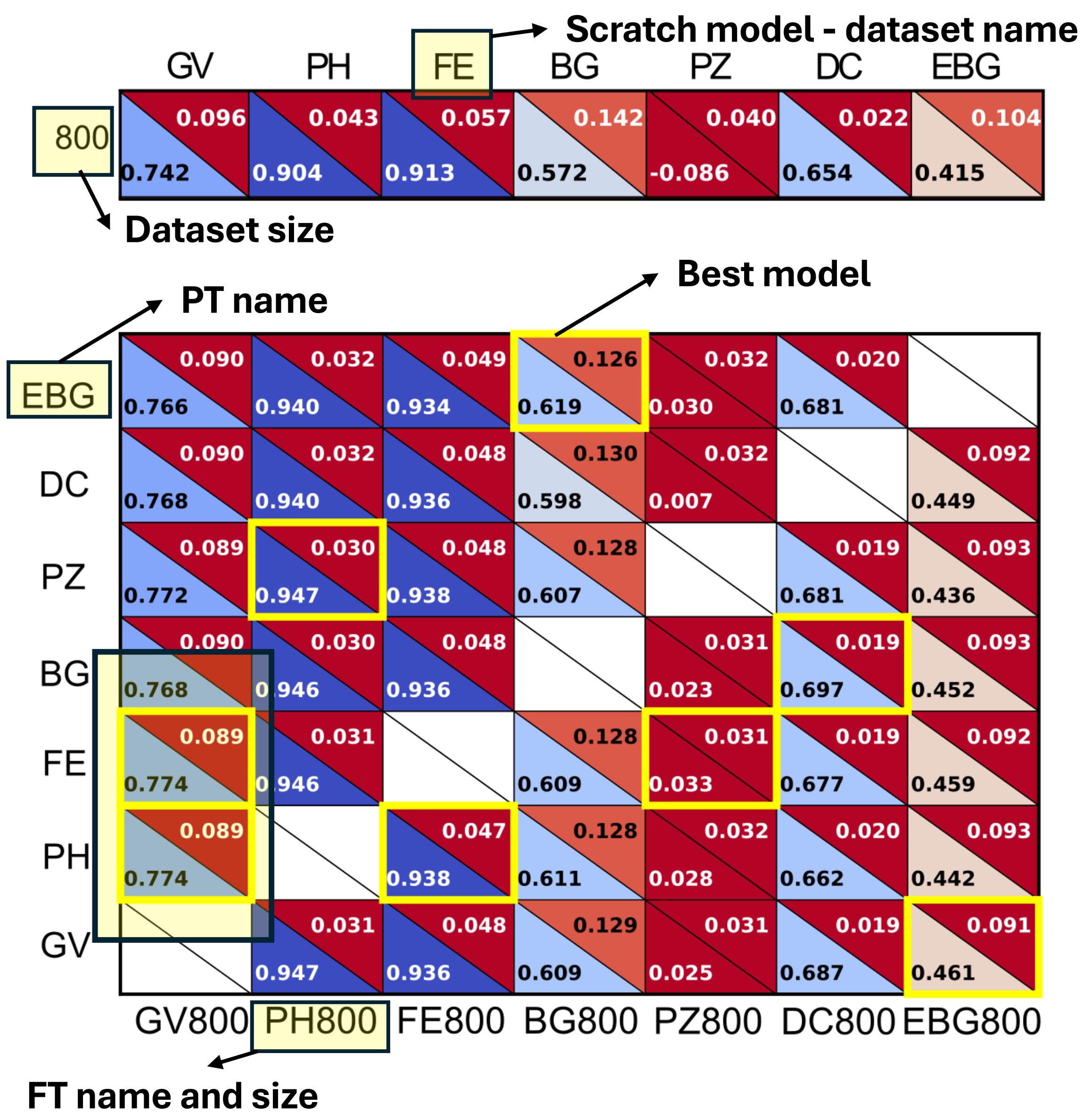
Unfreezing only the last layer offers the least R^2 score

Unfreezing all layers offer the best R^2 score

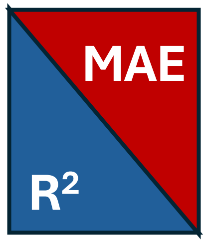
<u>Best strategy: Unfreezing all the layers</u>

Indicates that the PT model requires more re-training to generalize on the FT property

Pair-wise TL on all 7×6 combinations: Better performance at lower datapoints



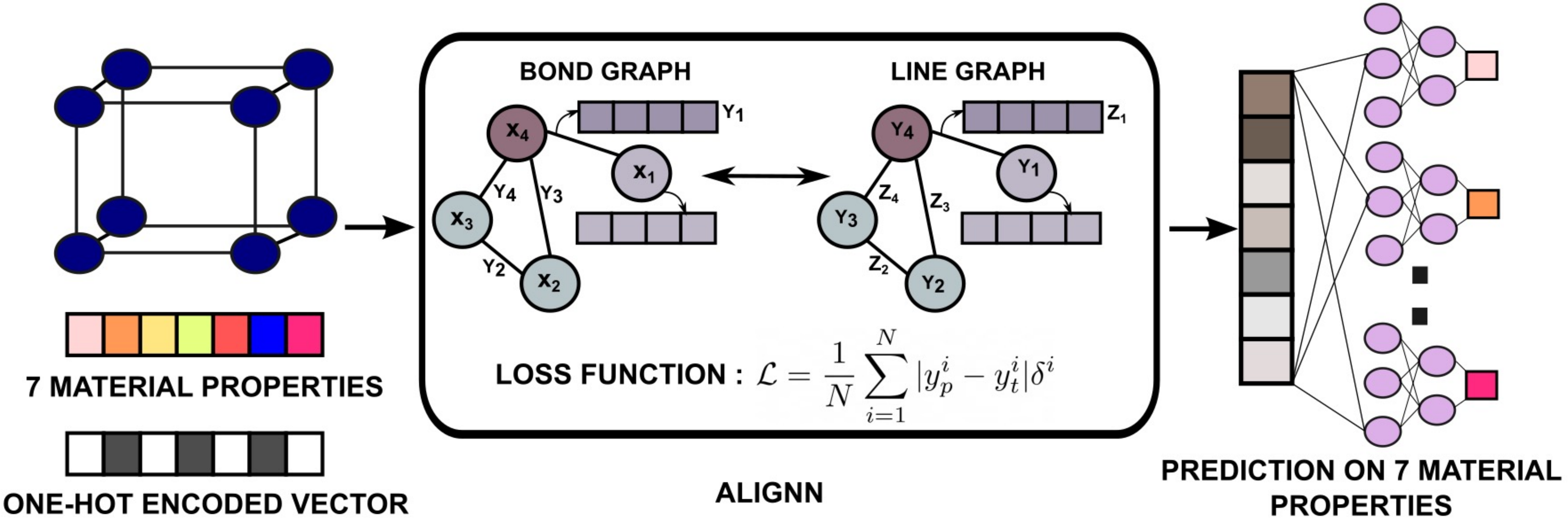
- All PT-FT models perform better than scratch
- Average increase in R^2 score and MAE is 28.4 % and 17.1% respectively
- The specific PT property has little influence on FT when the PT size is capped



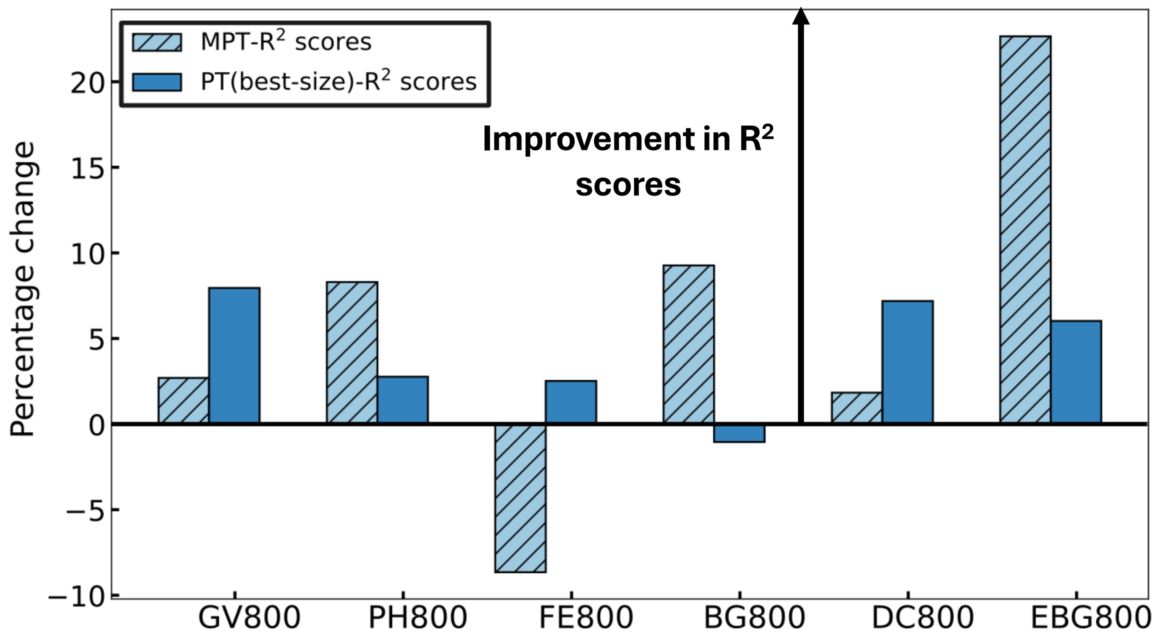
PT size: 941
FT strategy: Unfreeze all layers
FT size: 800
Experiments repeated for 5 different random trials and the mean results are plotted

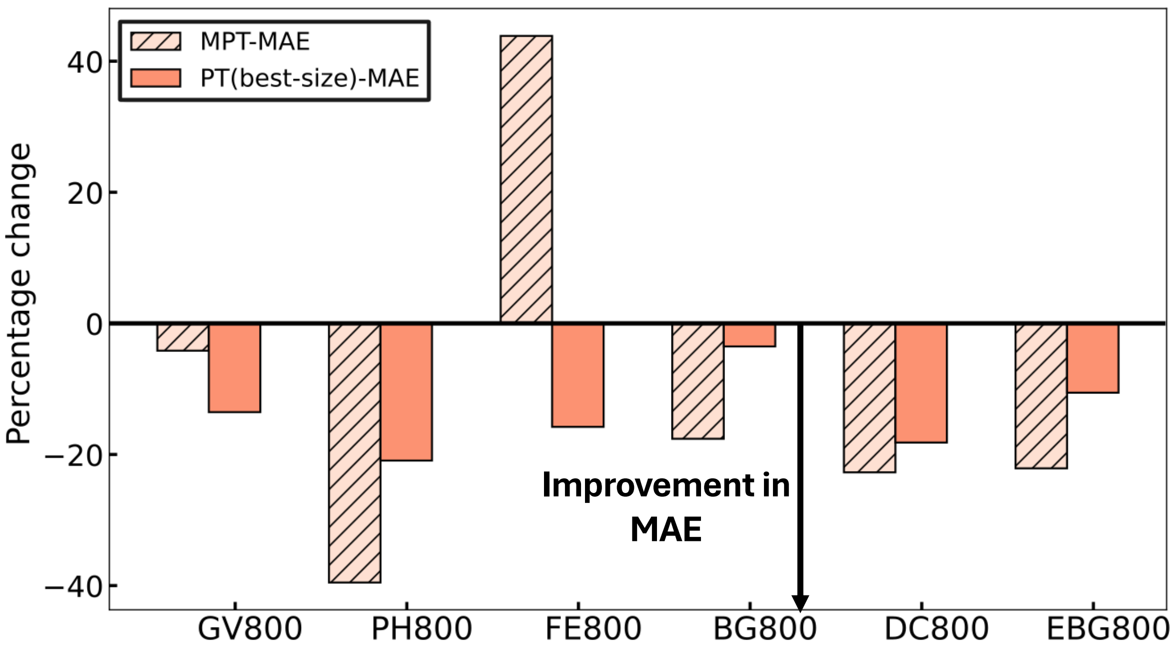
A step towards generalized models : MPT model

- Multi-property pre-trained (MPT) model: Trained with modified loss function on all the seven bulk properties simultaneously



MPT models: Improved R^2scores versus best pair-wise model



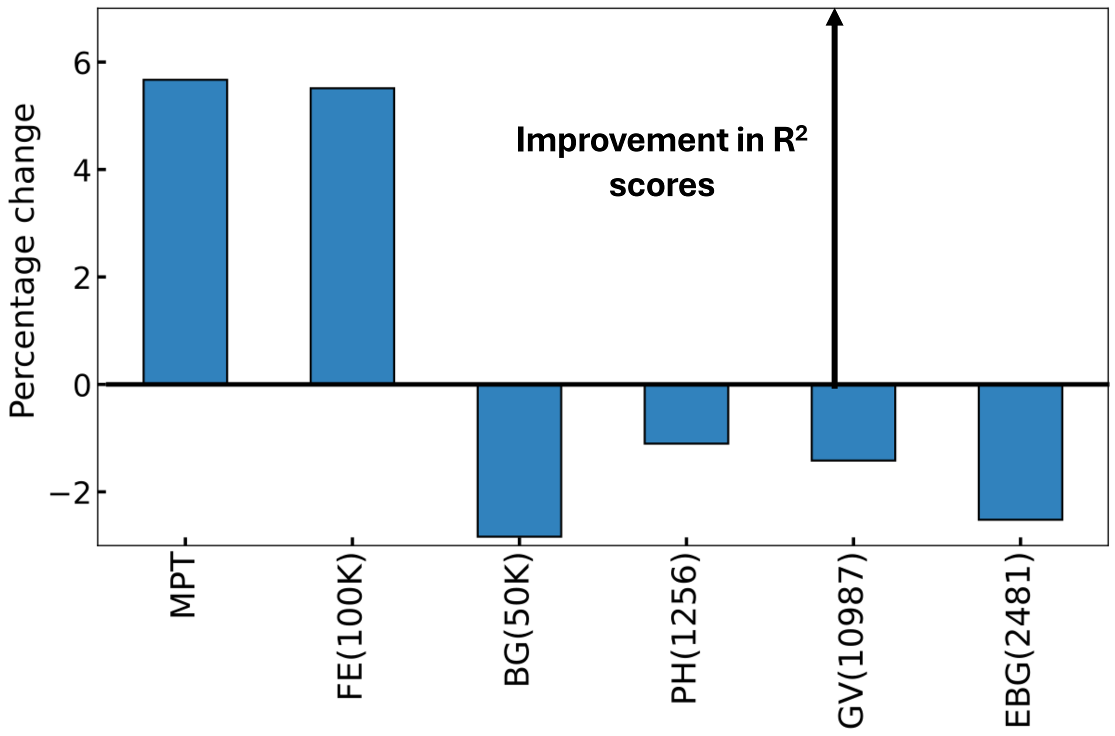


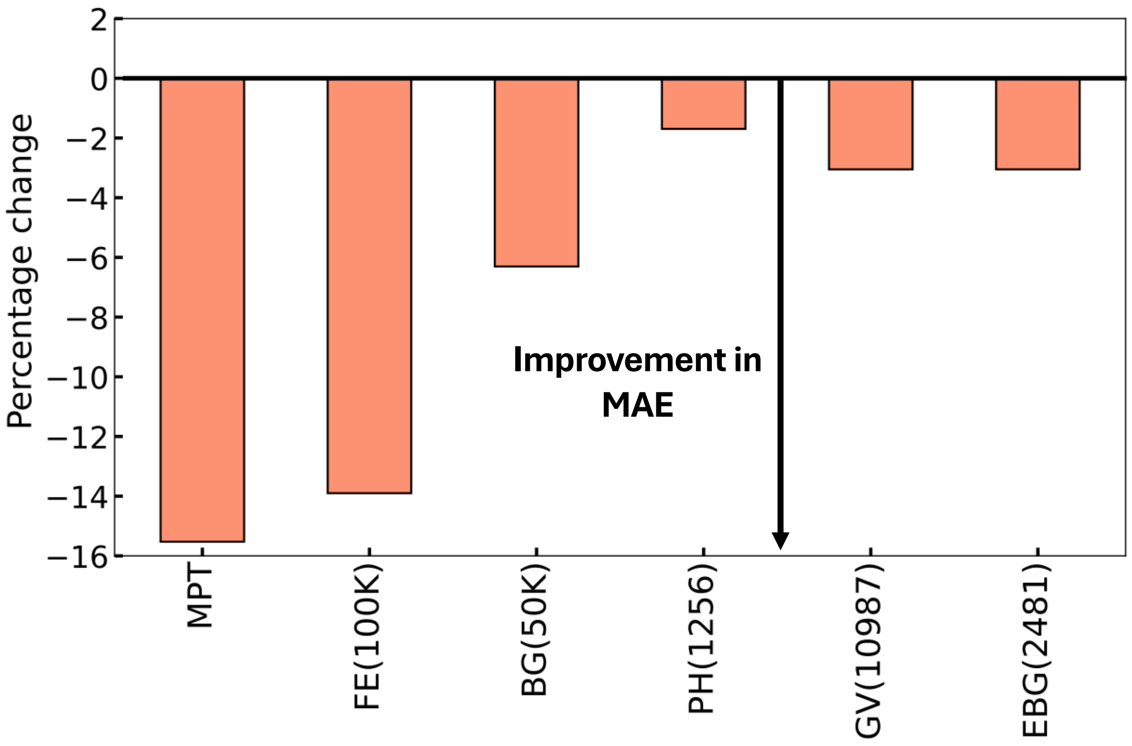
MPT offers best performance in 3/6 and 4/6 cases in terms of R^2scores and MAEs respectively, excluding FE

MPT-PT size: 132,270
Pair-wise PT size: Maxed-out best PT dataset
FT size: 800

MPT models: Improved R^2 scores versus best pair-wise model

Performance on a completely unrelated dataset: JARVIS 2D band gap



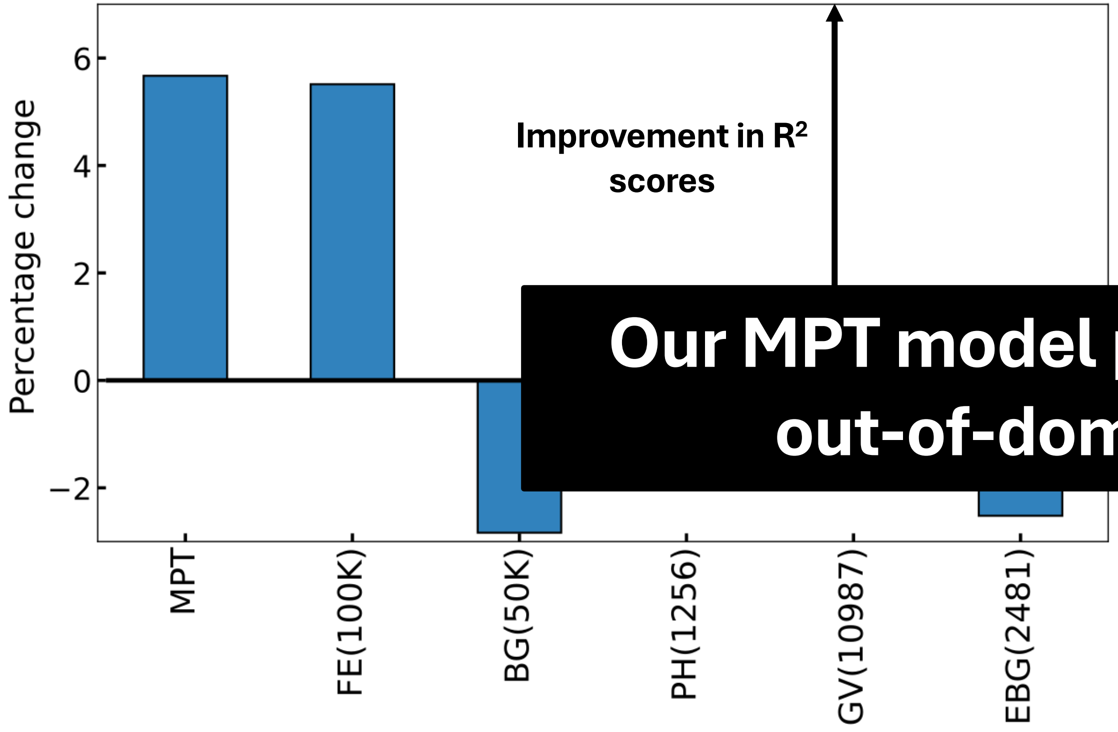


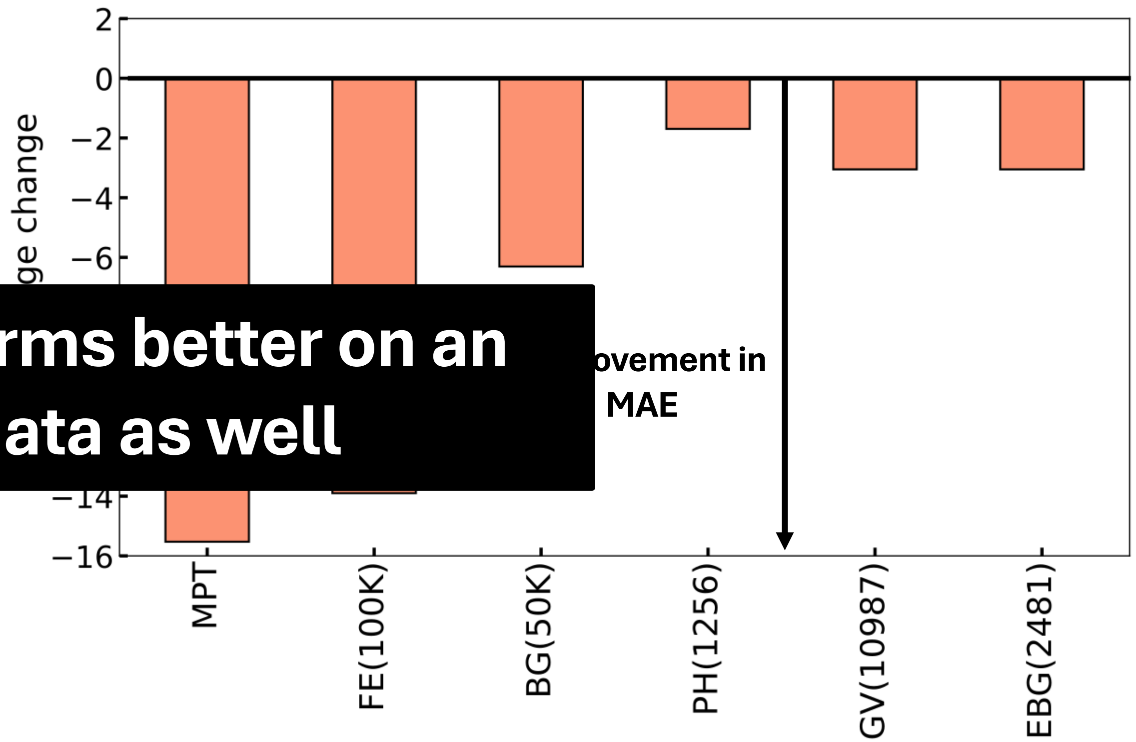
MPT-PT size: 132,270
Pair-wise PT size: Maxed-out best PT dataset
FT size: 800

Dataset size: 1103
PT: MPT model PT on all 7 properties
Pair-wise PT size: : Maxed-out best PT dataset

MPT models: Improved R^2 scores versus best pair-wise model

Performance on a completely unrelated dataset: JARVIS 2D band gap





Our MPT model performs better on an out-of-domain data as well

MPT-PT size: 132,270
Pair-wise PT size: Maxed-out best PT dataset
FT size: 800

Dataset size: 1103
PT: MPT model PT on all 7 properties
Pair-wise PT size: : Maxed-out best PT dataset

Q3 B: How do we construct a generalized model to predict E_m with all the insights gained so far?

Title: **Leveraging transfer learning for accurate estimation of ionic migration barriers in battery materials**

Authors: Reshma Devi, Keith T. Butler & Gopalakrishnan Sai Gautam

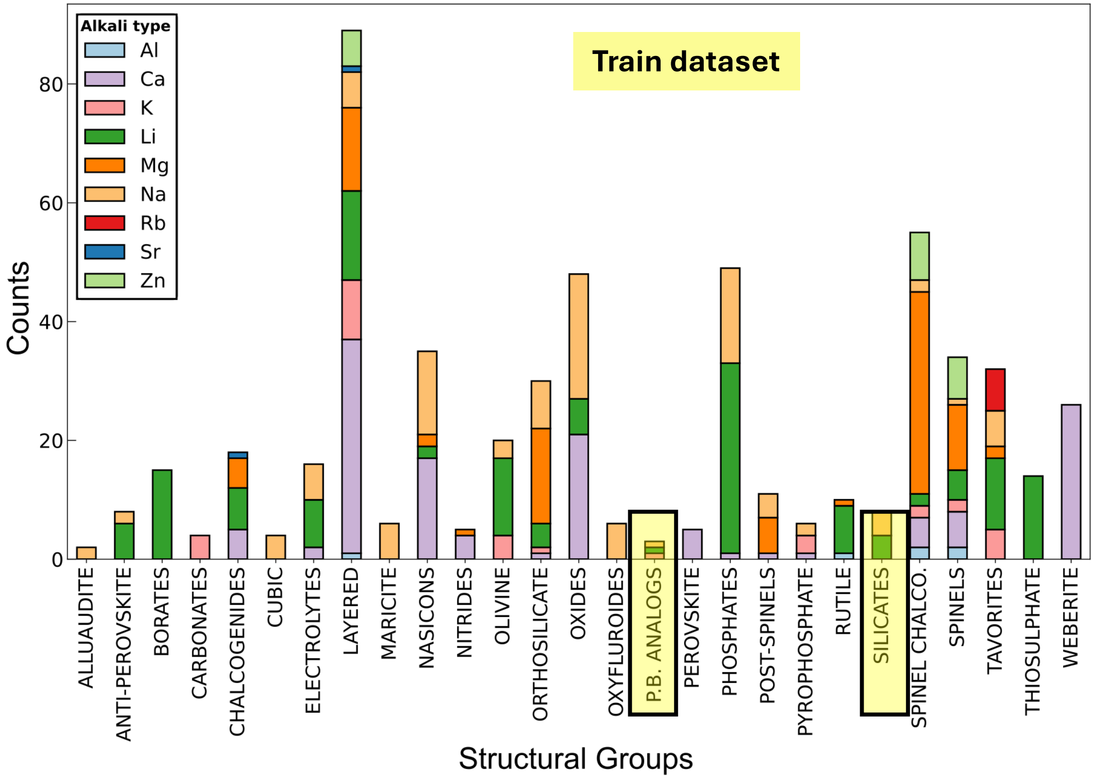
Journal: **To be submitted**

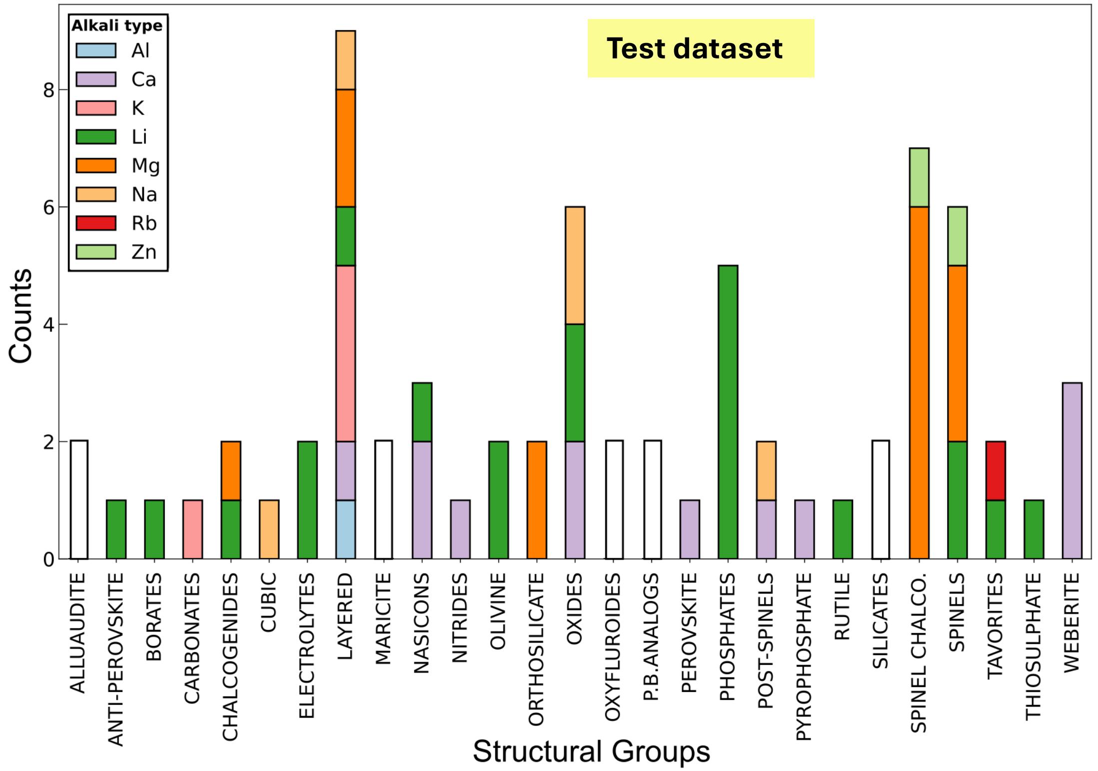
THE ROYAL SOCIETY

Keith T. Butler

UCL

Careful construction of the test dataset





- **Train-Test ratio was 559:60**

Test data construction (60 datapoints)

- Similar distribution as that of the train set
- Overcoming unfair penalization: Single datapoint in test set if the crystal groups constituted 1-2% of total distribution (less than 1% excluded)
- Random sampling within each group

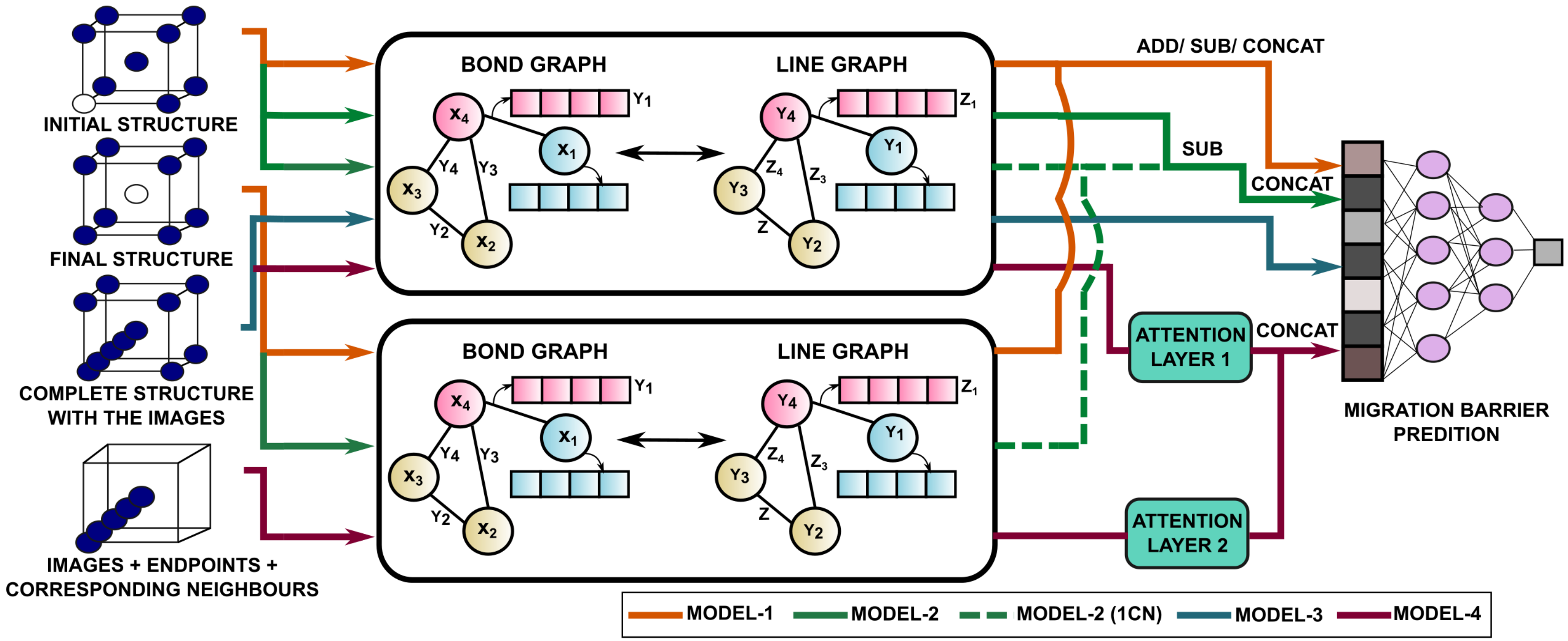
New FT architecture to capture multiple migration pathways

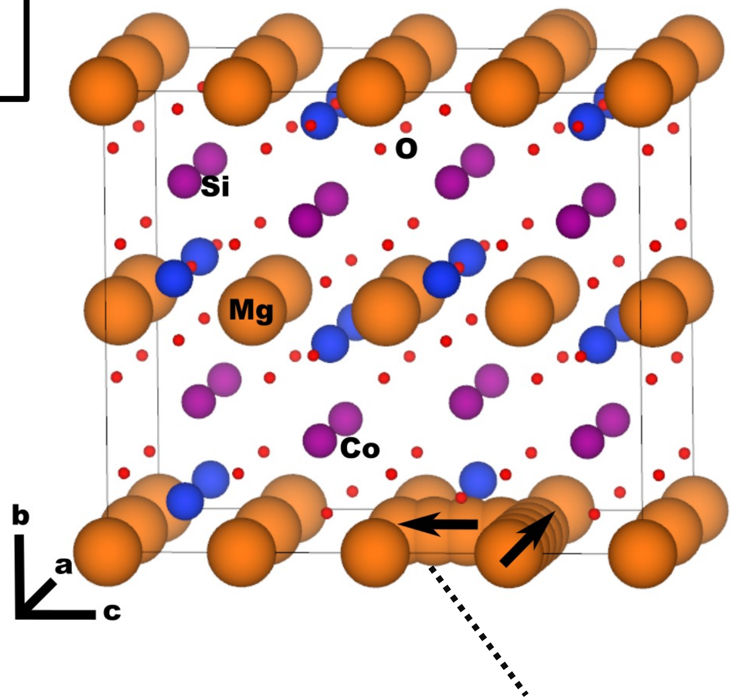
PT: MPT

FT: E_m

How do we make the FT-MPT model distinguish between different migration pathways?

- Initial and final configurations as input?
- Initial guess to the migration pathway in the form of interpolated images?
- Add attention based pooling strategies to learn about the local geometries

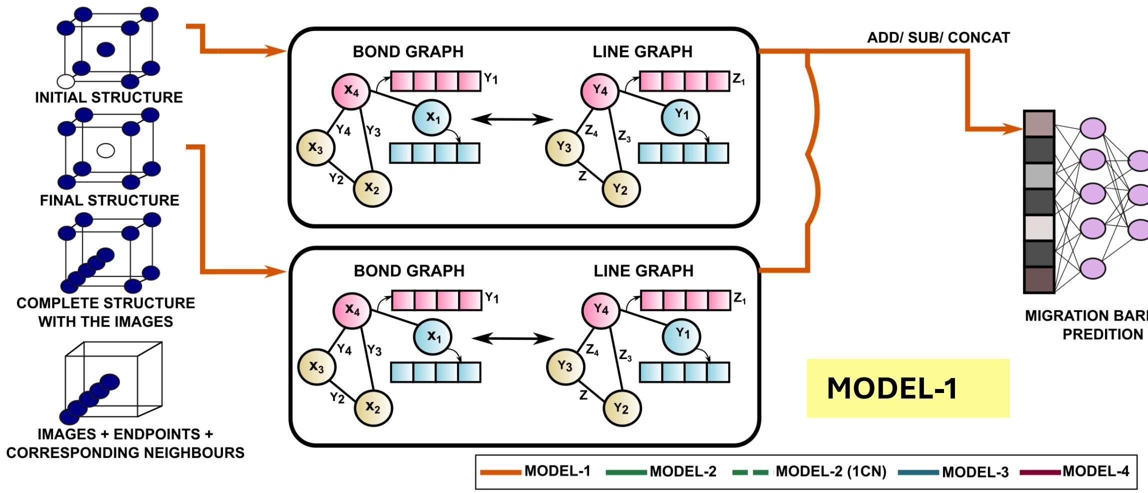




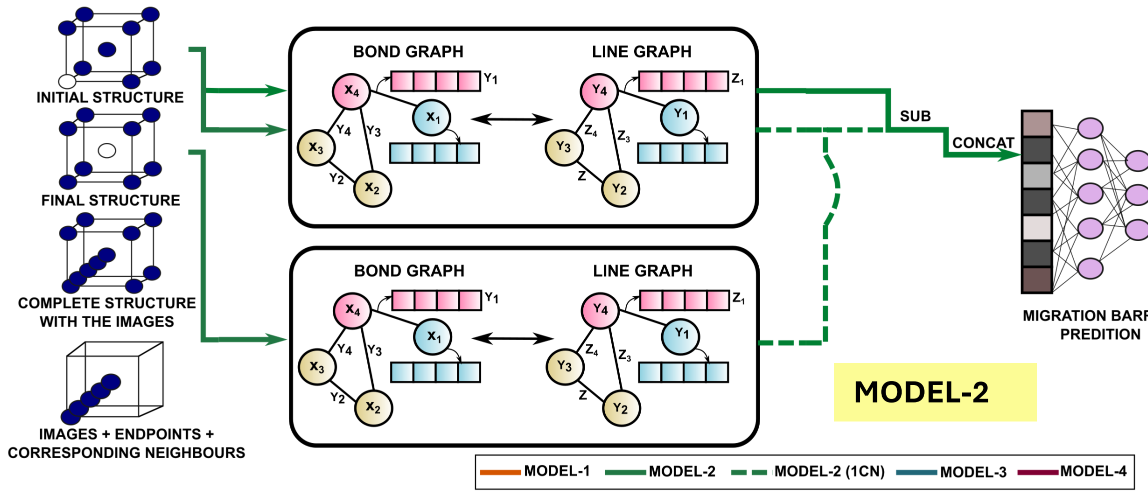
$MgMnSiO_4$ with two different pathways in the same structure

Four different FT architectures

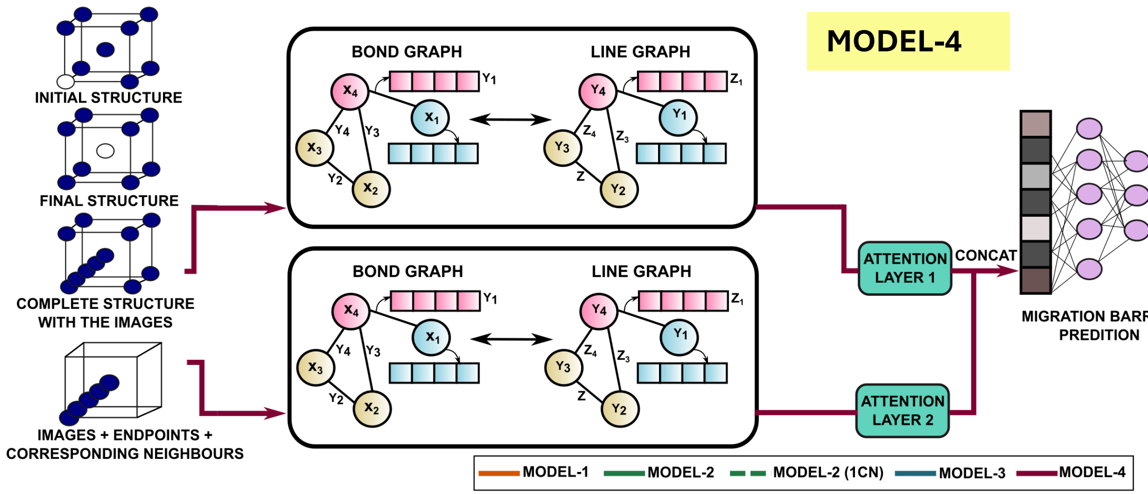
- Initial and final configurations as input: Direction of the pathway



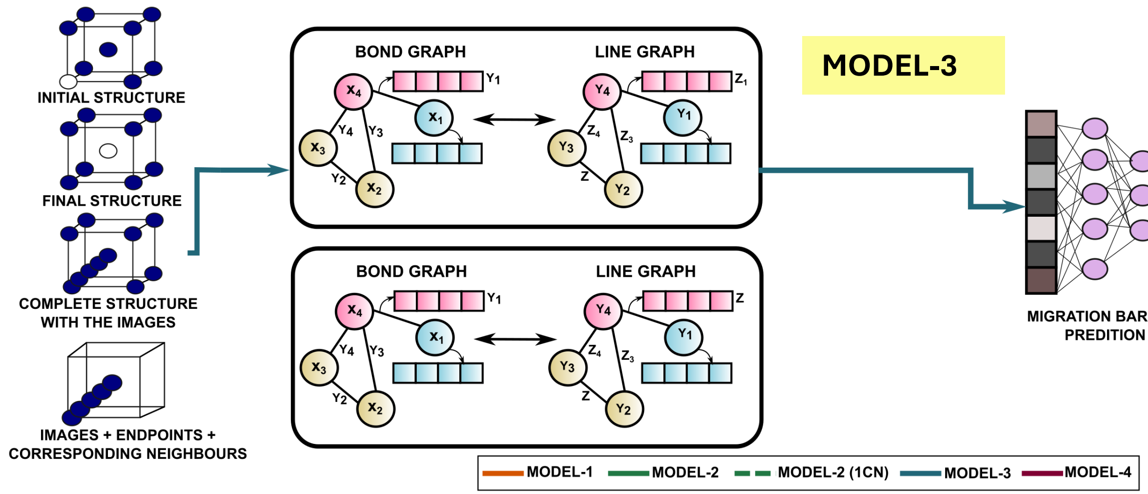
- Combination of initial/final configuration + Delta



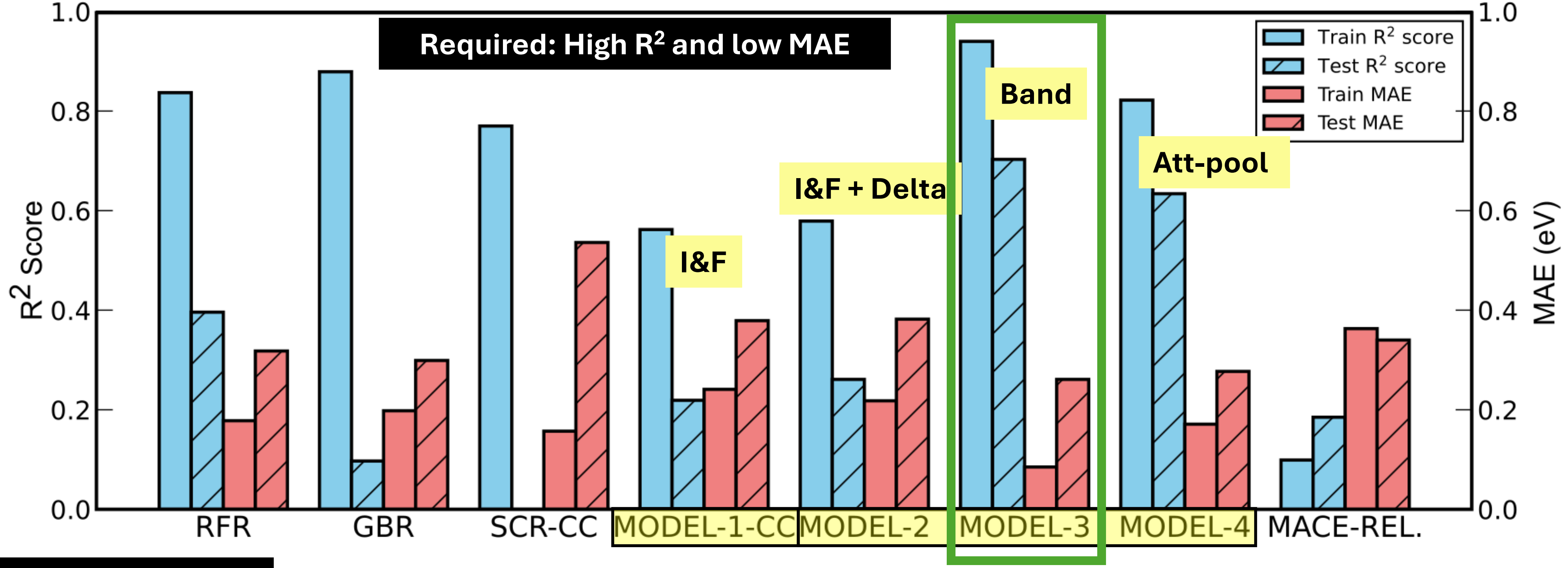
- Attention based pooling on the band



- Band: Transition state and complete pathway geometry



MODEL-3 outperforms with better R^2 score and MAE

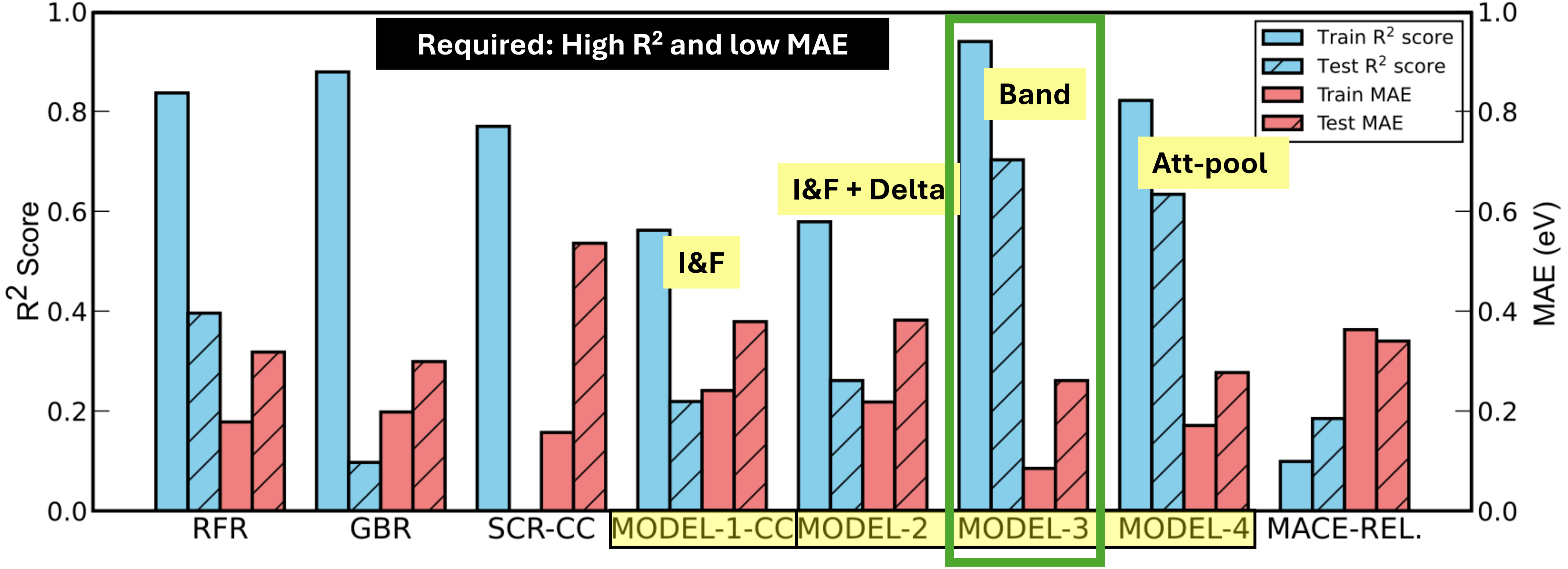


MODEL-3 Performance

- **Better than traditional ML and scratch model**
- **R^2 score: 0.703 and MAE: 0.261 eV**
- **MODEL-4: Comparable performance with respect to MODEL-3**
- **MACE-RELAX (Relaxed the endpoints before NEB calculation): Comparable MAE but poor R^2 score**

RFR: Random forest regressor
GBR: Gradient boost regressor
SCR-CC: Scratch with concatenated embedding
MACE-REL.: MACE-MP-0 with relaxed endpoints
I&F: Initial and final configuration
Att-pool: Attention based pooling

MODEL-3 outperforms with better R^2 score and MAE



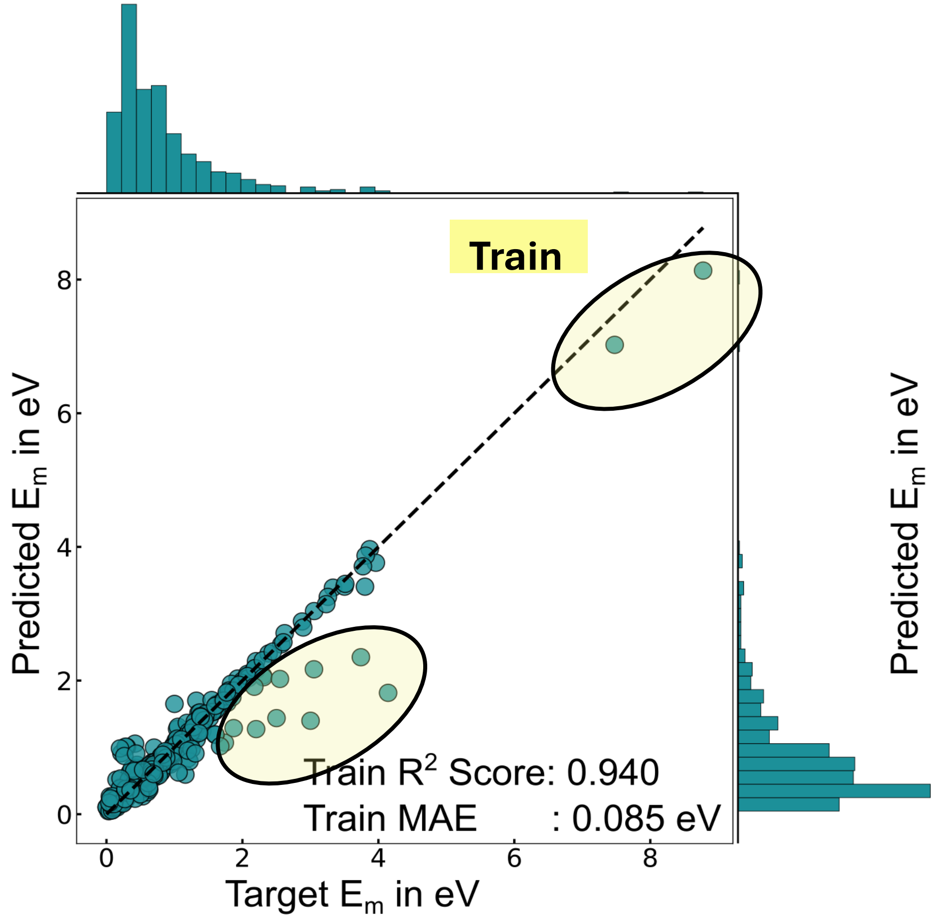
- **MODEL-3: 77.5% increase in R^2 score and 18% decrease in MAE with respect to RFR**
- **Good accuracy in identifying multiple migration pathways in the same structure**

RFR: Random forest regressor
GBR: Gradient boost regressor

SCR-CC: Scratch with concatenated embedding
MACE-REL.: MACE-MP-0 with relaxed endpoints

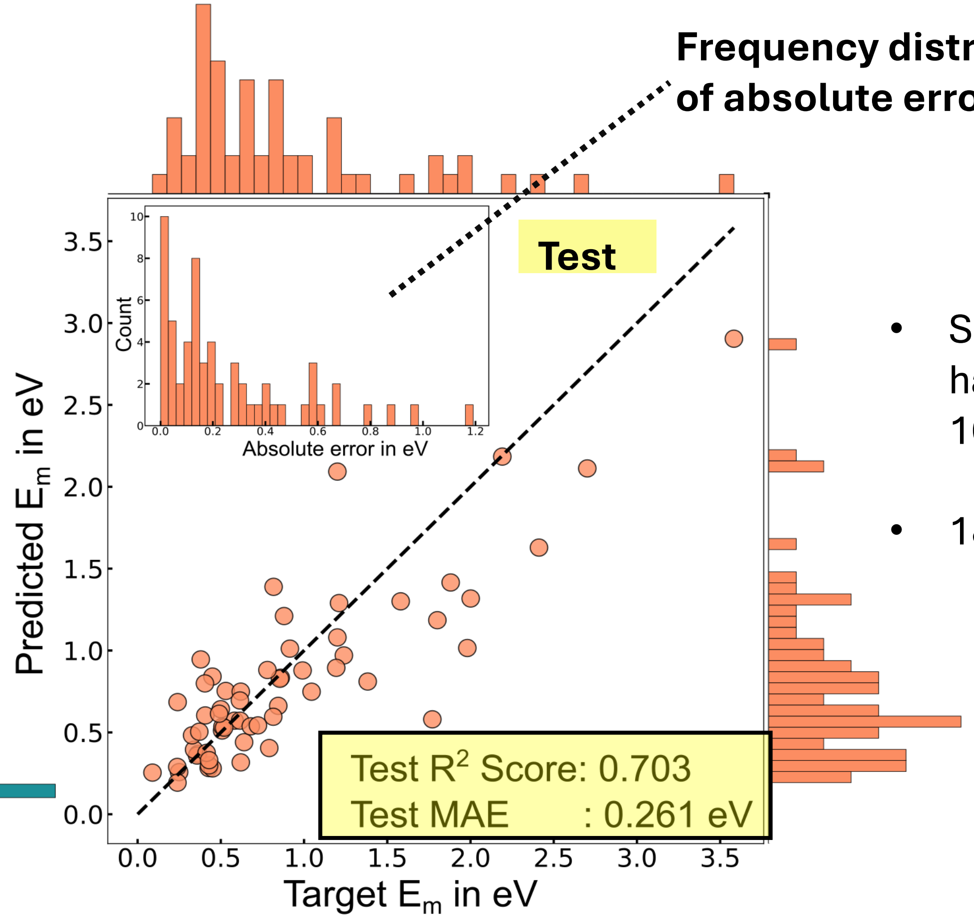
I&F: Initial and final configuration
Att-pool: Attention based pooling

70% of the test dataset have prediction errors less than 0.3 eV



Training Dataset

- Frequency of under and over predictions in comparable
- 12/19 datapoints: Under-prediction error greater than 0.5 eV
- 11/12 : Target E_m exceeding 1.5 eV, e.g., $CaCu_2O_3$ 1.82 eV vs 4.14 eV (target)

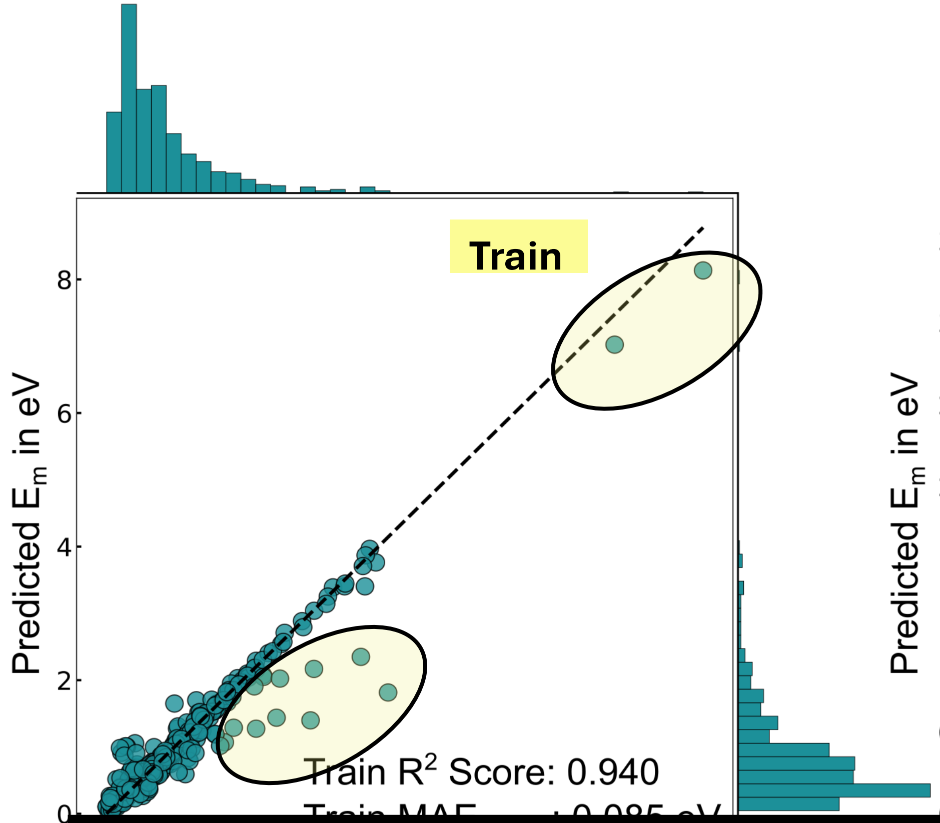


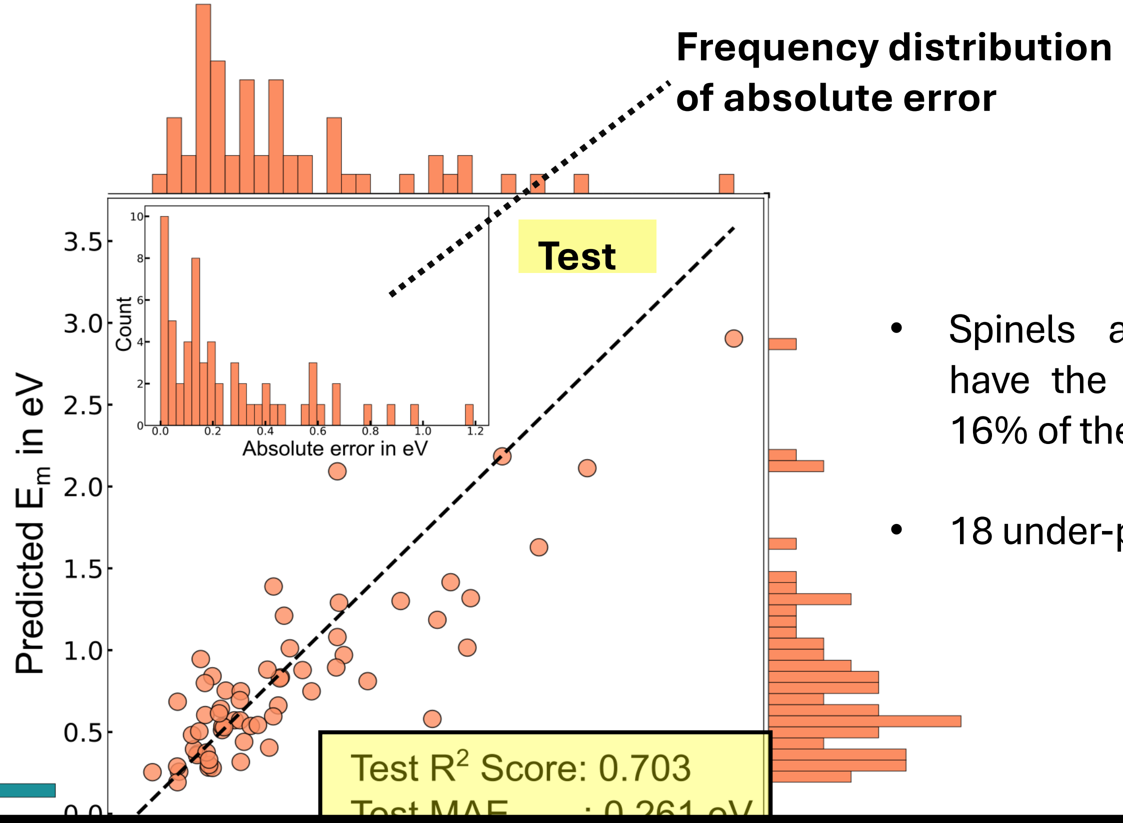
- Spinels and Spinel chalcogenides have the least error (<0.1 eV) ==> 16% of the training dataset
- 18 under-predicted with MAE of 0.6 eV

Test Dataset

- 32%: Absolute error <= 0.1eV (high accuracy)
- 38%: 0.1 < Absoluter error <= 0.3 eV (moderate accuracy)
- 30%: Absolute error > 0.3 eV (low accuracy)

70% of the test dataset have prediction errors less than 0.3 eV

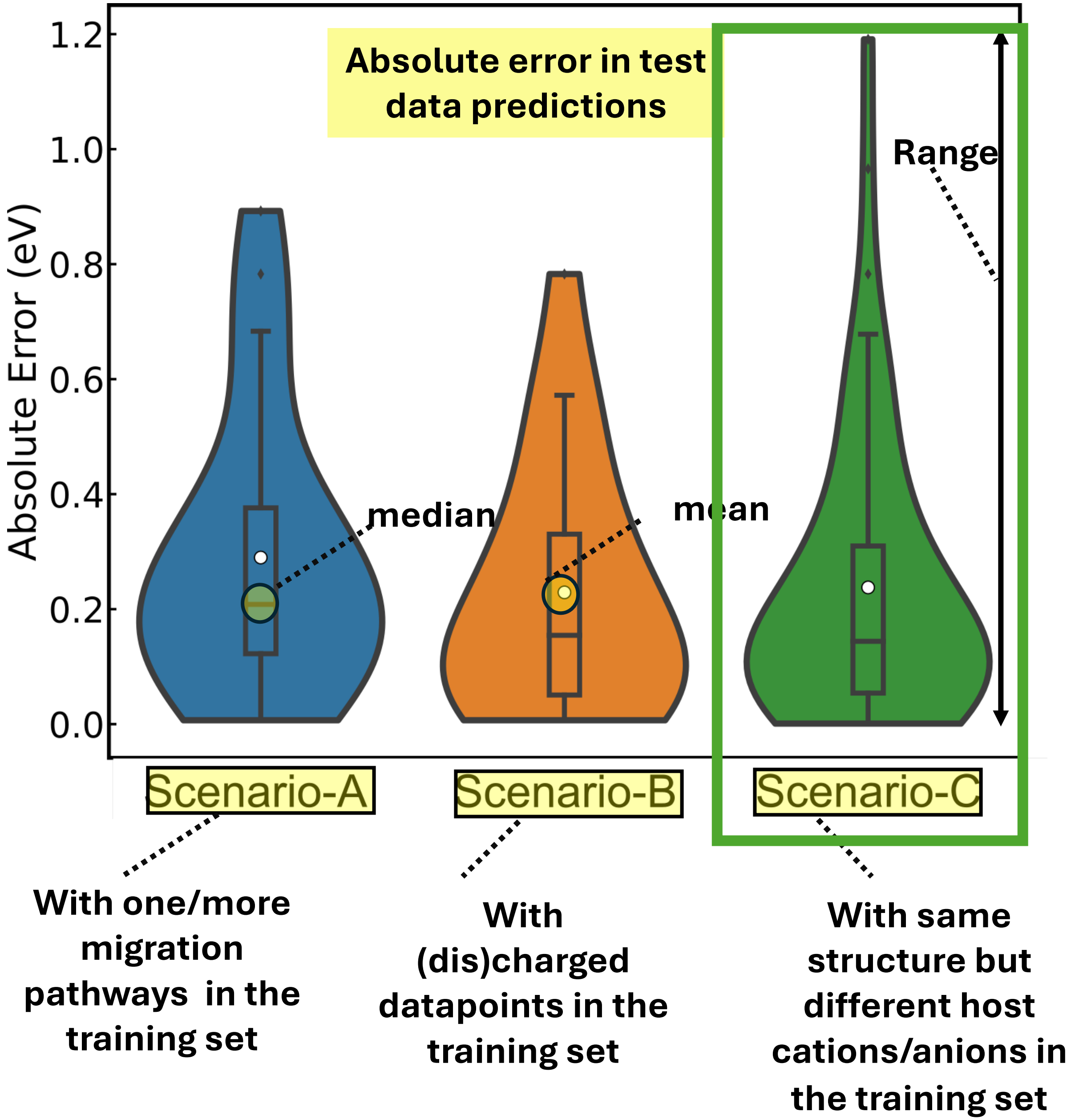




- Spinels and Spinel chalcogenides have the least error (<0.1 eV) ==> 16% of the training dataset
- 18 under-predicted with MAE of 0.6 eV

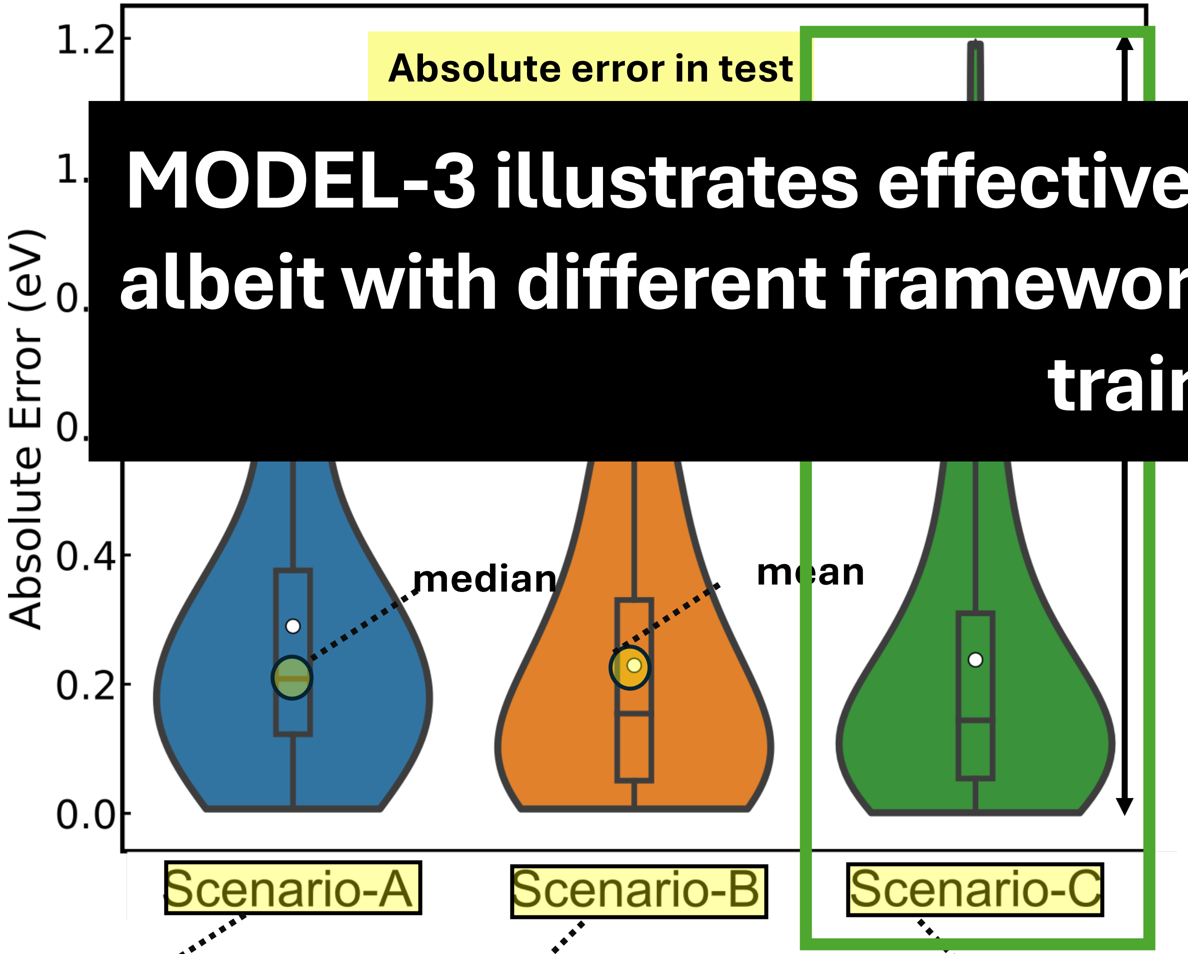
- **70% of the test data predictions have their absoluter errors in high or moderate accuracy range**
- **Better representation in the training dataset improvises the prediction accuracy**

Analysing the generalizability of MODEL-3



- Scenario A: Generalization across migration pathways
- Scenario B: Generalization across composition
- Scenario C: Generalization across Chemistry
- B & C have lower absolute error mean when compared to A
- Lower mean and median in Scenario C
- Scenario C: Datapoints in the high/moderate accuracy contribute to 68% of the test dataset
  - Identical pathways across compositions/chemistries
  - Important local structural motif

Analysing the generalizability of MODEL-3



With one/more migration pathways in the training set

With (dis)charged datapoints in the training set

With same structure but different host cations/anions in the training set

MODEL-3 illustrates effective E_m prediction if similar structure albeit with different framework cations/anions is present in the training set

- Lower mean and median in Scenario C
- Scenario C: Datapoints in the high/moderate accuracy contribute to 68% of the test dataset
  - Identical pathways across compositions/chemistries
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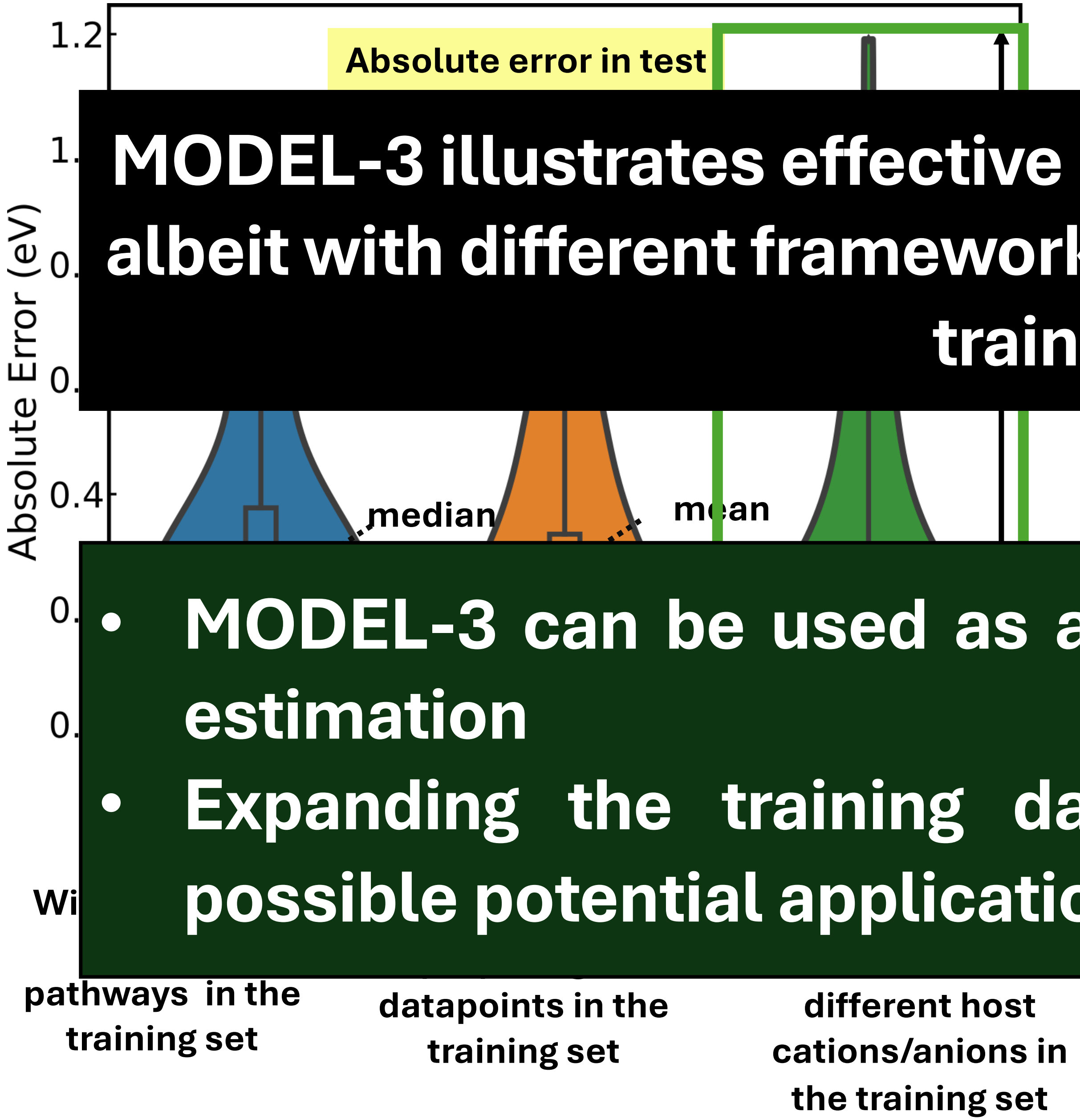
Analysing the generalizability of MODEL-3



MODEL-3 illustrates effective E_m prediction if similar structure albeit with different framework cations/anions is present in the training set

- Lower mean and median in Scenario C

- **MODEL-3 can be used as a potential screening tool for E_m estimation**
- **Expanding the training dataset: Boosted accuracy with possible potential applications in other relevant fields**

So, have we answered all the three questions?

YES!!

SCAN has better numerical accuracy

SCAN is computationally expensive

619 datapoints with diverse chemistries, compositions and structures

NELECT/CI doesn't affect accuracy

GGA can provide good qualitative trends

Efficient TL paradigm for knowledge transfer

Pair-wise TL models outperforms scratch models

MODEL-3 offers superior R^2 score and MAE

MODEL-3 can identify multiple migration pathways within same structure

MPT performs better in out of domain dataset

MODEL-3 has better generalization ability across different chemistries

MODEL-3 prediction accuracy outperform MACE-NEB E_m

Q1. How accurately can the current state-of-the-art techniques estimate E_m ?

Q2: Can we obtain a reliable dataset of E_m to construct an ML model?

Q3 A: How do we solve the data inadequacy issue in materials science?

Q3 B: How do we construct a generalized model with all the insights gained so far?

Publications

1. Devi, R. et al., **Effect of exchange-correlation functionals on the estimation of migration barriers in battery materials**, npj Computational Materials 8, 160 (2022).
2. Devi, R. et al., **Optimal pre-train/fine-tune strategies for accurate material property predictions**. npj Computational Materials 10, 300 (2024).
3. Devi, R. et al., **A literature-derived dataset of migration barriers for the investigation of transport properties in battery materials**. (Accepted in Scientific Data)
4. Devi, R. et al., **Leveraging transfer learning for accurate estimation of ionic migration barriers in battery materials**. (Under revision in npj Computational Materials)
5. Lawrence, E. A. et al., **Reversible Electrochemical Lithium Cycling in a Vanadium (IV)-and Niobium (V)-Based Wadsley–Roth Phase.** Chemistry of Materials 35, 3470–3483 (2023).
6. Verneker, D. et al., **Influence of Metastable Disorder in Titania Oxyhydroxides on High-Rate Sodium ion Storage Manuscript under preparation**. (Accepted in Chemistry of Materials)
7. Swathilakshmi, S., **Performance of the r^2scan functional in transition metal oxides**. Journal of chemical theory and computation 19, 4202–4215 (2023).
8. Devi, R. et al., **Predicting CO adsorption with transfer-learned graph neural networks to accelerate catalyst discovery** (To be submitted)

Accomplishments – Conferences and Workshops

- **Transfer learning for materials science (Hands-on)**

AI/ML for Materials Science Workshop at Department of Materials Engineering, Indian Institute of Science, Bengaluru, India — Tutorial, 8th January 2025

- **The effect of the exchange-correlation functionals on migration barrier estimation in battery materials <u>(Best oral)</u>**

18th Asian Conference on Solid State Ionics at Meenakshi College for Women, Chennai, India — Talk, 19th Feb 2024

- **Enhancing material property predictions by leveraging transfer learning techniques**

24th International Conference on Solid State Ionics at QEII Centre, London, UK — Talk, 18th July 2024

- **The effect of the exchange-correlation functionals on migration barrier estimation in battery materials**

11th International Conference on Materials for Advanced Technologies at Suntec Singapore Convention and Exhibition Centre, Singapore — Talk, 29th June 2023

- **Applications of machine learning to materials science (Hands-on)**

Namma Psi-k Workshop at Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, Karnataka, India — Tutorial, 25th July 2023

- **The effect of the exchange-correlation functionals on migration barrier estimation in battery materials**

American Physical Society March Satellite Meeting at International Centre for Theoretical Sciences, Bengaluru, India — Talk, 15th March 2022

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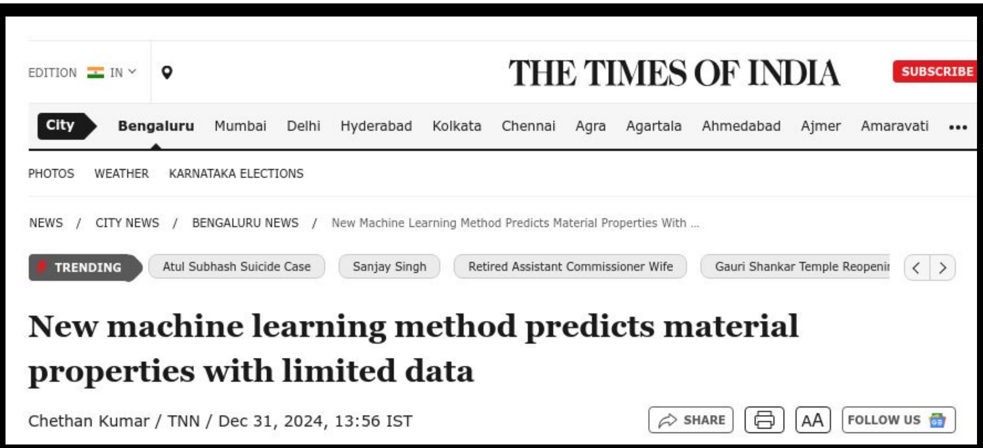
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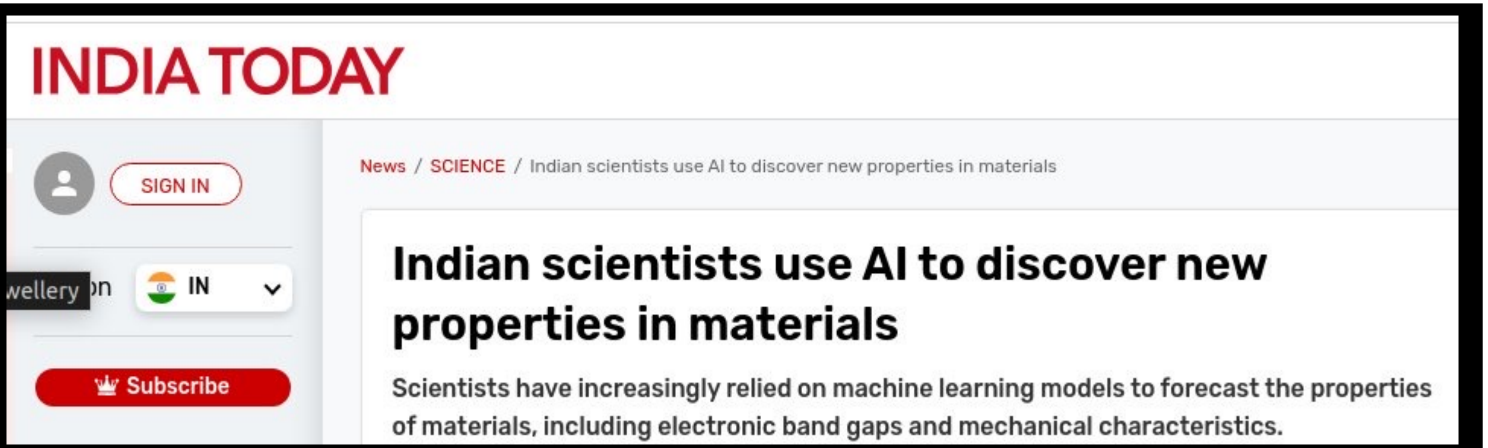
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Indian scientists use AI to discover new properties in materials

Scientists have increasingly relied on machine learning models to forecast the properties of materials, including electronic band gaps and mechanical characteristics.

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- United Kingdom Research and Innovation (UKRI)
- Engineering and Physical Sciences Research Council (EPSRC)
- Science and Engineering Research Board (SERB)

Supercomputing facilities :

- National Supercomputing Mission (NSM)
- Param Utkarsh at CDAC Knowledge Park
- ARCHER2 UK National Supercomputing Service
- National Supercomputing Center, Singapore,
- Param Pravega and Supercomputer Education and Research Center (SERC),IISc.