The role of computation in materials synthesis and characterization

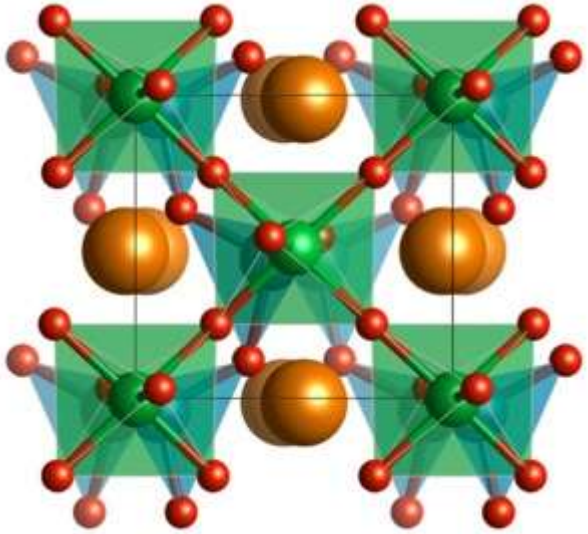
Nathan Szymanski

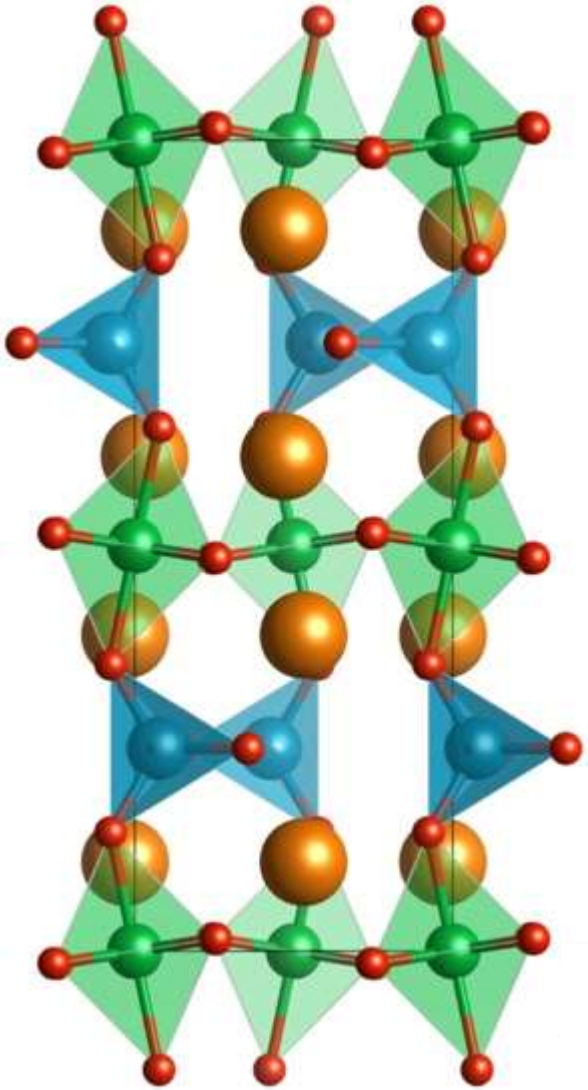
Design of Materials on Computers
DMC LAB
Bartel Research Group

bartel.cems.umn.edu
Chemical Engineering & Materials Science
University of Minnesota

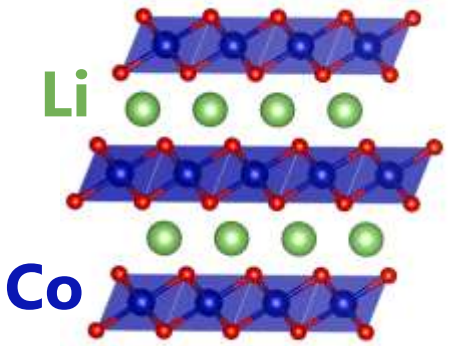
Research Seminar for Faculty Search 2025

Inorganic crystalline materials





Innovation is driven by materials with “just the right” properties



$LiCoO_2$ as a Li-ion cathode:

- Li can be reversibly (de)intercalated
- $Co^{3+/4+}$ redox occurs at high voltage

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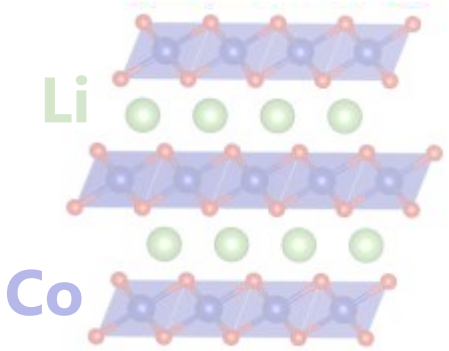

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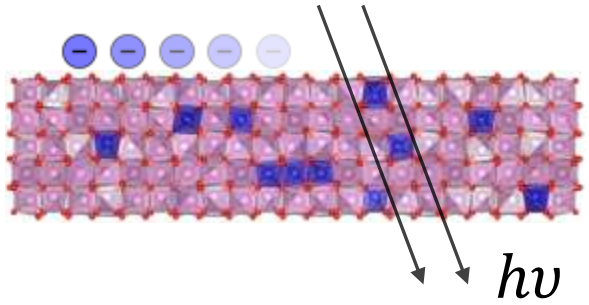
$In_{2-x}Sn_xO_3$ as a transparent conductor:

- High transparency to visible light
- Good electrical conductivity



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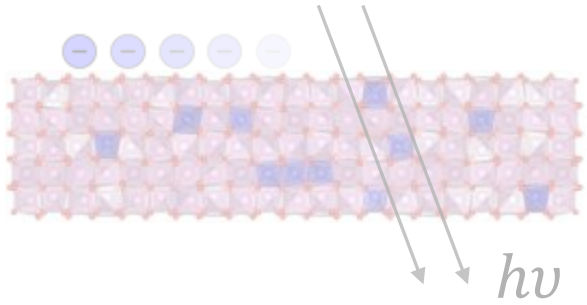
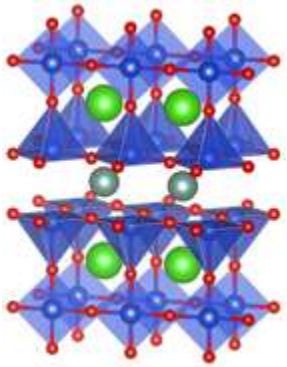




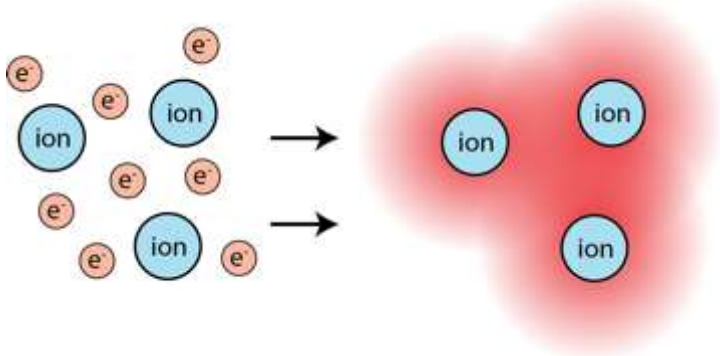
$YBa_2Cu_3O_{7-x}$ as a high-T_c superconductor:

- Superconductivity across CuO_2 planes
- Good tolerance to oxygen vacancies (x)

Computations can assist in designing new materials

CEMS Chemical Engineering & Materials Science

Density functional theory (DFT)



Internal **energy**
Electronic properties
Response functions

Provides an answer to the questions:

Is the material **stable?**

Does it have the properties we want?

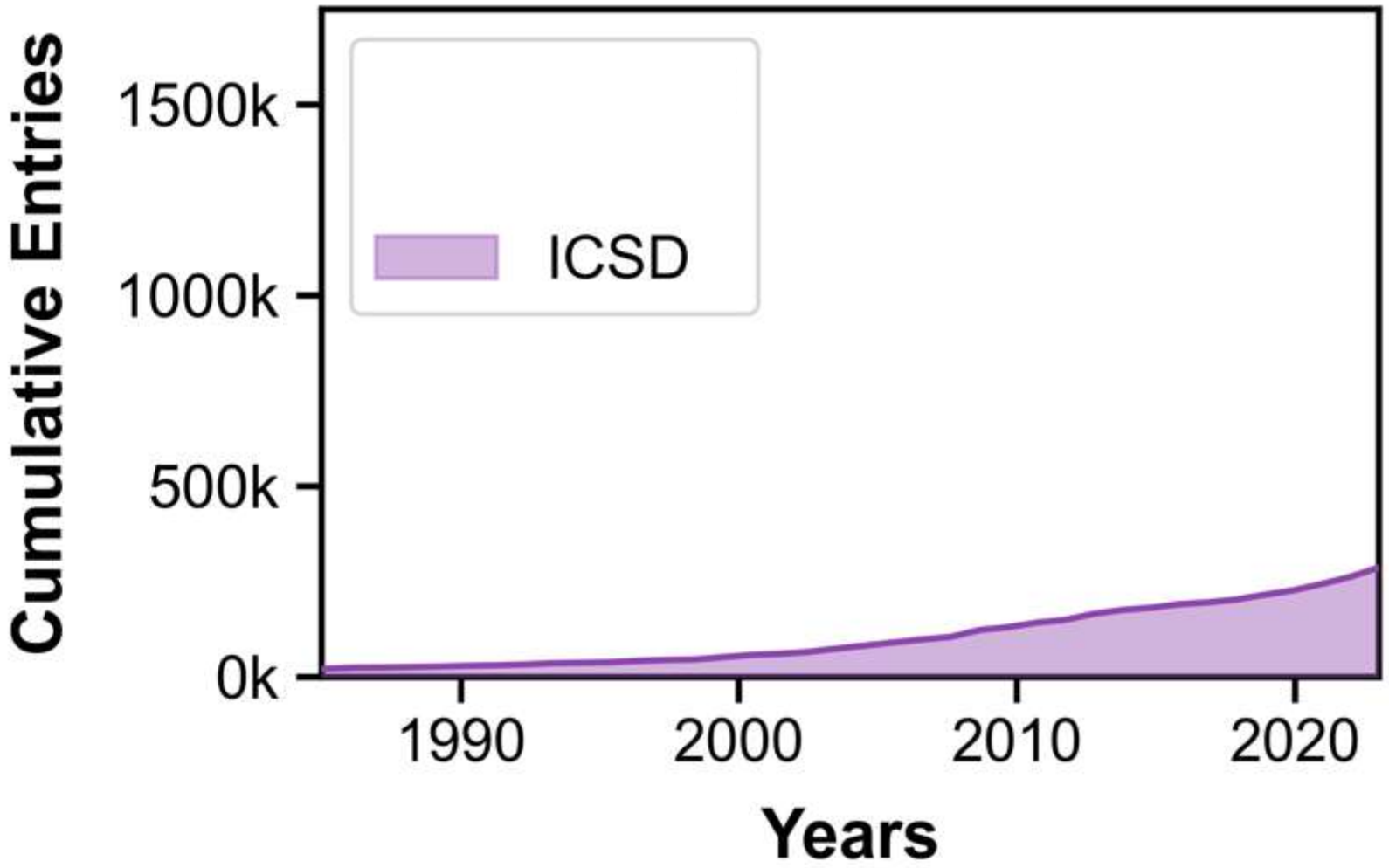
OQMD
The Open Quantum Materials Database

MATERIALS PROJECT

lexandria

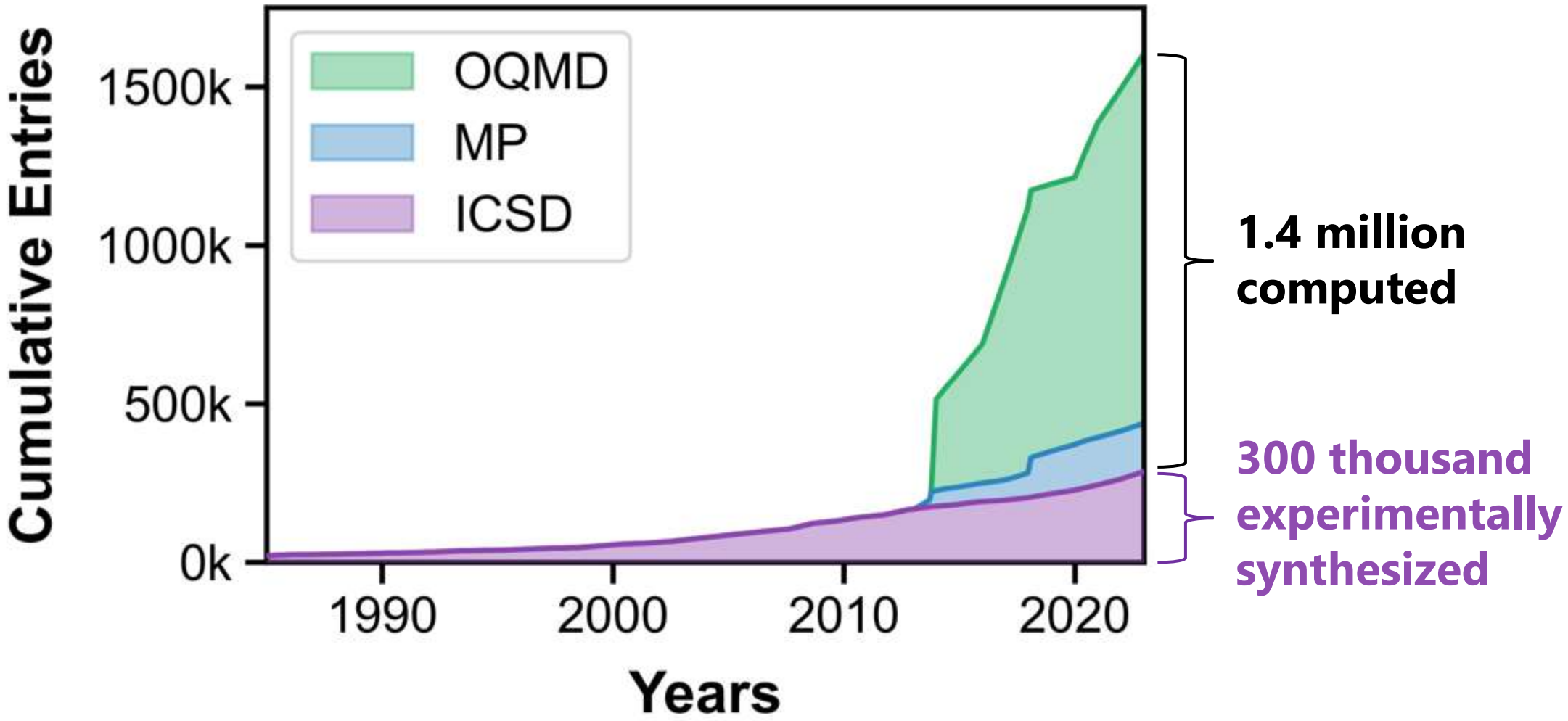
NOMAD
NOVEL MATERIALS DISCOVERY

There has been explosive growth in predicted materials



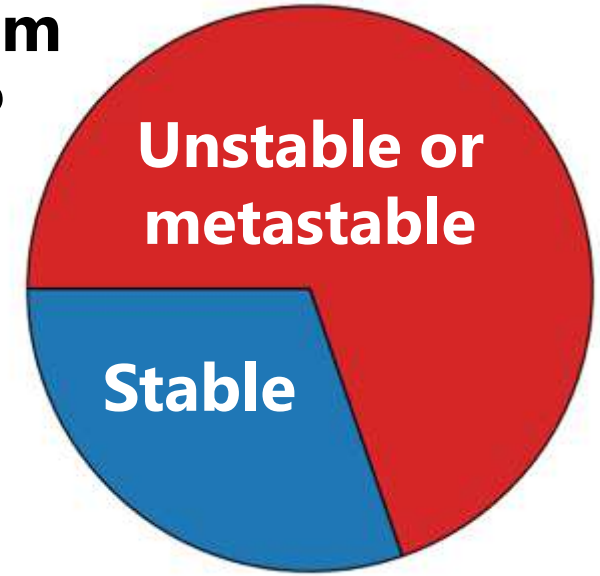
300 thousand experimentally synthesized

There has been explosive growth in predicted materials

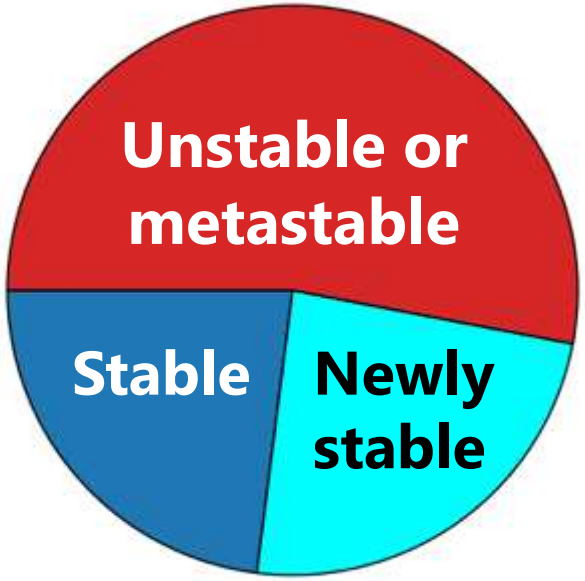


Only some of these materials are thermodynamically stable

From MP



The number of stable materials is growing fast



SCIENCE ADVANCES | RESEARCH ARTICLE

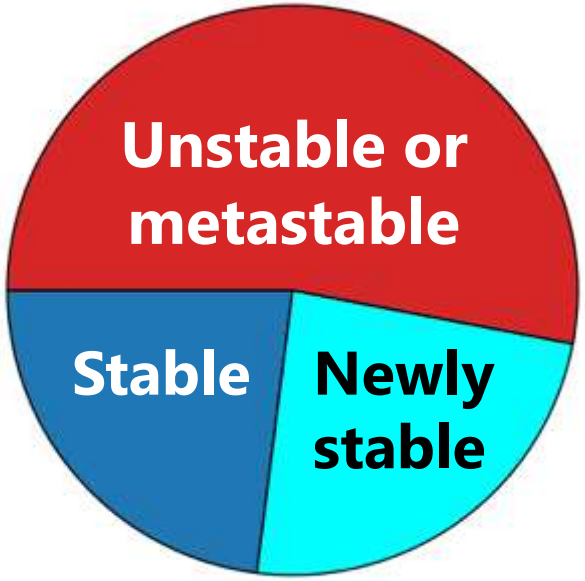
MATERIALS SCIENCE

Wide-ranging predictions of new stable compounds powered by recommendation engines

Sean D. Griesemer[1,2], Bianca Baldassarri[1], Ruijie Zhu[1], Jiahong Shen[1], Koushik Pal[1,3], Cheol Woo Park[1,4], Chris Wolverton[1]*

+60k predictions of stable materials!

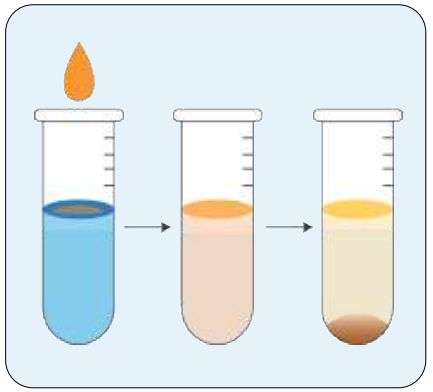
Synthesizing predicted materials remains challenging

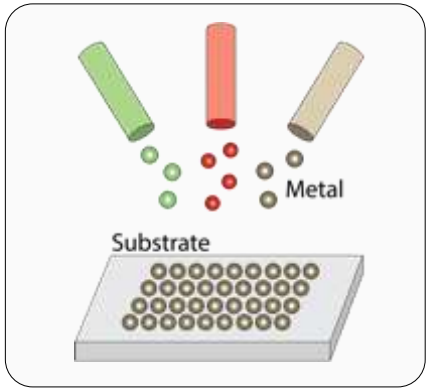


?

Solid-state

Solution

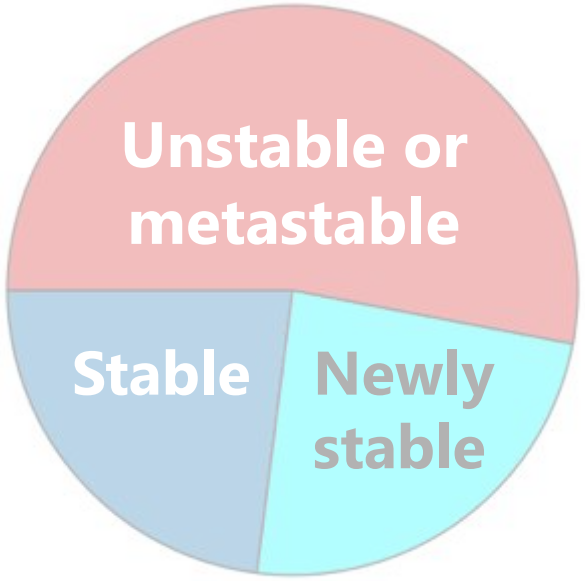




Thin film

So how do we synthesize these compounds?

Synthesizing predicted materials remains challenging



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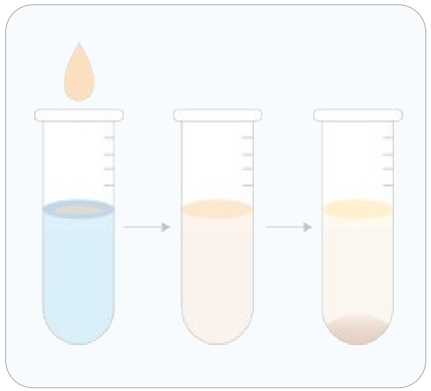
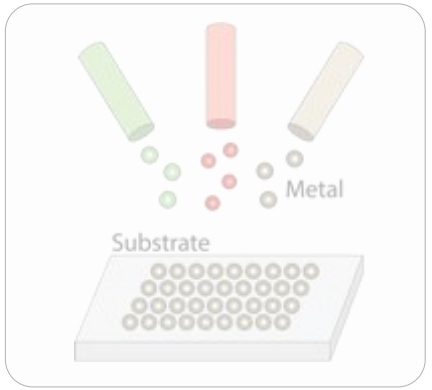




Thin film

Trial and error

What **precursors** and **conditions** to use? ⟶ The wrong answer may lead to:

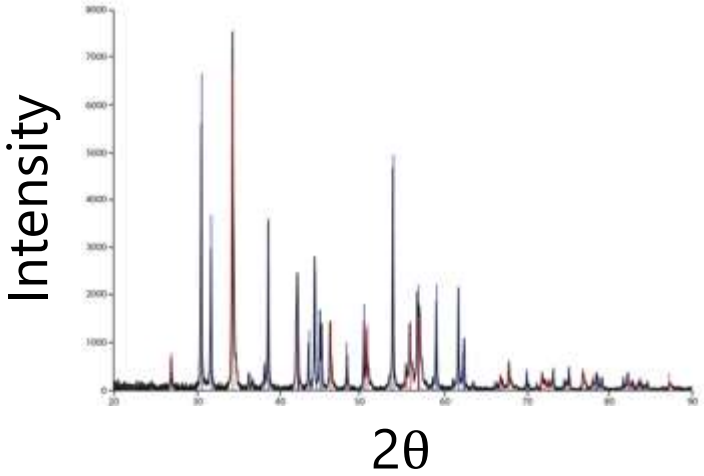
No target formed **Impurities**

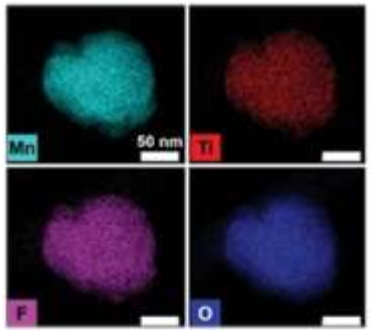
Loss of necessary elements

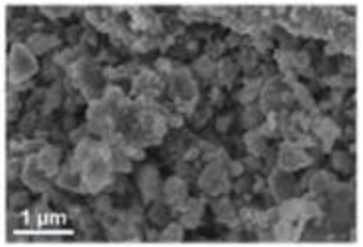
Characterization is a long and expertise-driven process

The **"cook-and-look"** process

Synthesis attempt ⇄ **Characterization and analysis**







Trial and error

What **precursors** and **conditions** to use? ⟶ The wrong answer may lead to:

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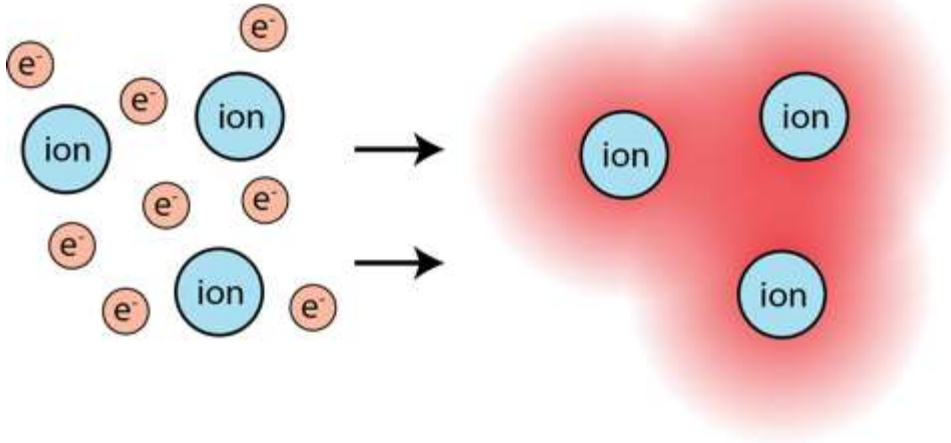
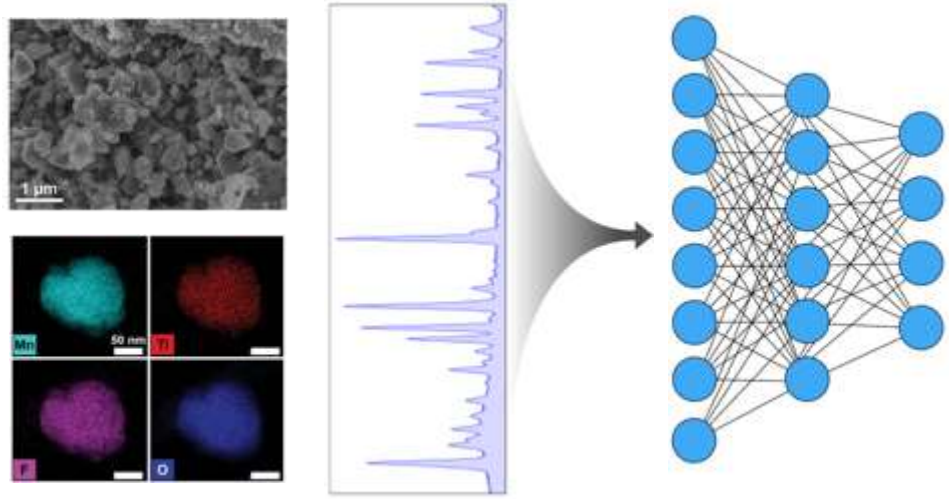
Computational tools for synthesis and characterization

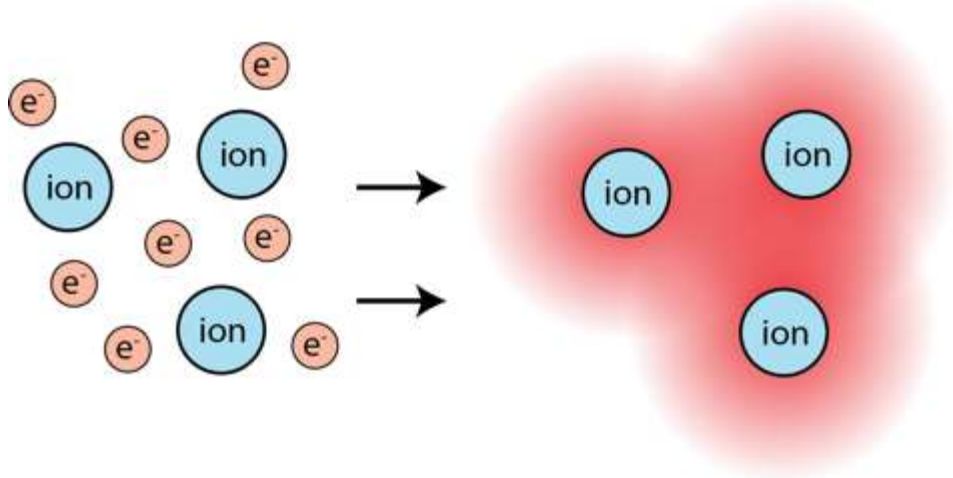




DFT for synthesis planning → **AI for characterization**

Integrate these two approaches for **closed-loop** experimental optimization

Computational tools for synthesis and characterization



DFT for synthesis planning

1) **What can we learn from computed thermodynamics?**

2) Using what we've learned: how can we design synthesis procedures?

Ab-initio calculation of the Gibbs free energy (G)

$$G(T,P) = E + PV - TS$$

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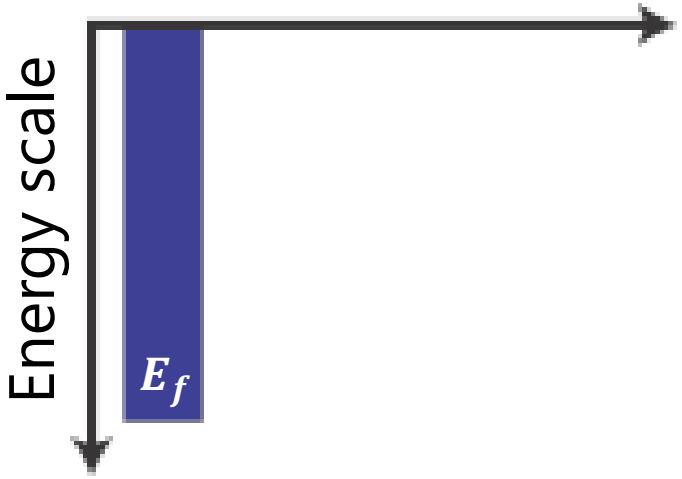
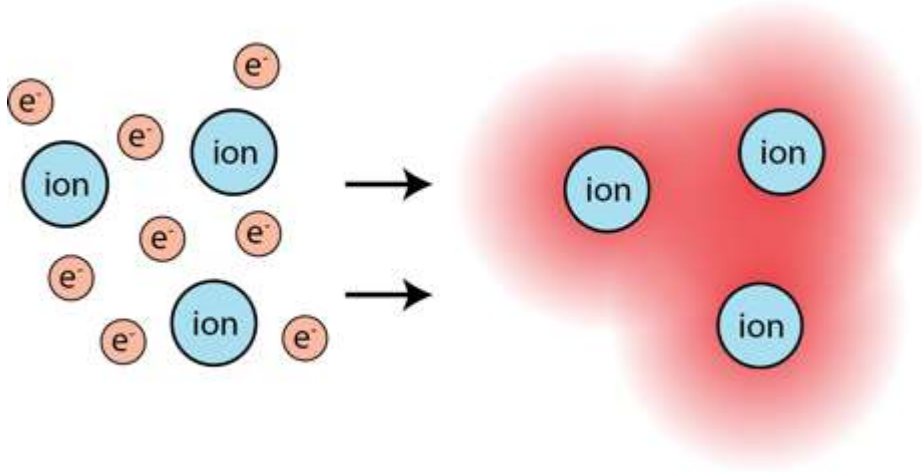


$$G(T,P) = E + PV - TS$$

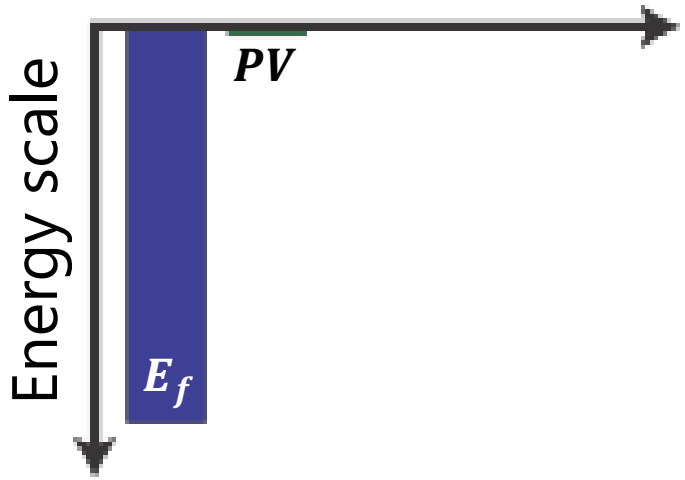
Internal energy (E) from DFT



Scale of E_f is usually a few eV/atom

Kirklin *et al.*, npj Computational Materials (2015).

Ab-initio calculation of the Gibbs free energy (G)

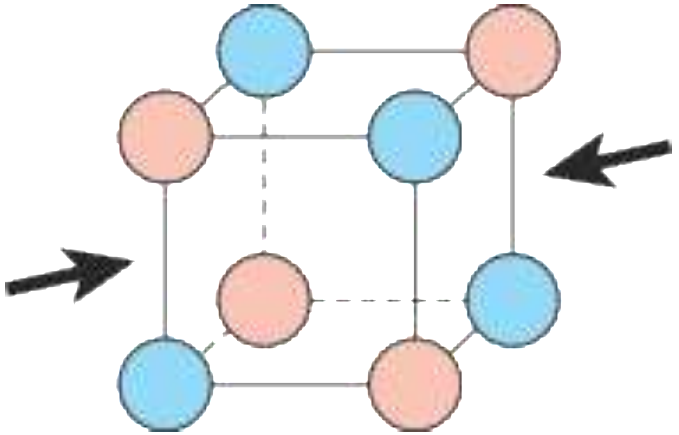


$$G(T,P) = E + PV - TS$$

Work term associated with volume change

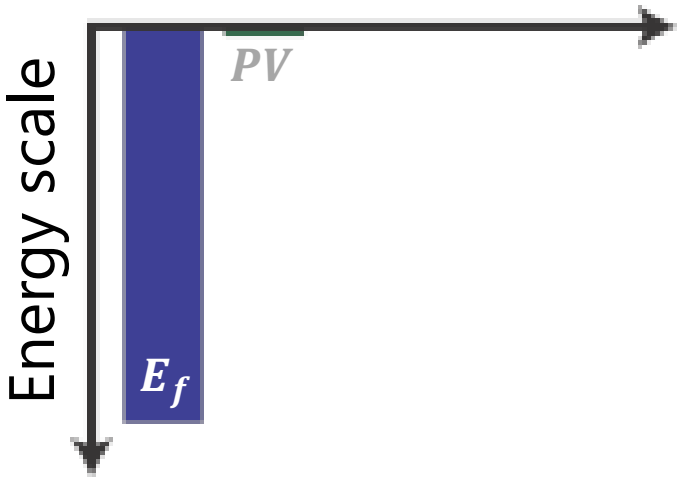
For most solids:

$P\Delta V \leq 0.01$ eV/atom



We can safely neglect this term under ambient pressure

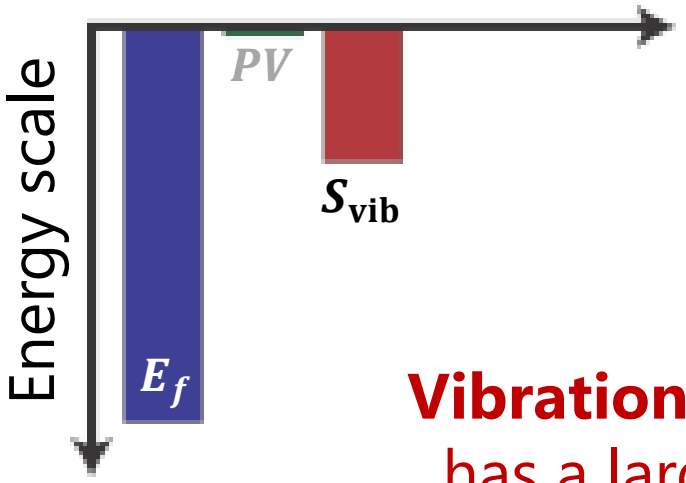
Ab-initio calculation of the Gibbs free energy (G)



$$G(T,P) = E + PV - TS$$

$$S_{\text{vib}} + S_{\text{elec}} + S_{\text{config}}$$

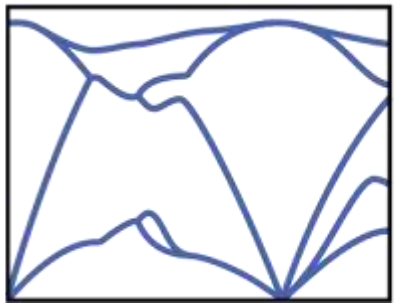
Ab-initio calculation of the Gibbs free energy (G)



$$G(T,P) = E + PV - TS$$

$$S_{vib} + S_{elec} + S_{config}$$

Vibrational entropy
has a large effect at
high temperature
(> 0.1 eV/atom)



Phonons
or ML*

*Schwalbe-Koda *et al.*, arXiv (2024).

*Bartel *et al.*, Nature Communications (2018).

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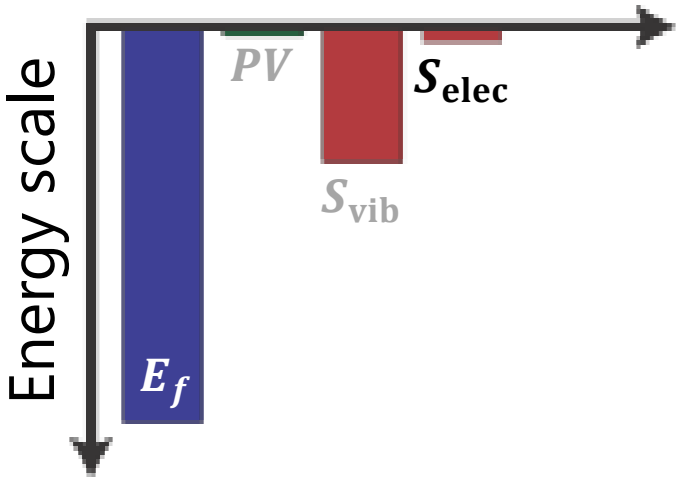
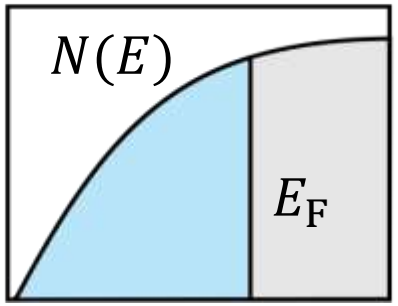


$$G(T,P) = E + PV - TS$$

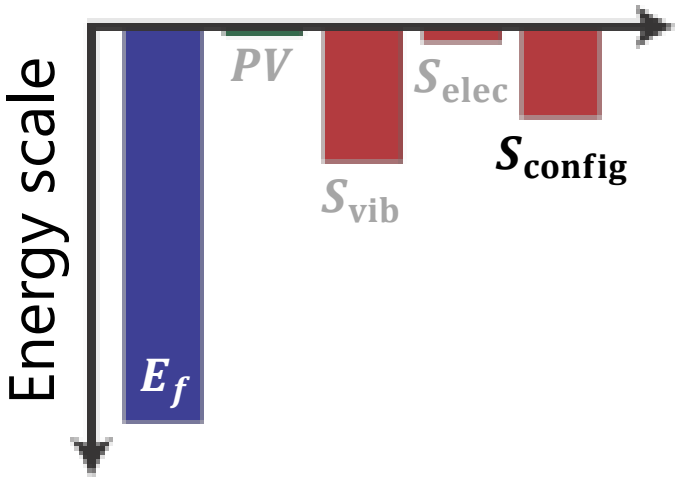
$$S_{\mathrm{vib}} + S_{\mathrm{elec}} + S_{\mathrm{config}}$$

Electronic entropy has a small effect on most solids (~ 0.01 eV/atom)



Density of states

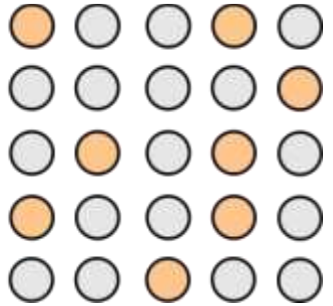
Ab-initio calculation of the Gibbs free energy (G)



$$G(T,P) = E + PV - TS$$

$$S_{vib} + S_{elec} + S_{config}$$

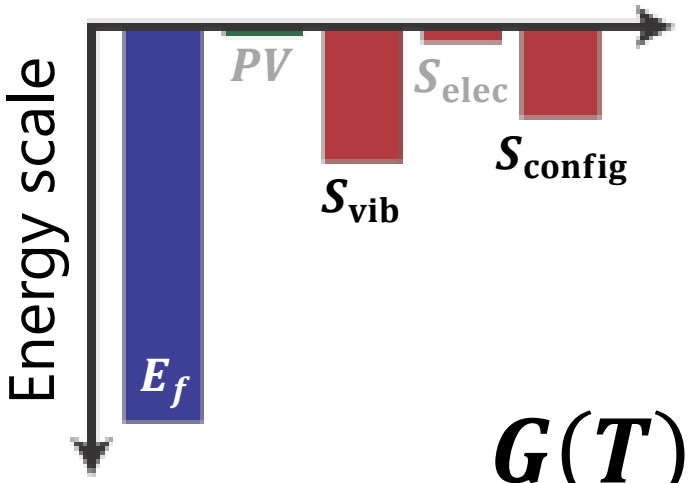
Configurational entropy has a large effect on disordered materials (~0.1 eV/atom)



$$S = -Nk_B \sum_i x_i \ln x_i$$

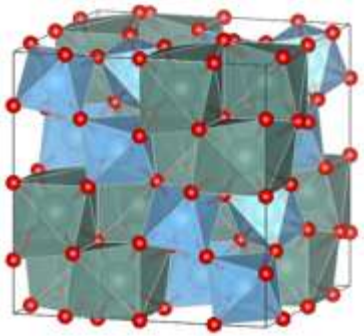
Statistical thermo.

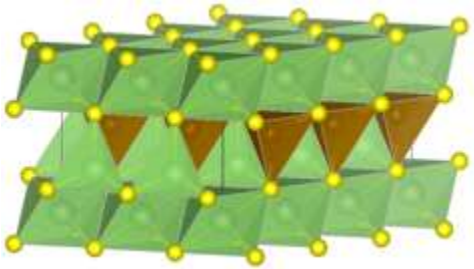
Ab-initio calculation of the Gibbs free energy (G)

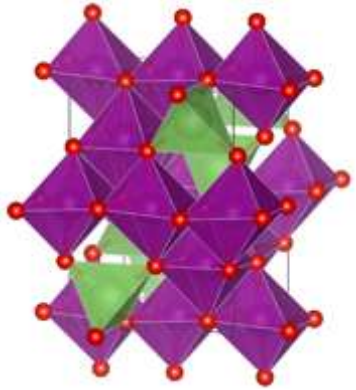


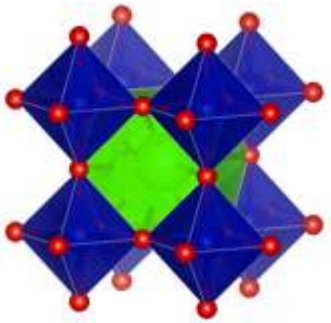
$$G(T,P) = E + PV - TS$$

$$G(T) = E - TS_{vib} + Nk_BT\sum_i x_i \ln x_i$$

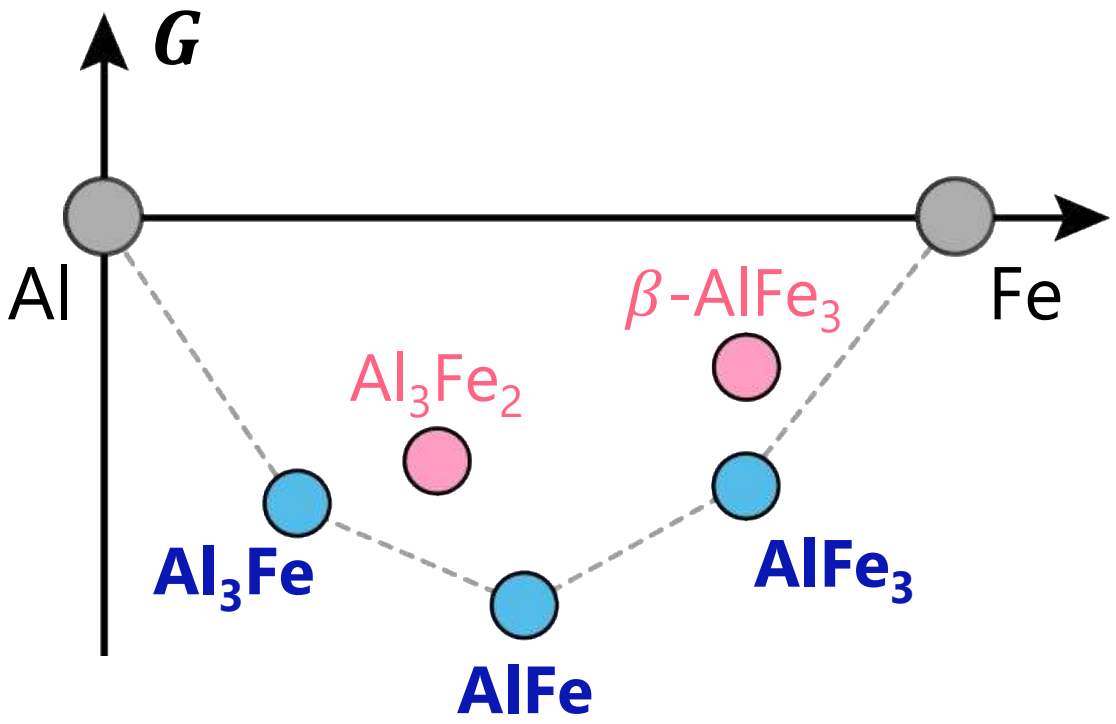




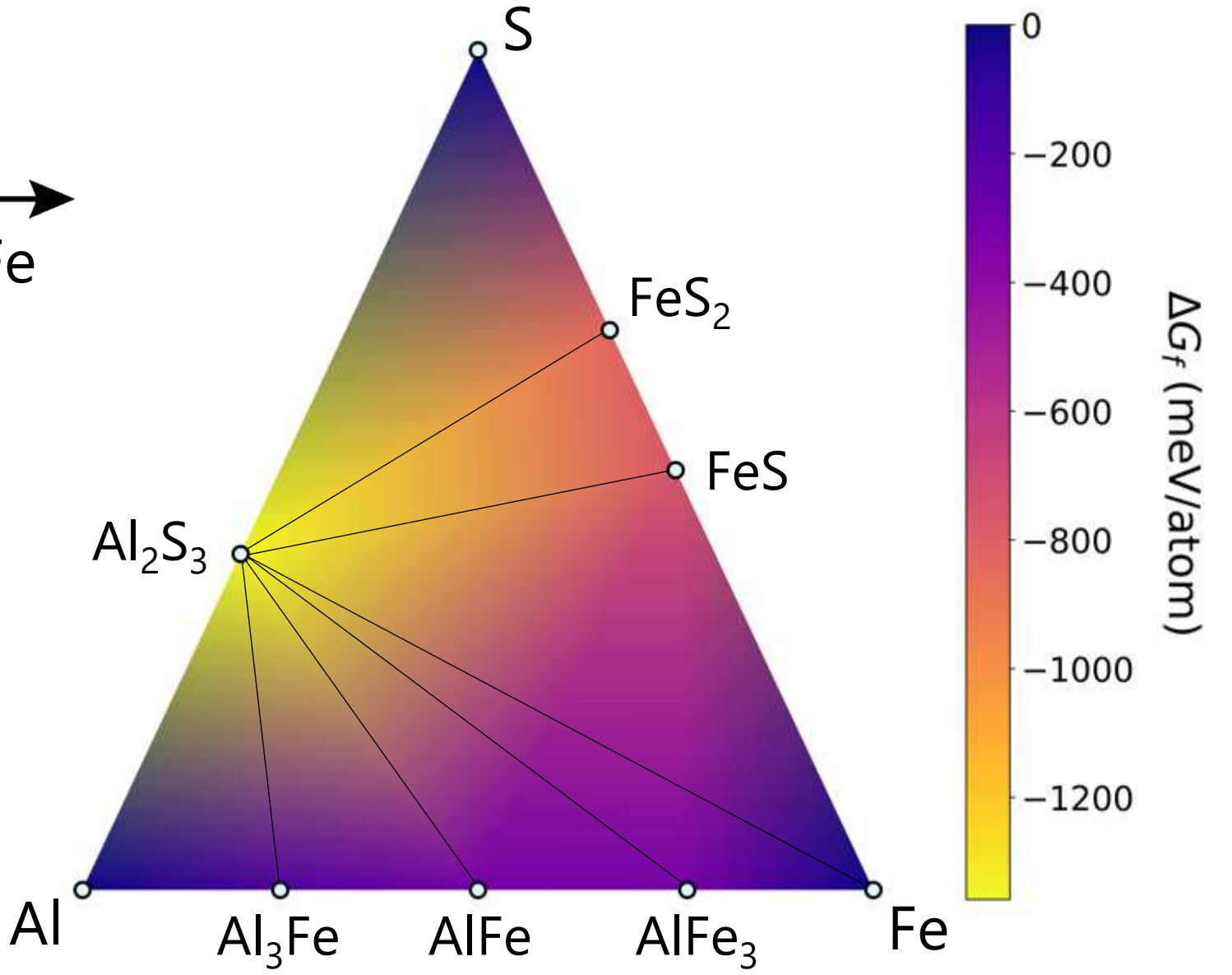




Using $G(T)$ to make computational phase diagrams



Ground states = lowest G
at a given composition



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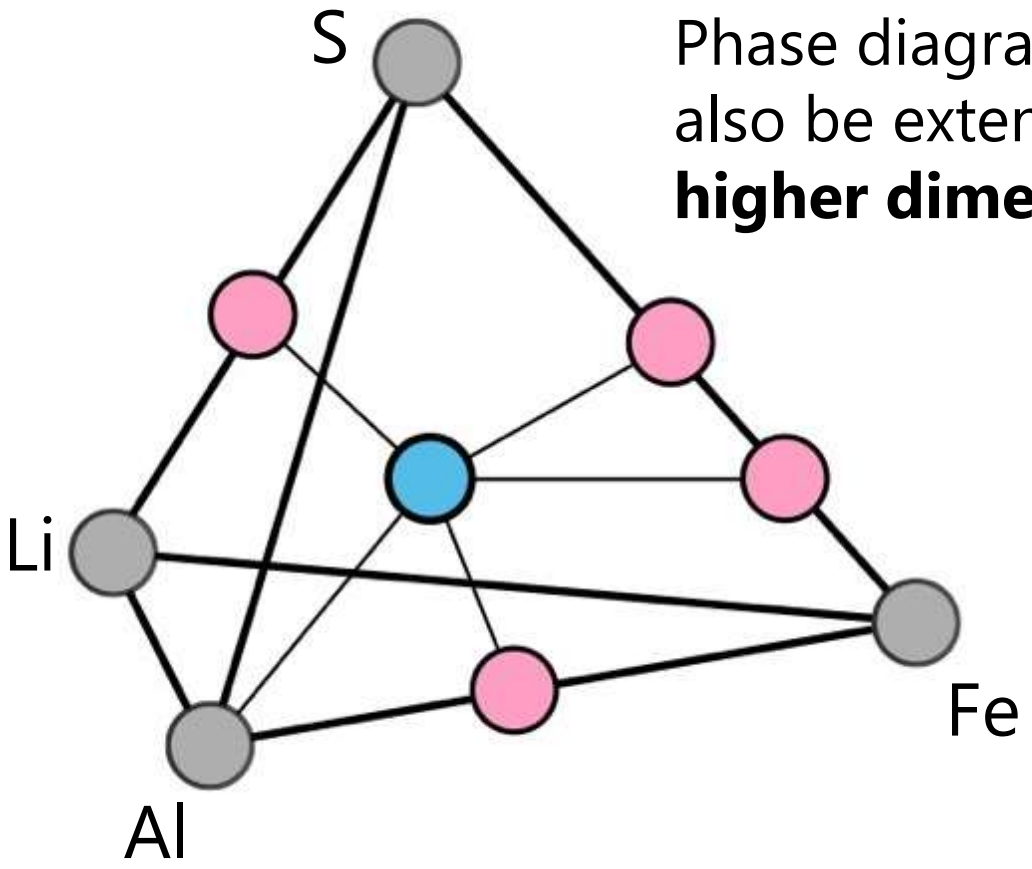
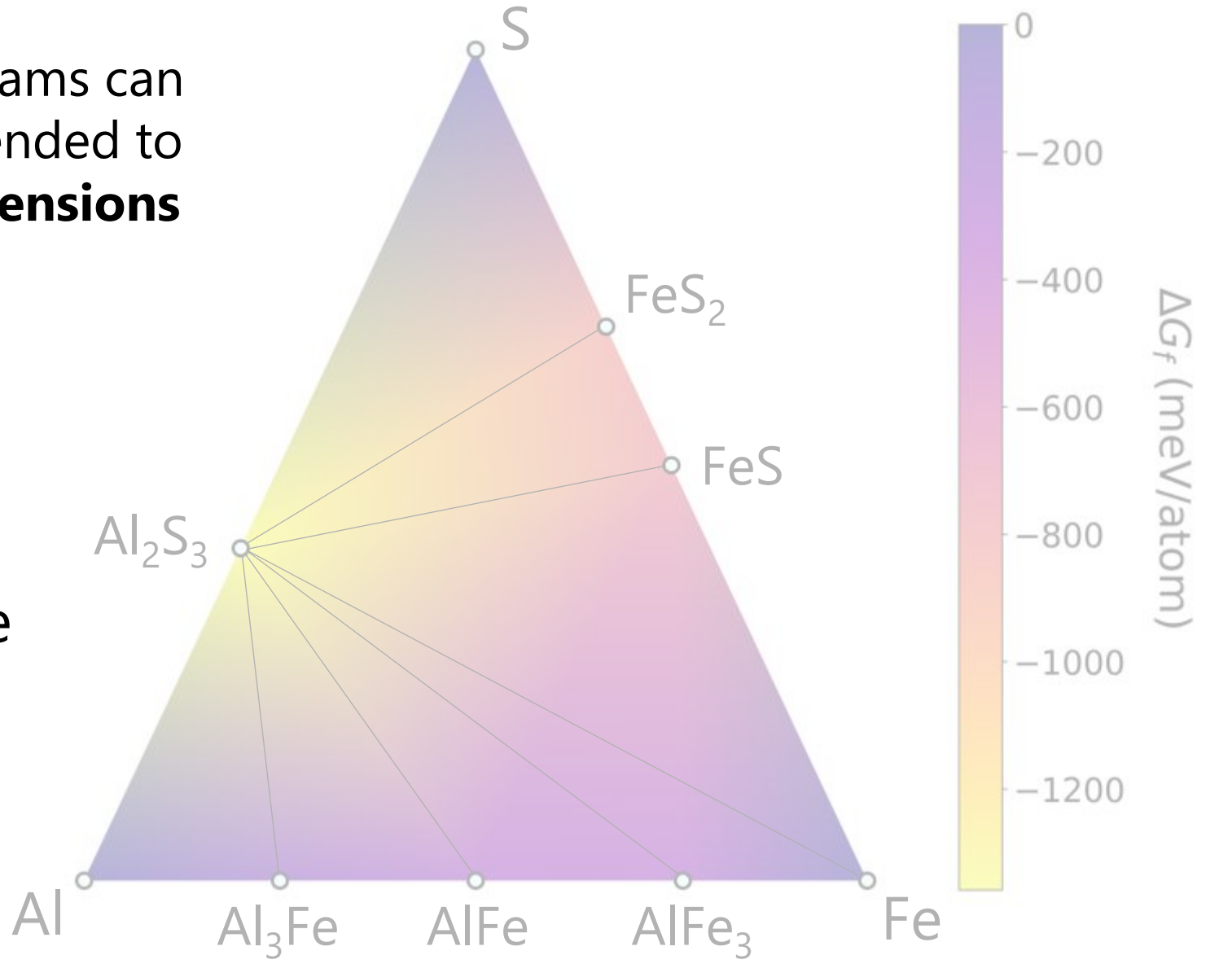
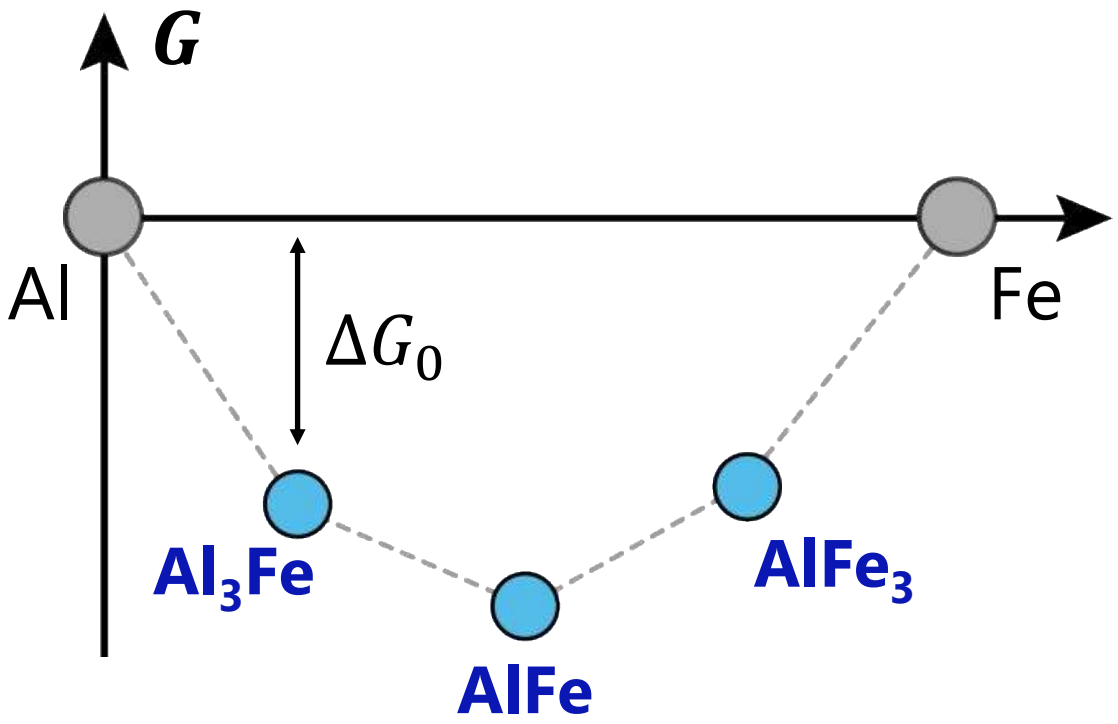
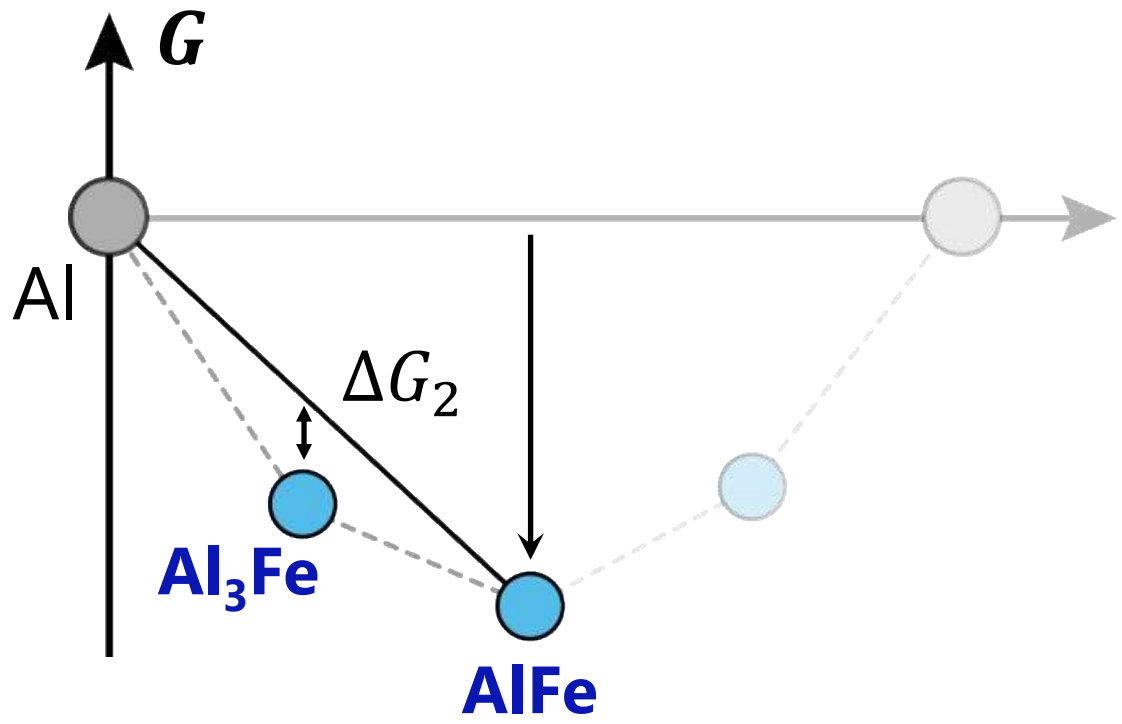


Phase diagrams can also be extended to **higher dimensions**



Computed phase diagrams don't always tell the whole story



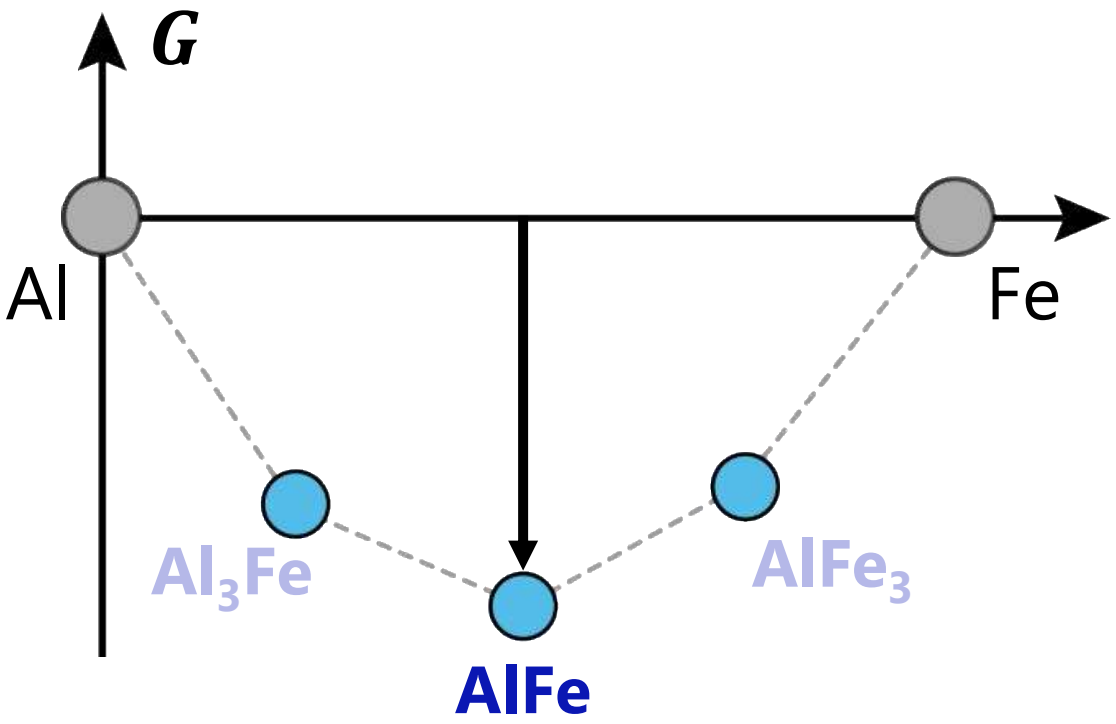


Desired reaction: $3\ \mathrm{Al} + \mathrm{Fe} \rightarrow \mathrm{Al_3Fe}\ (\Delta G_0 = -199\ \mathrm{meV/atom})$

Actual reactions: $\mathrm{Al} + \mathrm{Fe} \rightarrow \mathrm{AlFe}\ (\Delta G_1 = -327\ \mathrm{meV/atom})$

$\mathrm{AlFe} + 2\ \mathrm{Al} \rightarrow \mathrm{Al_3Fe}\ (\Delta G_2 = -83\ \mathrm{meV/atom})$

Computed phase diagrams don't always tell the whole story



Can we predict this initial reaction from the phase diagram alone?

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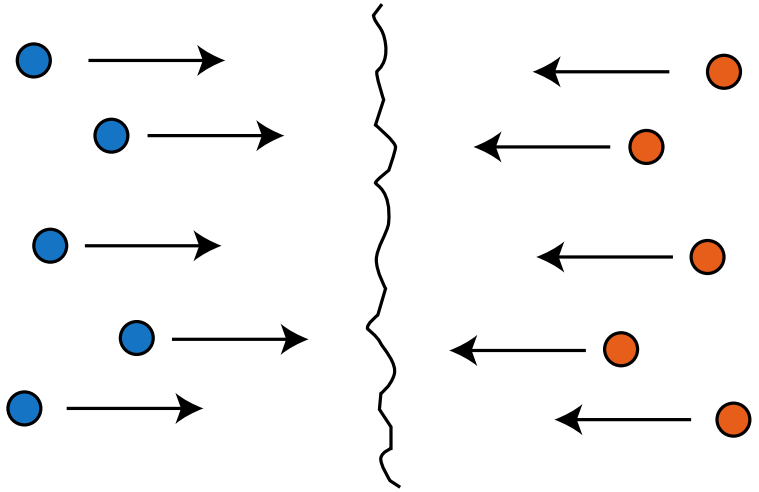
Actual reactions: $\mathrm{Al} + \mathrm{Fe} \rightarrow \mathrm{AlFe}\ (\Delta G_1 = -327\ \mathrm{meV/atom})$

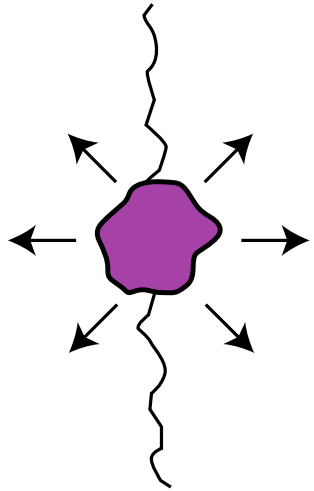
$\mathrm{AlFe} + 2\,\mathrm{Al} \rightarrow \mathrm{Al_3Fe}\ (\Delta G_2 = -83\ \mathrm{meV/atom})$

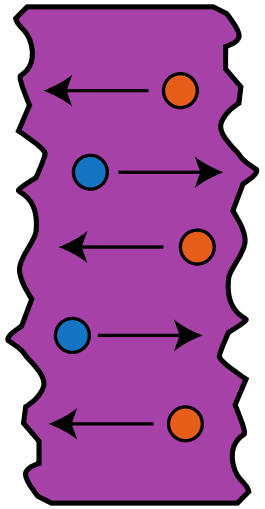
Reactions are inherently dictated by kinetics

Ions need to **diffuse** to the interface



A product needs to **nucleate**



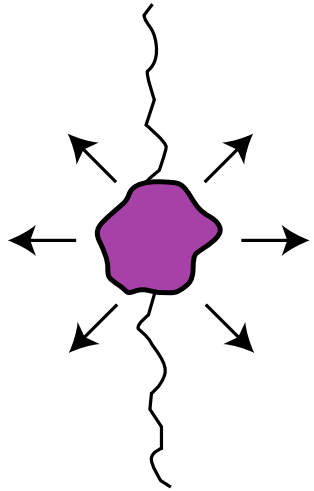


That product needs to grow *via* interdiffusion

Reactions are inherently dictated by kinetics

Ions need to **diffuse** to the interface

A product needs to **nucleate**



That product needs to grow *via* interdiffusion

Nucleation primarily depends on ΔG and σ

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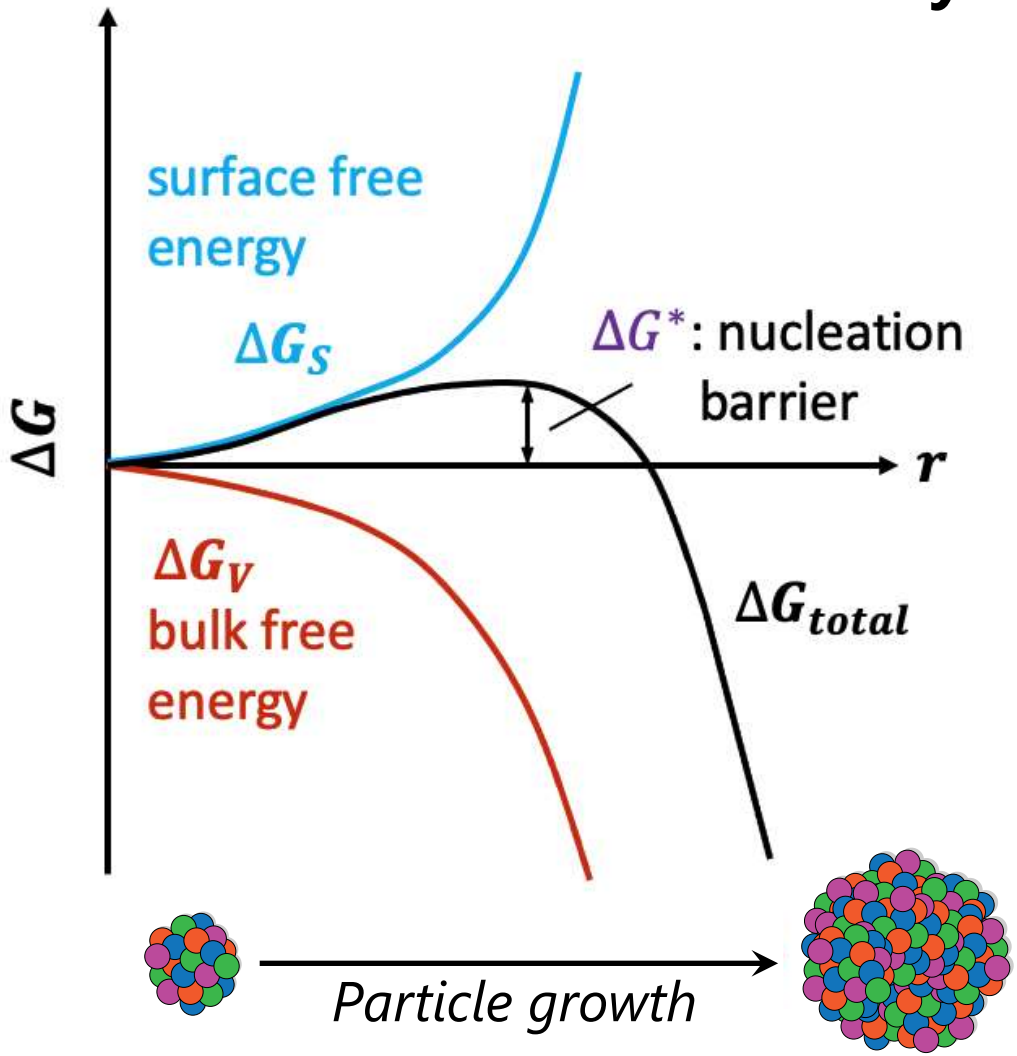
Classical nucleation theory



Nucleation rate:

$$Q = \mathrm{A}\exp\left(-\frac{\Delta G^*}{k_\mathrm{B}T}\right)$$

Nucleation barrier:

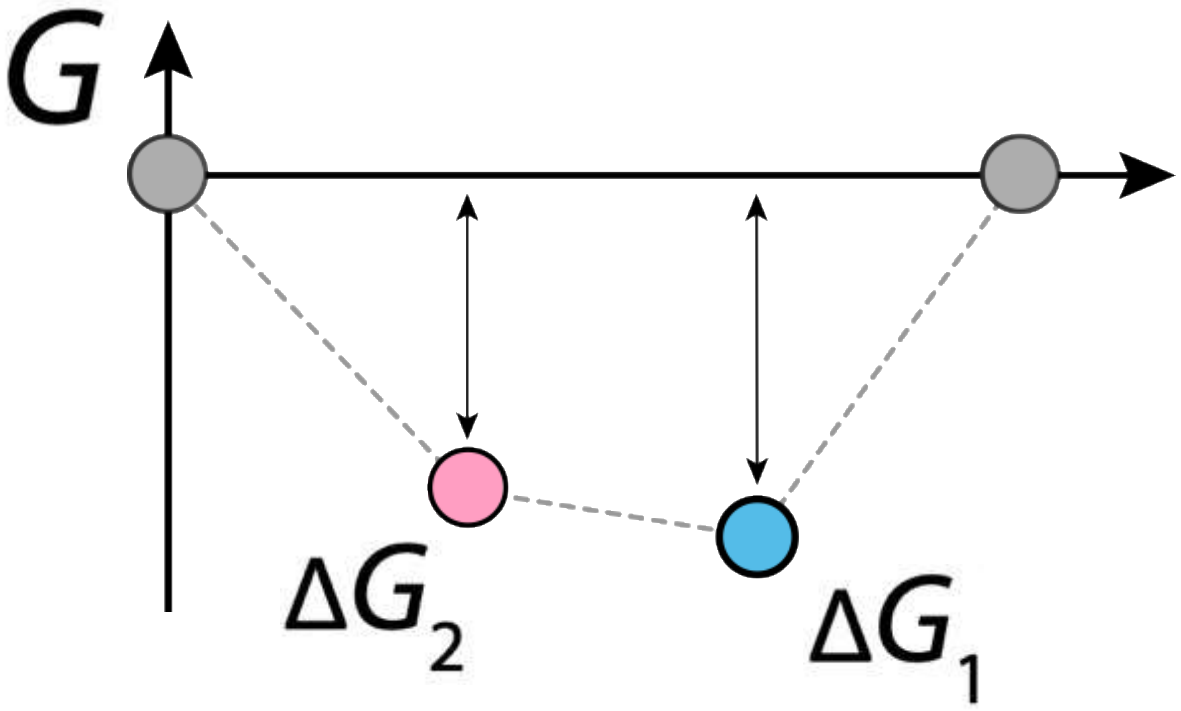
$$\Delta G^* = \frac{16\pi\sigma^3}{3(n\Delta G)^2}$$

Surface energy

Atomic density

Bulk reaction energy

Can we use ΔG to predict which phase will nucleate first?

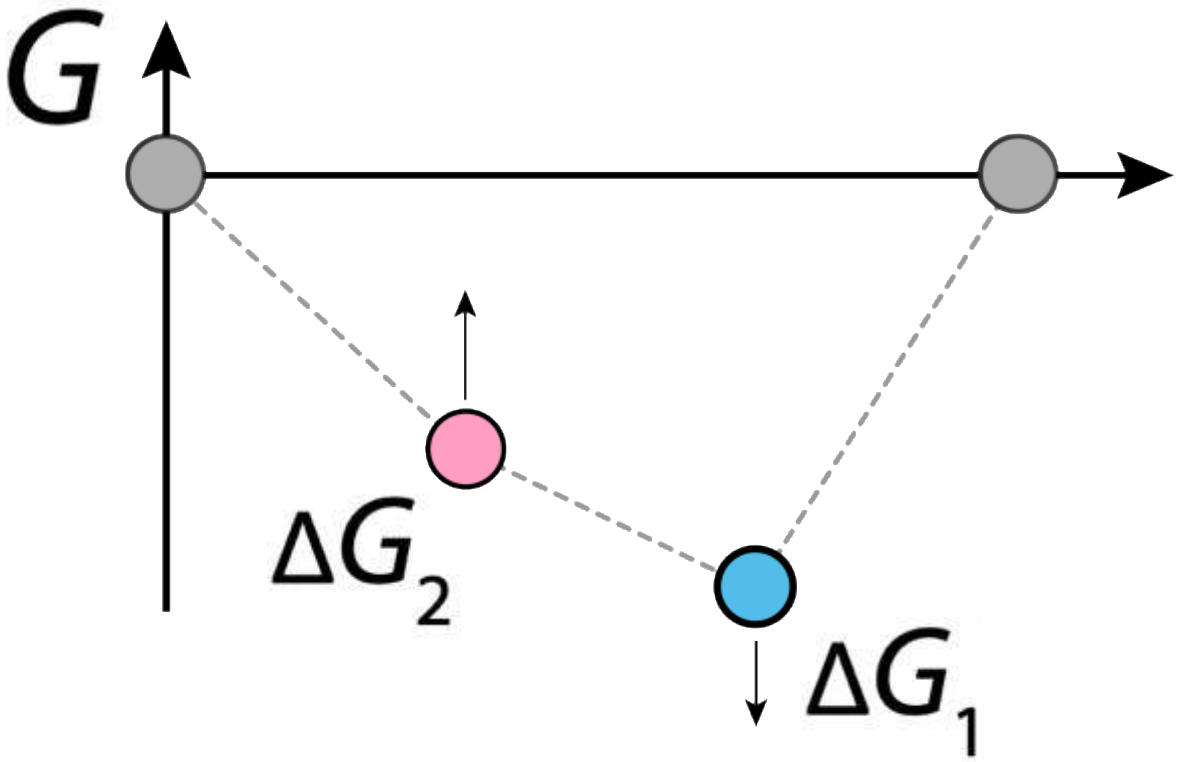


$$\ln(\boldsymbol{Q_1}/\boldsymbol{Q_2}) = \frac{16\pi}{3n^2 k_B T}\left(\frac{(\sigma_1)^3}{(\Delta G_1)^2} - \frac{(\sigma_2)^3}{(\Delta G_2)^2}\right)$$

Surface energy

Bulk reaction energy

Can we use ΔG to predict which phase will nucleate first?



Hypothesis:

If the difference between ΔG_1 and ΔG_2 is sufficiently large, it outweighs any difference between σ_1 and σ_2

$$\ln(\boldsymbol{Q_1}/\boldsymbol{Q_2}) = \frac{16\pi}{3n^2 k_B T}\left(\frac{(\sigma_1)^3}{(\Delta G_1)^2} - \frac{(\sigma_2)^3}{(\Delta G_2)^2}\right)$$

Surface energy

Bulk reaction energy

Can we use ΔG to predict which phase will nucleate first?

How large is "sufficiently large"

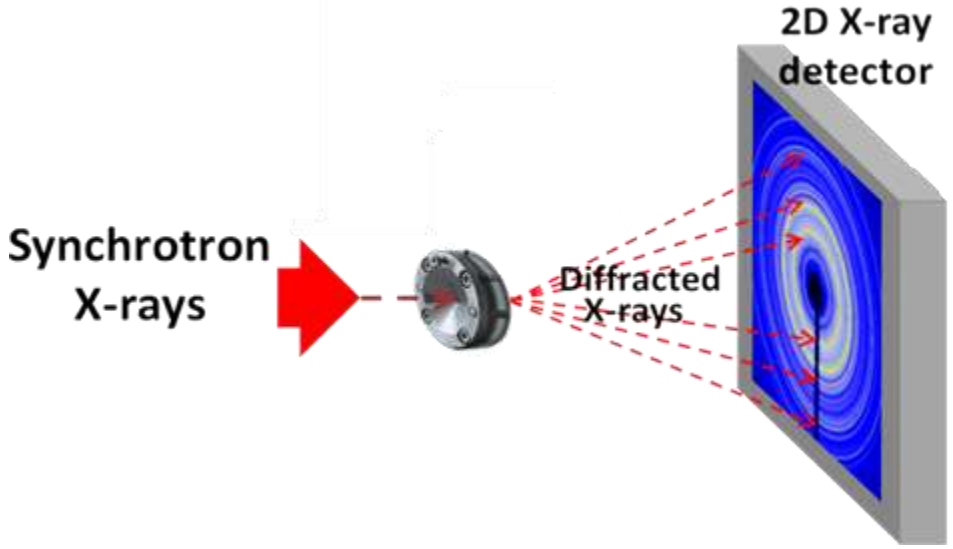
If the difference between ΔG_1 and ΔG_2 is **sufficiently large**, it outweighs any difference between σ_1 and σ_2

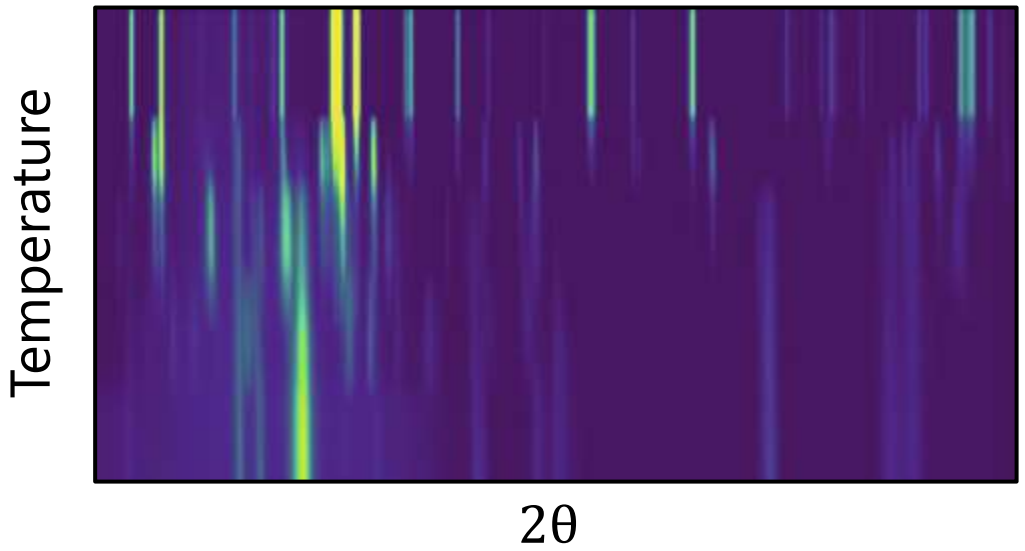
$$\ln(Q_1/Q_2) = \frac{16\pi}{3n^2 k_B T}\left(\frac{(\sigma_1)^3}{(\Delta G_1)^2} - \frac{(\sigma_2)^3}{(\Delta G_2)^2}\right)$$

Surface energy

Bulk reaction energy

Quantifying the limit using *in-situ* X-ray diffraction (XRD)





Given a pair of solid reactants, what is the **first product** that forms during heating?

Szymanski *et al.*, Science Advances (2024).

We used 37 ternary metal oxides (*A*-*M*-O) as a test case

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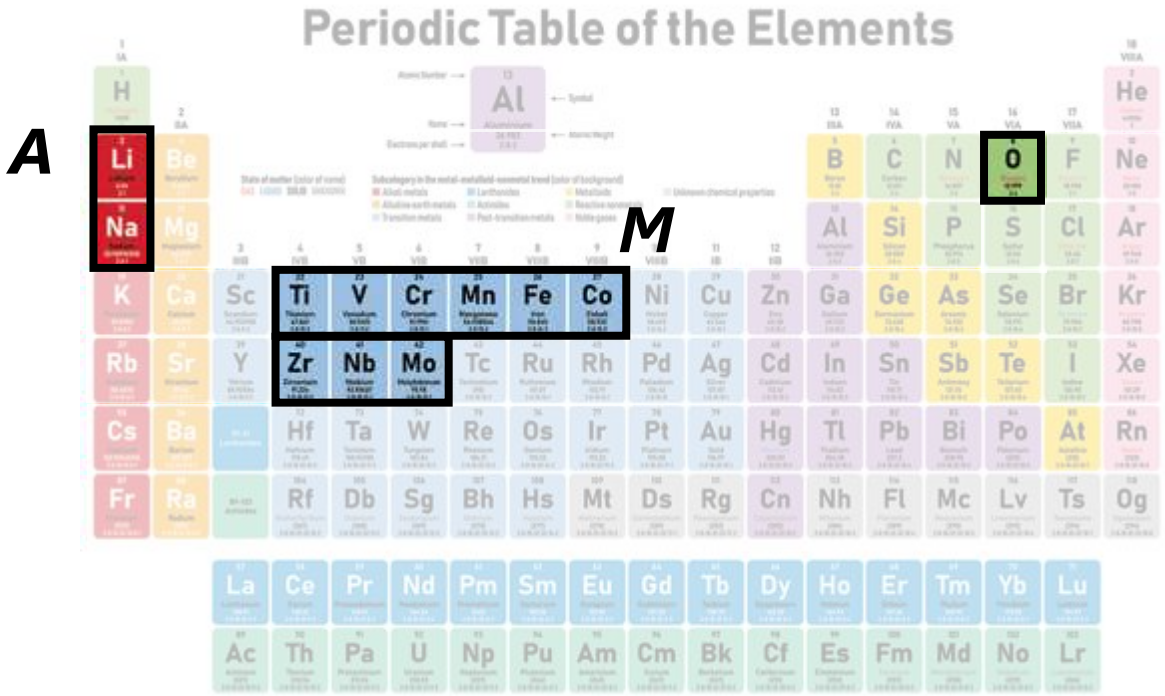
We took **alkali (*A*) precursors**:

Li_2CO_3, LiOH, Li_2O, $NaNO_3$, …

Mixed them with **metal (*M*) precursors**:

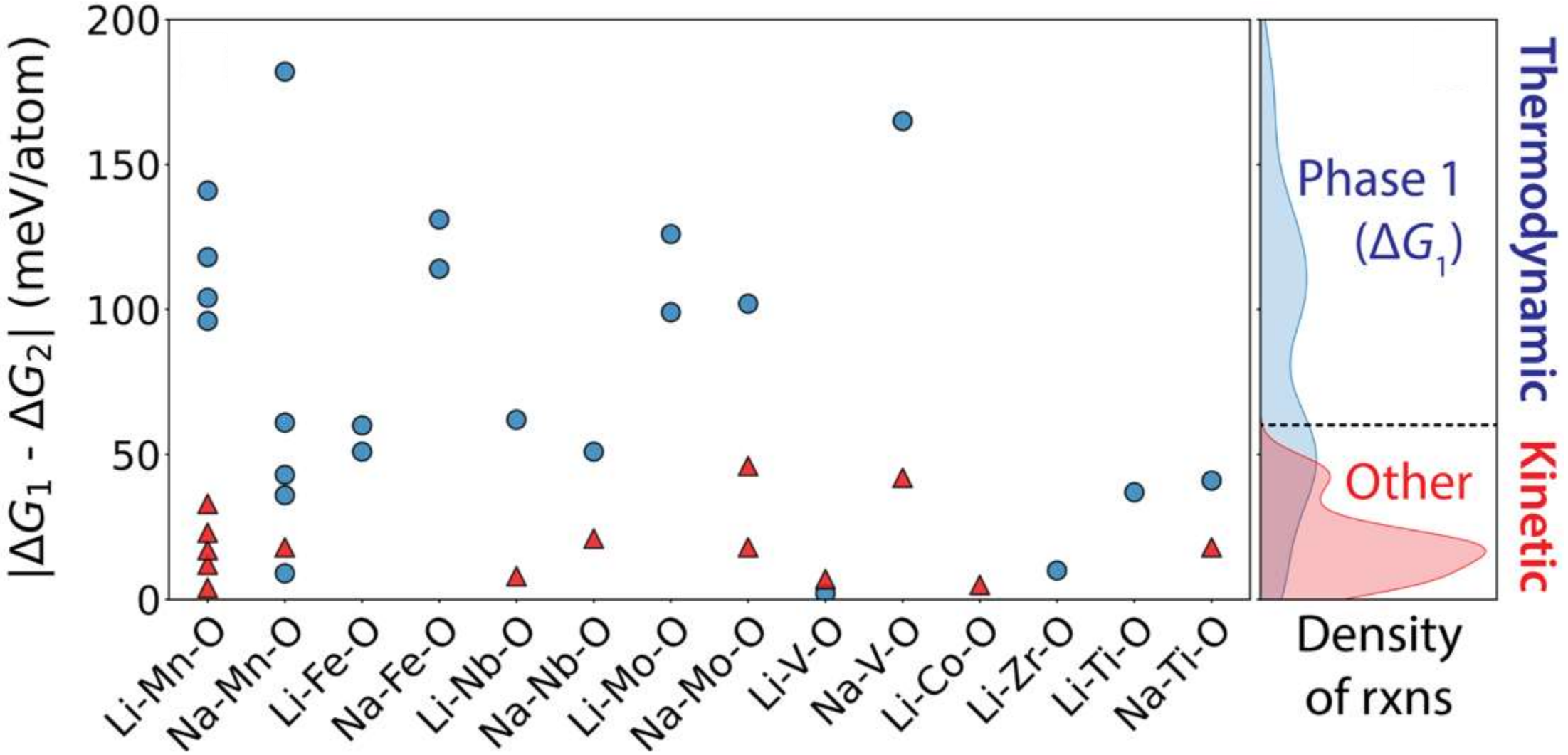
MnO, Mn_3O_4, MnO_2, Cr_2O_3, …

In a **1:1 ratio of *A*:*M*** for each sample, which was then **heated to 600 °C** while XRD scans were performed.



Szymanski *et al.*, Science Advances (2024).

Outcomes show a regime of thermodynamic (ΔG) control



Szymanski *et al.*, Science Advances (2024).

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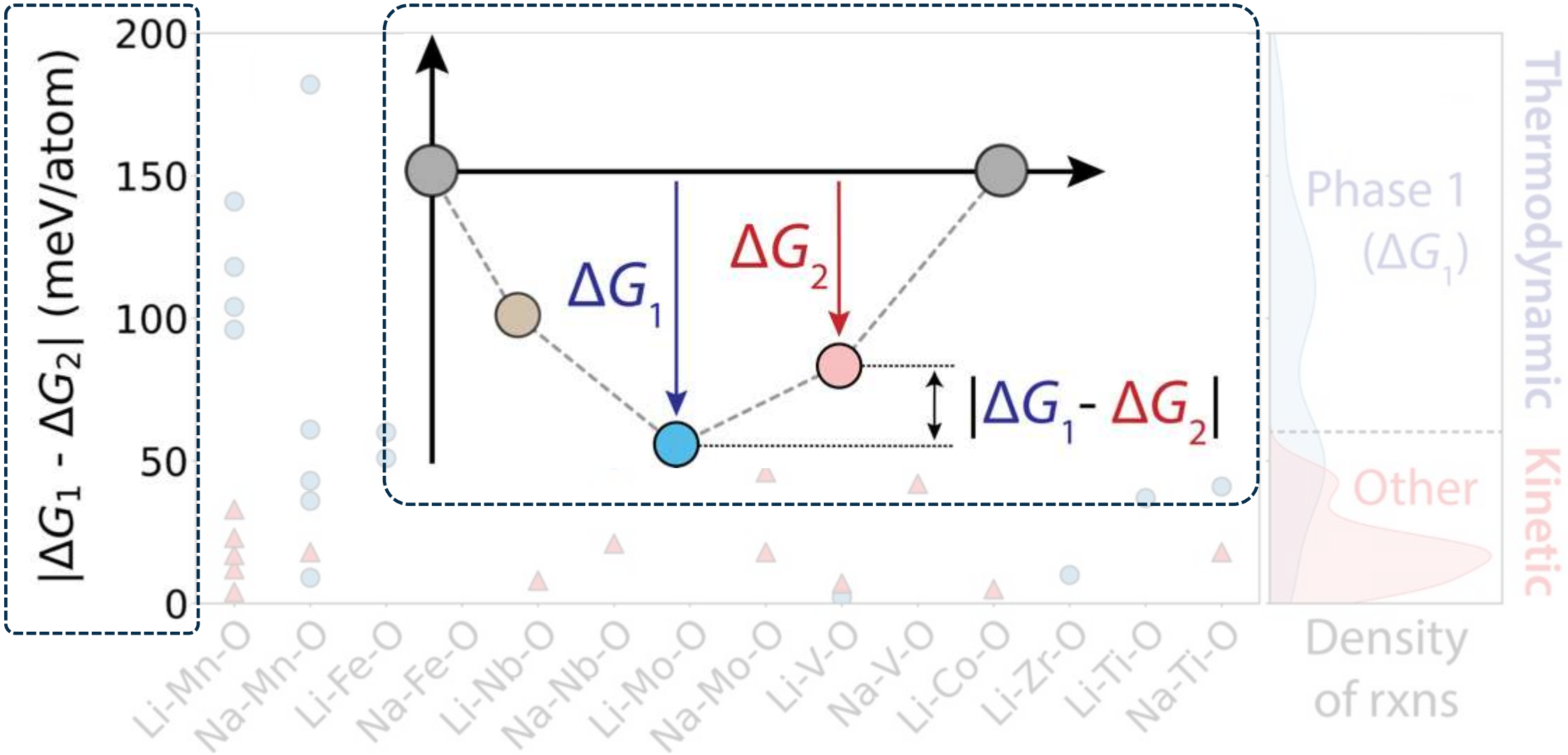

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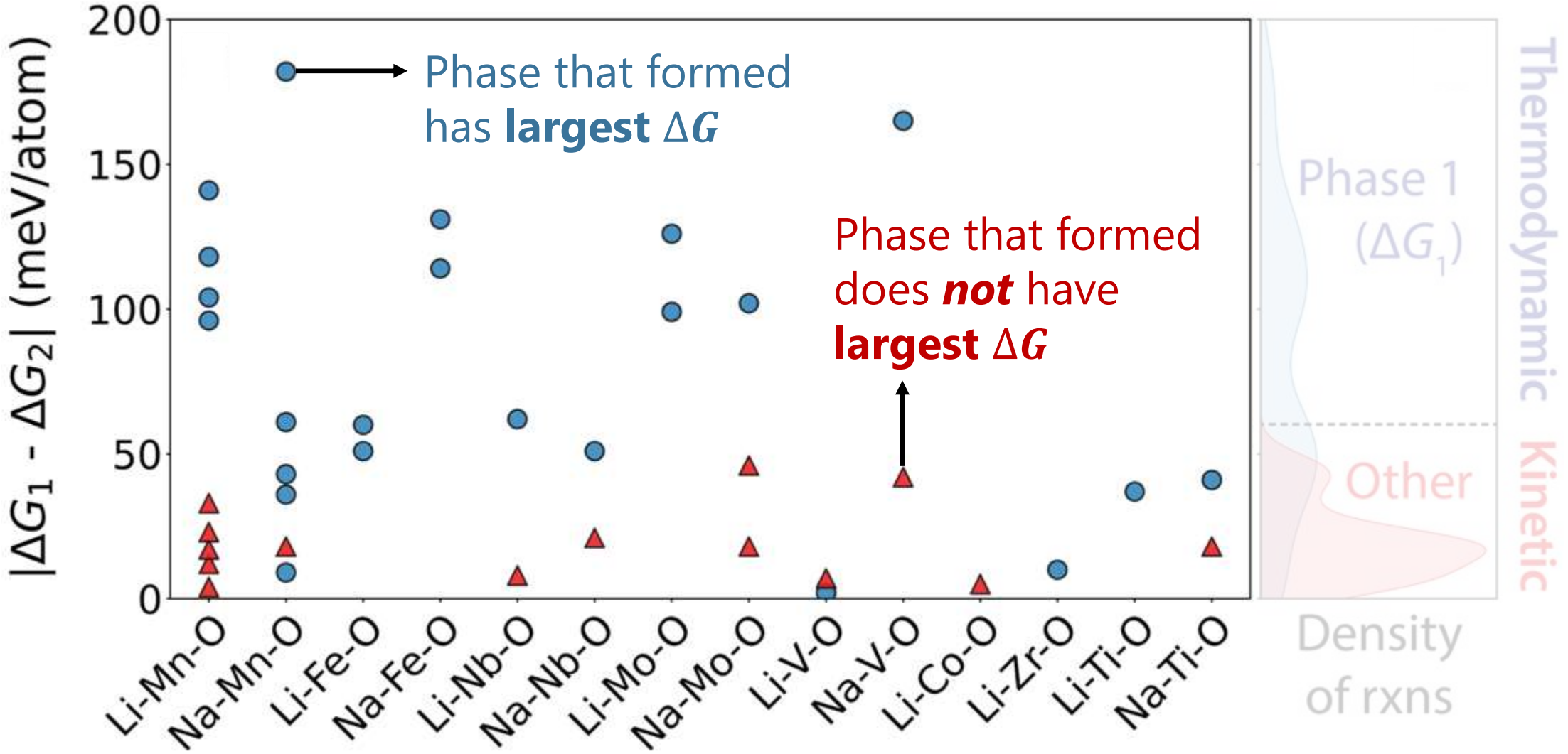

Szymanski *et al.*, Science Advances (2024).

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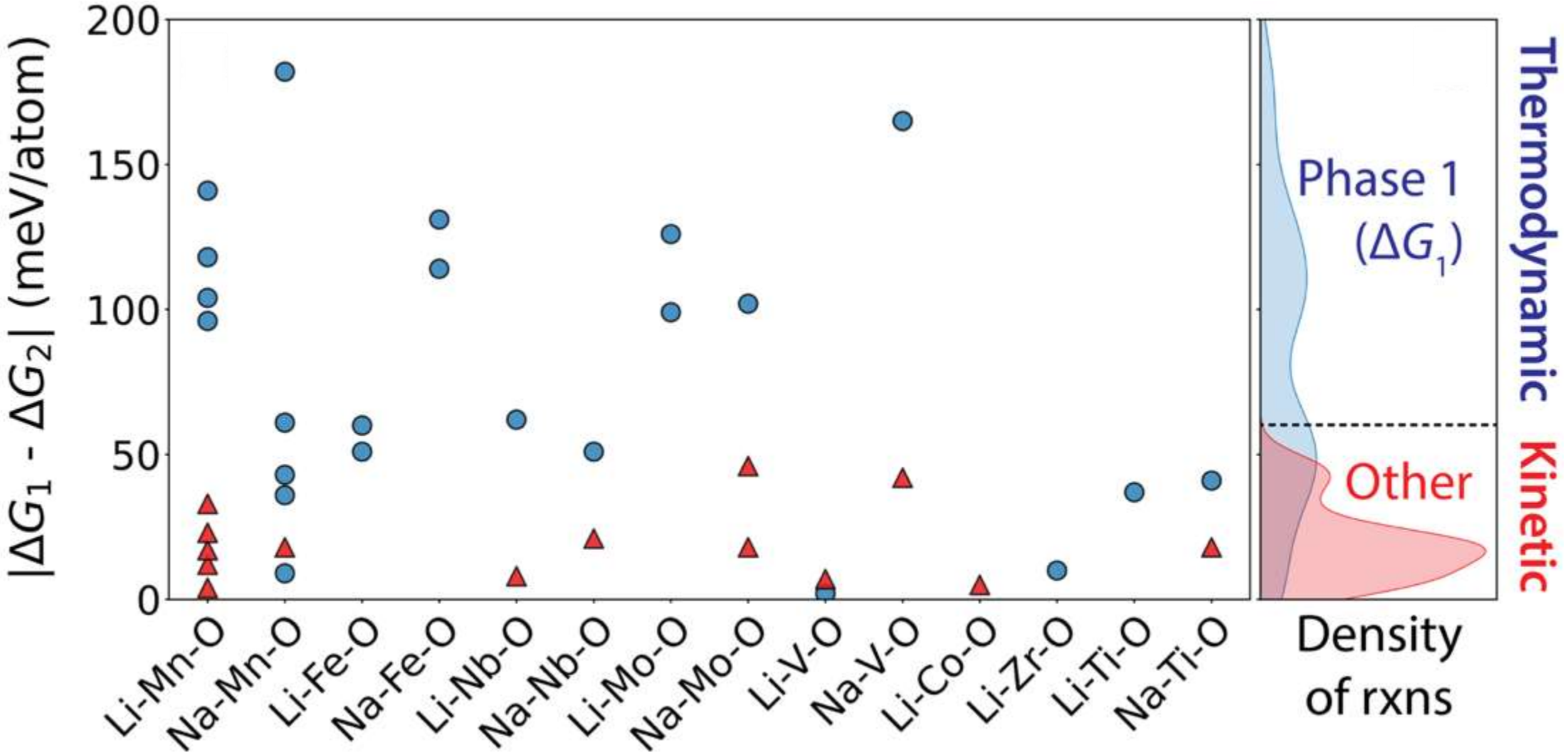
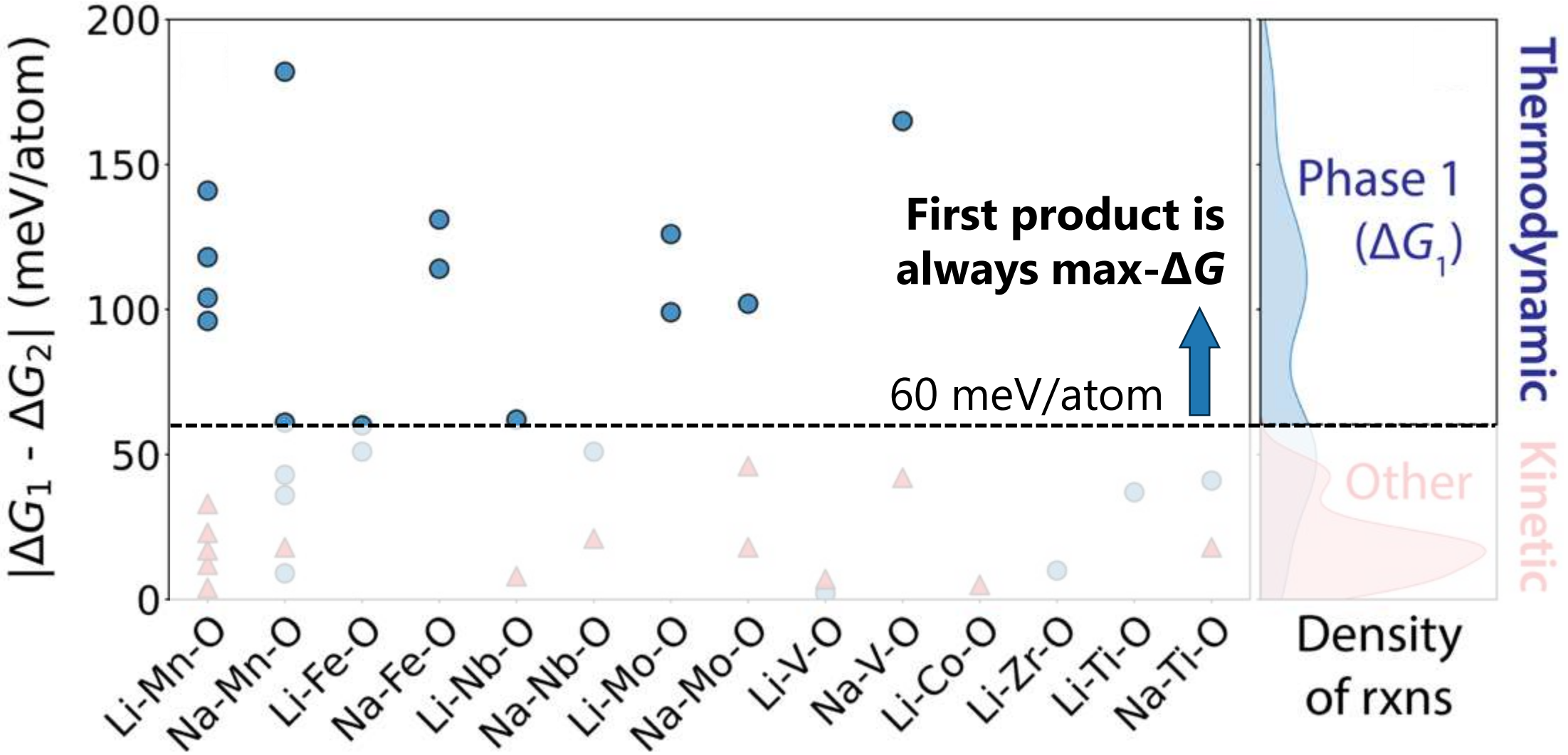


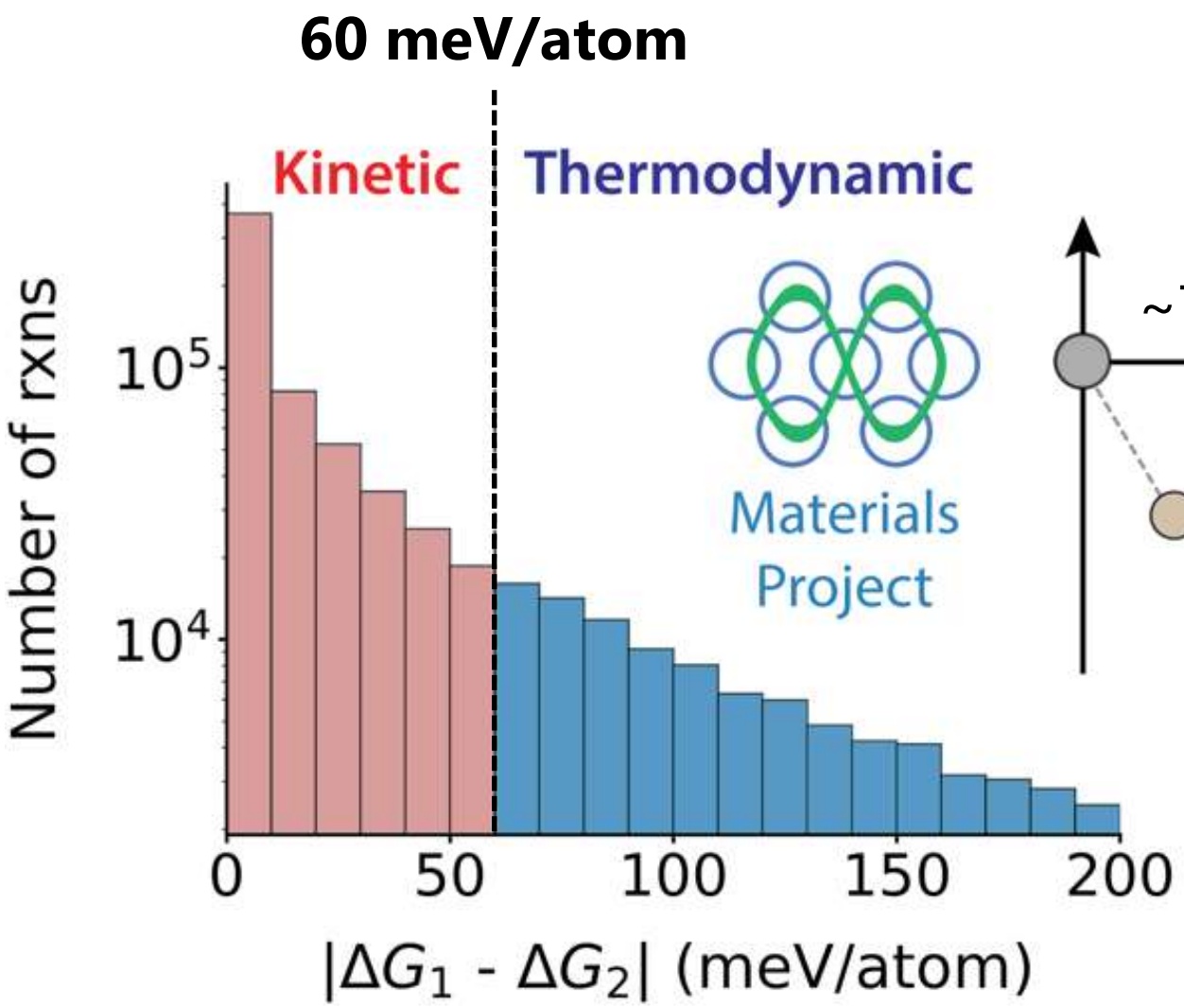
Szymanski *et al.*, Science Advances (2024).

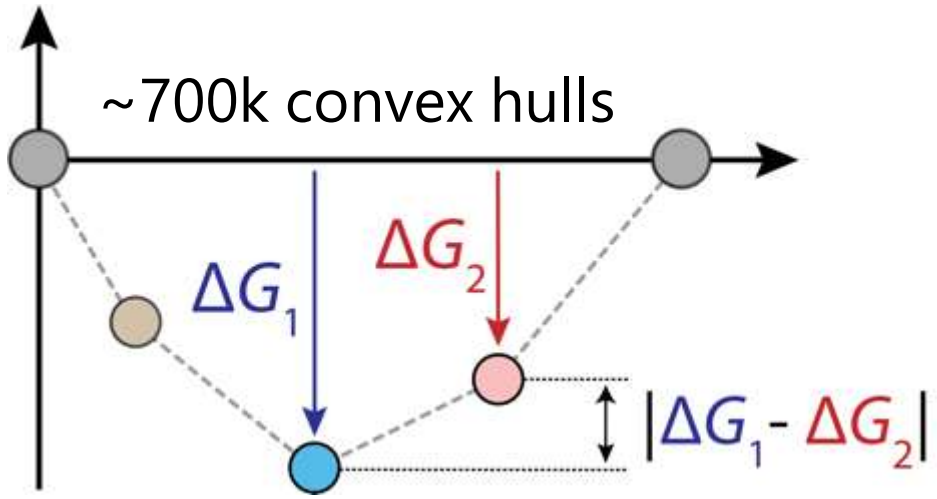
Outcomes show a regime of thermodynamic (Δ*G*) control



Szymanski *et al.*, Science Advances (2024).

But most reactions are *not* in a thermodynamic regime





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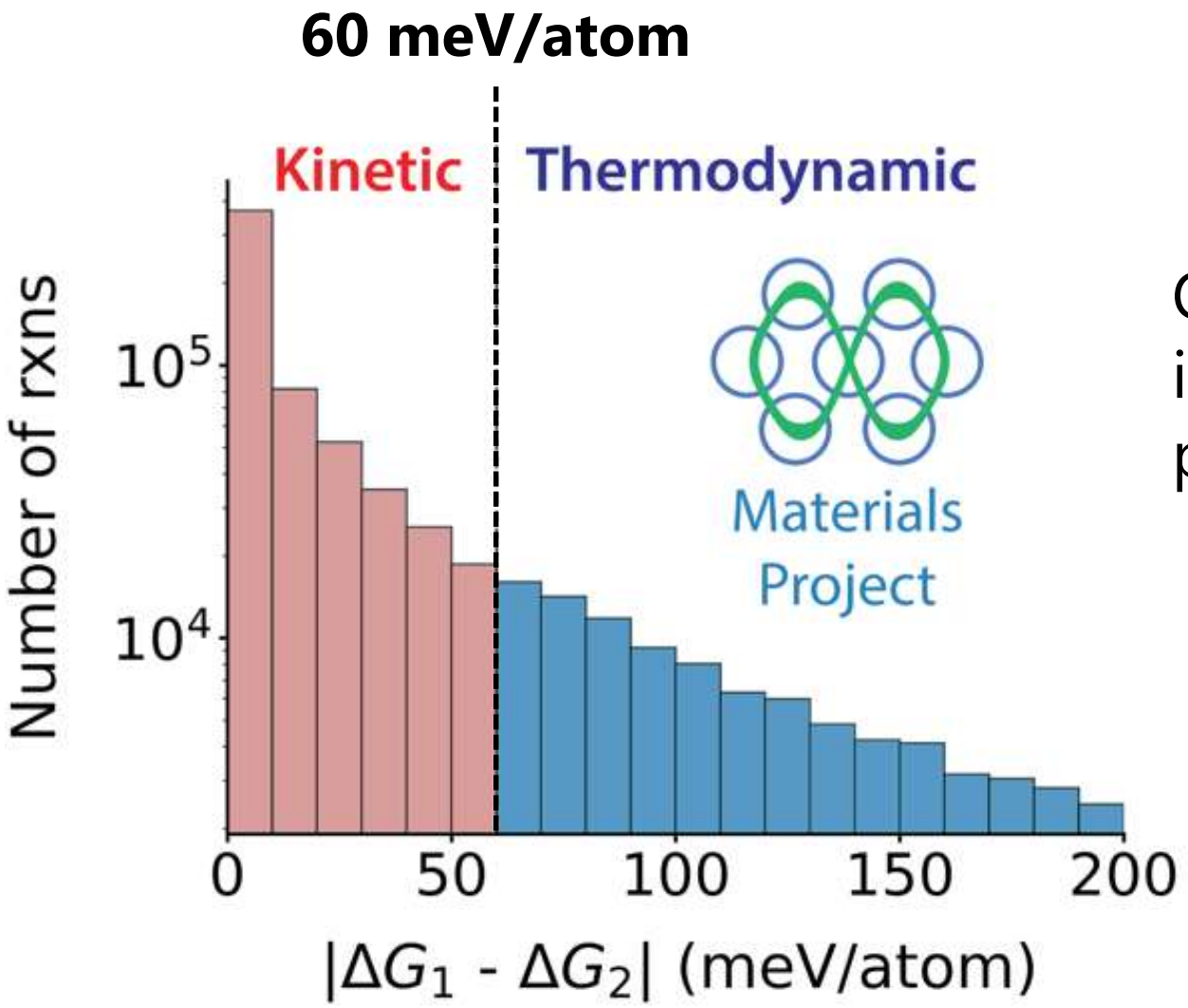
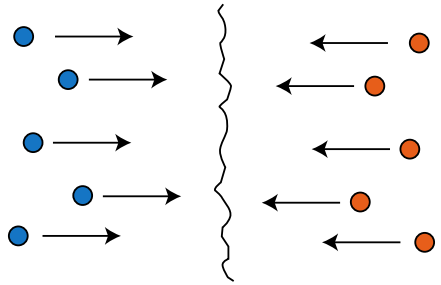


Only **15% of the binary convex hulls** in the Materials Project fall above the proposed threshold of 60 meV/atom

Szymanski *et al.*, Science Advances (2024).

How to deal with the remaining 85% of reactions?

Recall the two factors we neglected:

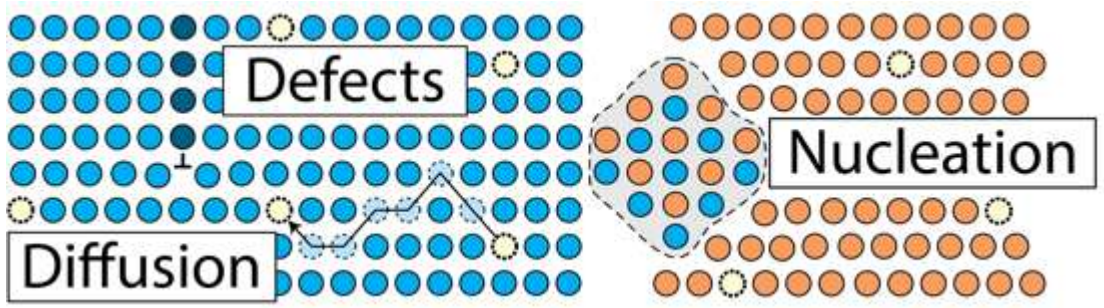


Diffusion

$$\Delta G^* = \frac{16\pi\sigma^3}{3(n\Delta G)^2}$$

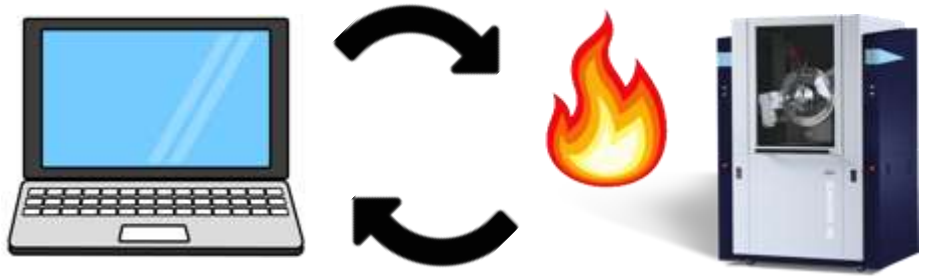
Surface energy

Option 1:
Simulate these processes directly

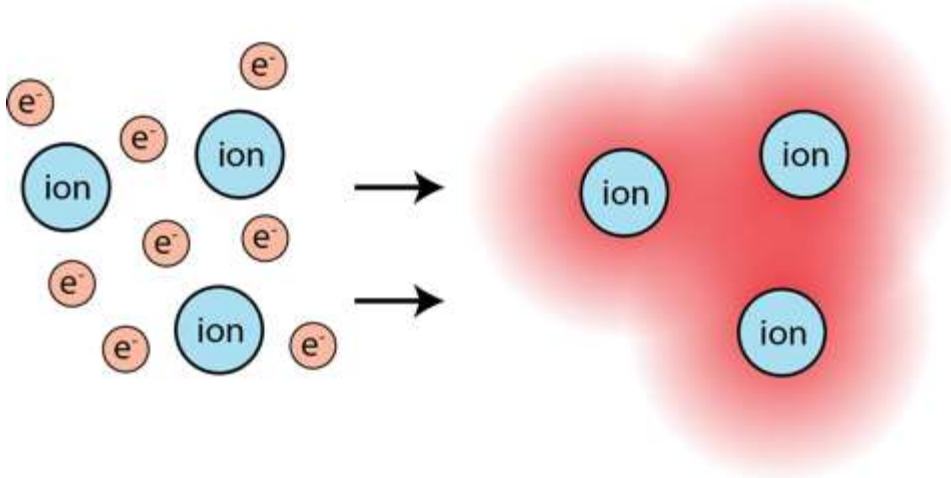


Existing computational models of kinetics are too costly

Option 2:
Integrate our starting predictions (based on ΔG) with experiment and update them accordingly



Computational tools for synthesis and characterization



DFT for synthesis planning

1) What can we learn from computed thermodynamics?

2) **Using what we've learned: how can we design synthesis procedures?**

Combining predictions with experiments to optimize synthesis

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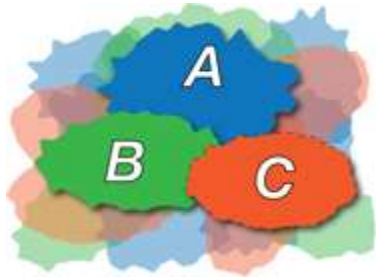
ARROWS^3

Autonomous Reaction Route Optimization With Solid-State Synthesis

Given a target material, find the **best precursors and conditions**



How to deal with mixtures of > 2 phases?

Figure adapted from: A. Miura *et al.*, Advanced Materials (2021).

Combining predictions with experiments to optimize synthesis

CEMS Chemical Engineering & Materials Science

ARROWS^3

Autonomous Reaction Route Optimization With Solid-State Synthesis

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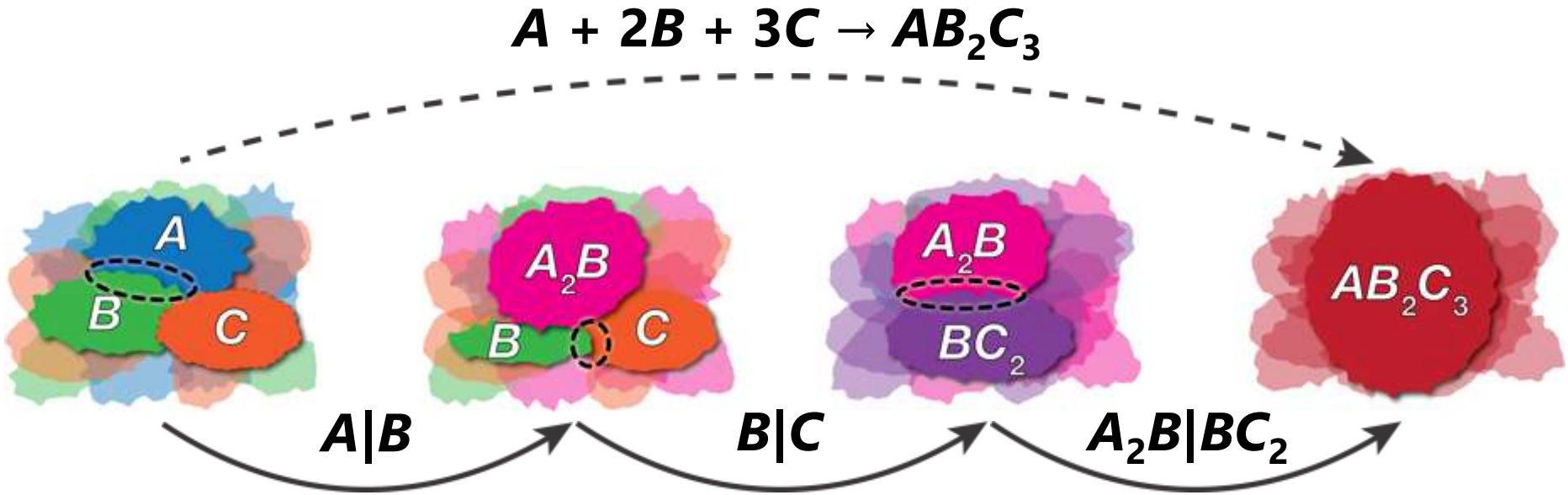

Figure adapted from: A. Miura *et al.*, Advanced Materials (2021).

Combining predictions with experiments to optimize synthesis

CEMS Chemical Engineering & Materials Science

ARROWS[3]

Autonomous Reaction Route Optimization With Solid-State Synthesis

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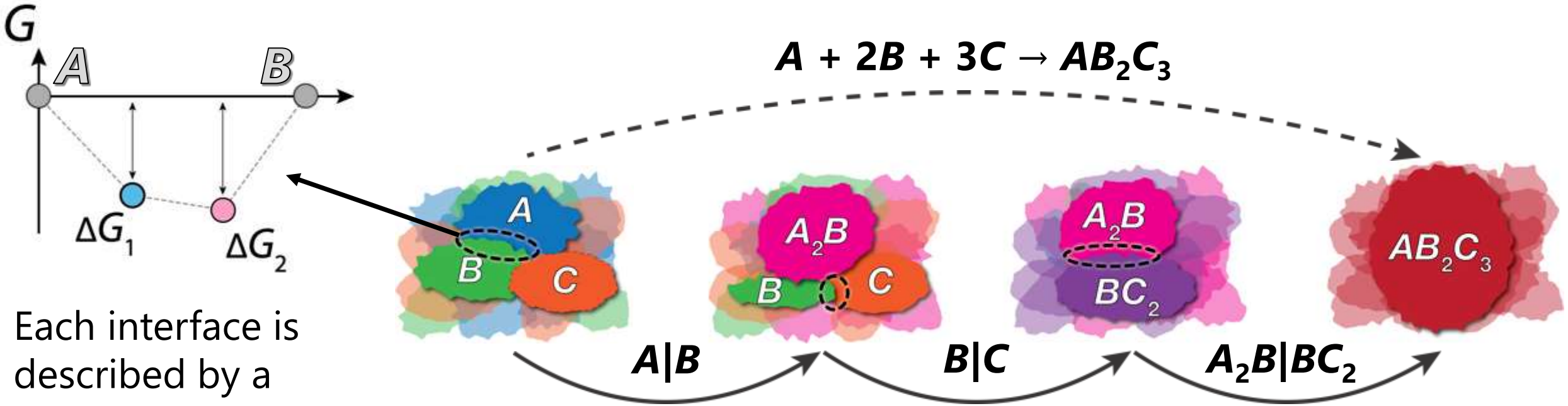
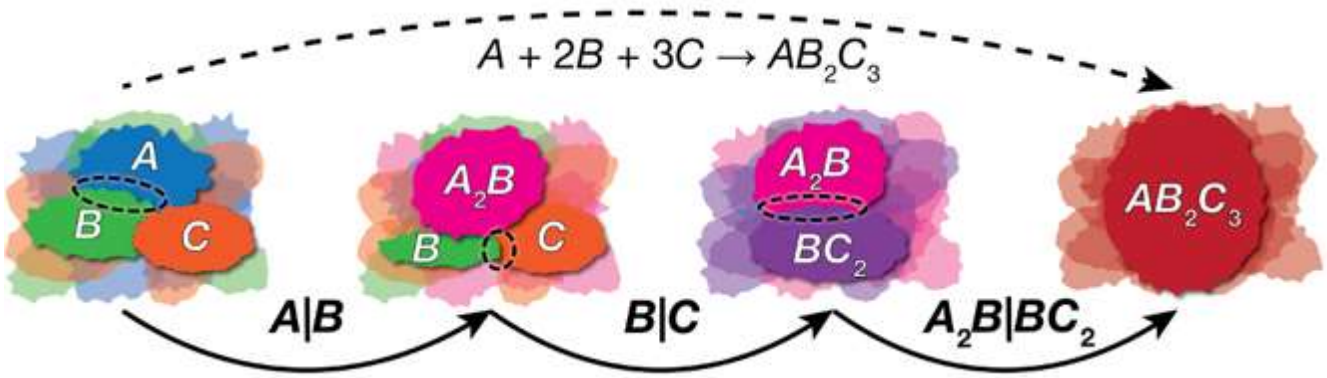
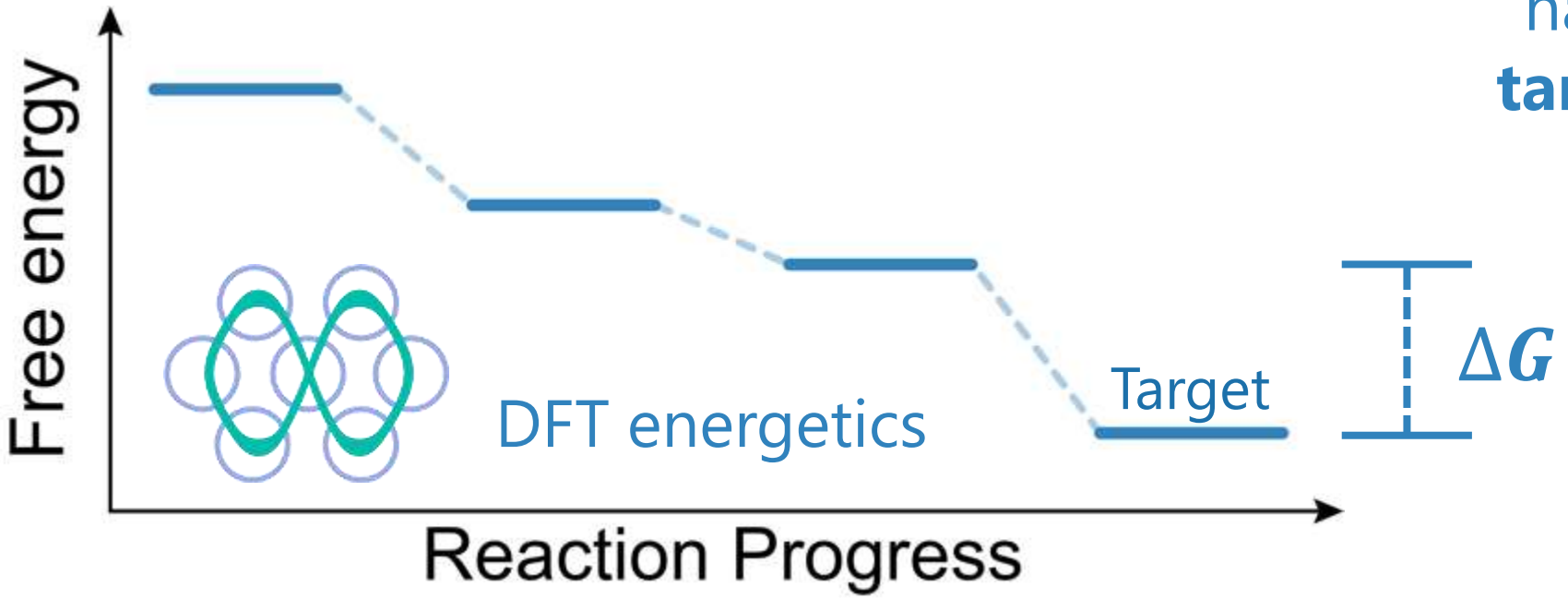


Each interface is described by a **binary convex hull**

Figure adapted from: A. Miura *et al.*, Advanced Materials (2021).

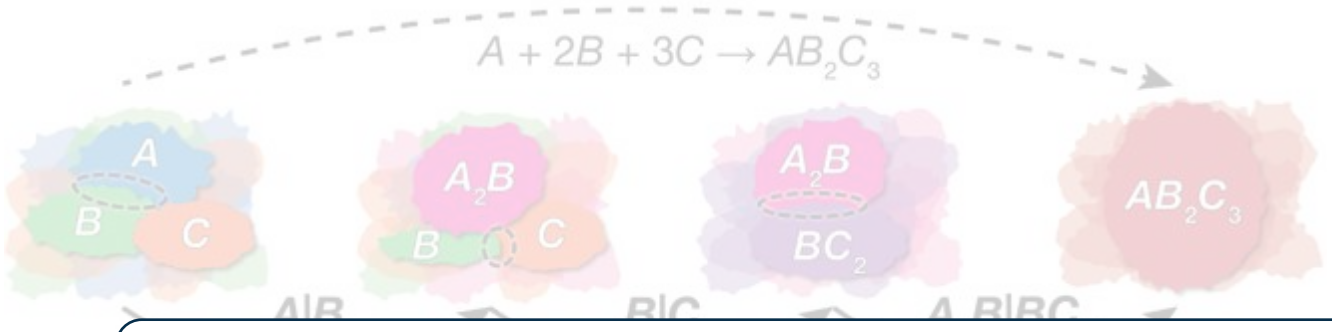
Computed thermodynamics (ΔG) guide the optimization





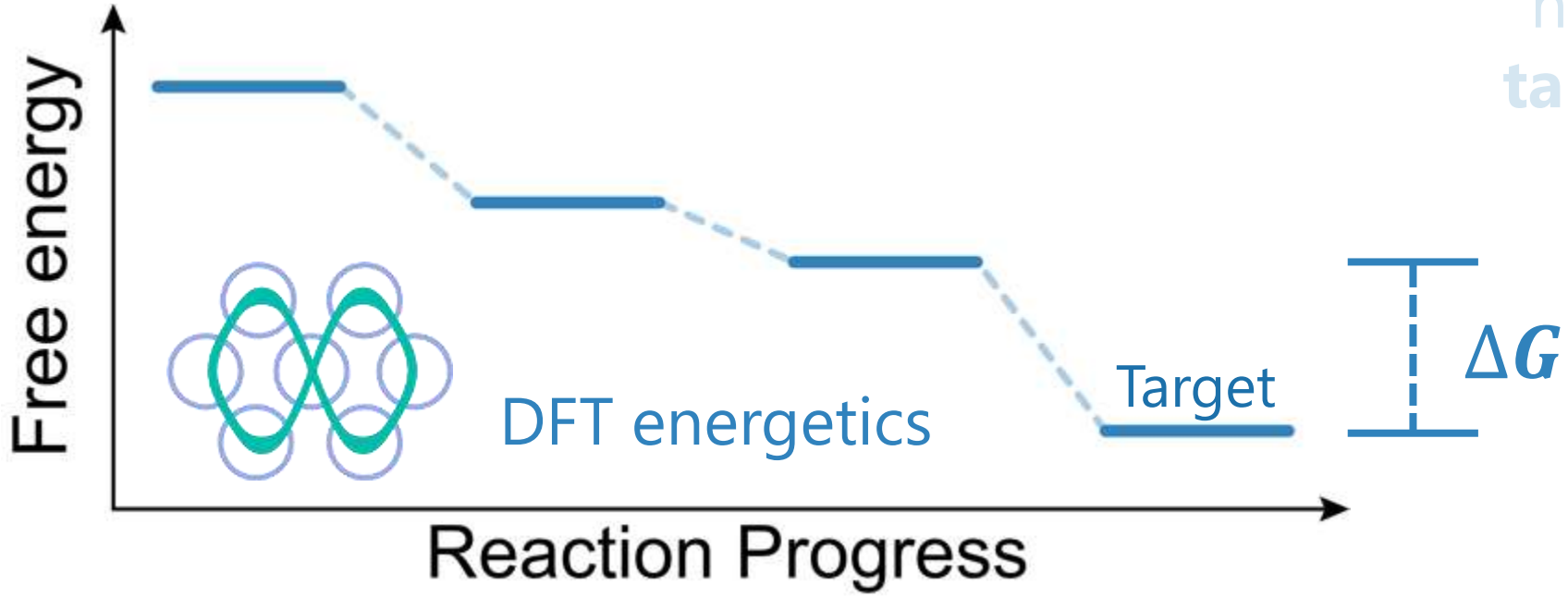
An ideal reaction pathway has **large ΔG** at the **target-forming step**

Computed thermodynamics (ΔG) guide the optimization



But how do we know what these pathways will be?

hway
has **large** ΔG at the
target-forming step



ARROWS learns the reaction pathways

CEMS Chemical Engineering & Materials Science

MATERIALS PROJECT

DFT-calculated energetics

Prioritize precursor sets with **large ΔG**

Precursors

Target

ΔG

Predict reaction outcomes of new precursor sets

Perform experiments using suggested precursors

ARROWS learns the reaction pathways

CEMS Chemical Engineering & Materials Science

MATERIALS PROJECT

DFT-calculated energetics

Prioritize precursor sets with **large ΔG**

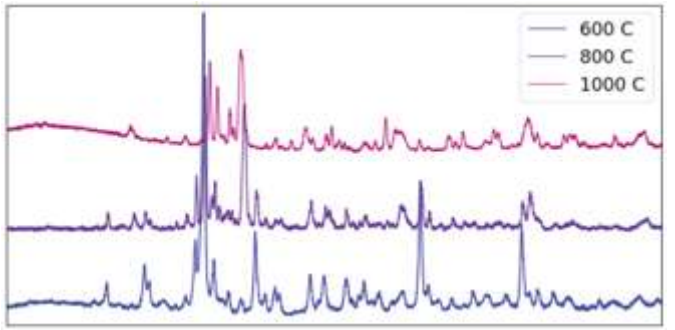
Intermediates

ΔG

Target

Perform experiments using suggested precursors

Learn what pairwise reactions occurred and **re-compute ΔG**



Predict reaction outcomes of new precursor sets

ARROWS learns the reaction pathways

CEMS Chemical Engineering & Materials Science

MATERIALS PROJECT

DFT-calculated energetics

Prioritize precursor sets with **large ΔG**

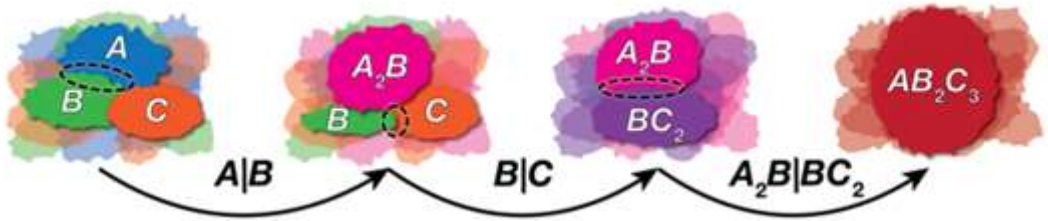
Intermediates

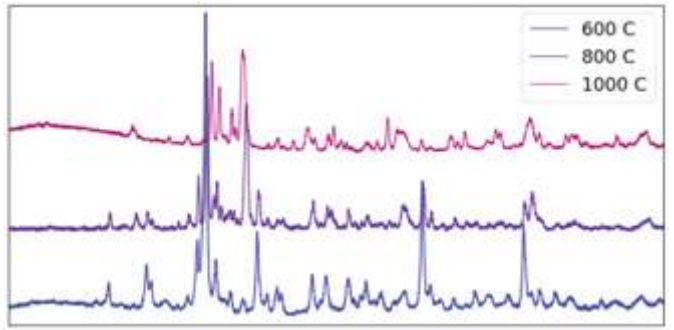
ΔG

Target

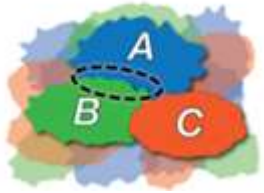
Perform experiments using suggested precursors

Predict reaction outcomes of new precursor sets





ARROWS learns the reaction pathways



Avoid pairs that form highly stable intermediates

Prioritize precursor sets that ***retain*** large ΔG

Update ranking

Iterate to success!

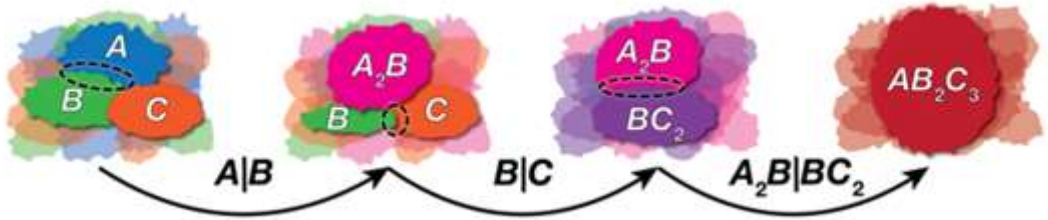
Predict reaction outcomes of new precursor sets

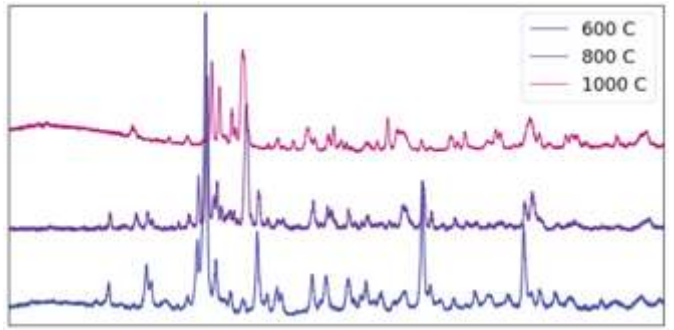
Perform experiments using suggested precursors

Intermediates

ΔG

Target





Finding improved synthesis routes for a high-T_c superconductor

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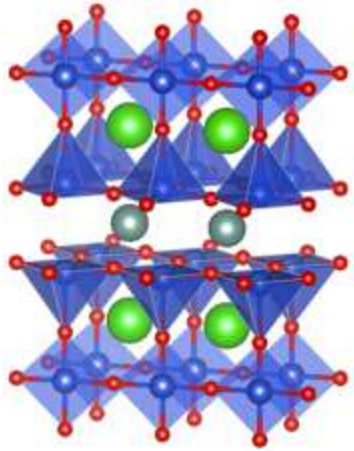
$YBa_2Cu_3O_{7-x}$
(YBCO)



Traditional synthesis of YBCO:

4 $BaCO_3$ + Y_2O_3 + 6 CuO @ **950 °C for > 12 h**

With intermittent regrinding and reheating

Common impurities: $BaCuO_2$ and Y_2BaCuO_5

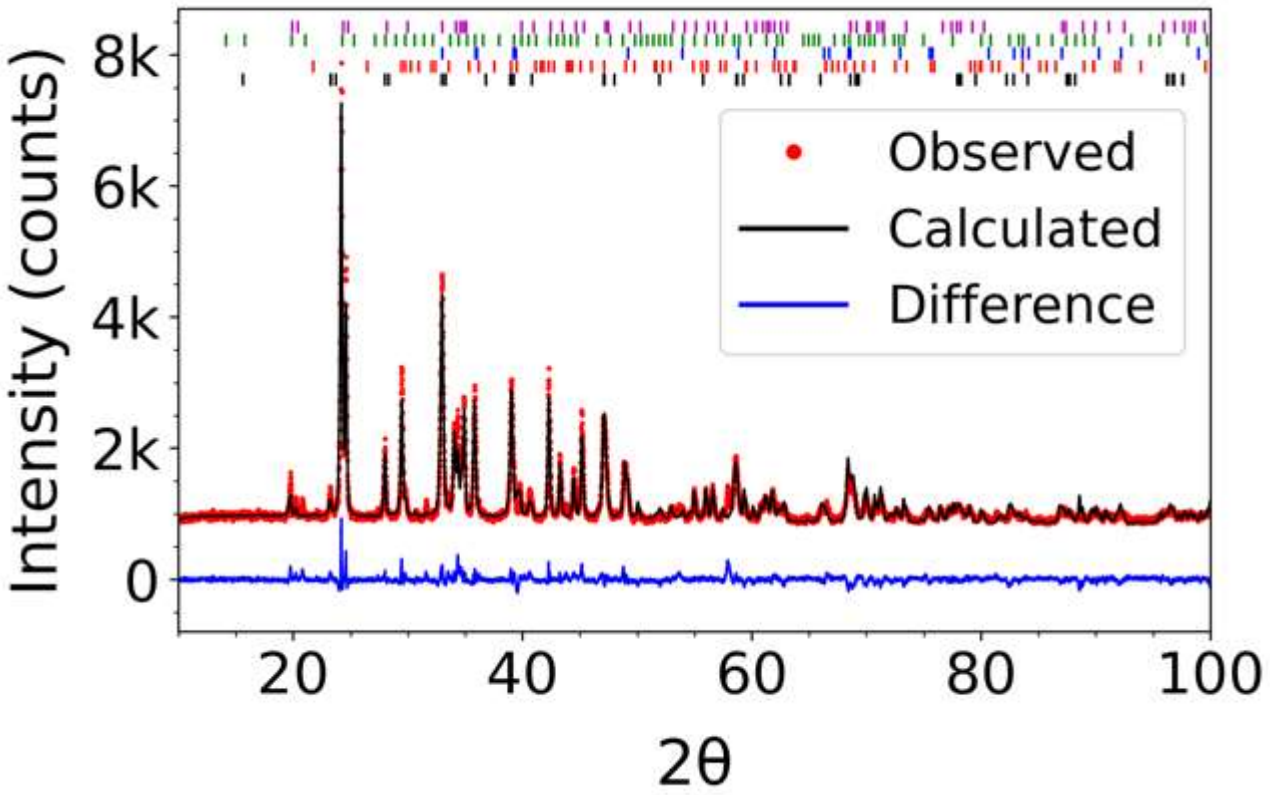
ARROWS^3
Autonomous Reaction Route Optimization With Solid-State Synthesis

Objective:
Find synthesis routes that yield
~pure YBCO in 4 h at ≤ 900 °C

N. J. Szymanski *et al.*, Nature Communications (2024).

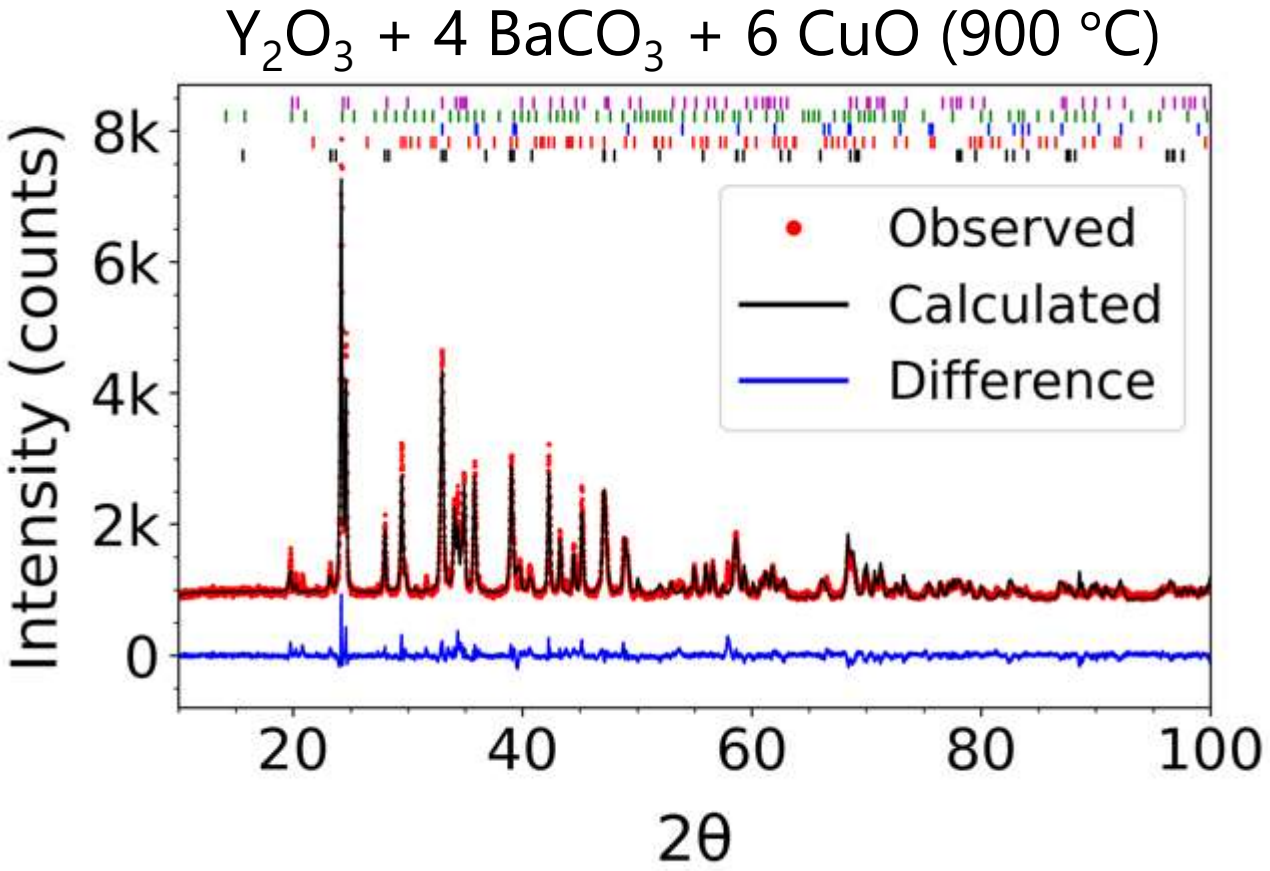
Traditional precursors lead to many impurities after 4 h

Y_2O_3 + 4 $BaCO_3$ + 6 CuO (900 °C)



47.8% $BaCO_3$
9.7% $BaCuO_2$
27.1% CuO
6.5% Y_2BaCuO_5
8.9% YBCO ⟶ Low target yield

Traditional precursors lead to many impurities after 4 h



47.8% $BaCO_3$ ⟶ **$BaCO_3$ is slow to react before its decomposition (> 1000 °C)**

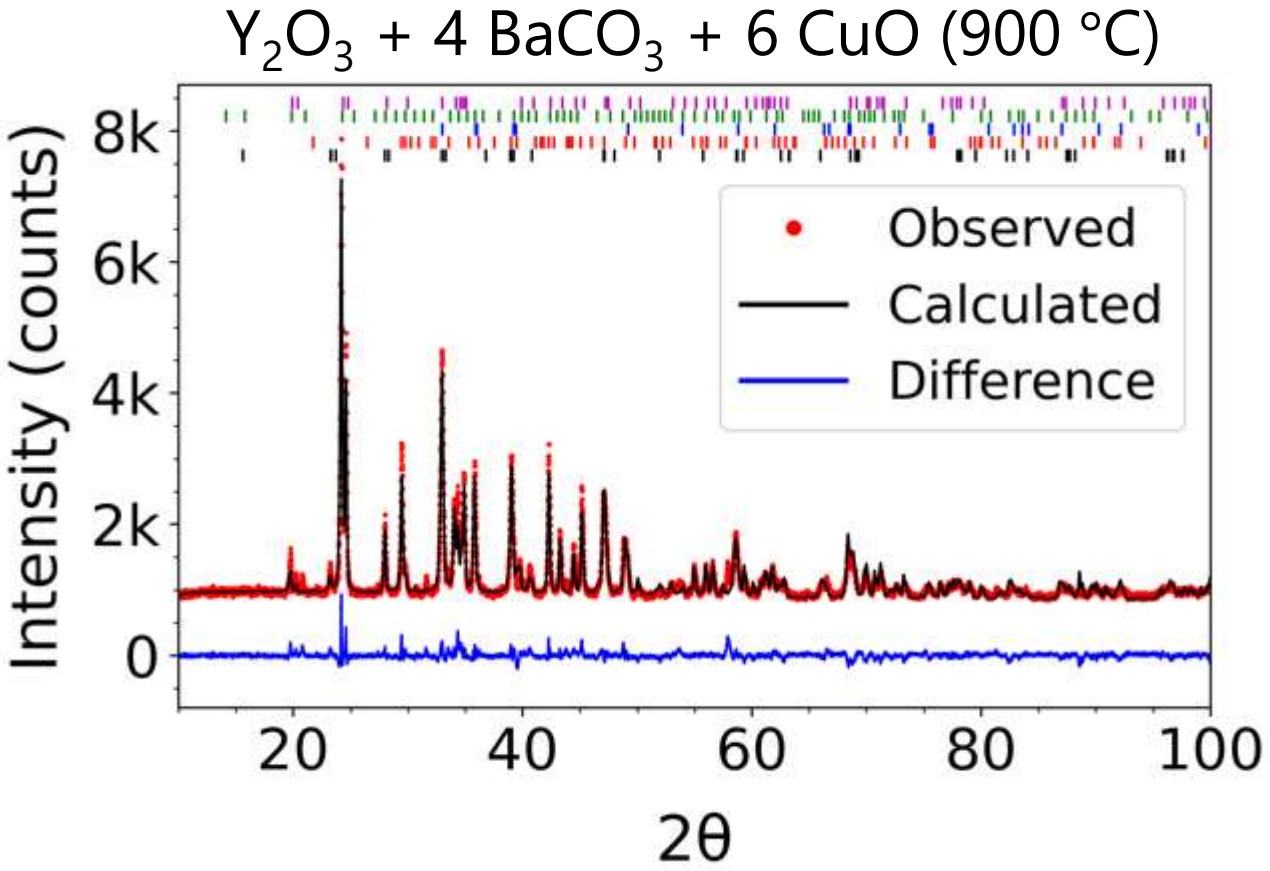
9.7% $BaCuO_2$

27.1% CuO

6.5% Y_2BaCuO_5

8.9% YBCO

Traditional precursors lead to many impurities after 4 h



47.8% $BaCO_3$

9.7% $BaCuO_2$ → **$BaCuO_2$** and subsequently

27.1% CuO

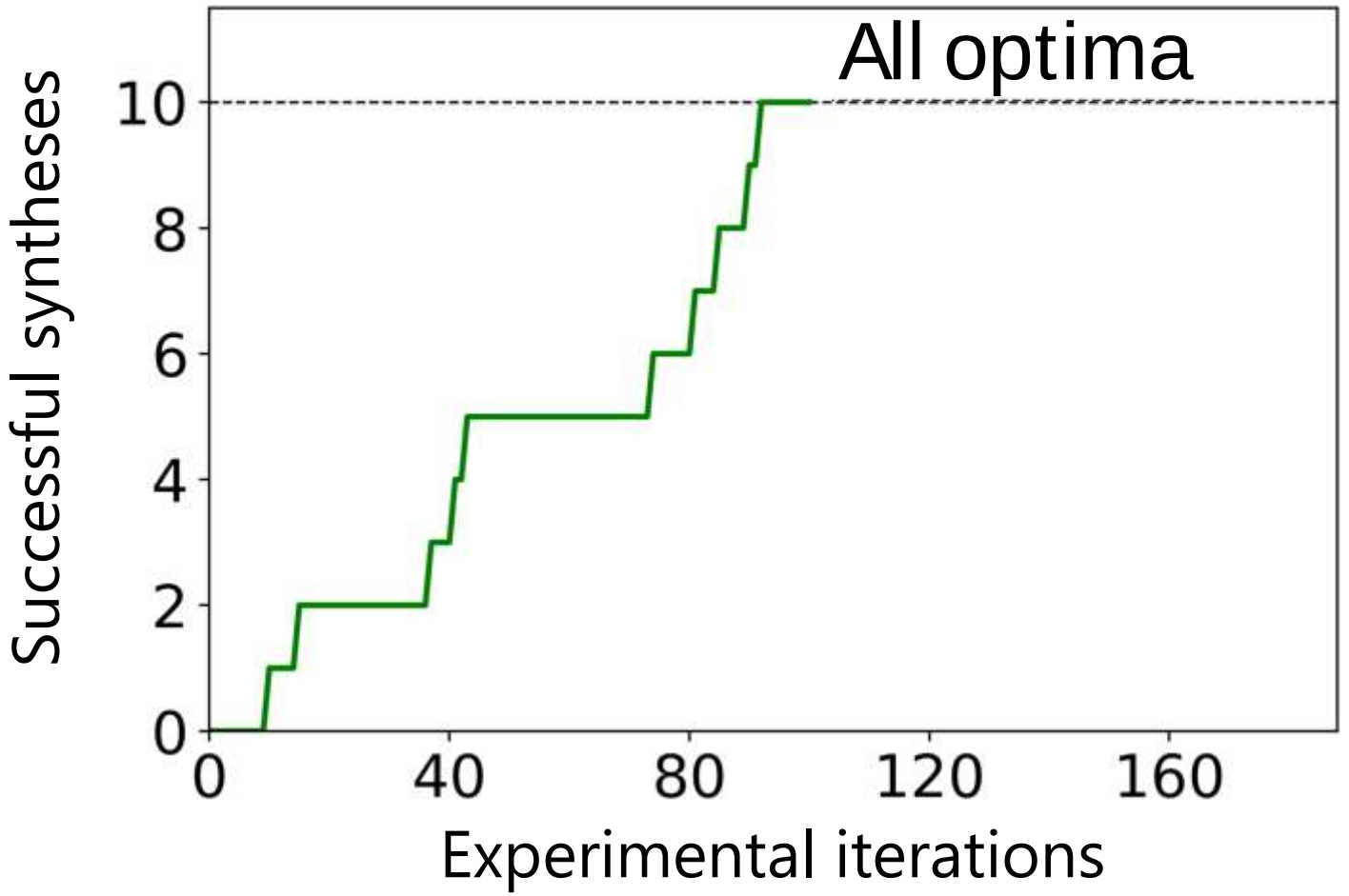
6.5% Y_2BaCuO_5 → **Y_2BaCuO_5**

8.9% YBCO

When $BaCO_3$ reacts, it forms **$BaCuO_2$** and subsequently **Y_2BaCuO_5**

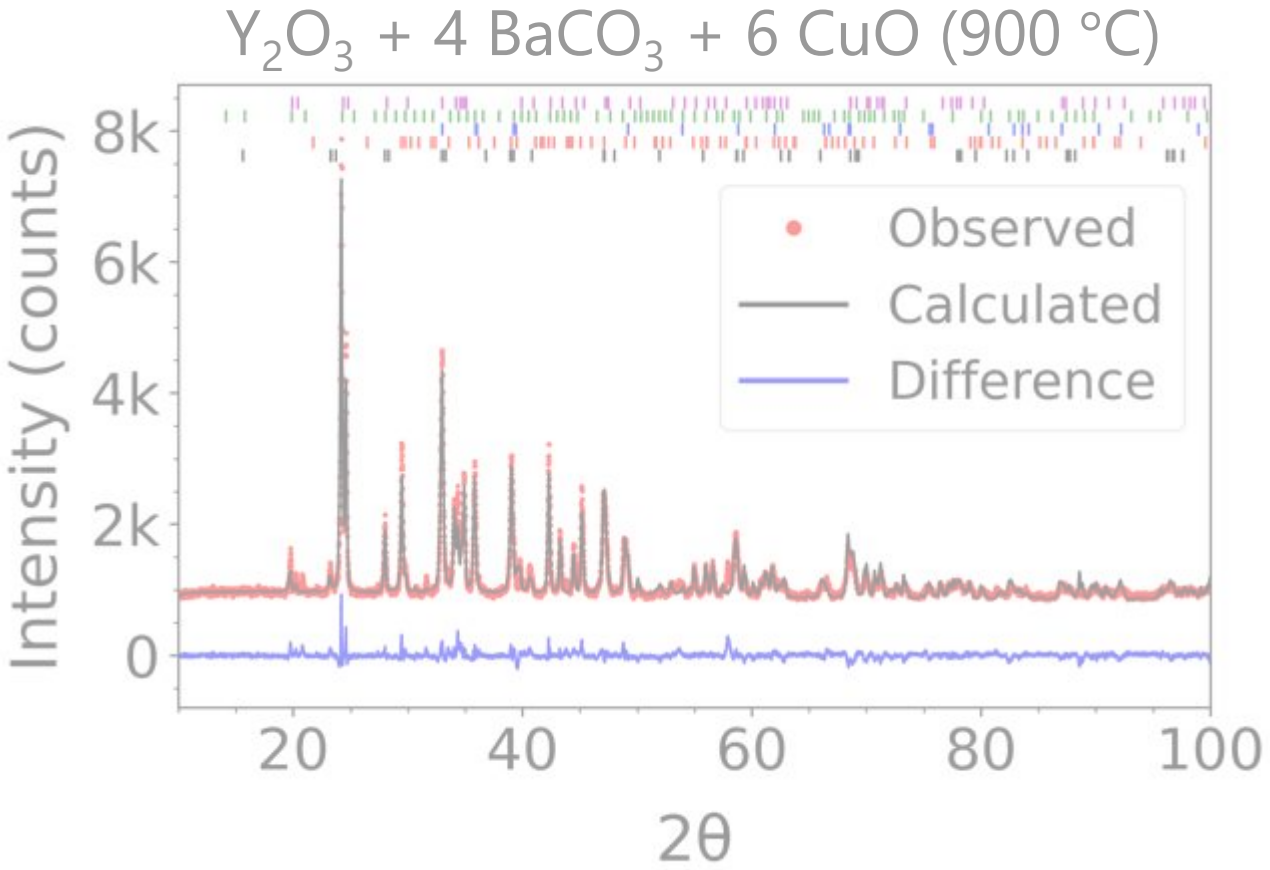
These are **impurities we'd like to avoid**

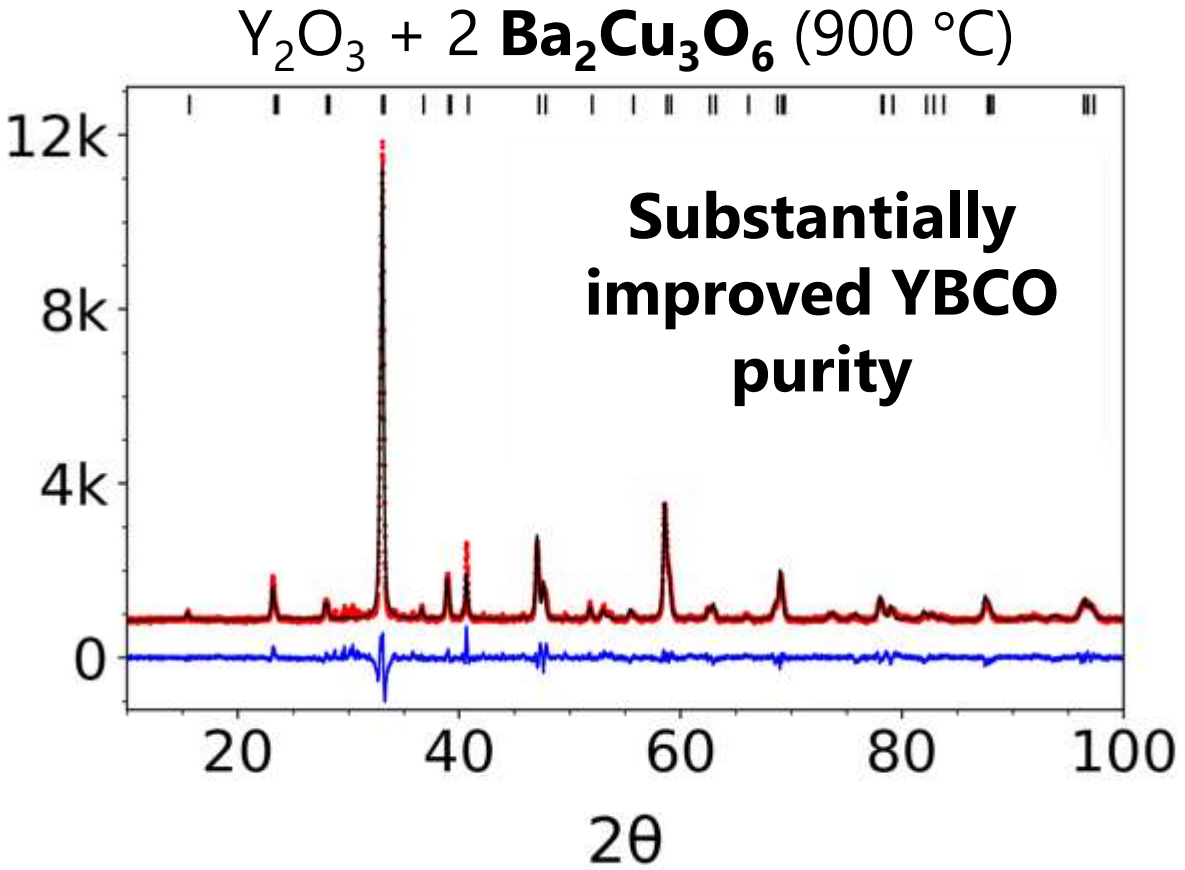
ARROWS succeeds in identifying fast synthesis routes



In **87 iterations**, ARROWS found **10 synthesis routes** that produce YBCO with **high yield in ≤ 4 h**

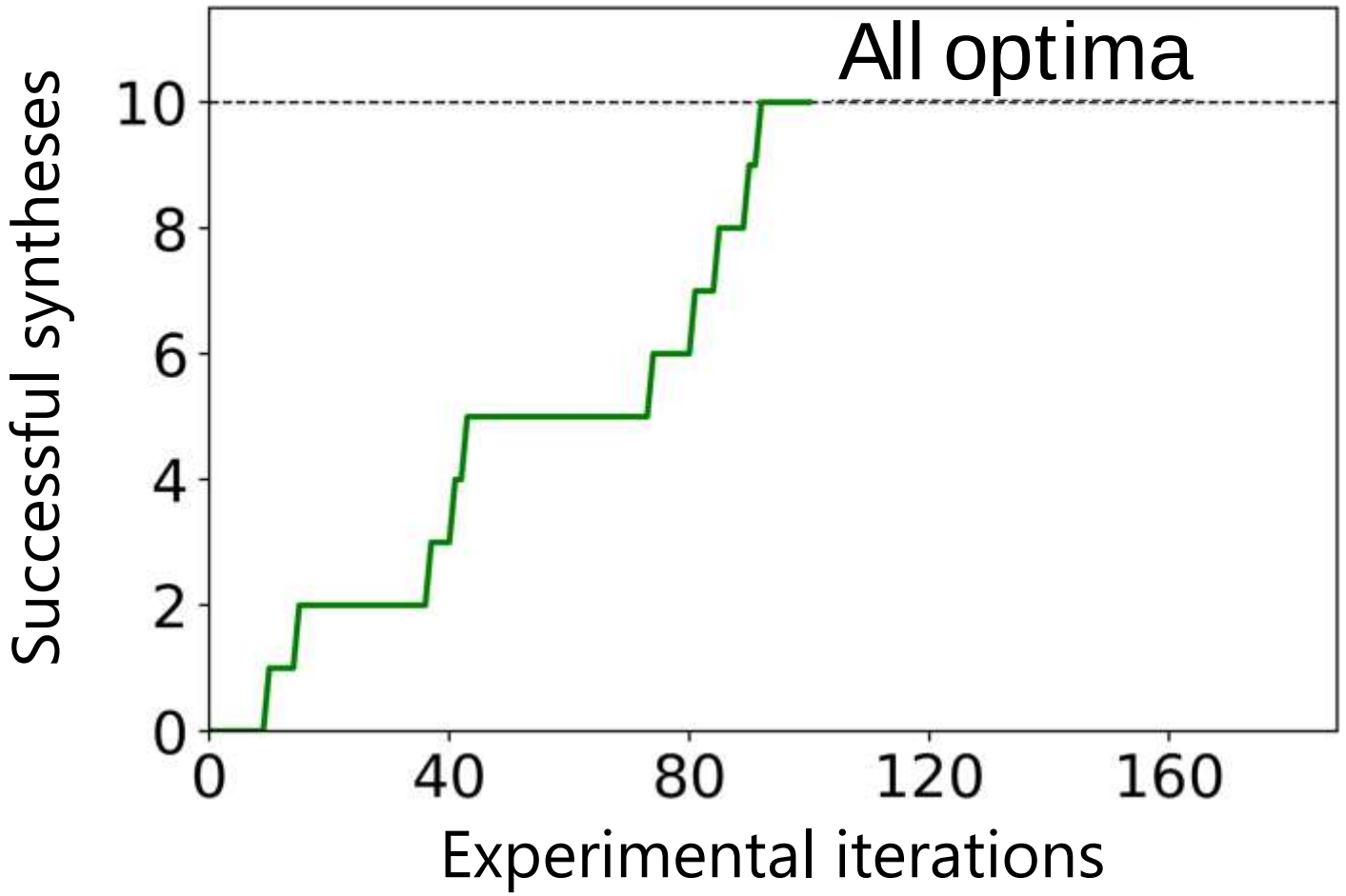
The optimized precursors lead to much higher purity





$Ba_2Cu_3O_6$ and Y_2O_3 react directly to form YBCO at $T \leq 900$ °C

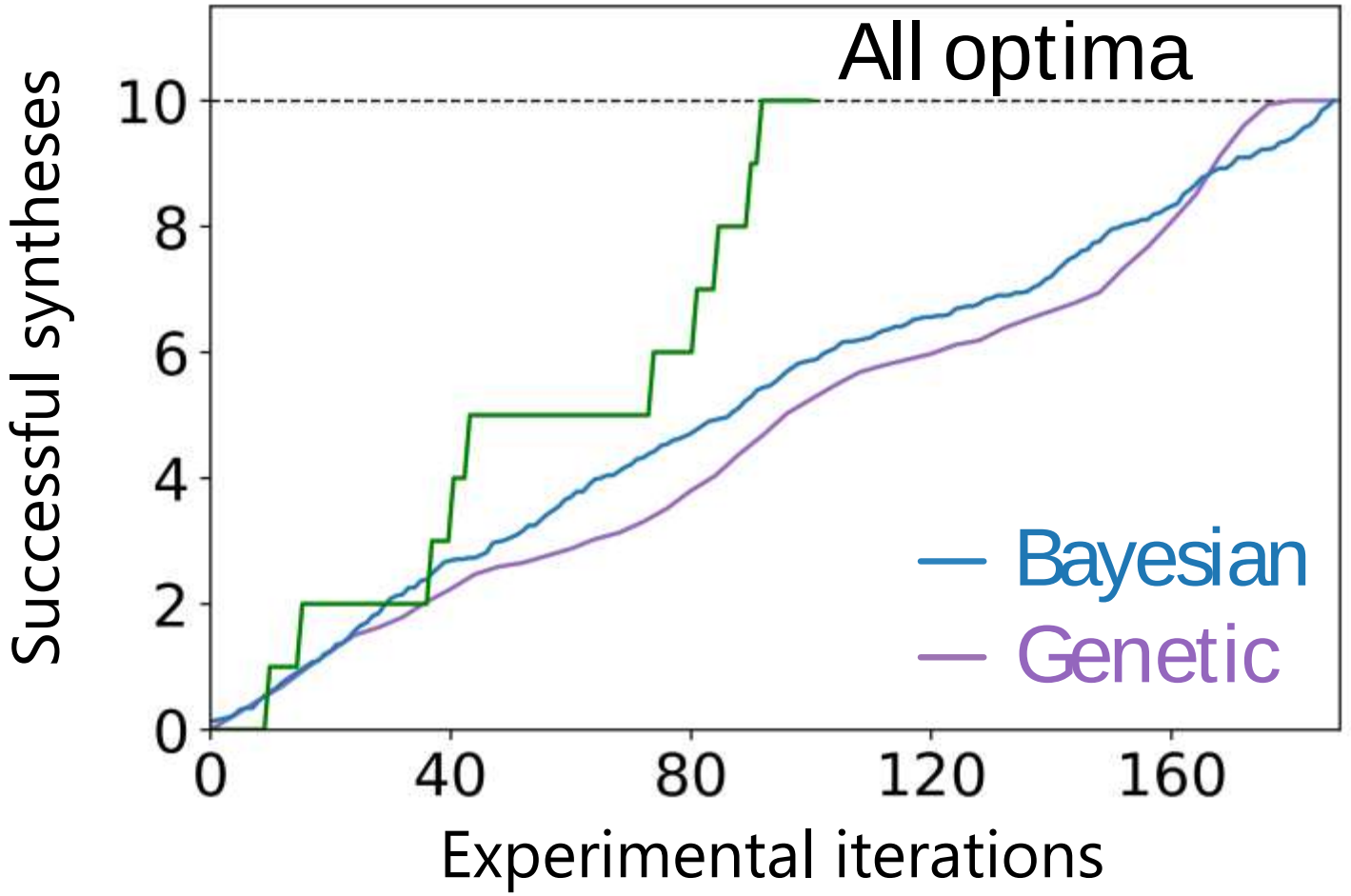
ARROWS succeeds in identifying fast synthesis routes



In **87 iterations**, ARROWS found **10 synthesis routes** that produce YBCO with **> 95% yield in ≤ 4 h**

Is ARROWS efficient?

ARROWS outperforms black-box optimization



In **87 iterations**, ARROWS found **10 synthesis routes** that produce YBCO with **> 95% yield in ≤ 4 h**

For comparison:
Bayesian optimization and genetic algorithms required **> 160 iterations**

Computational tools for synthesis and characterization

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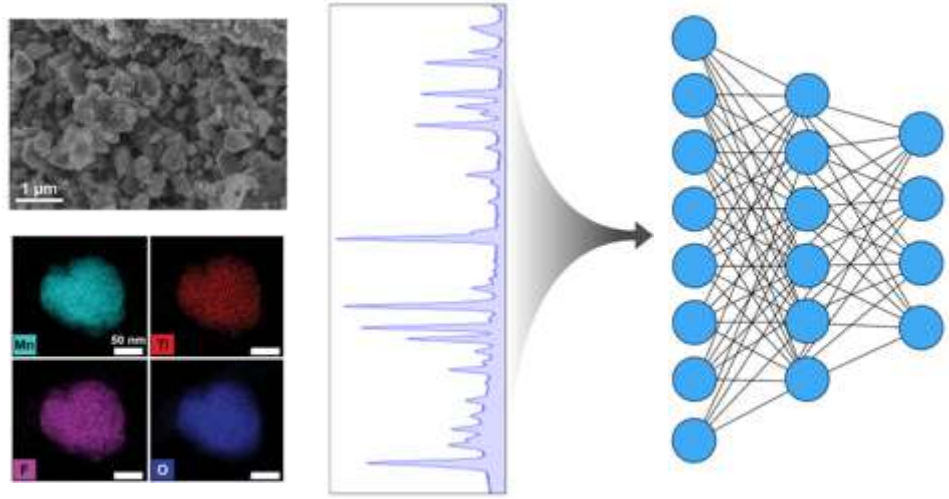
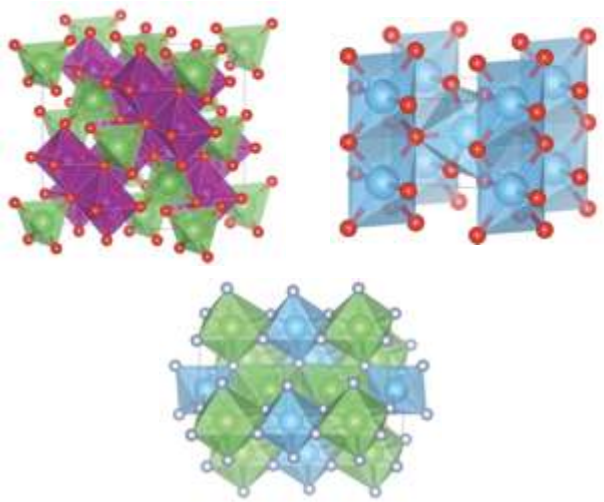
With automated decision making,
analysis of characterization data becomes the bottleneck



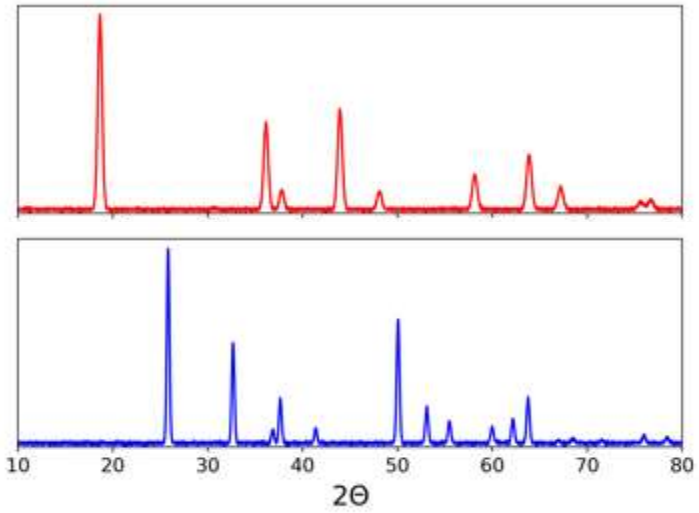
AI for characterization

Powder X-ray diffraction (XRD)
→ what phases are present

Simulating XRD is easy, but *solving* XRD is hard



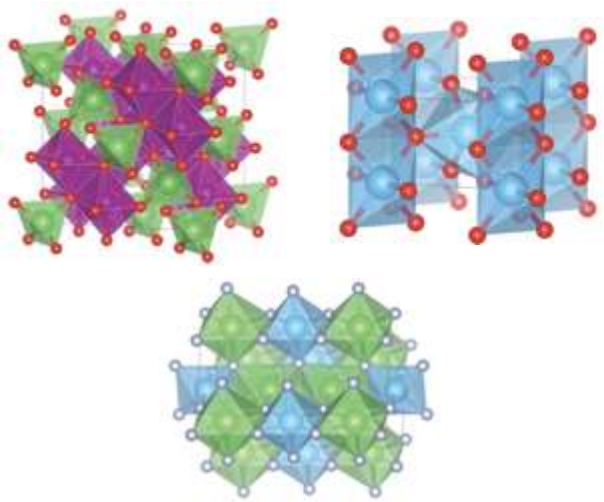
$$F_{hkl} = \sum_{j=1}^{N} f_j e^{-2\pi i(hx_j + ky_j + lz_j)}$$



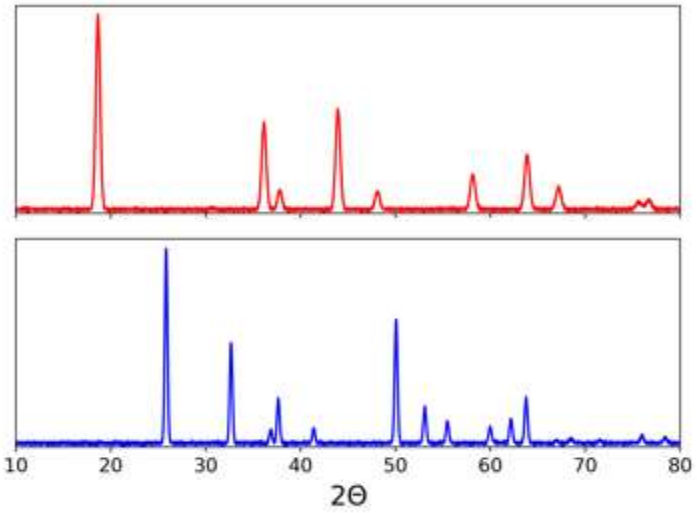
How to go from XRD to structure?

- **Experimental artifacts** modify peaks
- **Multi-phase mixtures** are common
- The pattern **may not be unique**

Simulating XRD is easy, but *solving* XRD is hard



$$F_{hkl} = \sum_{j=1}^{N} f_j e^{-2\pi i(hx_j + ky_j + lz_j)}$$



Train ML to solve reverse problem!

- **Experimental artifacts** modify peaks
- **Multi-phase mixtures** are common

} These can be ***simulated*** and used to train ML models

- The pattern **may not be unique** → ML can be ***probabilistic***

Neural networks are trained on simulated XRD patterns

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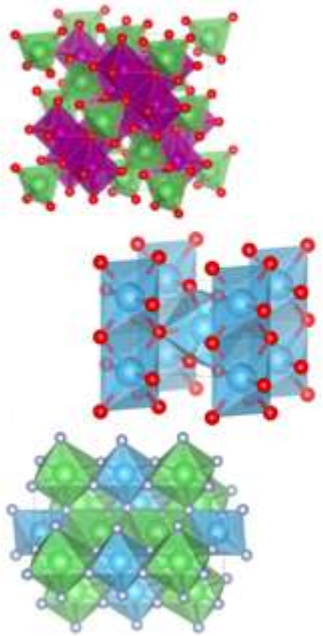
Known structures

ICSD FIZ Karlsruhe

Materials Project



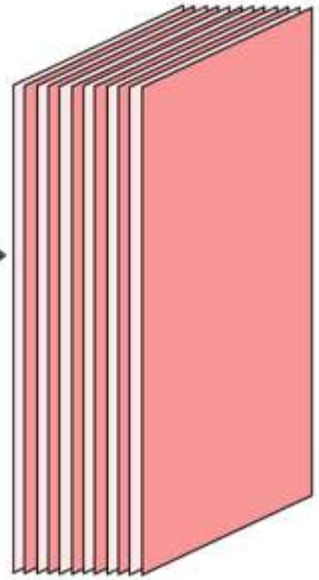
Simulated patterns

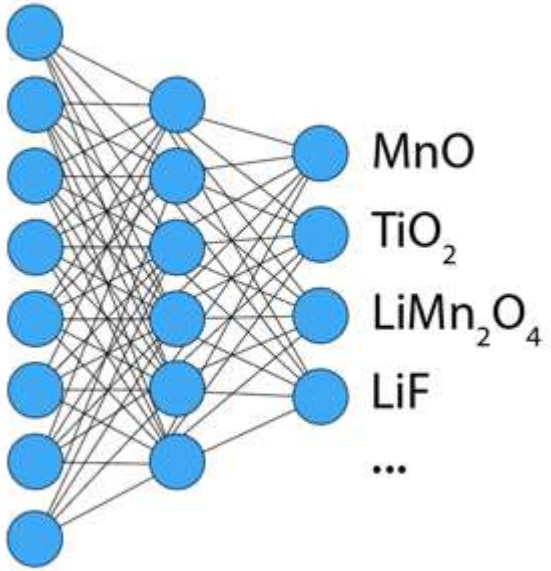
Shifts in 2θ

Intensity changes

Broad peaks

Convolutional neural networks

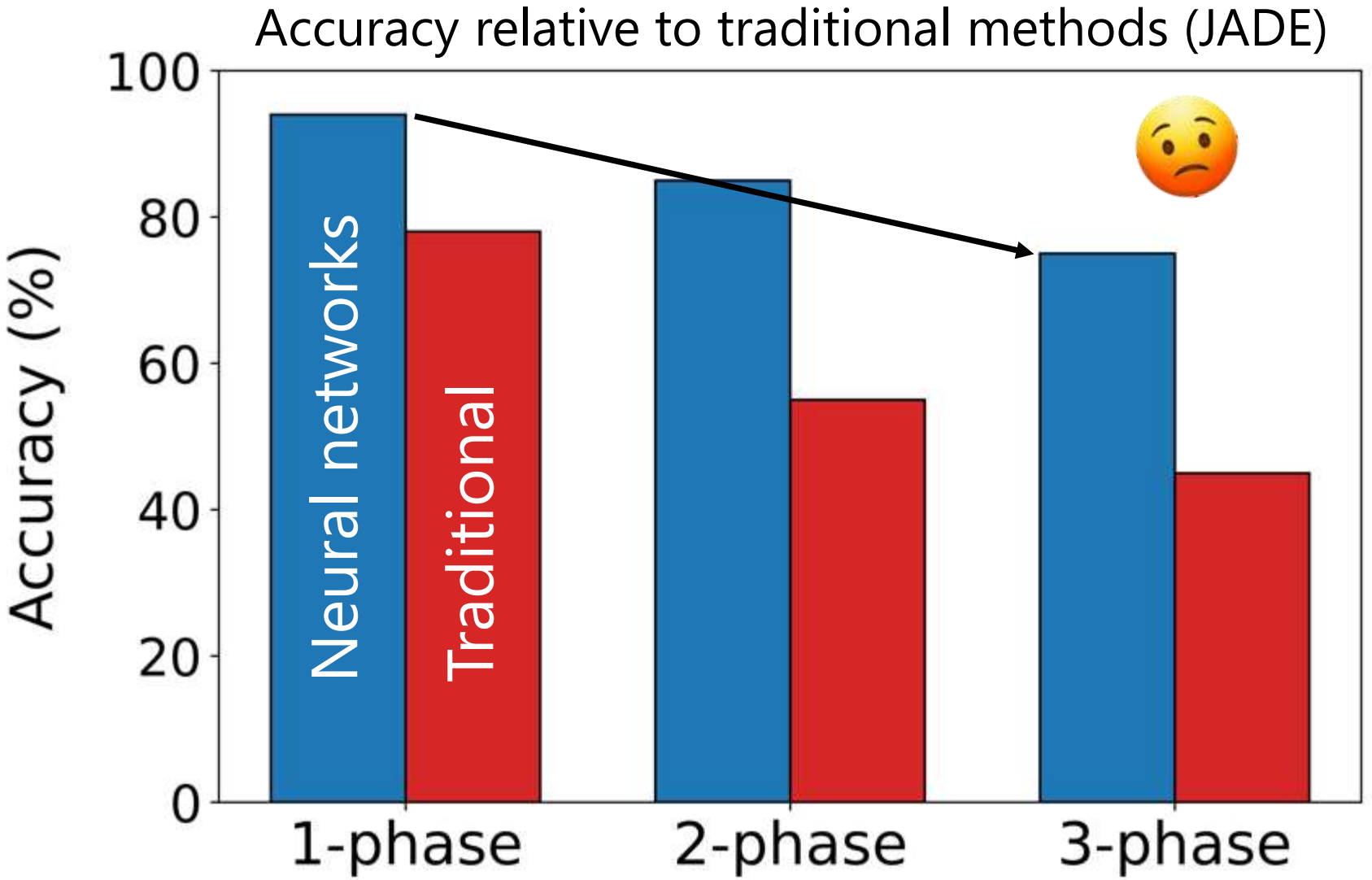




Data augmentation
from strain, texture, and poor crystallinity

N. J. Szymanski *et al.*, Chemistry of Materials (2021).

ML outperforms traditional methods, but limitations persist



Mixtures are difficult to characterize reliably

Simulated test data:

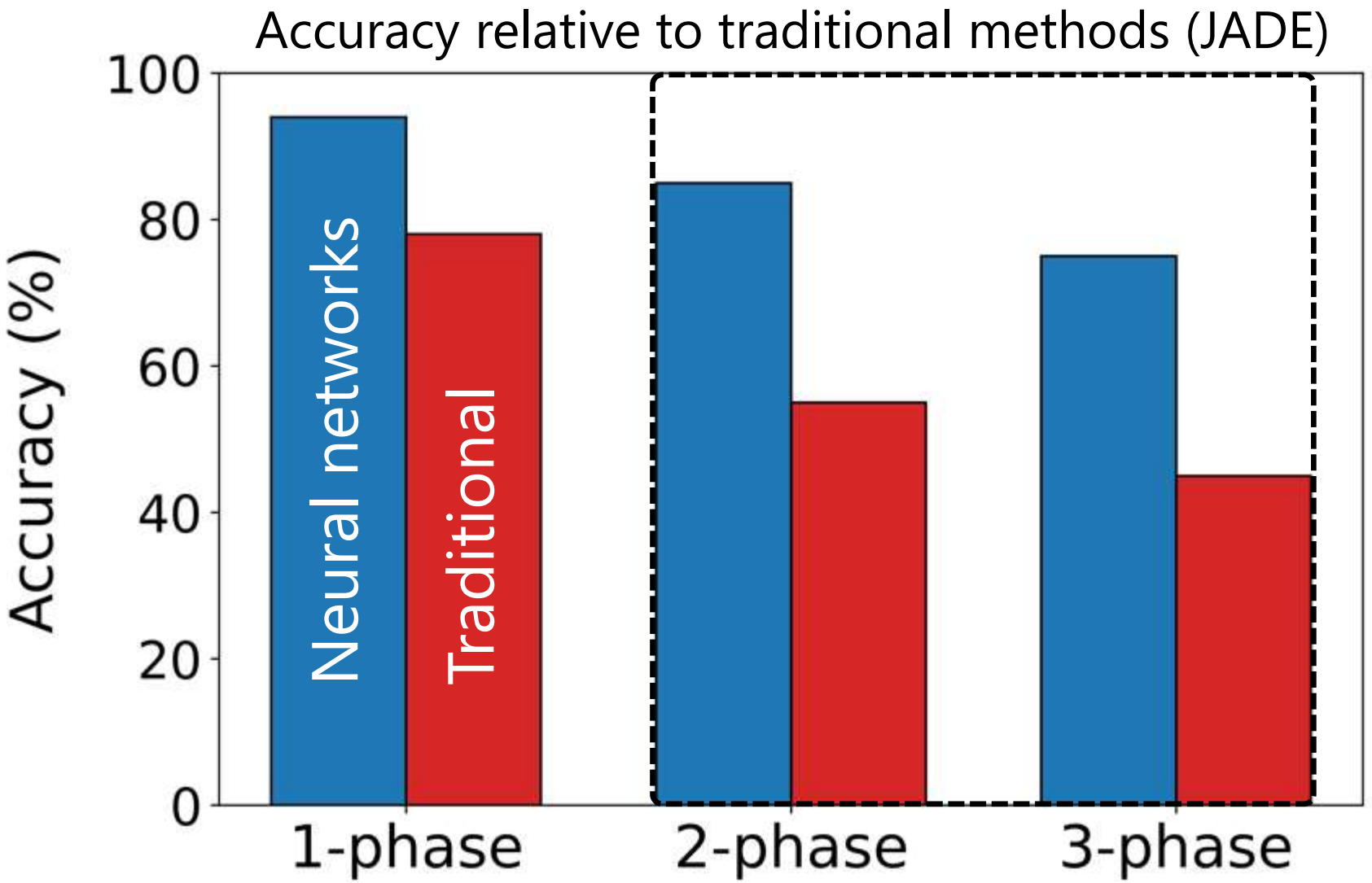
4k patterns augmented with exp artifacts

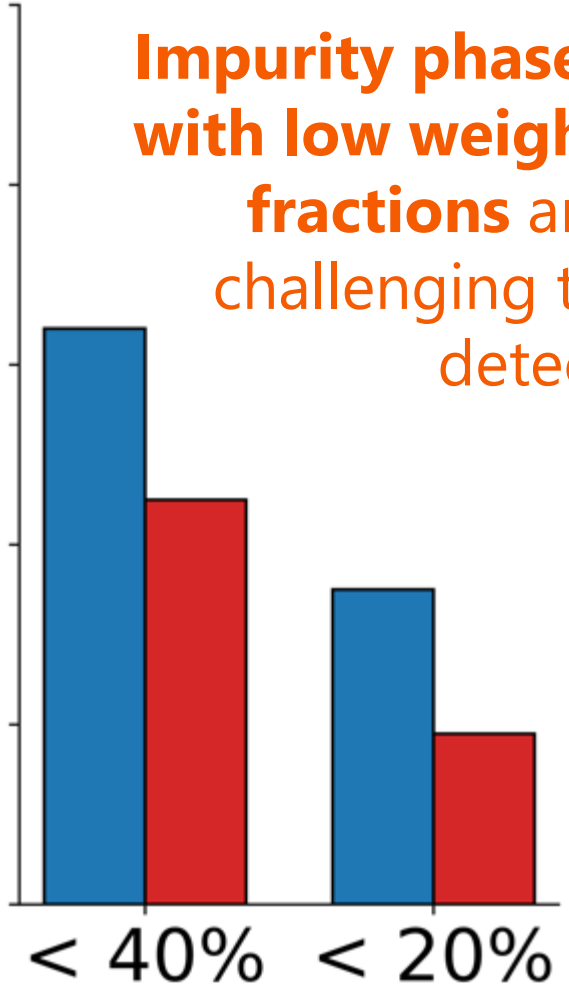
Experimental test data:

80 patterns augmented with exp artifacts

(Li-Mn-Ti-O-F)

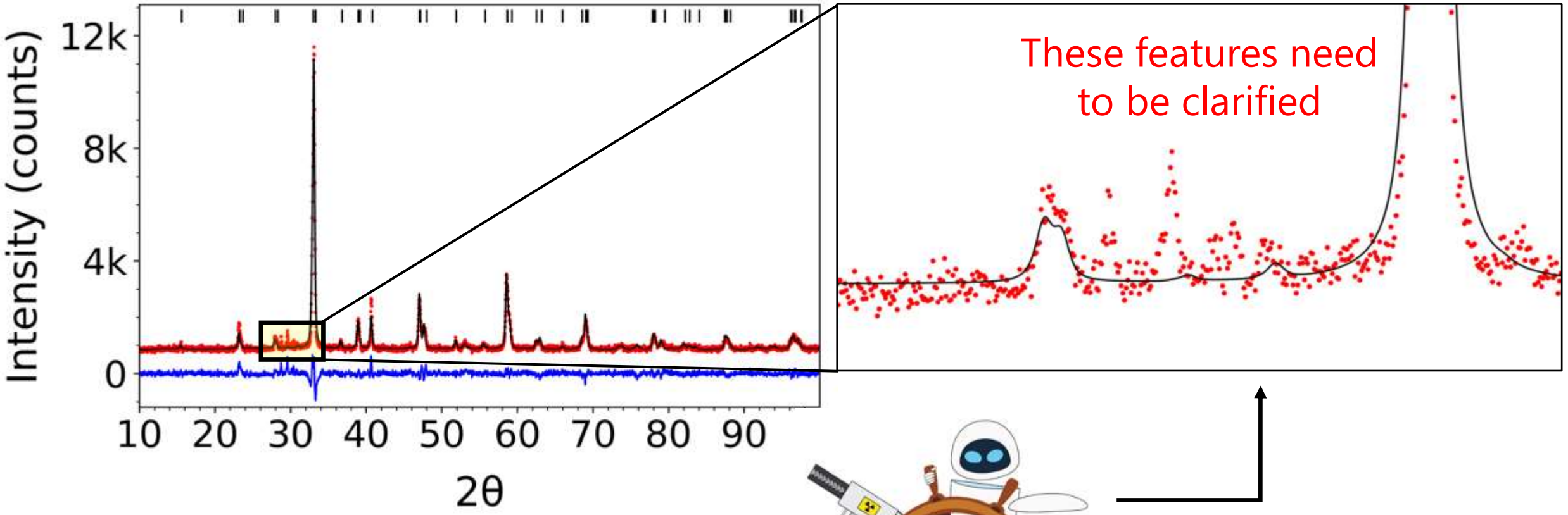
ML outperforms traditional methods, but limitations persist



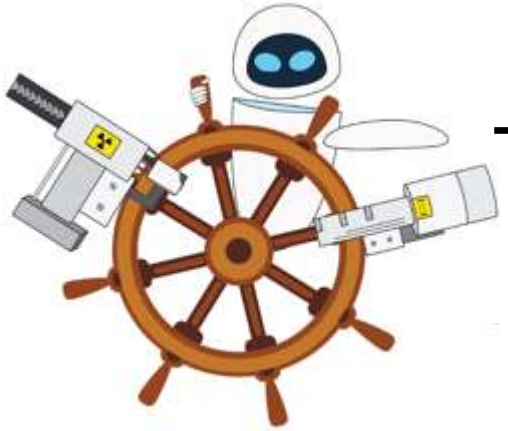


Impurity phases with low weight fractions are challenging to detect

Can we *adaptively* control XRD to focus on impurities?

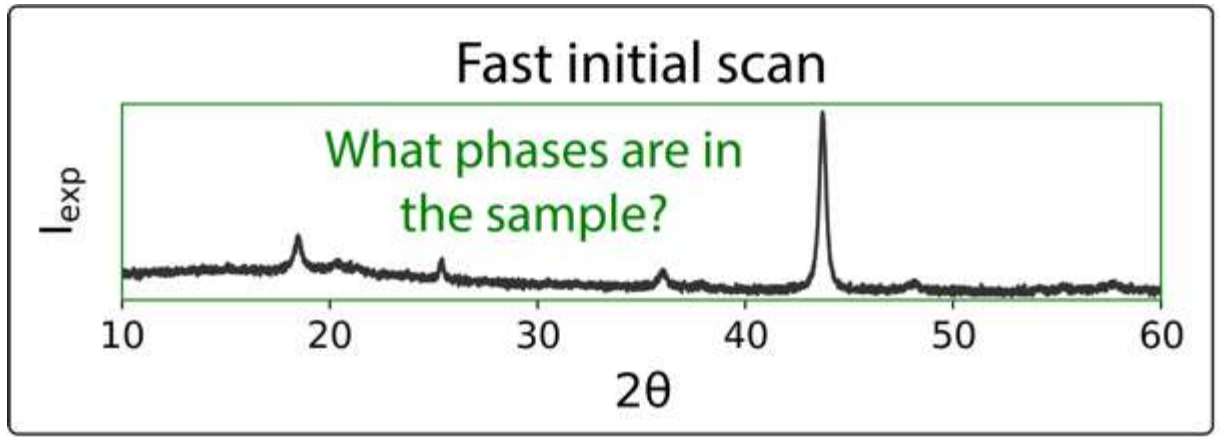


What impurity phases are present?



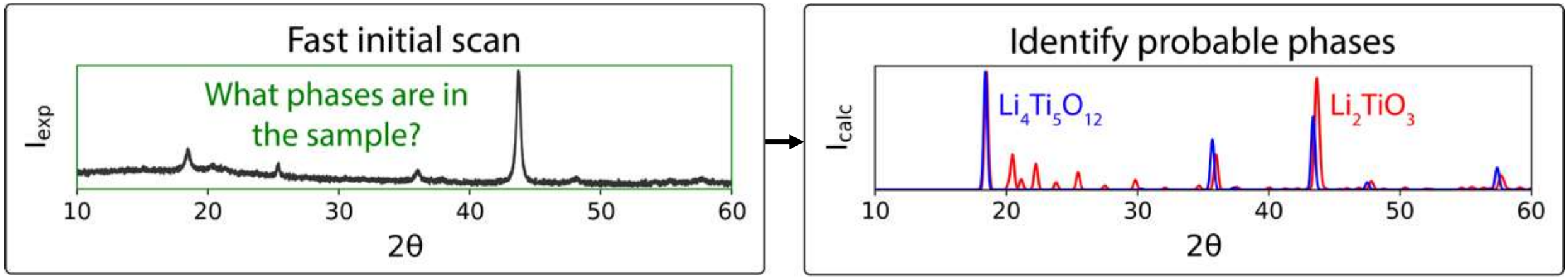
Steer diffractometer toward region of interest

Adaptive XRD workflow: initial scan is fast and noisy



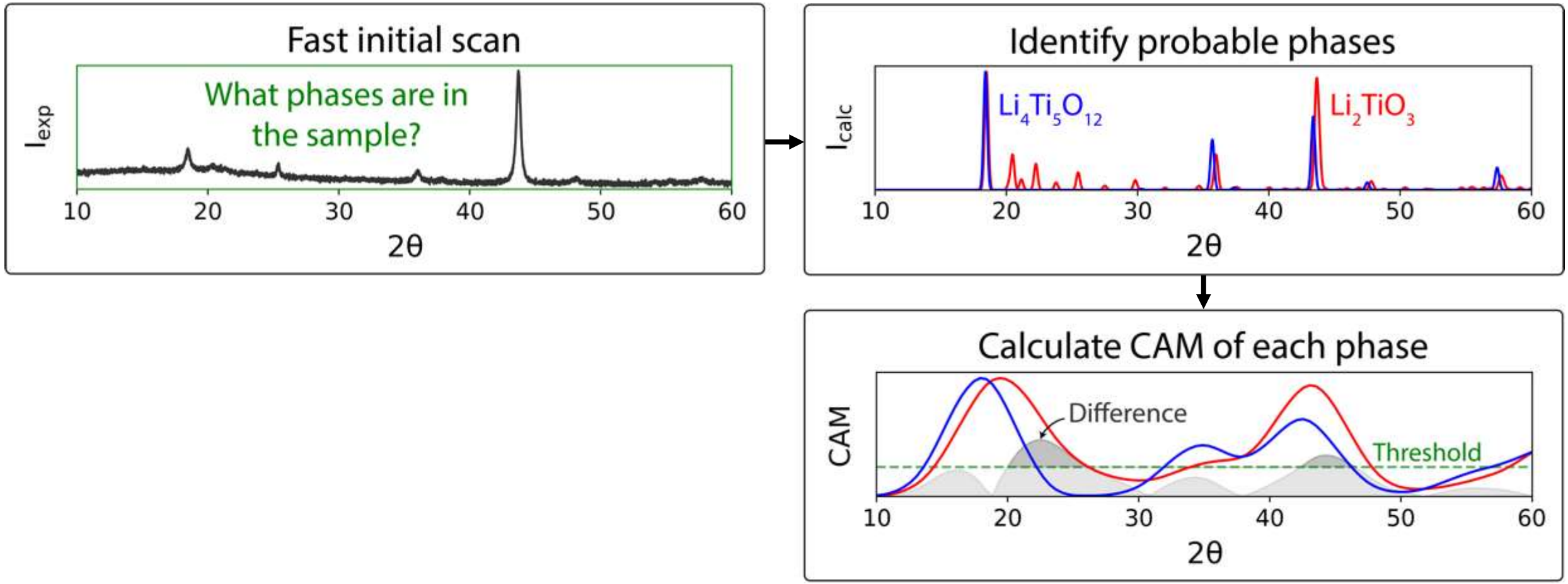
N. J. Szymanski *et al.*, npj Computational Materials (2023).

Adaptive XRD workflow: CNN predicts likely phases



N. J. Szymanski *et al.*, npj Computational Materials (2023).

Adaptive XRD workflow: CAMs highlight areas of interest



N. J. Szymanski *et al.*, npj Computational Materials (2023).

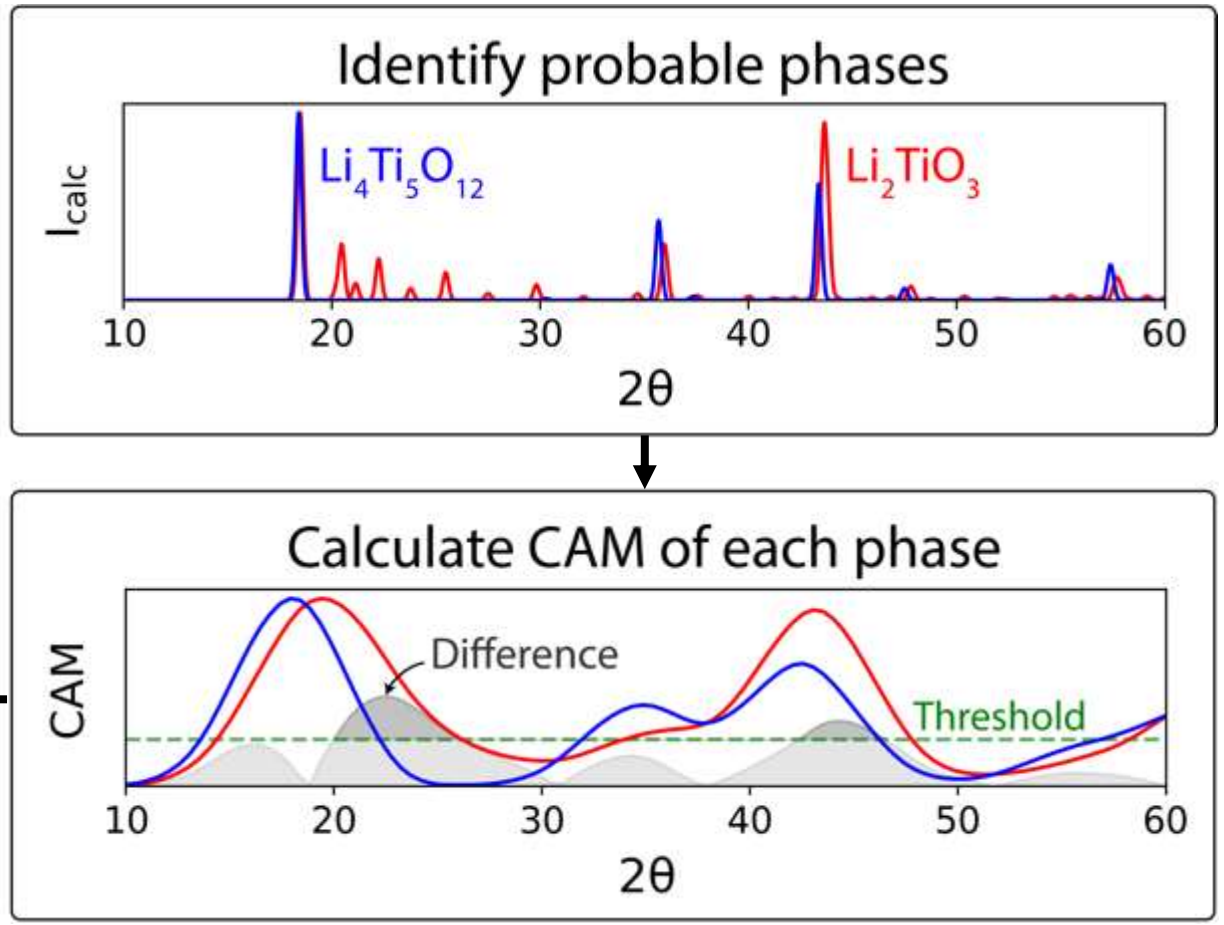
Adaptive XRD workflow: CAMs highlight areas of interest

Model predicts **dog**

Model predicts **cat**

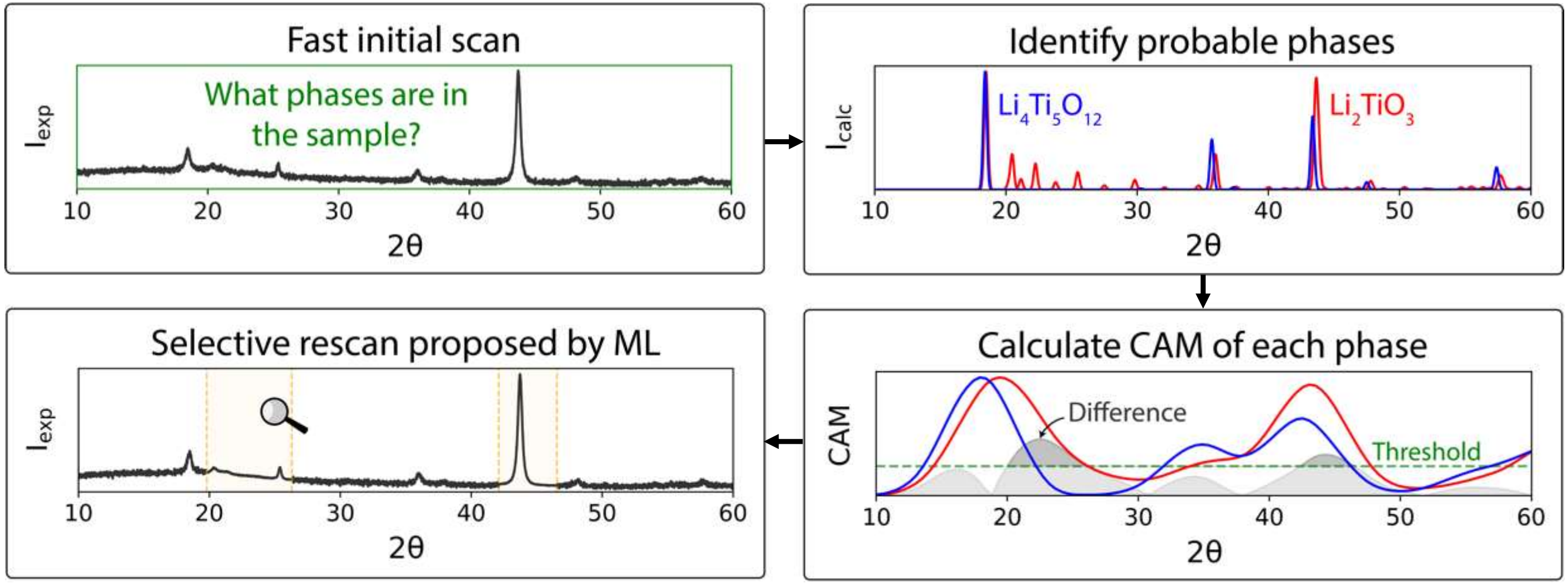
Example from Keras tutorials

Class activation map (CAM)



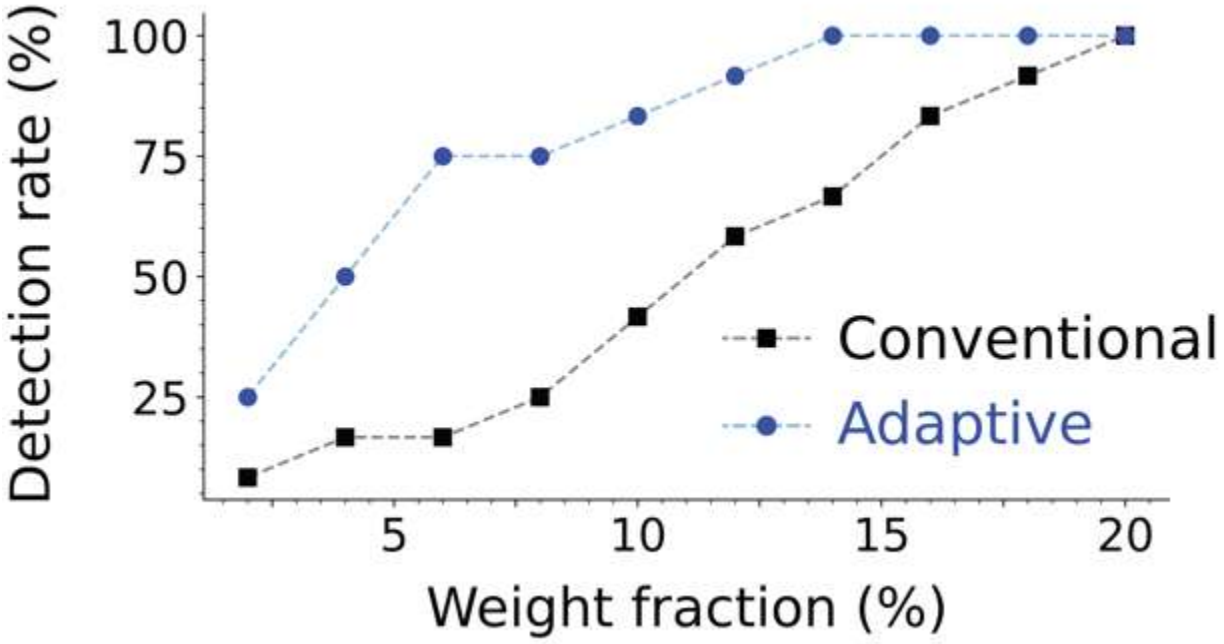
N. J. Szymanski *et al.*, npj Computational Materials (2023).

Adaptive XRD workflow: slower rescans clarify key features



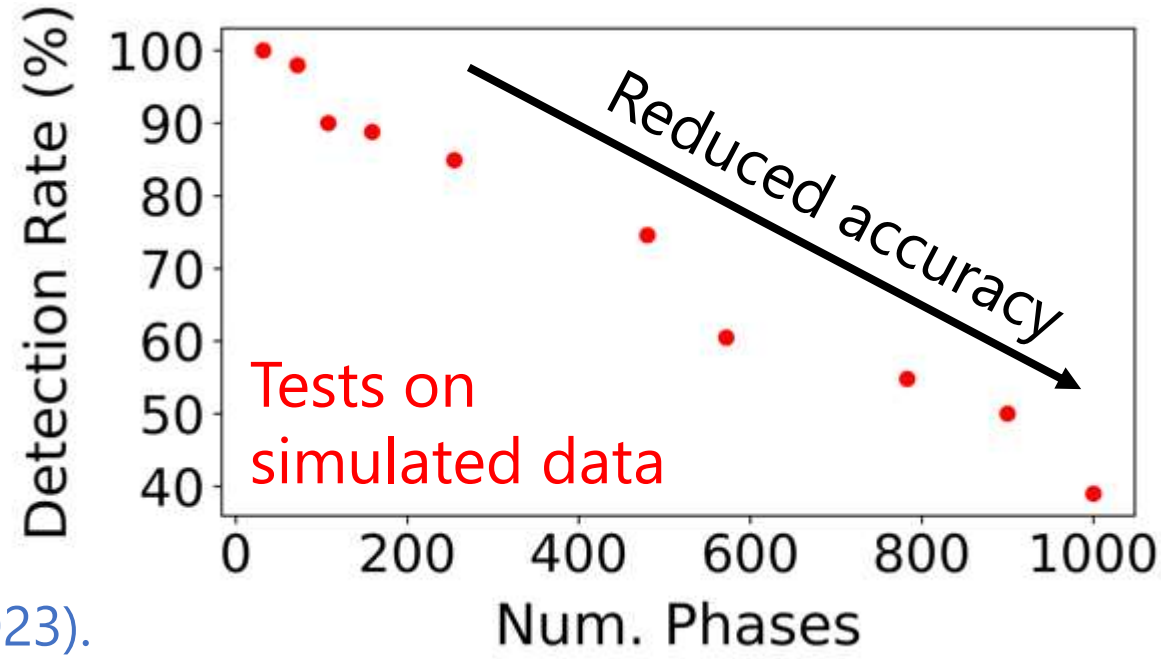
N. J. Szymanski *et al.*, npj Computational Materials (2023).

Adaptive scans more effectively detect secondary phases



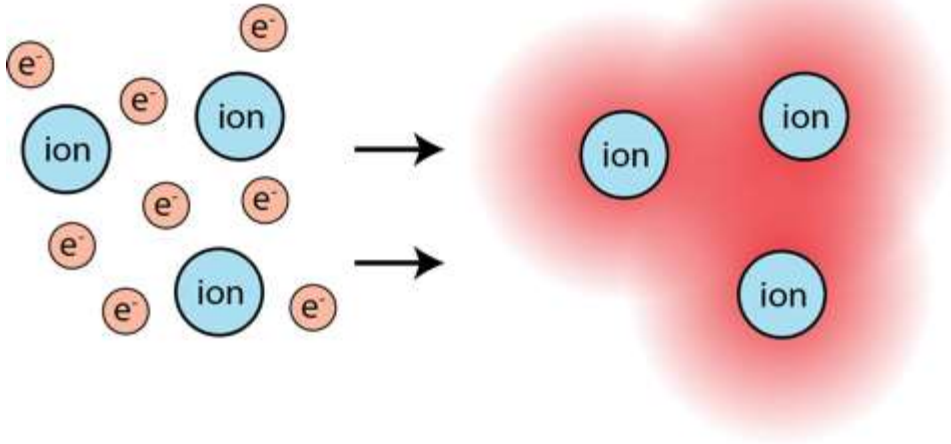
- XRD performed on **120 mixtures** in the **Li-La-Zr-O space**, prepared with varied impurity amounts
- **Adaptive scans show improved accuracy in impurity detection**

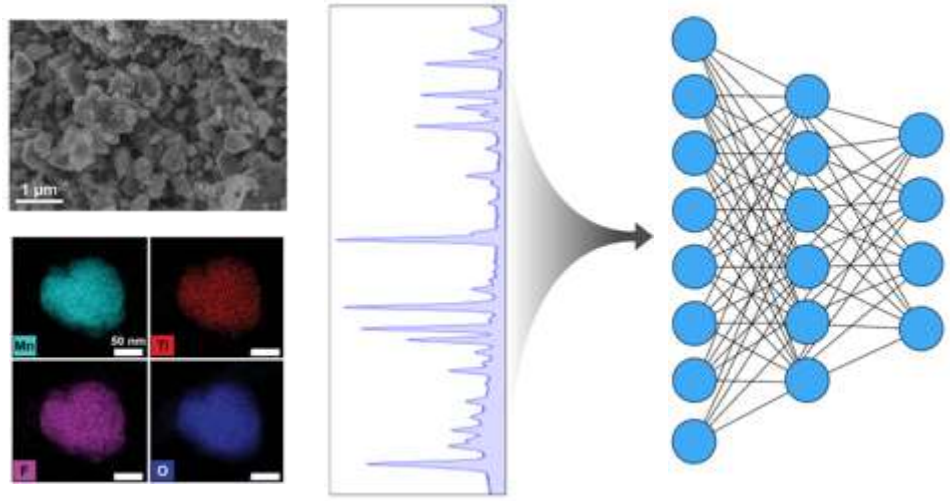
However, impurity detection remains **challenging when there are more phases to choose from**



N. J. Szymanski *et al.*, npj Computational Materials (2023).

Computational tools for synthesis and characterization

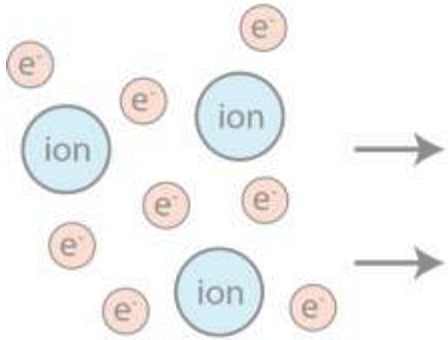


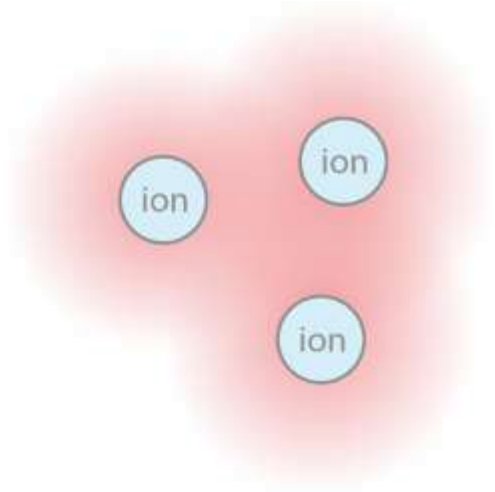


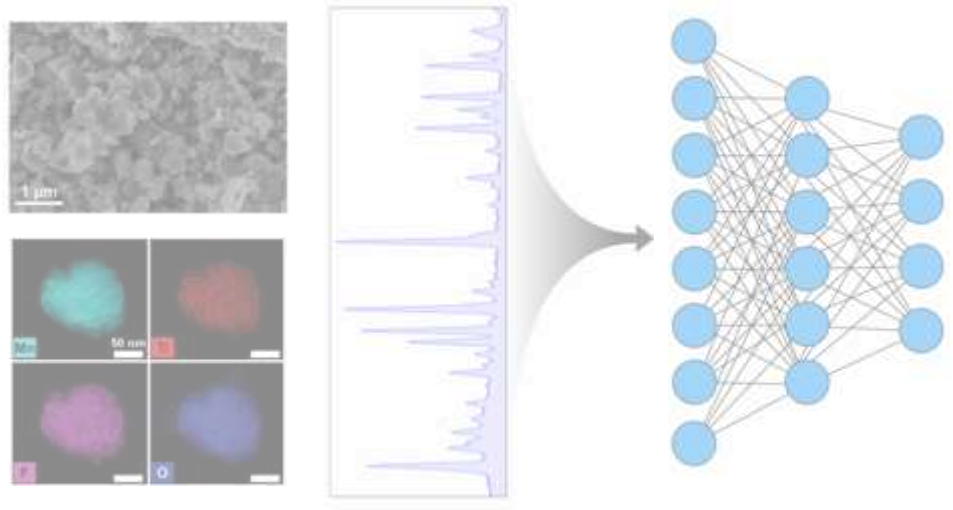
DFT for synthesis planning

AI for characterization

Computational tools for synthesis and characterization





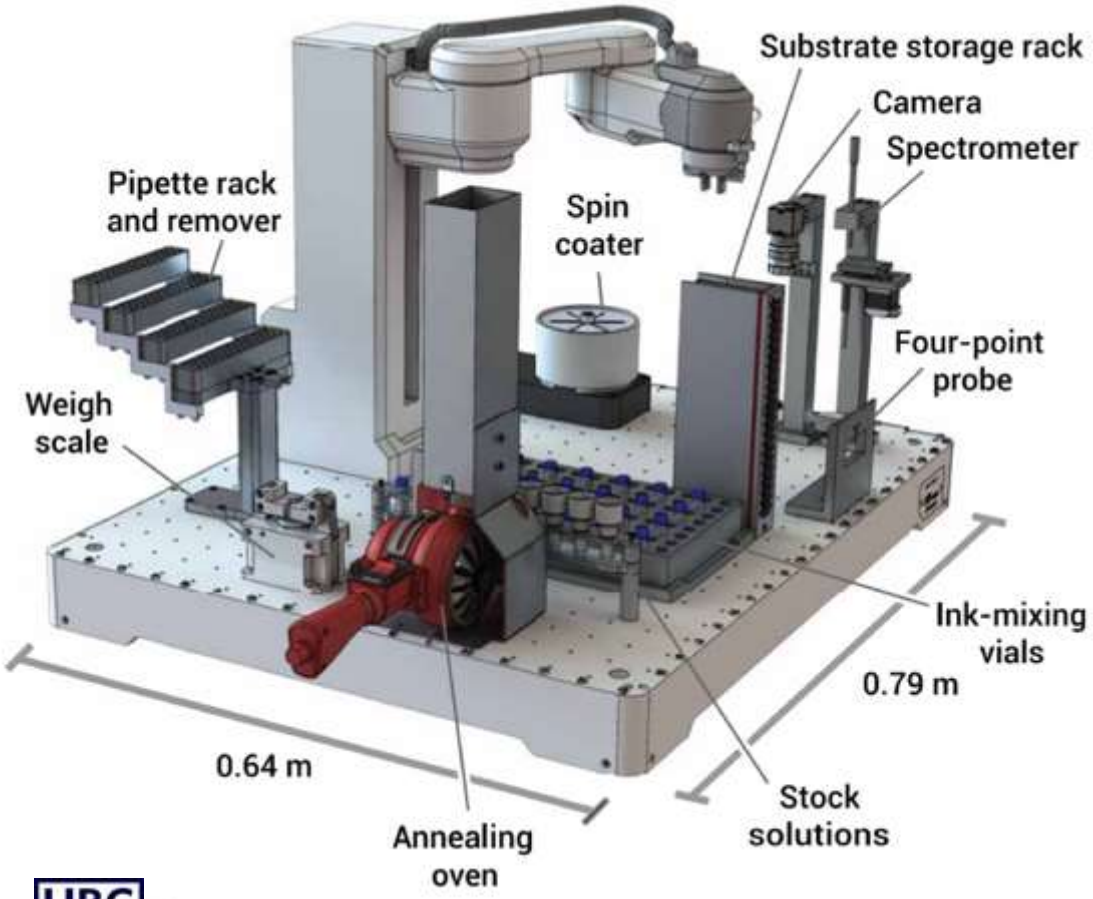


DFT for synthesis planning → AI for characterization

Integrate these two approaches for **closed-loop** experimental optimization

Self-driving labs

Self-driving labs are being developed around the globe



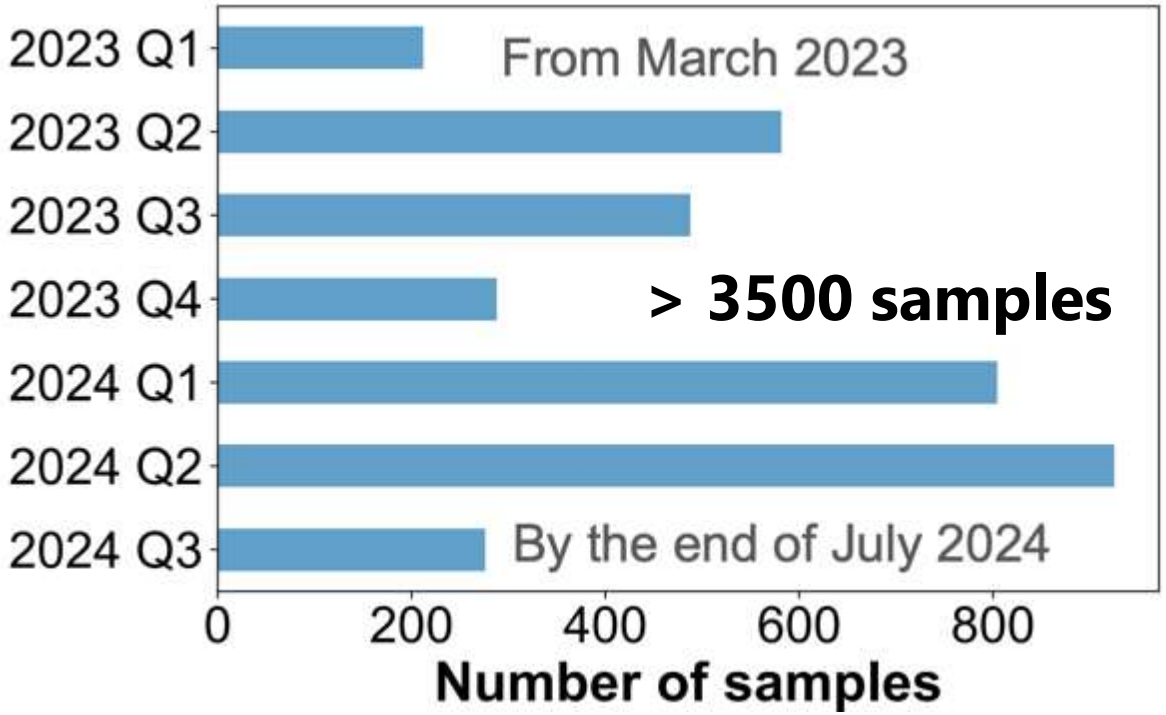
Automated thin film growth

Automated solution-based synthesis

MacLeod *et al.*, Science Advances (2020).

Burger *et al.*, Nature (2020).

Automated solid-state synthesis for inorganic materials

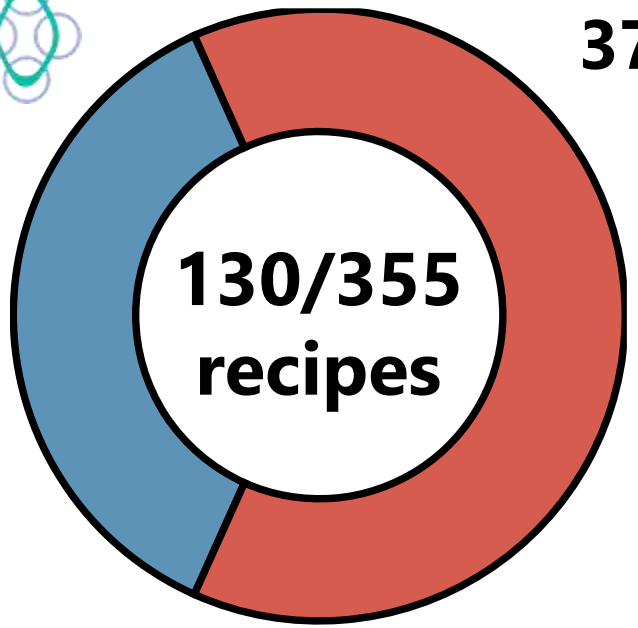


Sample prep → **Heating** → **Extraction** → **XRD**

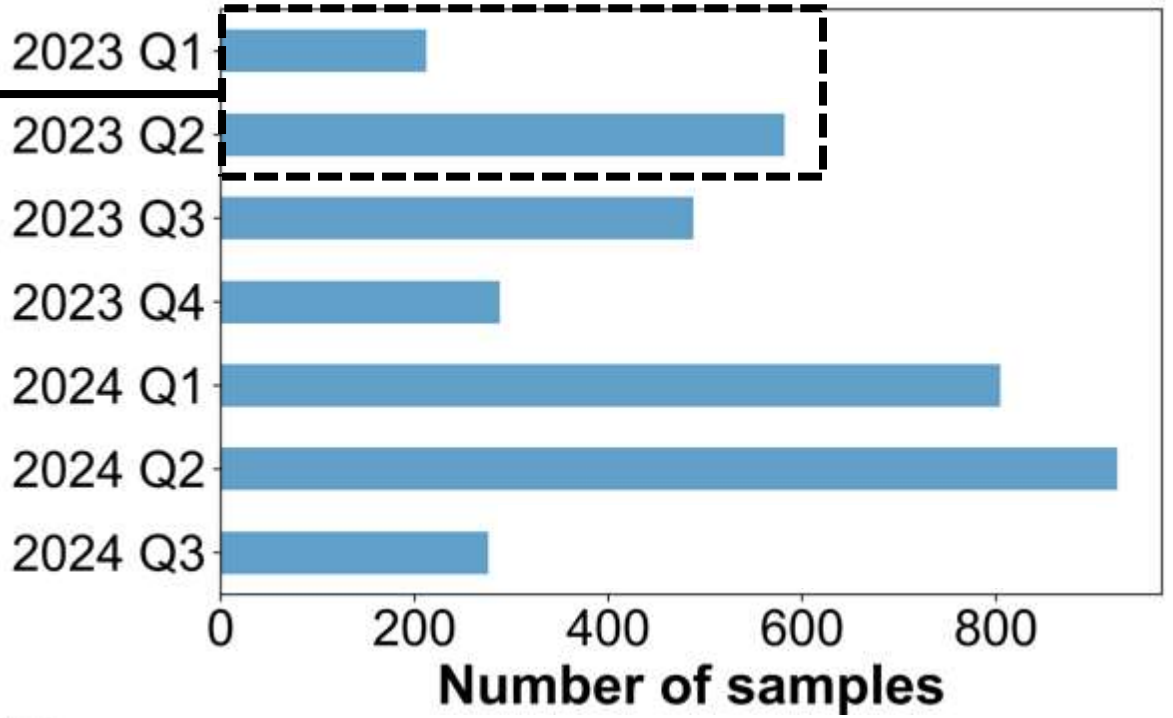
N. J. Szymanski *et al.*, Nature (2023).

Y. Fei *et al.*, Digital Discovery (2024).

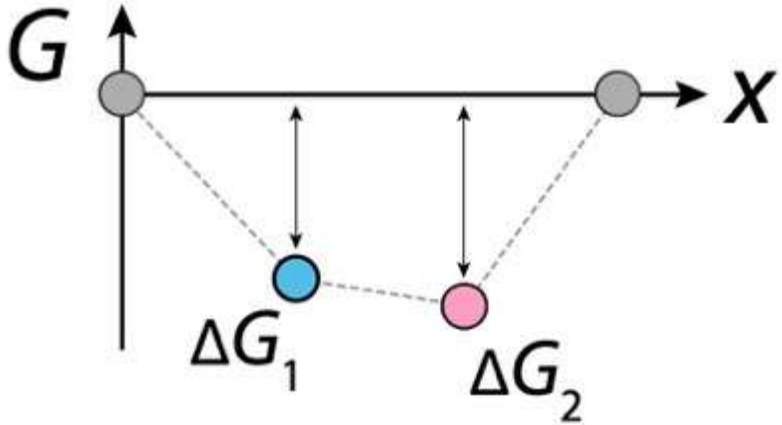
Challenge #1: most experimental iterations fail



37% success per recipe



Computed phase diagrams only get us so far

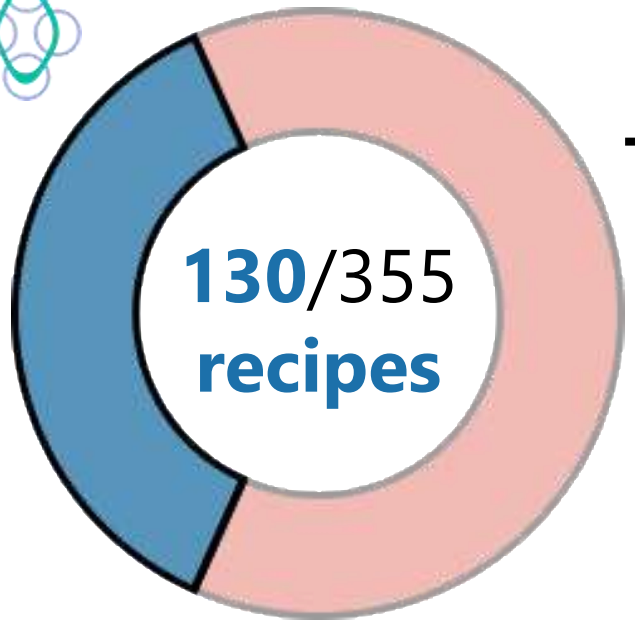


ARROWS[3]

Autonomous Reaction Route Optimization With Solid-State Synthesis

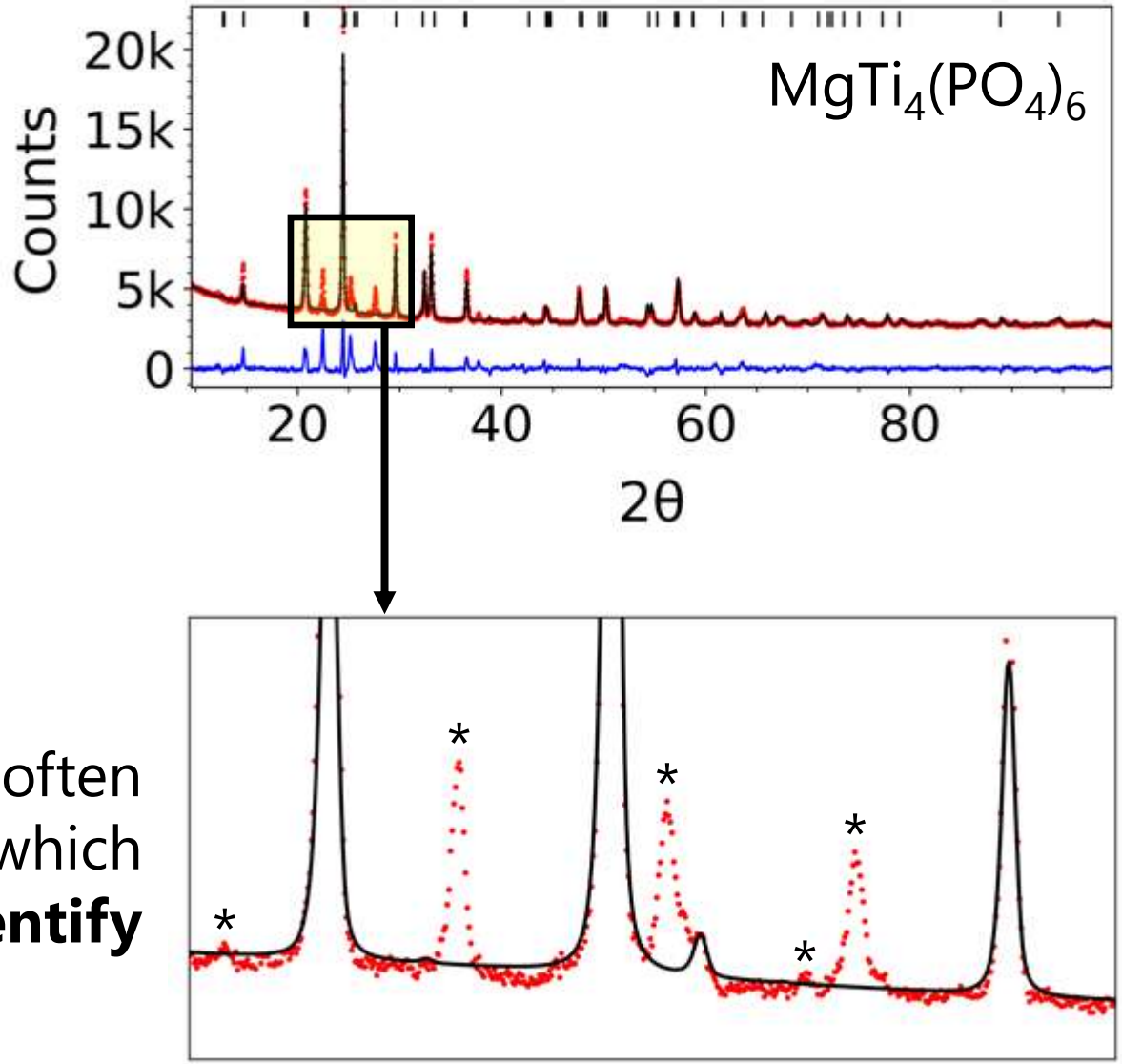
N. J. Szymanski *et al.*, Nature (2023).

Challenge #2: materials characterization remains difficult



Conventional

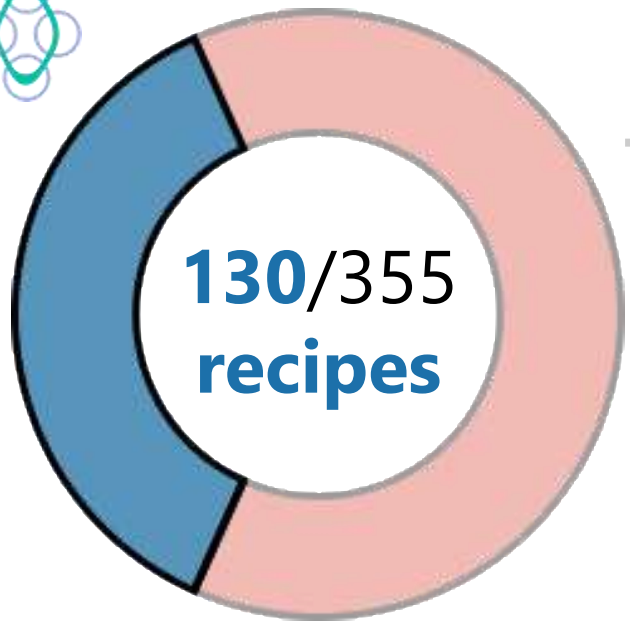
(*ex-situ*) XRD



Successful syntheses often still contain **impurities**, which the **AI struggles to identify**

Leeman *et al.*, PRX Energy (2024).

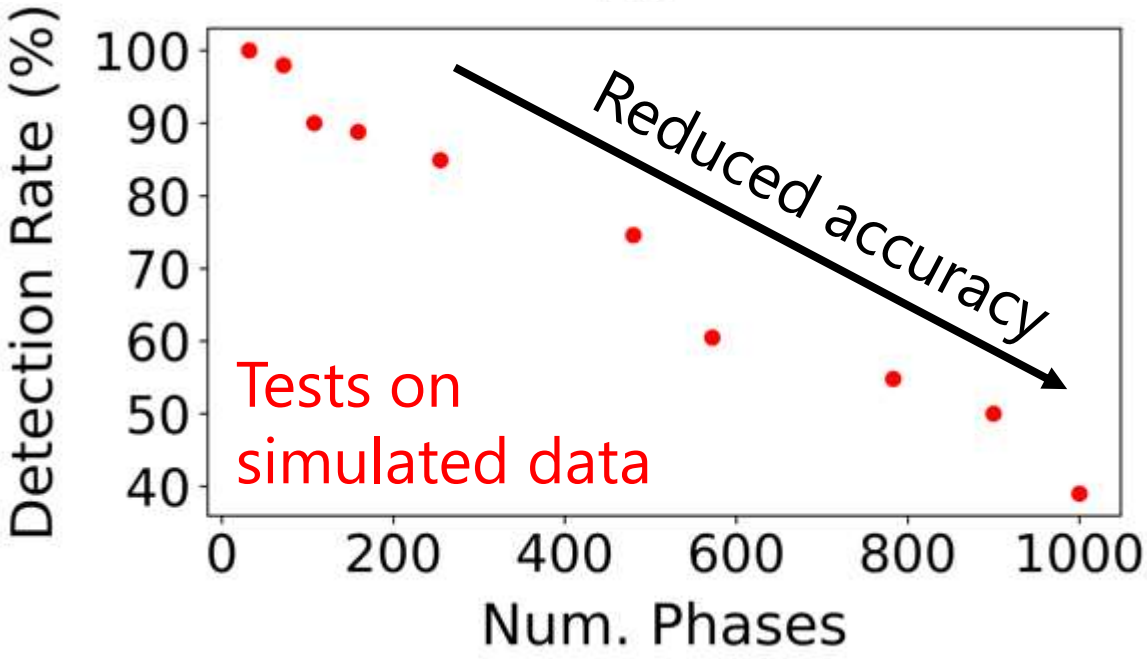
Challenge #2: materials characterization remains difficult



Conventional
(*ex-situ*) XRD

Adaptive XRD can help with impurity detection, but its accuracy still decreases in many-component chemistries

***Ex-situ* XRD only gets us so far**



Future: additional characterization, with a focus on *in-situ*

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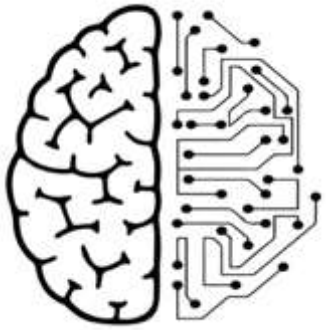
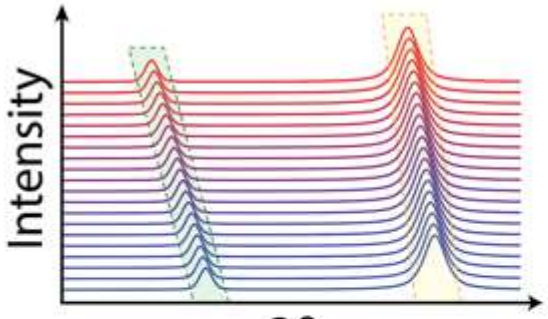
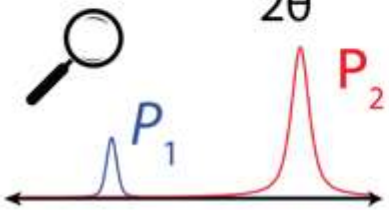
High-throughput *in-situ* XRD



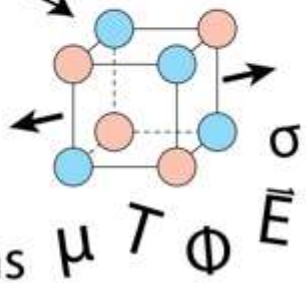


$$\approx \begin{bmatrix} P_1 \\ \dots \\ P_N \end{bmatrix} \times \begin{bmatrix} w_1 & \dots & w_N \end{bmatrix}$$

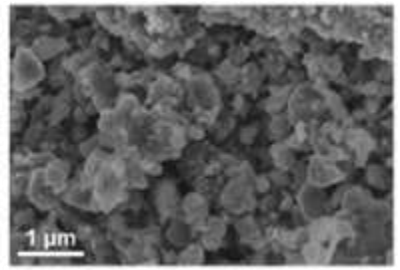
Factorization

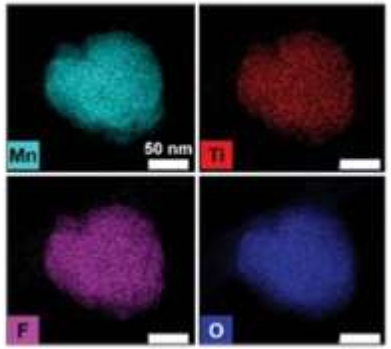


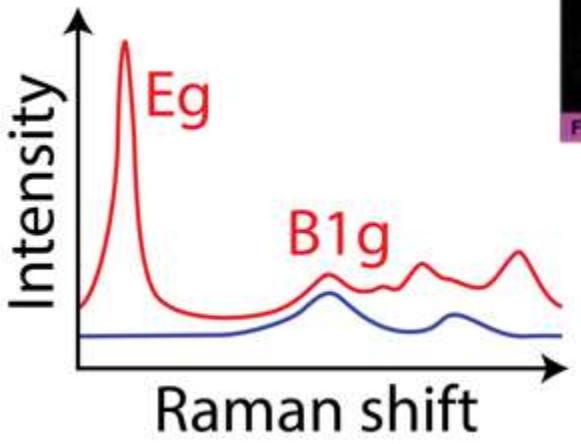
Informed by DFT-calculated **reponse** functions



ML for complementary techniques

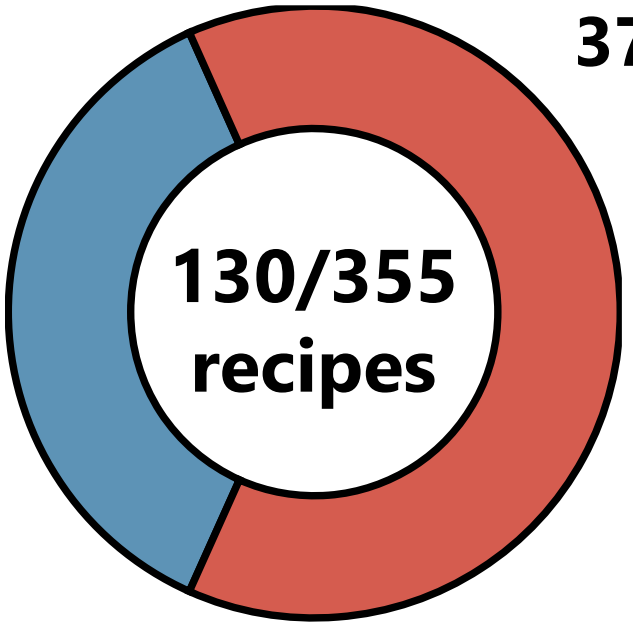






Open-source

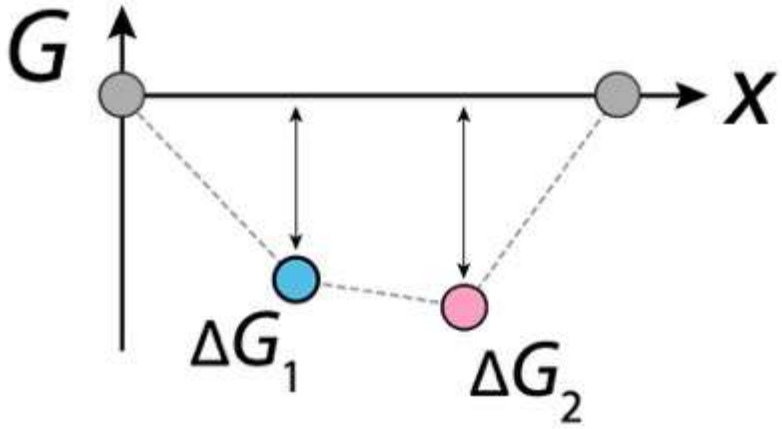
Challenge #1: most experimental iterations fail



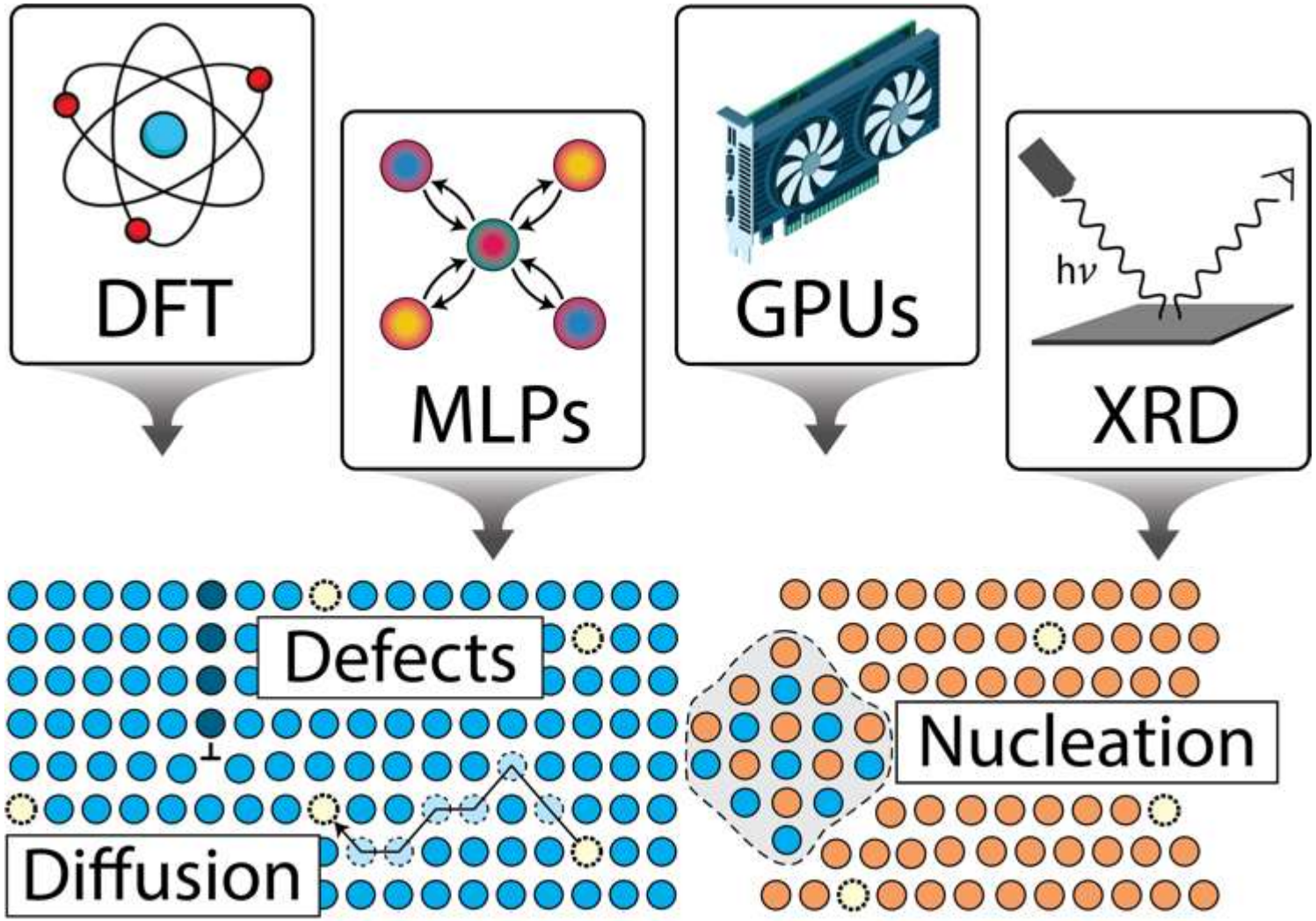
37% success per recipe

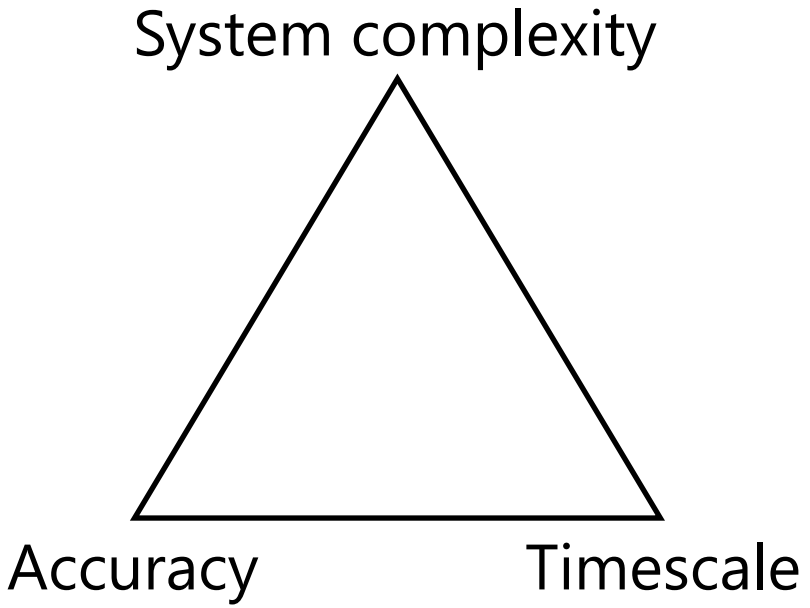
How to overcome the low success rate of thermodynamic-based synthesis design?

Computed phase diagrams only get us so far

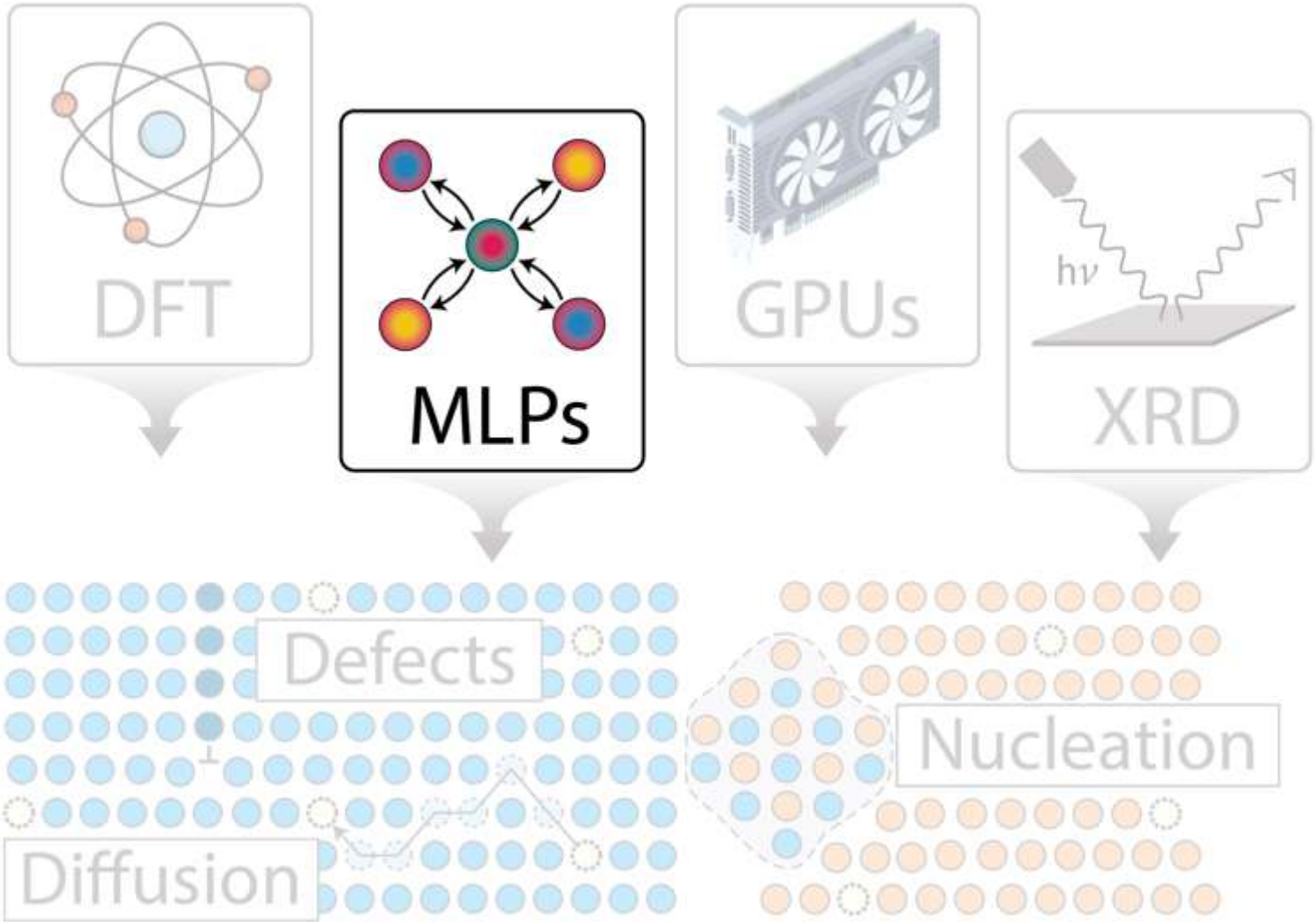


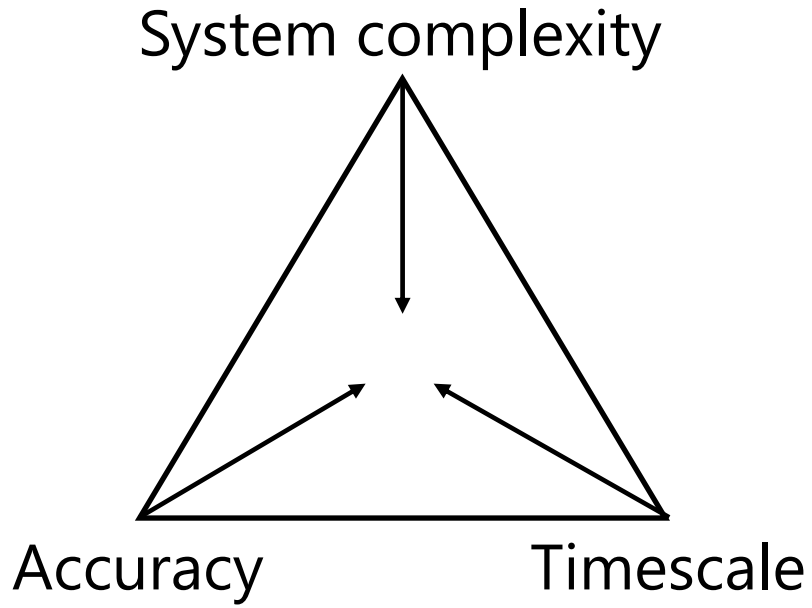
Future: directly simulate the *kinetics* of solid-state reactions





Future: directly simulate the *kinetics* of solid-state reactions





Leverage **machine learning** to bridge this gap in the simulation of kinetics

Acknowledgements

CEMS
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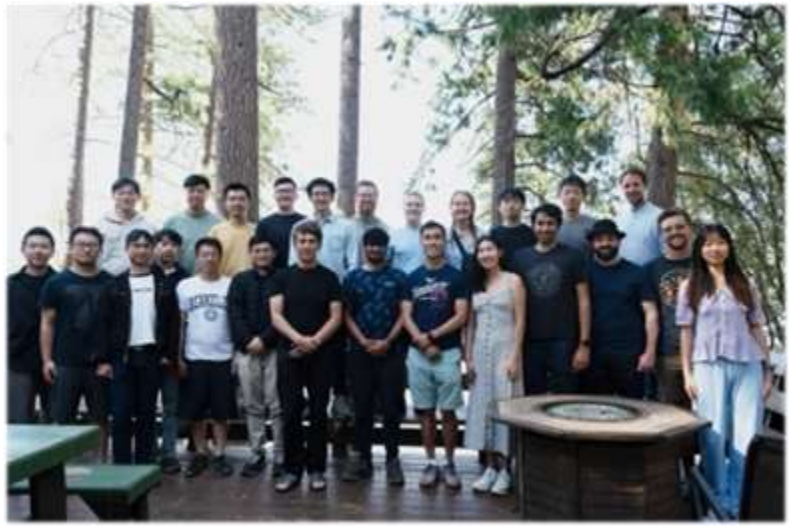
& Materials Science









umicore