ET-AL: Entropy-targeted active learning for bias mitigation in materials data

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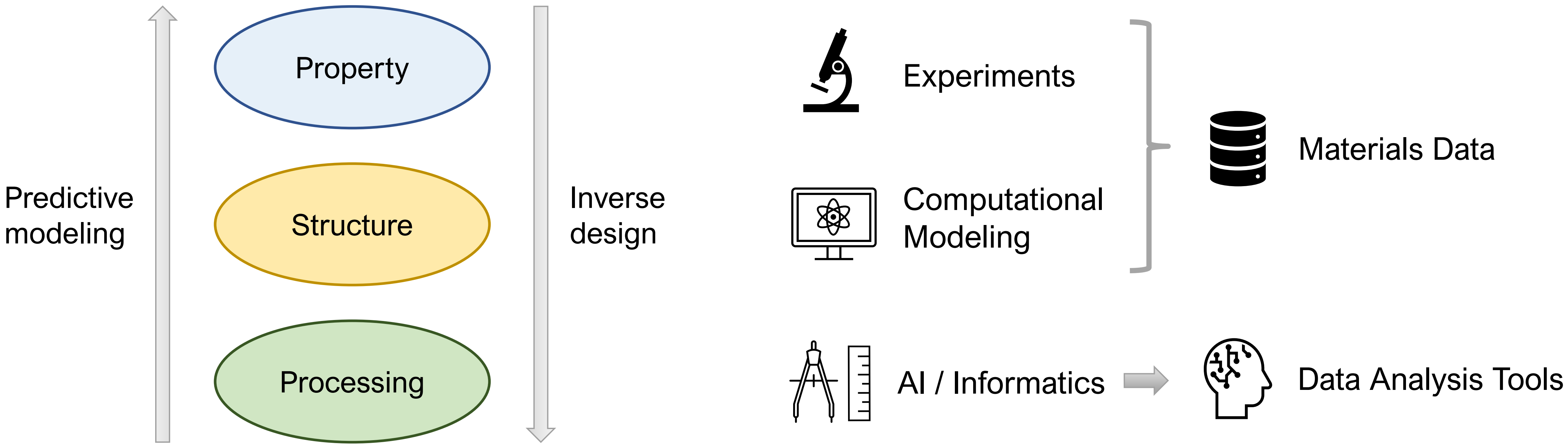
IDEAL Integrated DEsign Automation Laboratory

MATERIALS THEORY AND DESIGN GROUP

Materials Science with Data

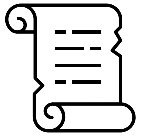


Growing materials data + data-driven methods →

- Accurate predictive modeling
- Efficient, on-demand materials design

Data Sources

Where materials informatics / data-driven design researchers get data



Published literature

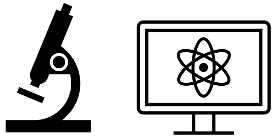
Materials receiving more focus

Easy to synthesize or simulate

OQMD The Open Quantum Materials Database

Materials databases

Built upon known structural prototypes (not balanced)



Experiments and computation

Data acquisition

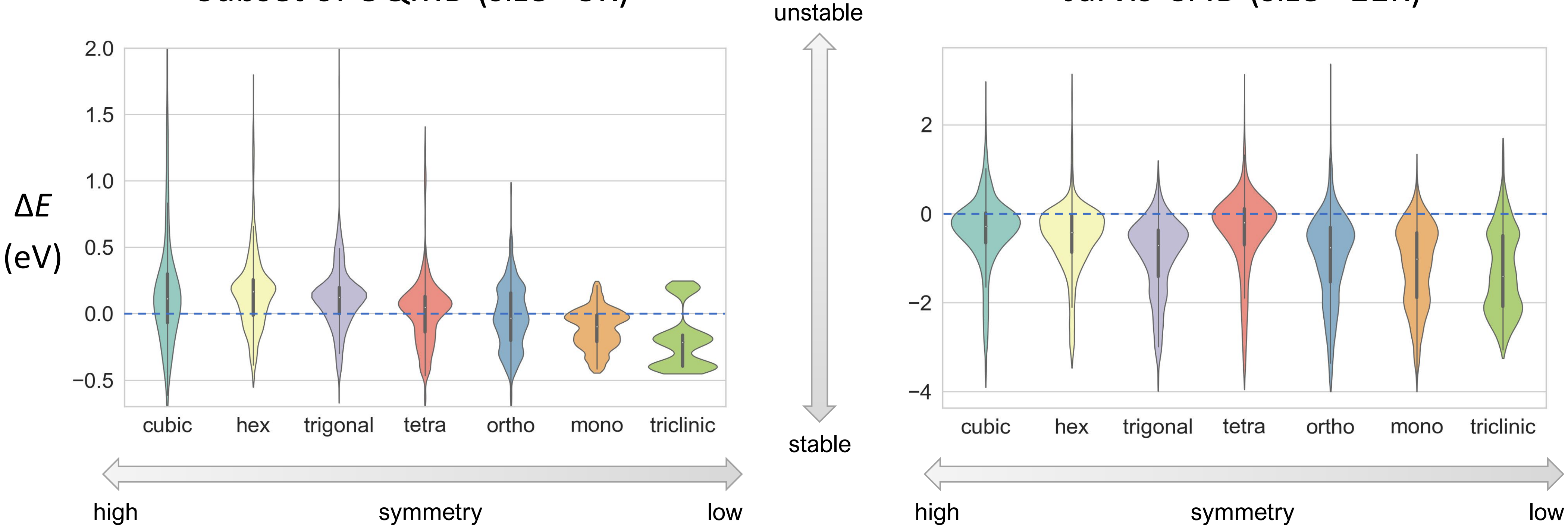
Can mitigate the bias

These data sources are often biased

Bias in Materials Databases

Subset of OQMD (size ~3K)

Jarvis-CFID (size ~11K)



Symmetry ↑ { Coordination number ↑ / More close-packed ↑ } Stability ↑

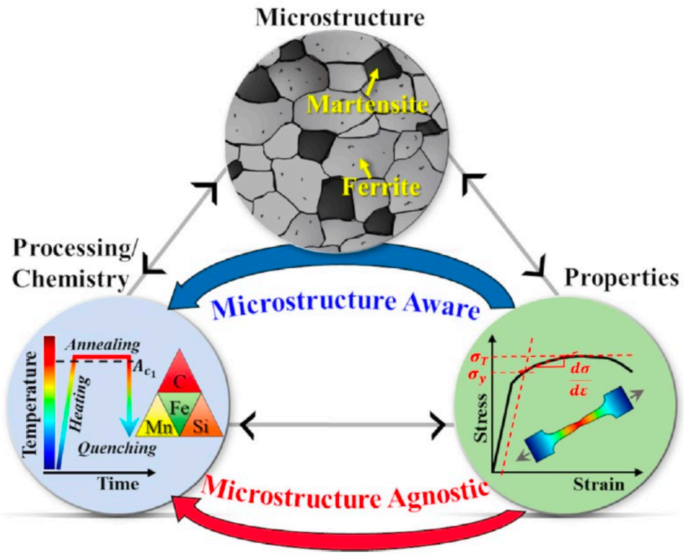
We see the opposite in the data

➡ The "structure–stability bias"

Why is bias a problem?

From a materials science perspective

- Microstructure information helps modeling materials properties
- Microstructure relies on ΔE of phases
- Bias in ΔE → problematic property models



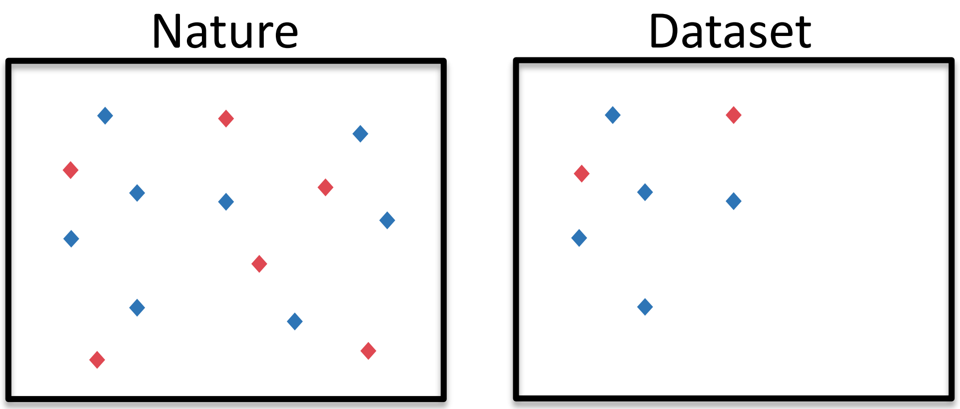
From a data science perspective

- Lower bias → better coverage of the design space → better generalizability of models

A. Molkeri, D. Khatamsaz, R. Couperthwaite et al. *Acta Materialia* 223, 117471 (2022)

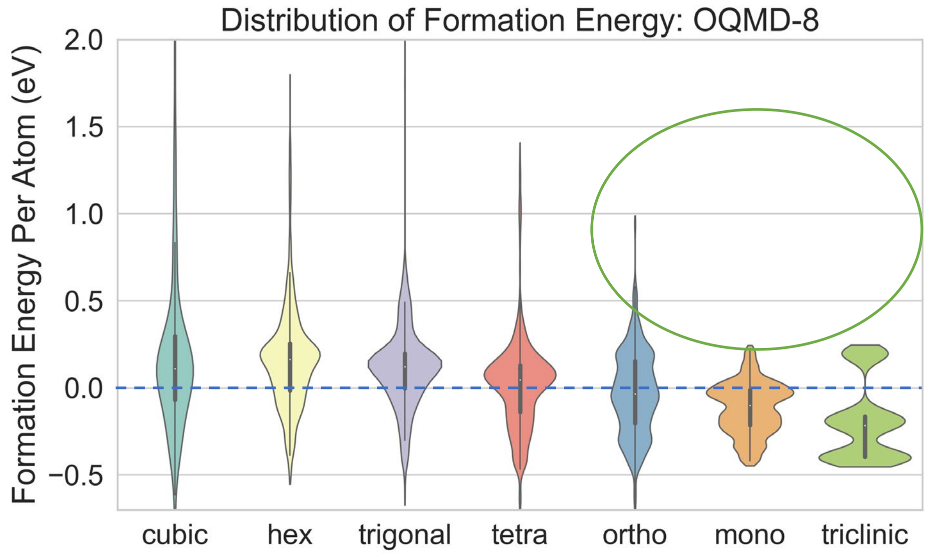
Problem Formulation

- Data bias in properties of interest
  - Deviates from known nature
  - Lack of representativeness
- Bias is ubiquitous in materials data, but its **level** can be reduced



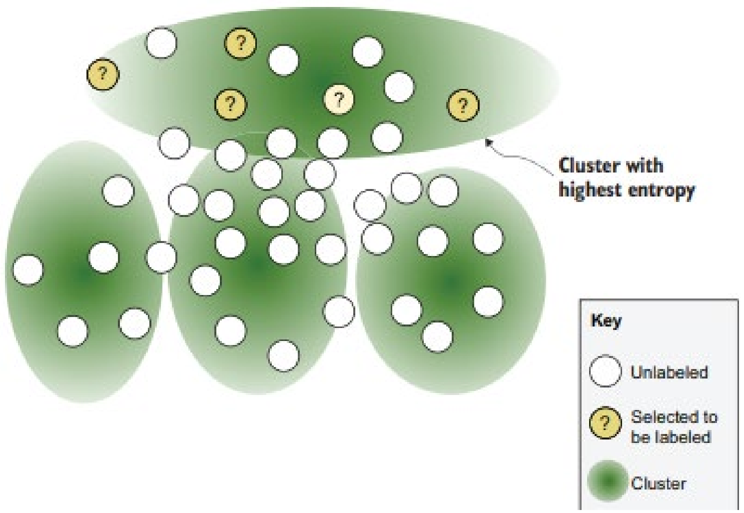
Goals:

- Detect (quantify) bias
- Reduce bias by adding new data



Information Entropy as a Bias Metric

Define bias among groups



Here, use crystal system (a natural, trivial grouping)

Information entropy

$$h(Y) = -\int p(y) \ln p(y) \, \mathrm{d}y$$

→ Diversity of a set of Y values.

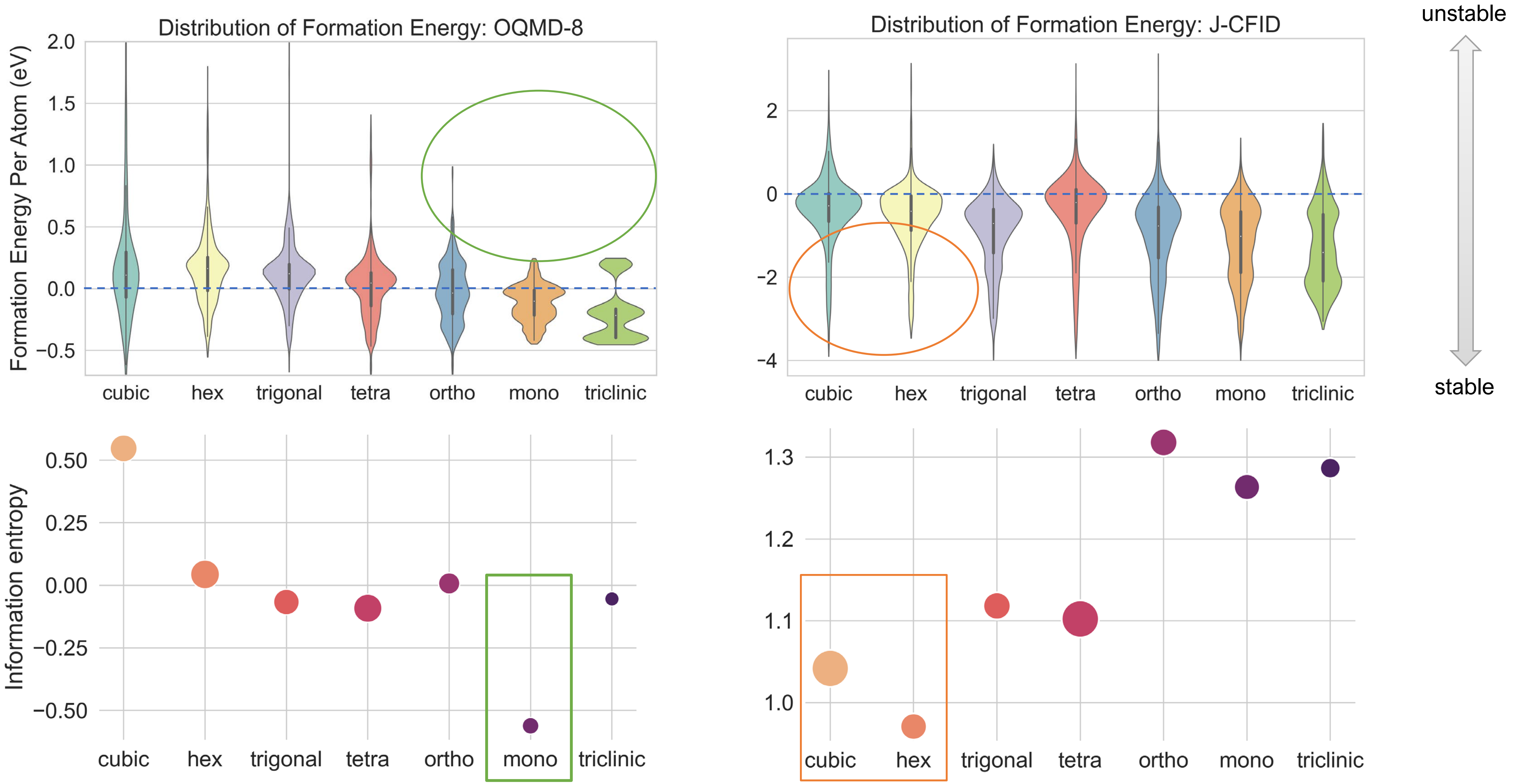
Here we consider $h(\Delta E)$ in each system

- Diversity of ΔE in a crystal system
- If low, the system is underrepresented

Fairness metric

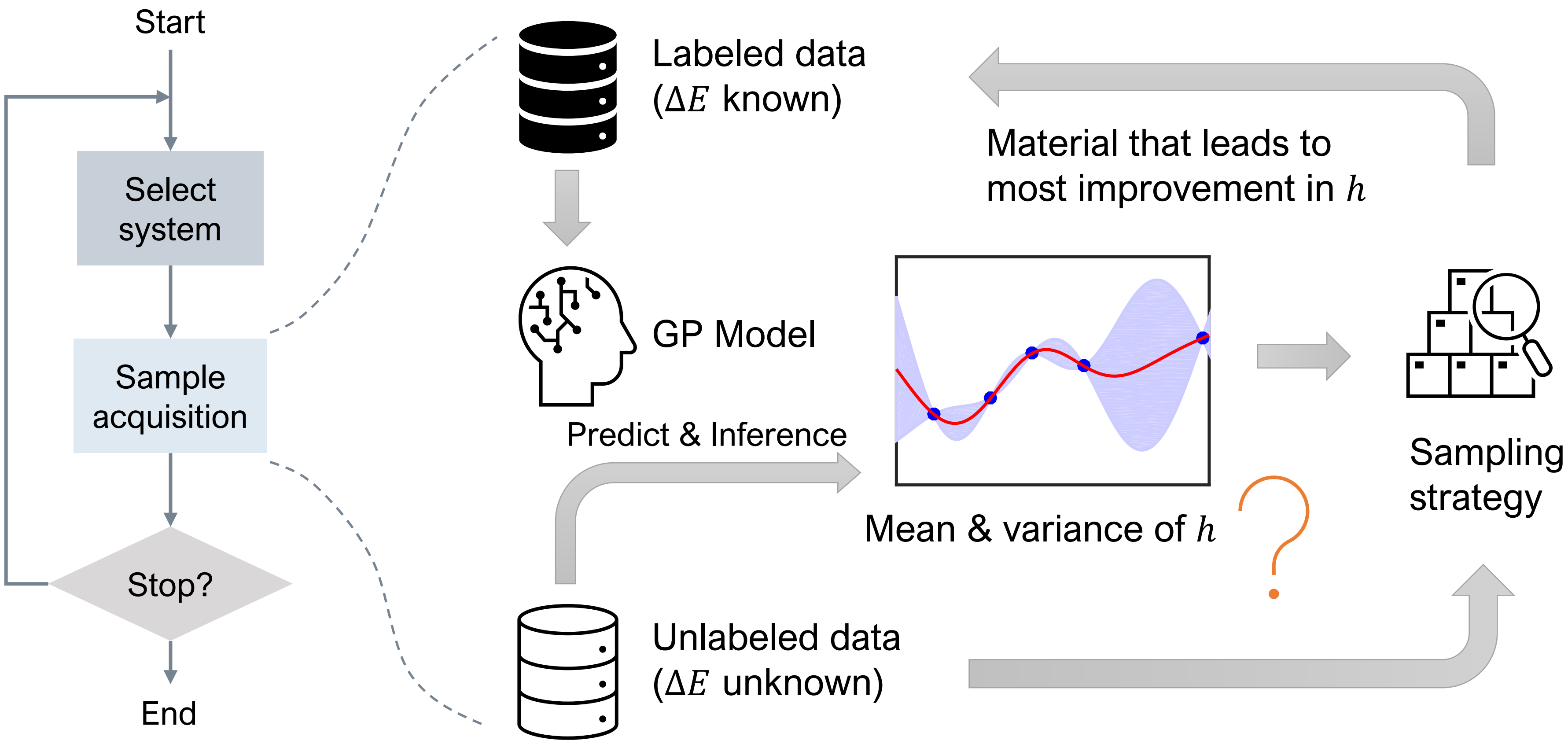
- Difference of h among groups → bias

Demonstration of the Bias Metric



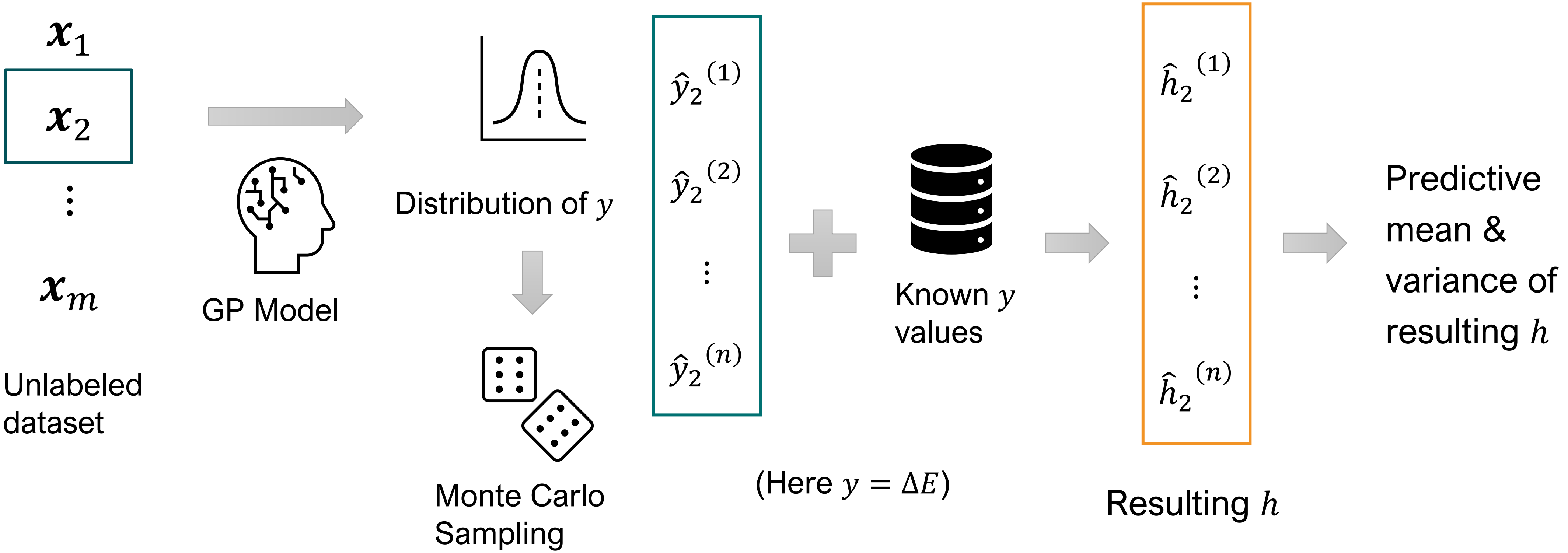
ET-AL: Entropy-Targeted Active Learning

To mitigate bias: add data in underrepresented crystal system to increase h.



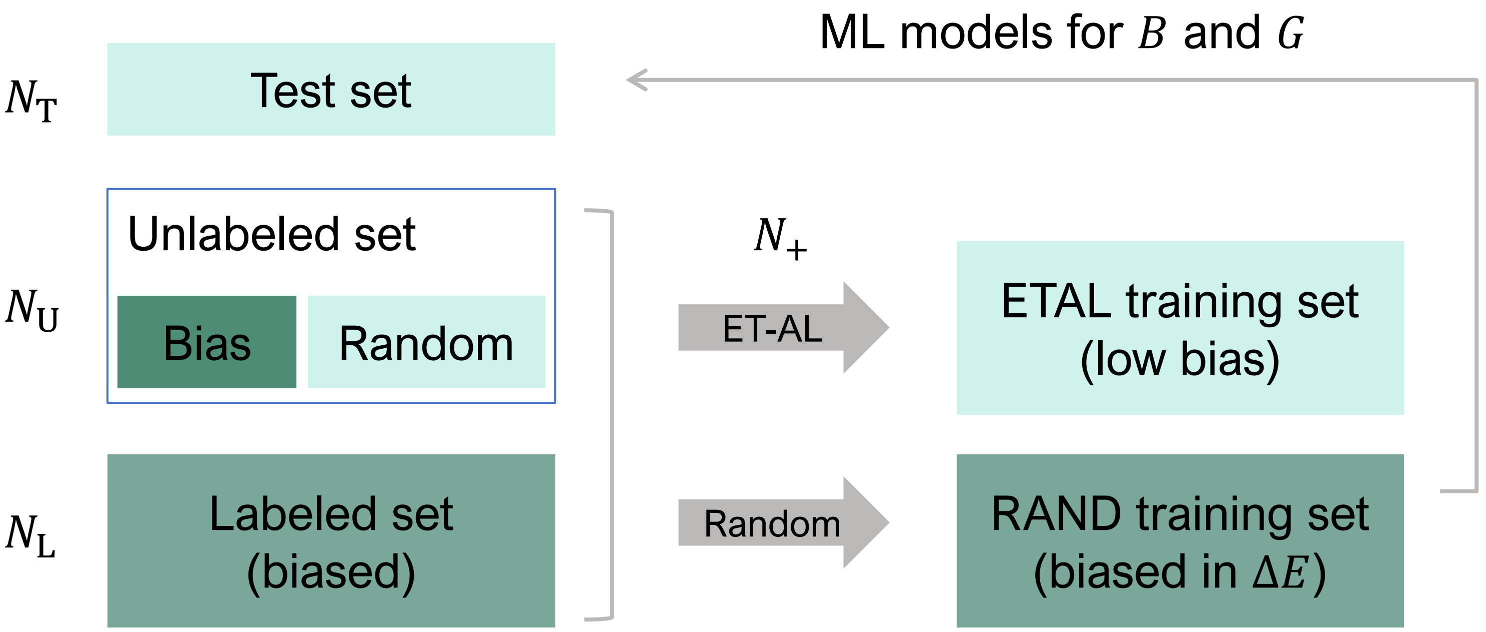
H. Zhang et al. ET-AL: Entropy targeted active learning for bias mitigation in materials data. *Applied Physics Reviews*, 2023.

Uncertainty Estimation for h



For every $\boldsymbol{x}$ in the unlabeled sample pool, we can calculate expected improvement (EI) in h.

Experiments for Demonstration



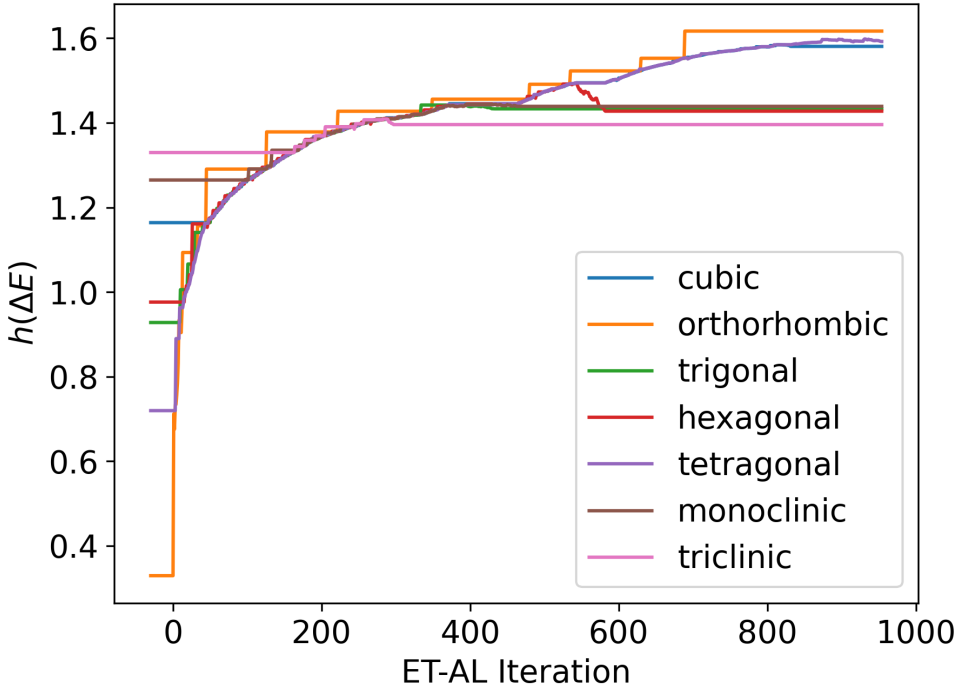
1. Mitigate artificial structure–stability bias
2. ML: bulk & shear moduli (B & G), important mechanical properties

Testbed: Jarvis dataset (~11K)

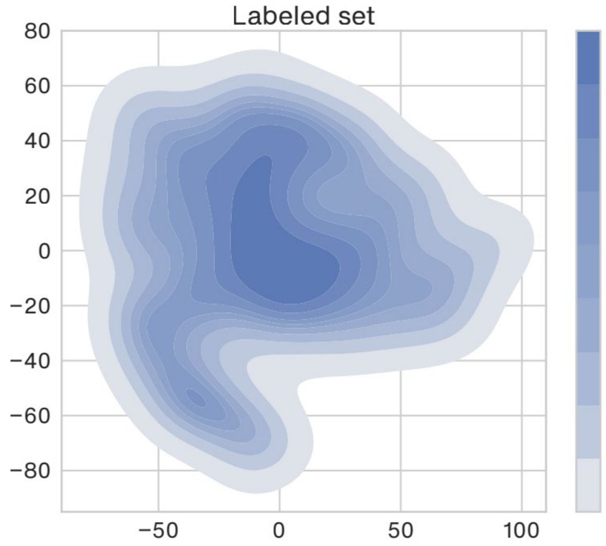
- remove H, VIIA, VIII, and radioactive elements
- $N_L = 1000, N_U \sim 5000, N_T = 5000$

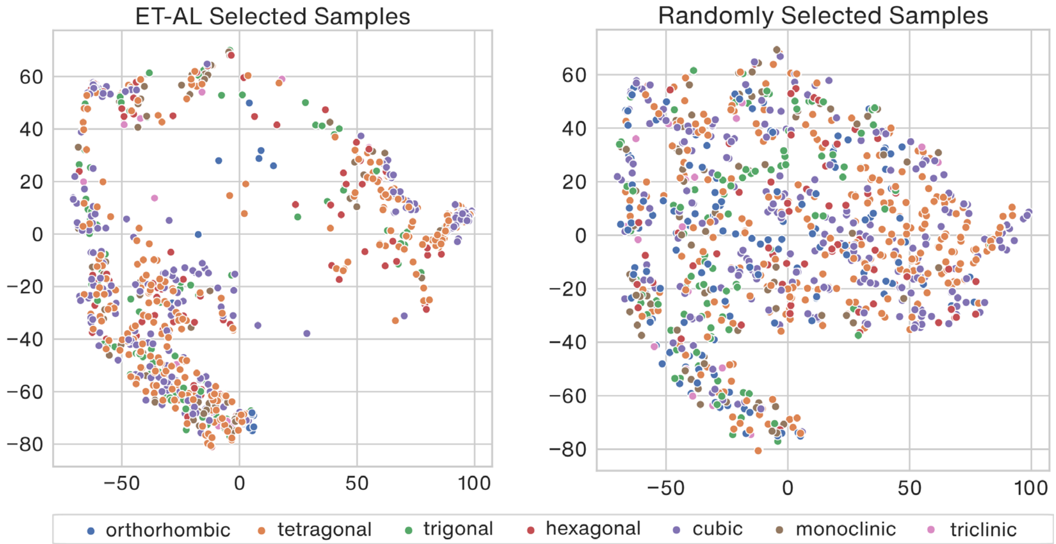
Experimental Results

ET-AL successfully fixed the artificially created bias.

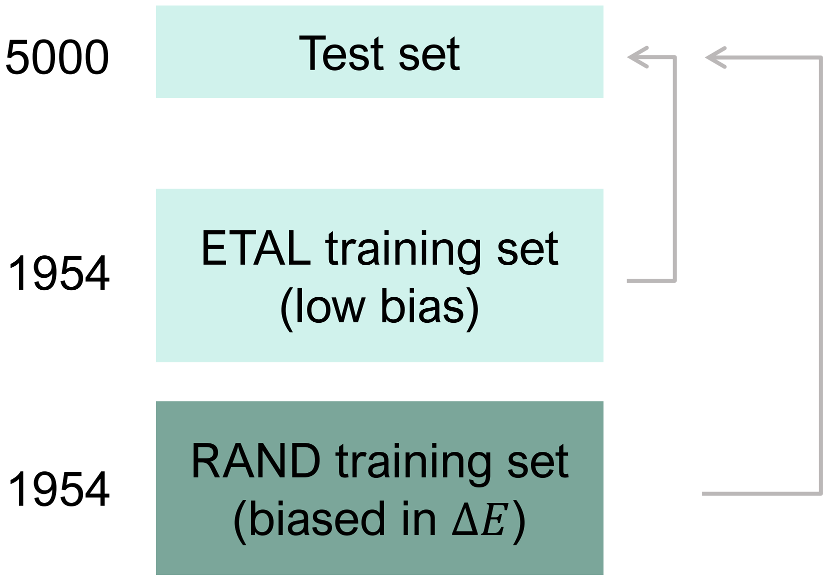


ET-AL samples in underrepresented regions.





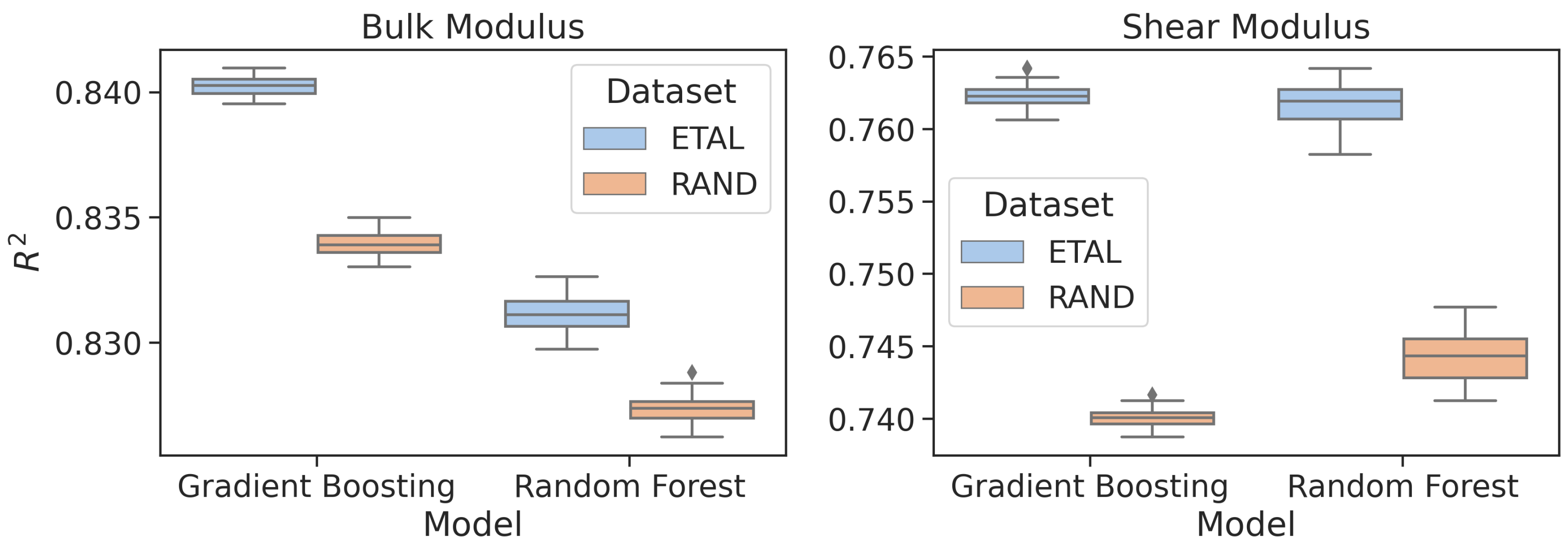
Experimental Results



Compare ML models for B and G

Tried multiple different ML models: NN, trees, SVM, …

- Hyperparameters are tuned
- Tree-based ensemble models perform better
- ETAL dataset shows systematic advantage



Conclusions

- We developed and presented
  - A metric for measuring bias in (materials) data
  - ET-AL framework to mitigate bias by guiding data acquisition

- ET-AL can mitigate data bias, thus benefiting data-driven informatics

Help improve dataset quality

Guide database construction

Applicable to other scientific domains

is there bias in materials science databases? what are the problems it may cause?

Searching for: **bias in materials science databases**

Generating answers for you…

Yes, there can be bias in materials science databases. Researchers have different focuses and preferences of what materials to study; some experiments and simulations are easier to conduct than others which can contribute to bias [1].

However, there are methods to mitigate that bias such as developing an entropy-targeted active learning method [1].

The bias can cause problems such as limiting the scope of research and development [2].

Are there ways to solve this problem?

Searching for: **methods to mitigate bias in materials science databases**

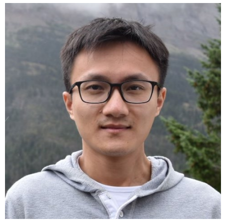
Generating answers for you…

Yes, there are methods to mitigate bias in materials science databases such as developing an entropy-targeted active learning method [1]. The team settled on information entropy as a metric to measure bias [1]. Using this metric, they organized existing data into regions in a materials space and constructed their algorithm to more heavily prioritize regions that received less attention [1]. They also identified regions that would most benefit from future research efforts to reduce data bias [1].

Other methods include pre-processing techniques such as sampling, massaging, reweighing to more complex methods like optimized data transformation which reduces bias and the predictability of the protected or sensitive attribute [2].

Acknowledgments

- **Collaborators** (the "et al.")



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CHiMaD NIST arpa·e CHANGING WHAT'S POSSIBLE DIFFERENTIATE

Thanks for your attention!

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