UCLA

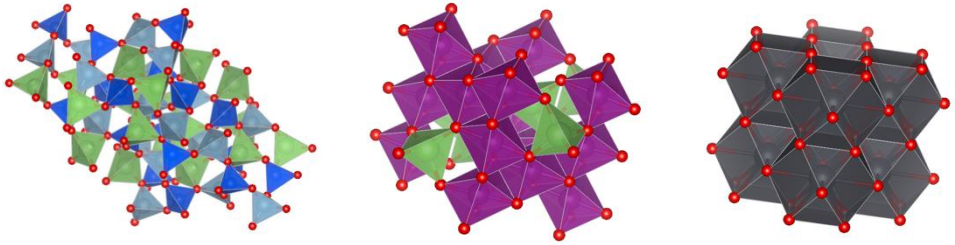
# How effective is generative AI for "materials discovery"

Nathan Szymanski
University of California, Los Angeles
MLCM, May 18th, 2026

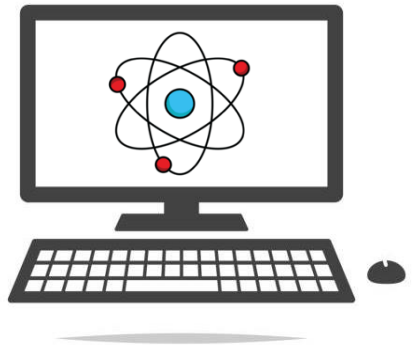
MD² LAB
MATERIALS DESIGN THROUGH DYNAMICS

Samueli
School of Engineering

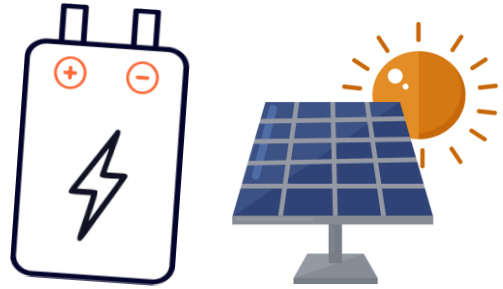
# Finding materials through *inverse design*



**Inorganic crystalline materials**

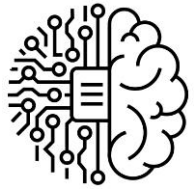


**Quantum chemistry (DFT)**



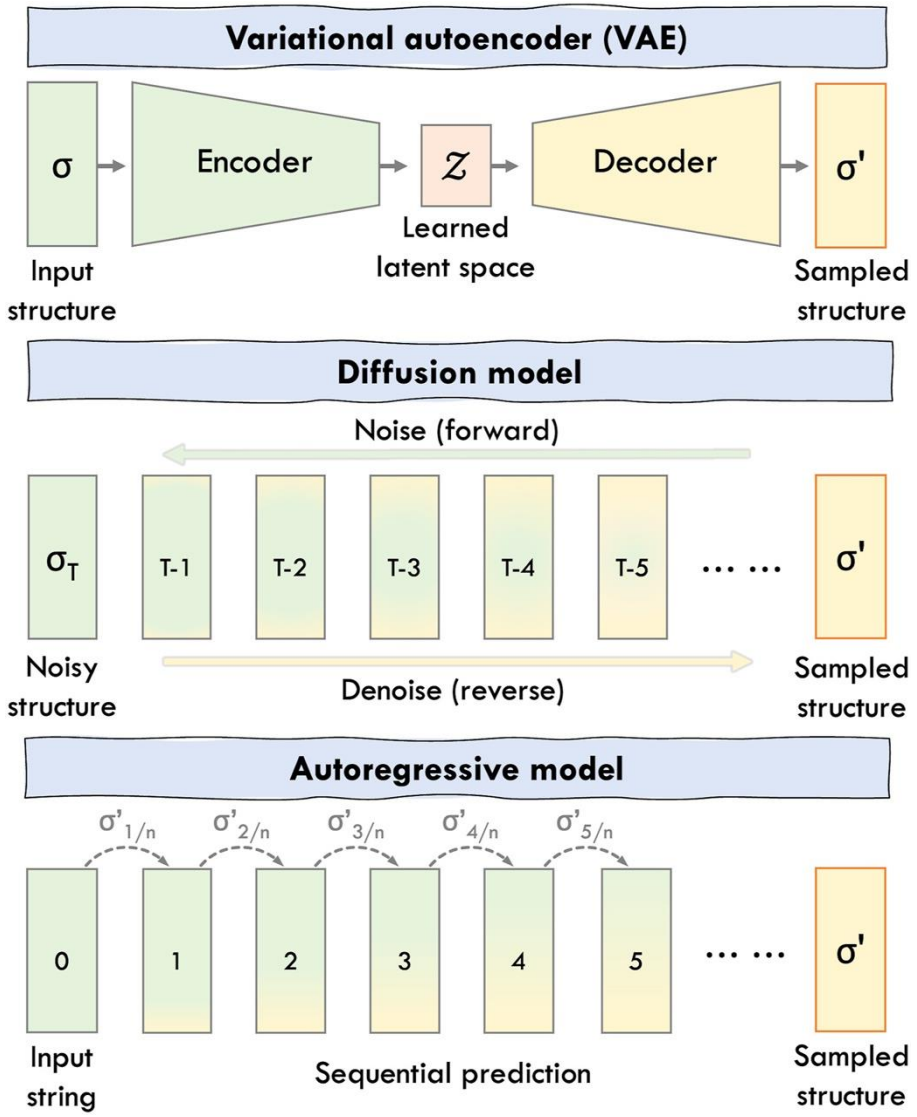
**Predicted functionality**

**Generative AI may help us solve the *inverse problem***



Given a desired functionality:
propose hypothetical materials

# Many genAI models out there! We tested four




Park, Li, and Walsh, *Matter*, 2024.

**Matter**

Article

An invertible crystallographic representation for general inverse design of inorganic crystals with targeted properties

Zekun Ren, Siyu Isaac Parker Tian, Juhwan Noh, ..., Kedar Hippalgaonkar, Yousung Jung, Tonio Buonassisi

**FTCP**

Published as a conference paper at ICLR 2022

CRYSTAL DIFFUSION VARIATIONAL AUTOENCODER FOR PERIODIC MATERIAL GENERATION

Tian Xie, Xiang Fu, Octavian-Eugen Ganea, Regina Barzilay, Tommi Jaakkola

**CDVAE**

**A generative model for inorganic materials design**

**nature**

Claudio Zeni[1,8], Robert Pinsler[1,8], Daniel Zügner[2,8], Andrew Fowler[1,8], Matthew Horton[3,8], Xiang Fu[1], Zilong Wang[4], Aliaksandra Shysheya[1], Jonathan Crabbé[1], Shoko Ueda[1], Roberto Sordillo[1], Lixin Sun[1], Jake Smith[3], Bichlien Nguyen[3], Hannes Schulz[2], Sarah Lewis[1], Chin-Wei Huang[5], Ziheng Lu[6], Yichi Zhou[7], Han Yang[6], Hongxia Hao[6], Jielan Li[6], Chunlei Yang[4], Wenjie Li[4], Ryota Tomioka[1,8] & Tian Xie[1,8]

**MatterGen**

**nature communications**

Received: 22 December 2023

Article

Luis M. Antunes[1], Keith T. Butler[2] & Ricardo Grau-Crespo[1]

https://doi.org/10.1038/s41467-024-54639-7

**Crystal structure generation with autoregressive large language modeling**

**CrystaLLM**

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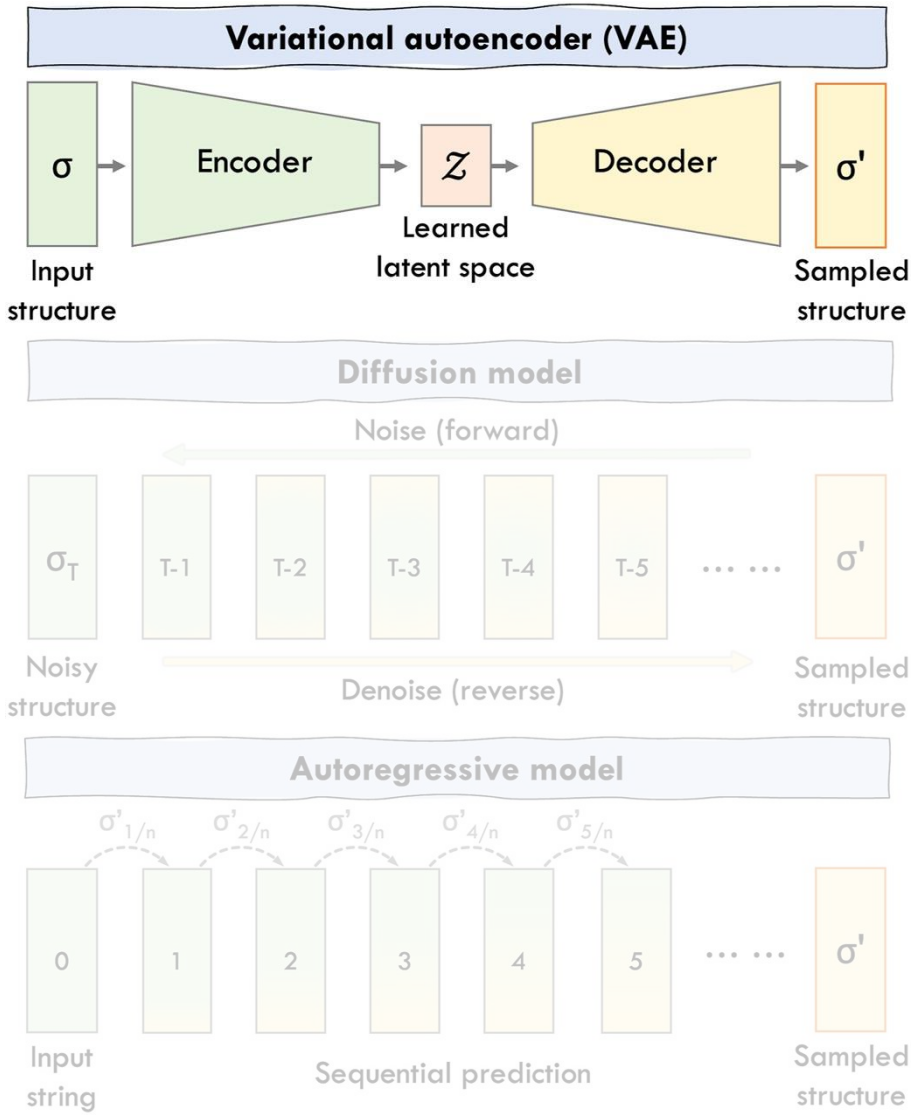


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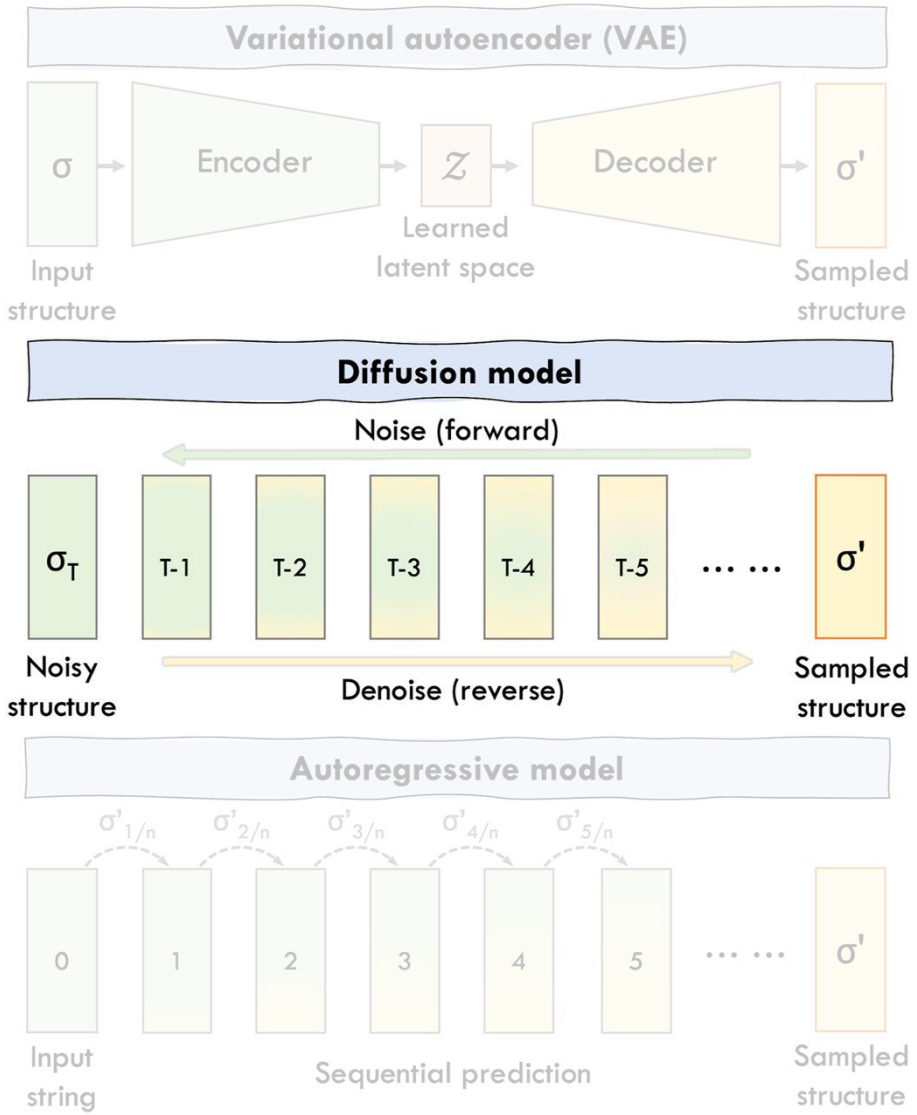


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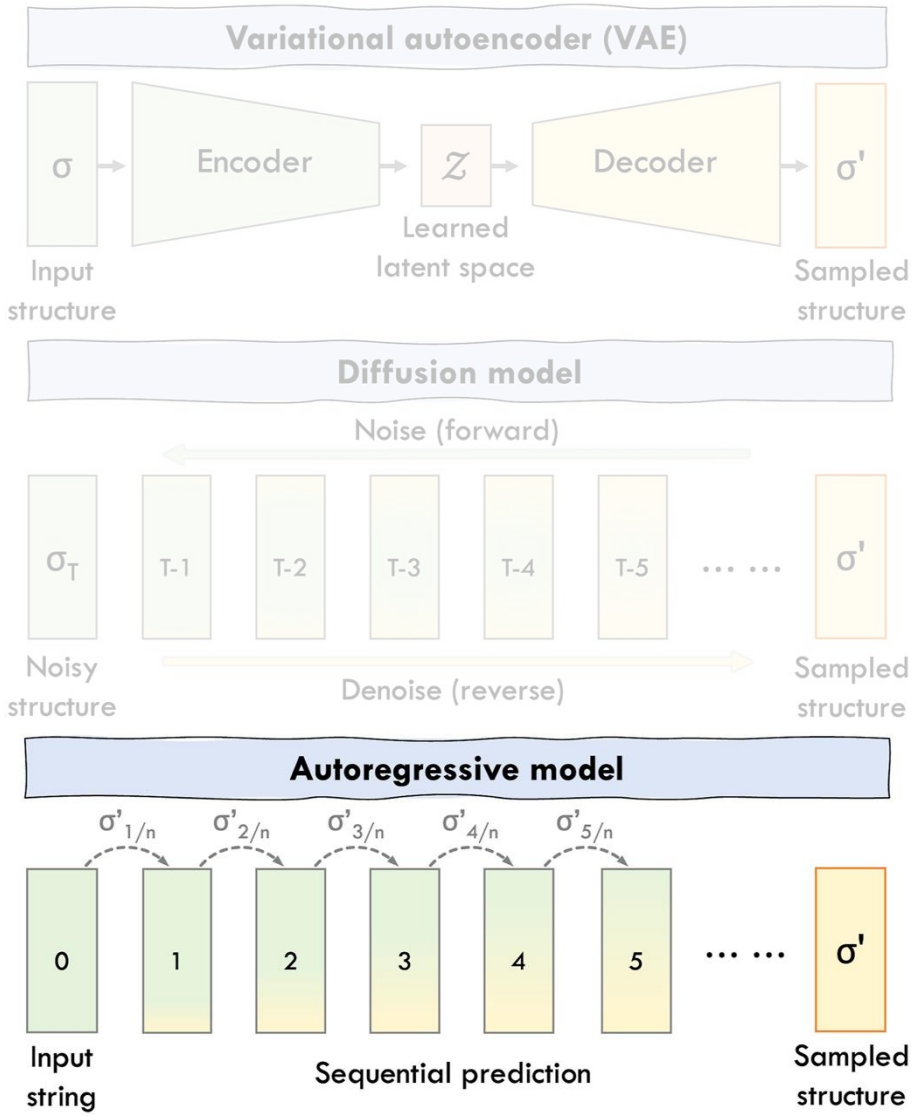


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**Can we actually make the materials proposed by these models?**

**Or does the AI hallucinate?** 😬

Matter

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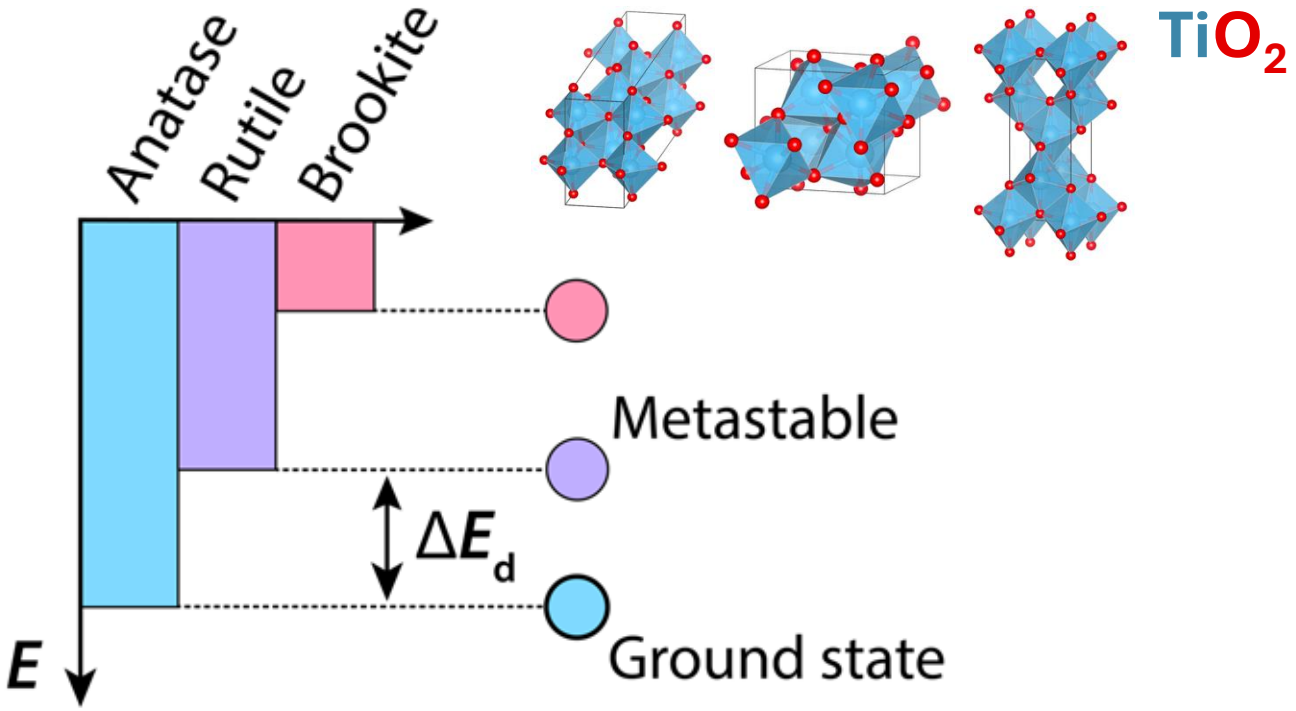
Crystal structure generation with autoregressive large language modeling

CrystaLLM

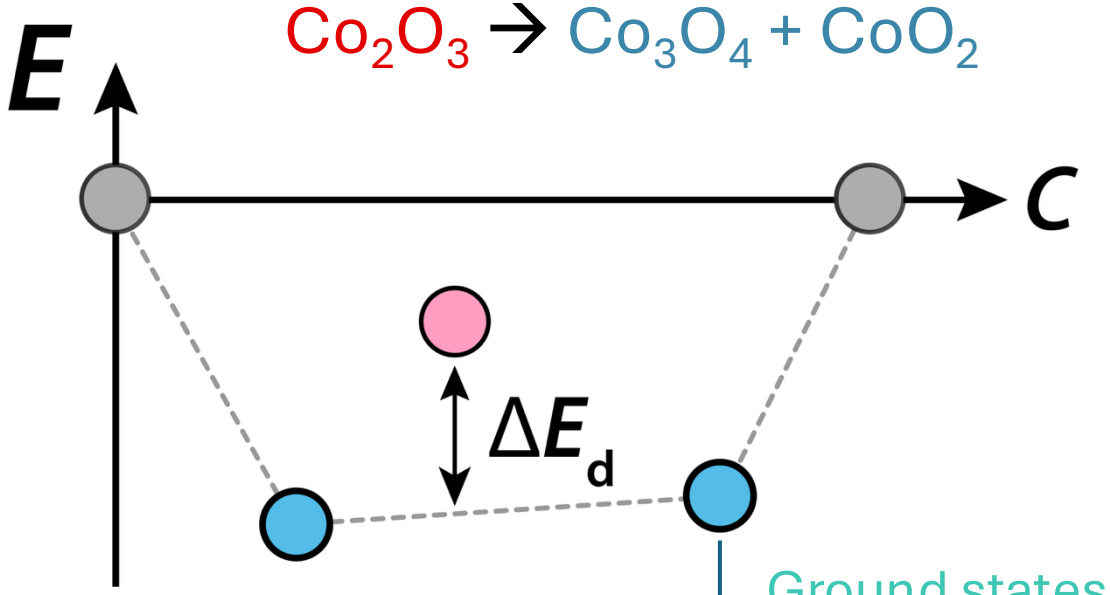
# We can assess thermodynamic stability



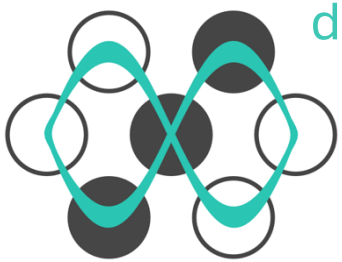

$TiO_2$

**Example:**

$Co_2O_3 \rightarrow Co_3O_4 + CoO_2$




Ground states from online datasets



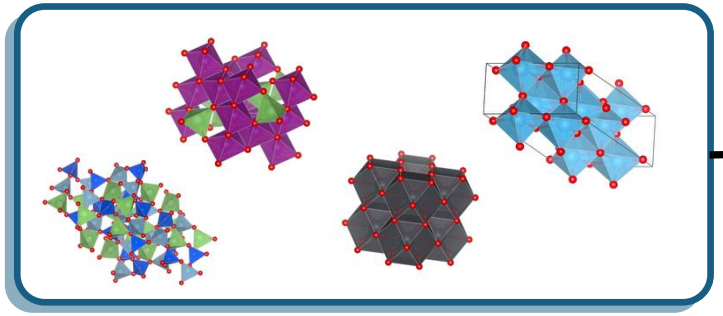
MATERIALS PROJECT

$\Delta E_d$ is the **decomposition energy**, which we can get from density functional theory (DFT) calculations

**Smaller $\Delta E_d$ → better chance of synthesis**

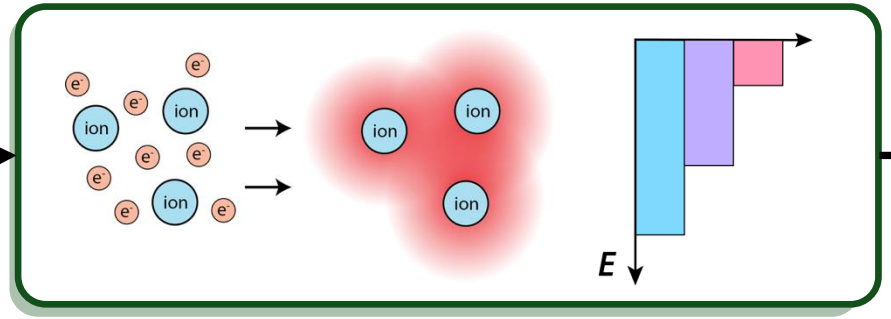
# $\Delta E_d$ provides "sanity check" for GenAI

**Generate new* materials**



500 per model, ***not in MP**

**Calculate energy with DFT**

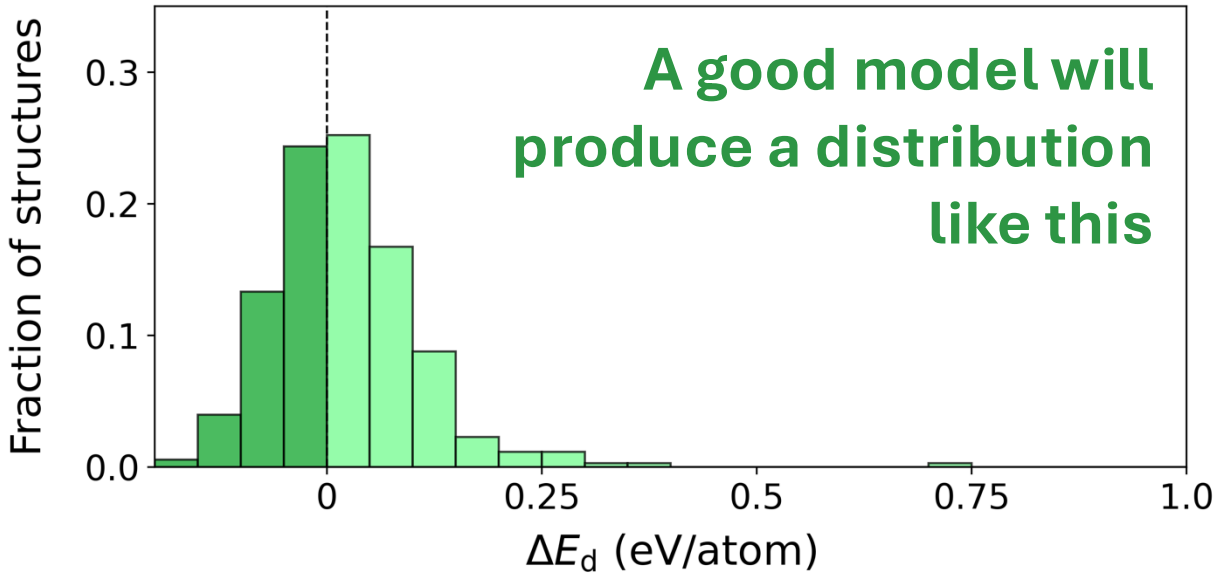


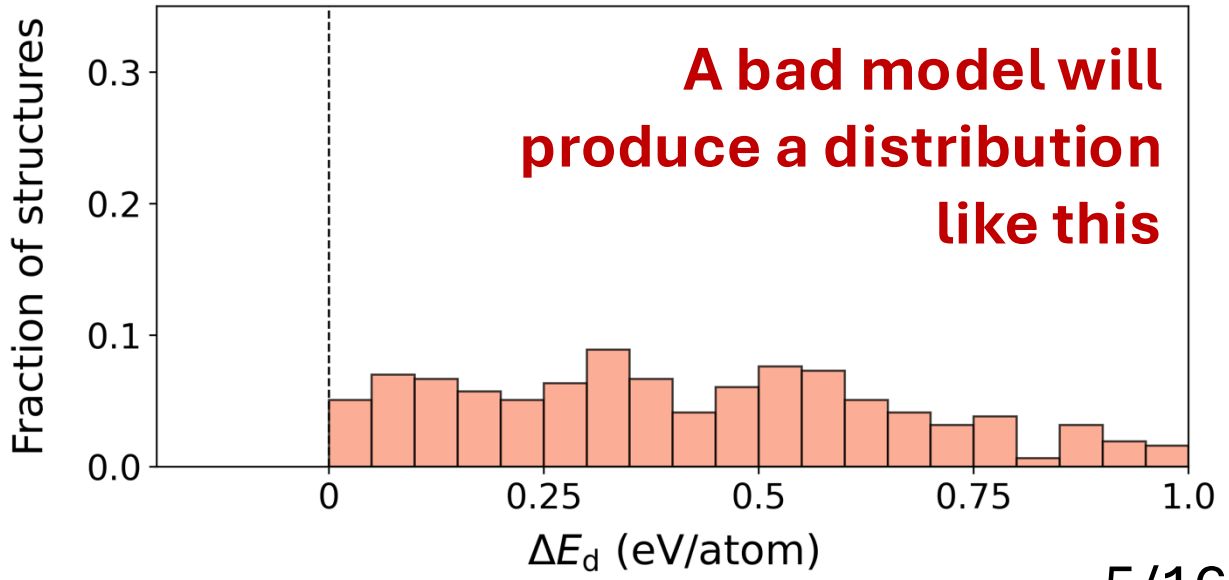

**Compare to ground states**

MATERIALS PROJECT

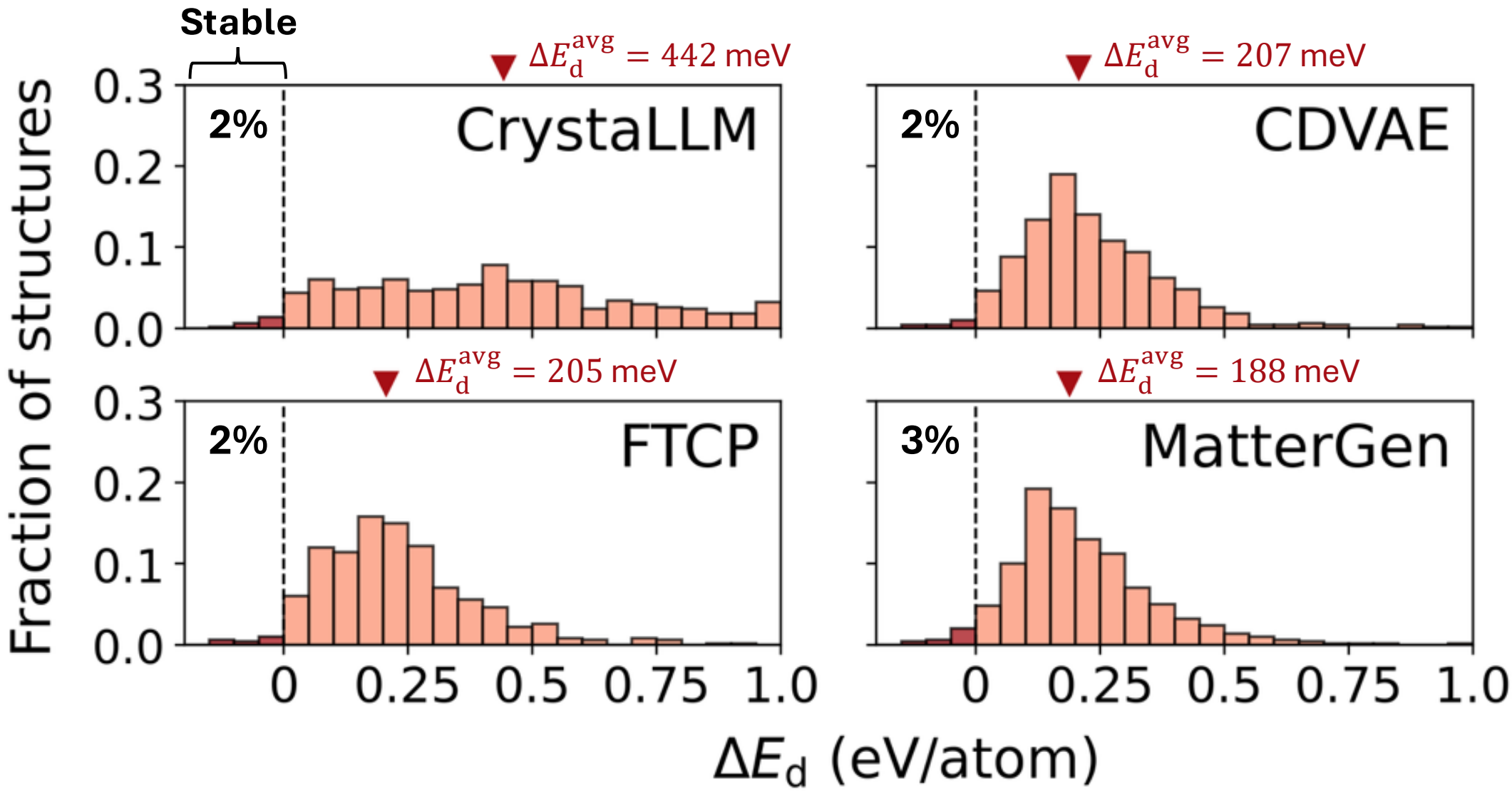
~200k compounds

## MatGen-Baselines

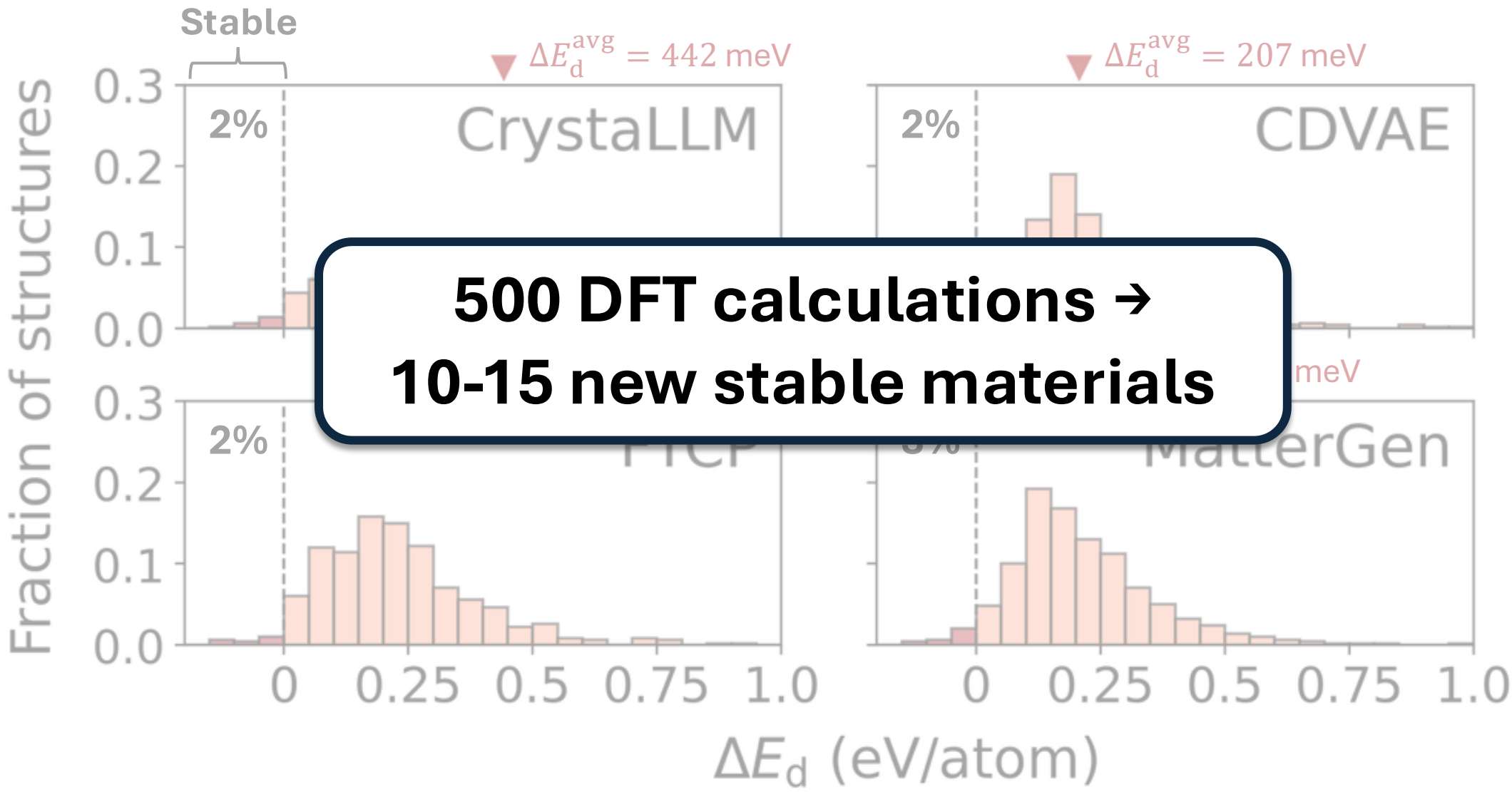


# GenAI-predicted materials have limited stability



# Is this a “good” success rate?




**500 DFT calculations →**
**10-15 new stable materials**

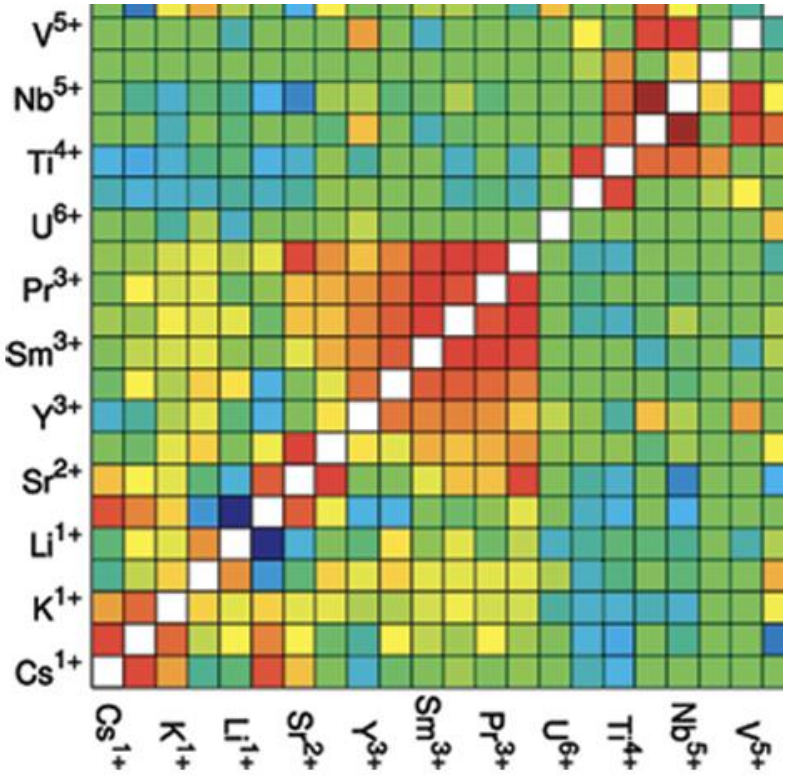
# Ion substitution provides a baseline

New materials are often designed **through analogy** to known materials

**e.g., $MgTi_2S_4$ → $MgCr_2S_4$**

**3.2. Ionic Pair Substitution Analysis.** The tendency for a pair of ions to substitute for each other can be estimated by computing the pair correlation:

$$g_{ab} = \frac{p(X_1 = a,\ X_1' = b)}{p(X_1 = a)p(X_1 = b)}$$




**"DMSP"**

$g_{ab} \rightarrow 1$

$g_{ab} \rightarrow 0$

G. Hautier *et al.*, *Inorganic Chemistry*, 2010.

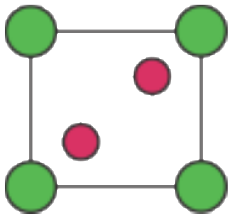
# The baseline outperforms genAI on stability

New materials are often designed **through analogy** to known materials

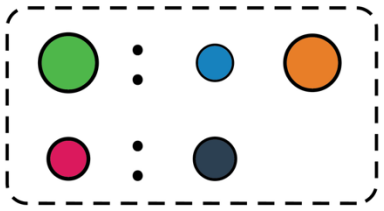
**e.g., $MgTi_2S_4$ → $MgCr_2S_4$**

Choose known materials **that are stable**

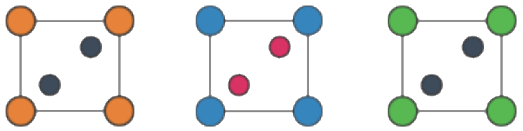
MATERIALS PROJECT

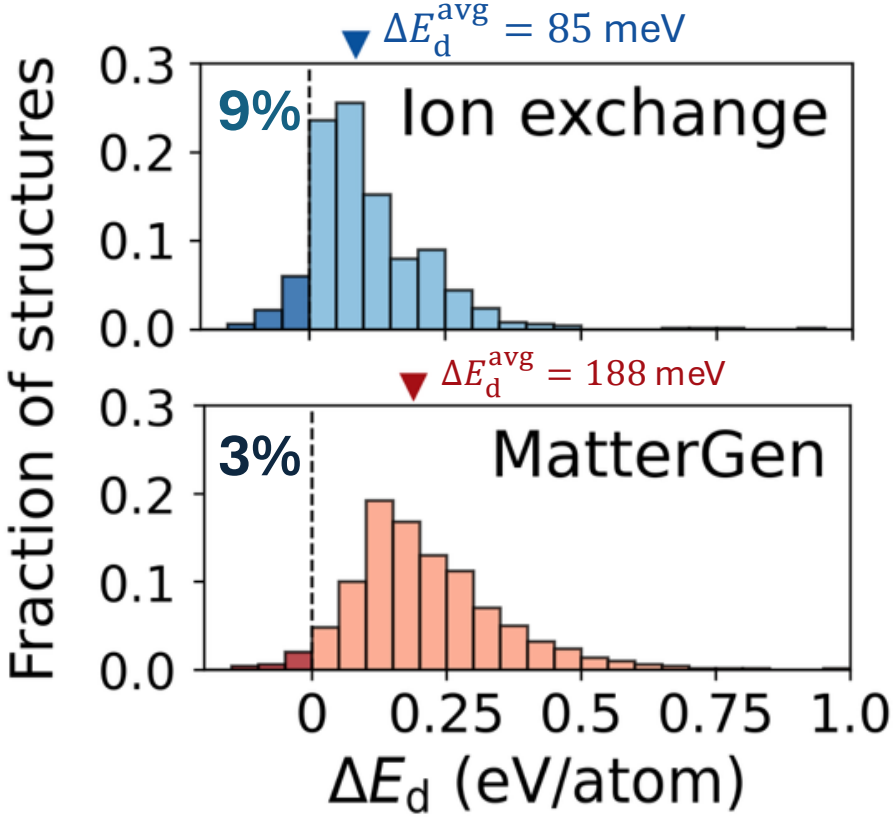


Then perform **data-driven ion exchange**

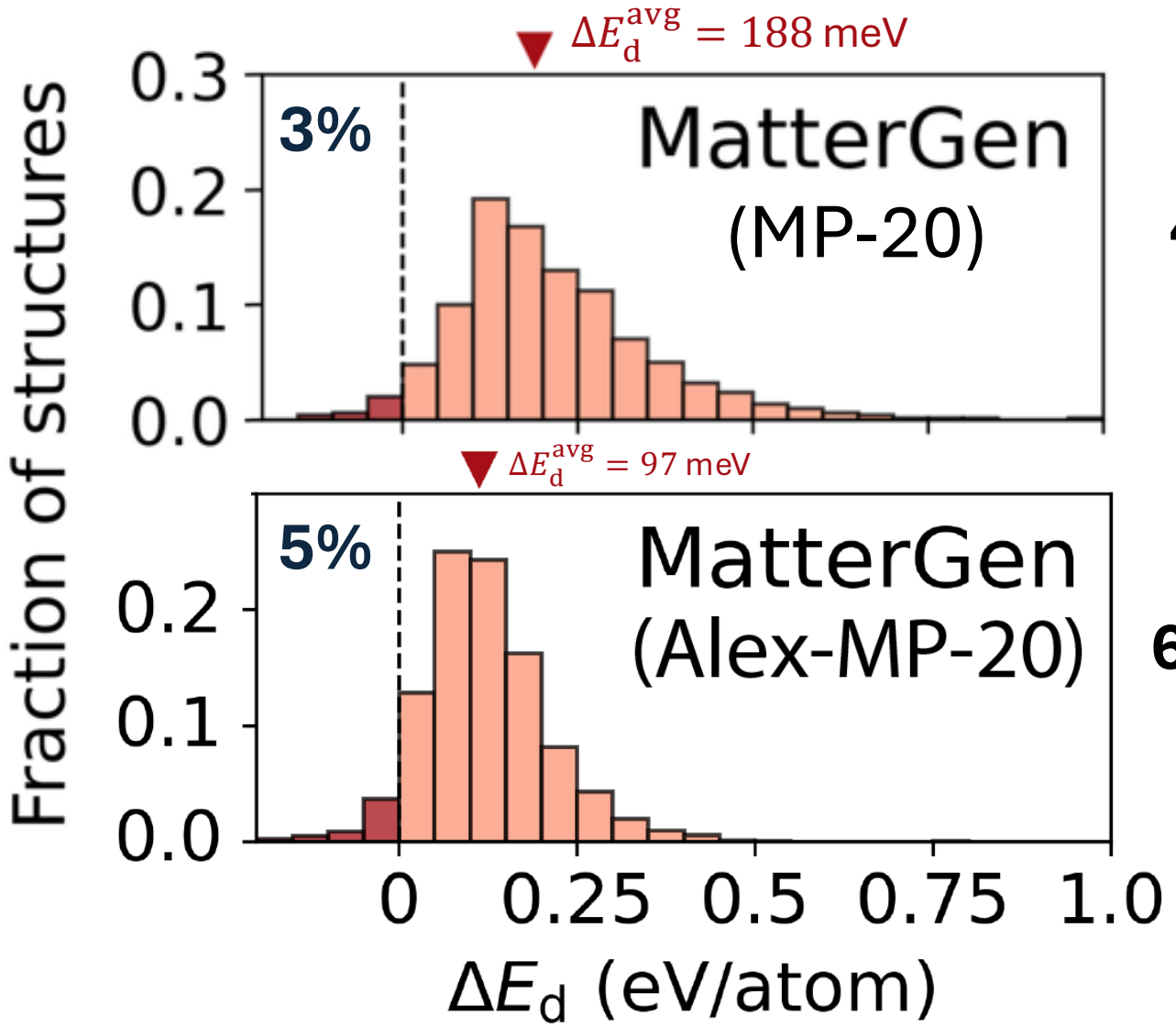


e.g., $Cr^{3+}$ for $Ti^{3+}$





# But there is room for genAI optimism



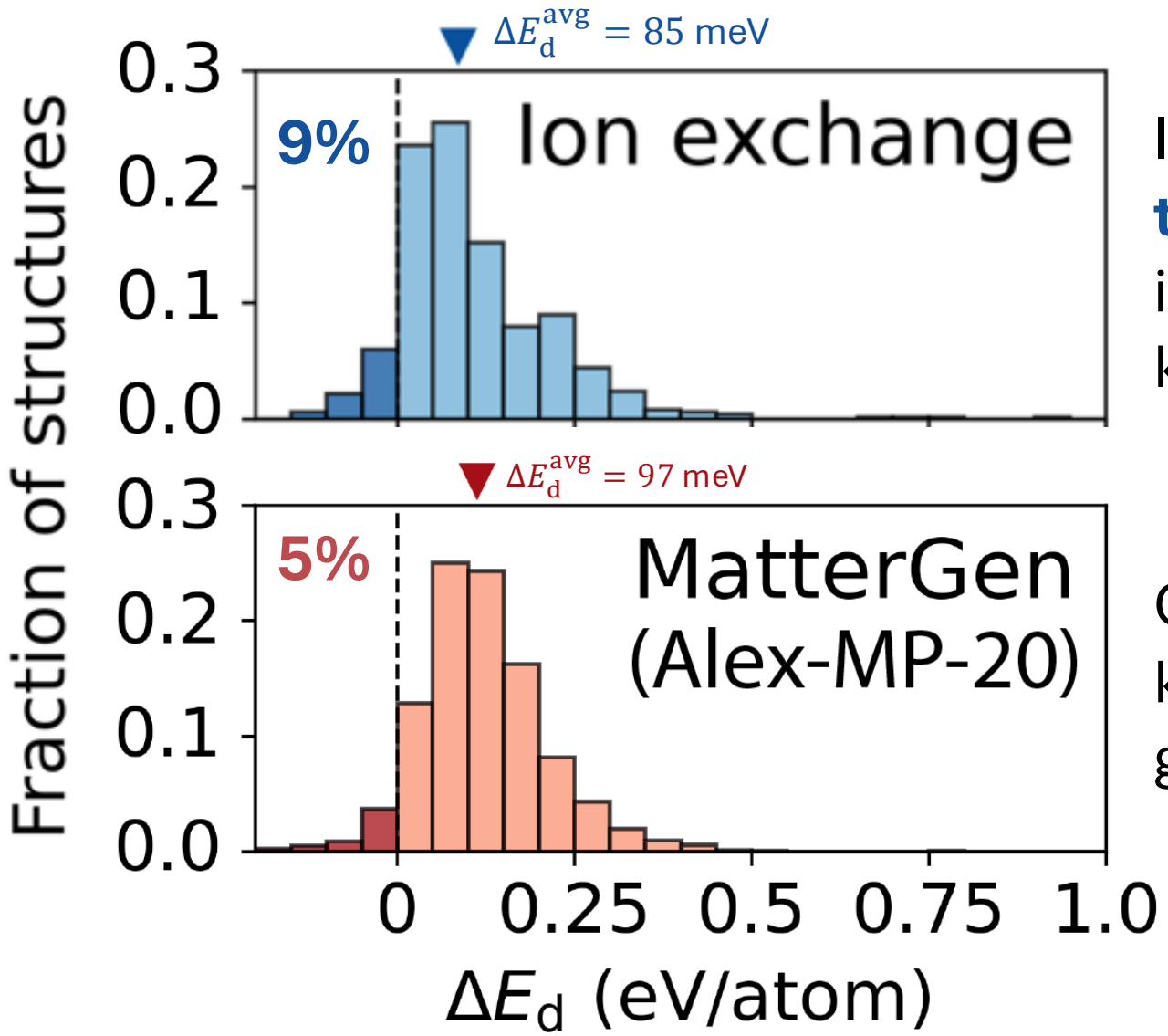

MATERIALS PROJECT

**45k training examples**

**600k training examples**

+ lexandria

# GenAI can also “think outside the box”



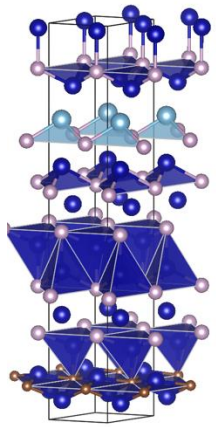

Ion exchange is a **template-based** method; it will only generate known structures

GenAI is not restricted to known templates; it can generate **new prototypes**

# GenAI can also “think outside the box”

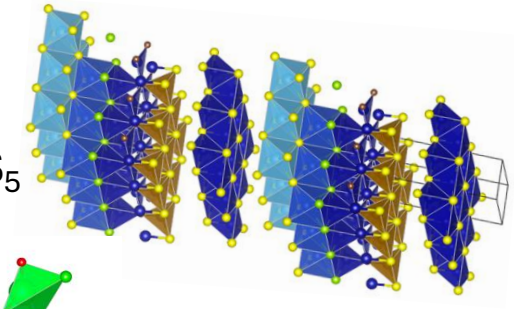
| Method | Novel prototype rate (%) |
|---|---|
| CrystaLLM | 1.0 |
| CDVAE | 8.2 |
| FTCP | 1.8 |
| MatterGen | 7.2 |

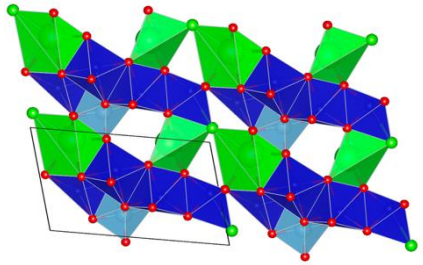
**36/500 structures cannot be mapped to a known prototype**



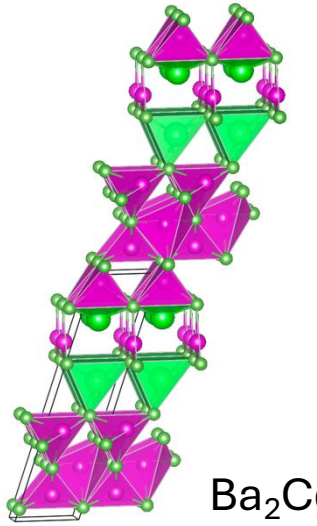
$AlCr_{10}P_6C$

$TiCrFeCo_4CuCSeS_5$

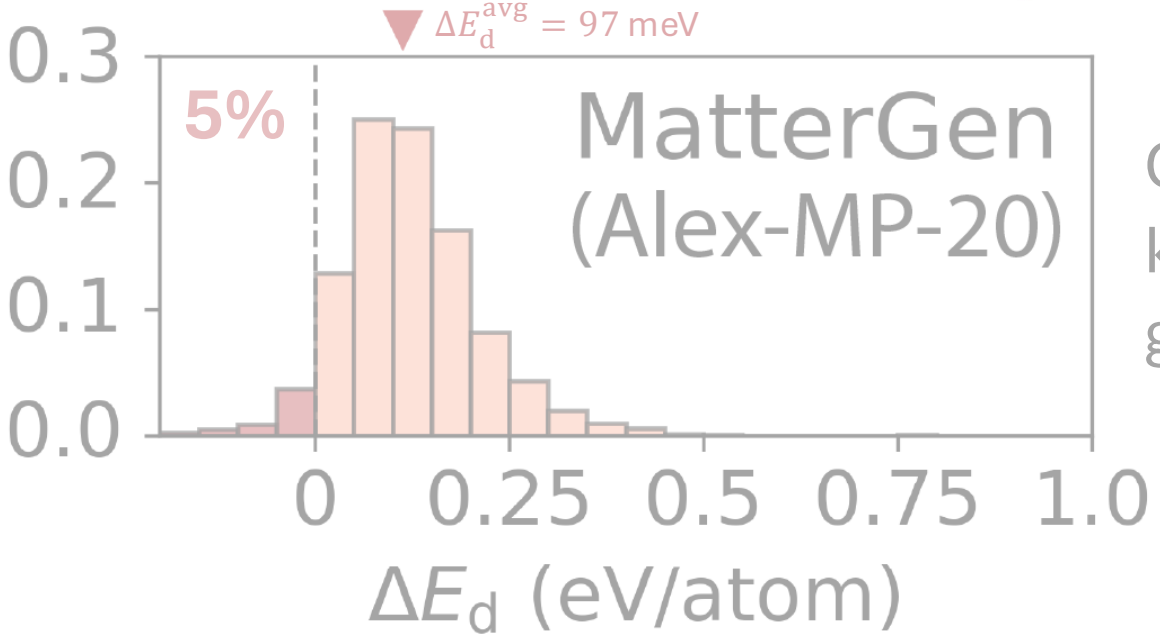




$Ba_2Tm_4TiO_{10}Cl$



$Ba_2Cd_5As_6$




GenAI is not restricted to known templates; it can generate **new prototypes**

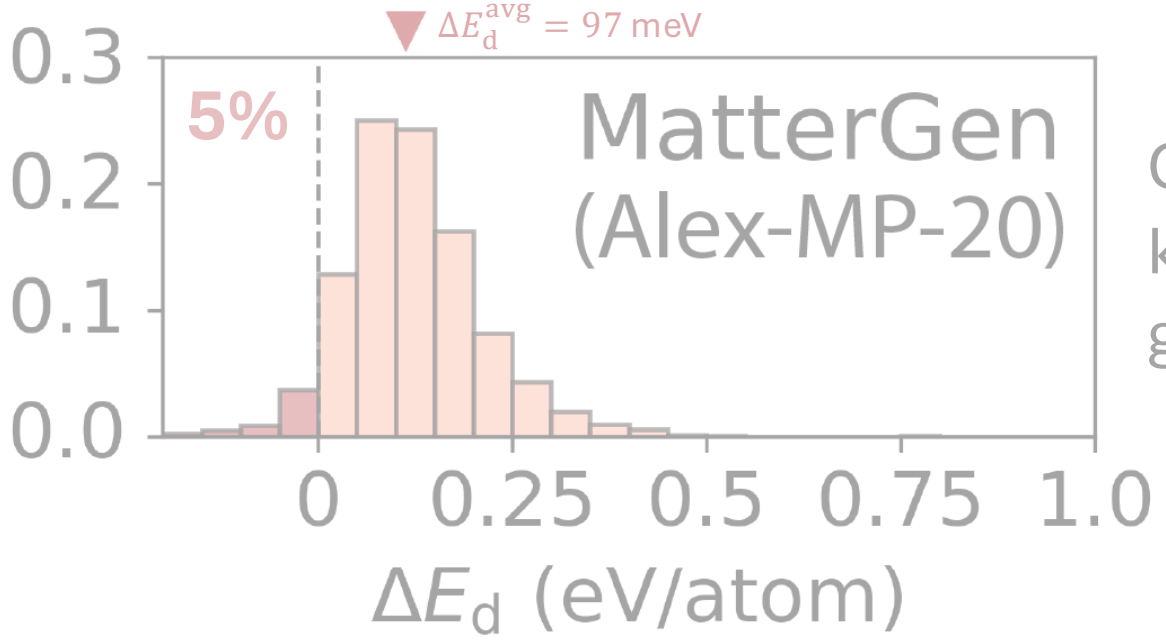
# GenAI can also “think outside the box”

| Method | Novel prototype rate (%) | Novel prototype stability rate (%) |
|---|---|---|
| CrystaLLM | 1.0 | 0 |
| CDVAE | 8.2 | 0 |
| FTCP | 1.8 | 0 |
| MatterGen | 7.2 | 0 |

**Unfortunately, *none* of the new structures from GenAI are thermodynamically stable**



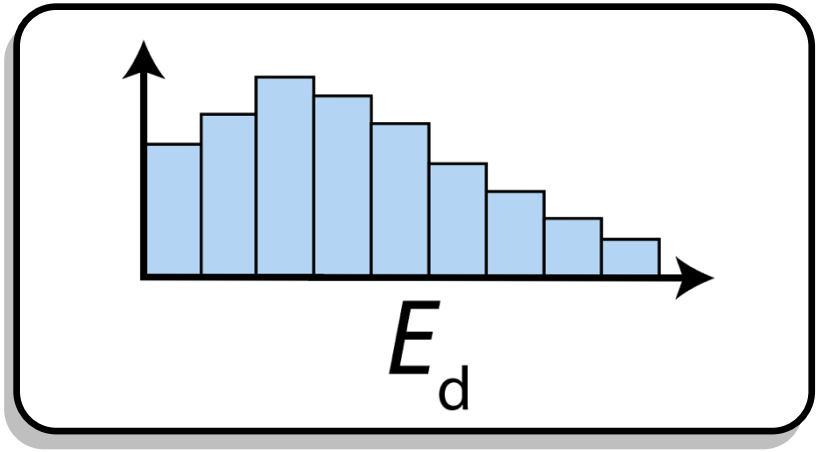
**36/500 structures cannot be mapped to a known prototype**

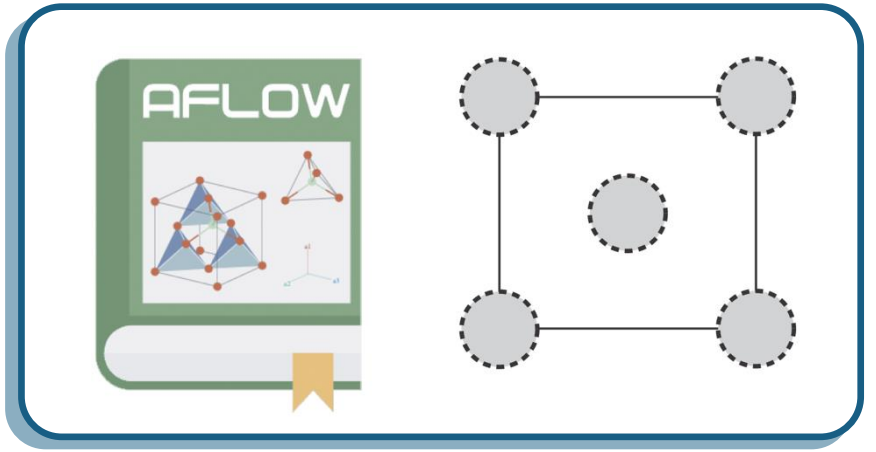

GenAI is not restricted to known templates; it can generate **new prototypes**

# These is a strict tradeoff: stability *vs.* novelty

**Thermodynamic stability**




**Structural novelty**

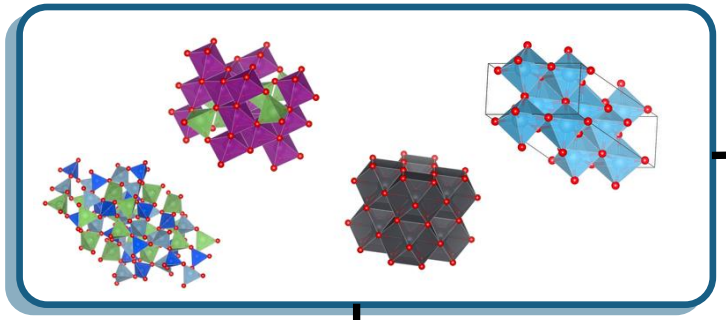



Template-based methods (ion substitution) yield **more ground states**

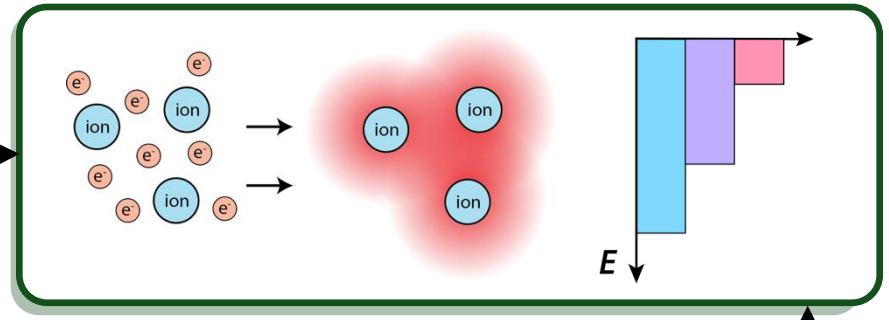
GenAI can generate **entirely new structures** but they lack stability

# Can we reach a balance with MLIPs?

Materials generation



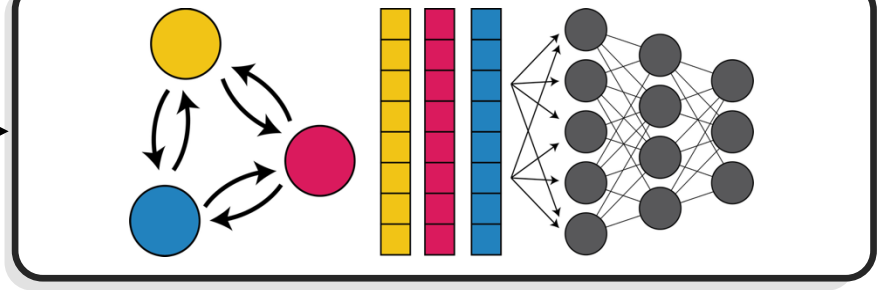
DFT calculations




Can take hours-to-days for each material

*Is it stable?*

MLIPs



Once trained, models make predictions in a matter of seconds

UMA

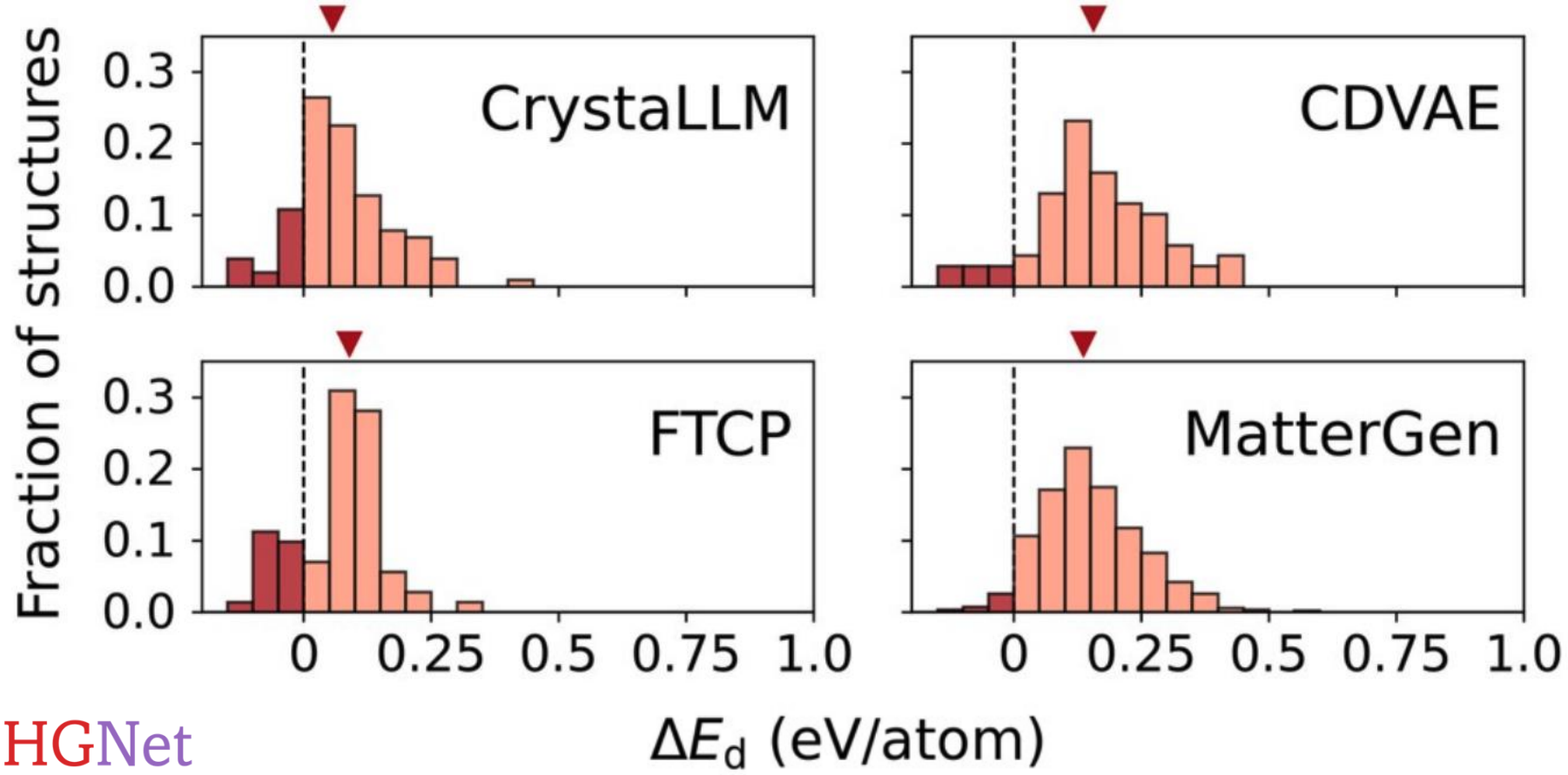
CHGNet

Orbital Materials

SevenNet

# CHGNet filtering → higher stability rates

DFT calculations were performed ***only*** **on structures predicted stable by CHGNet**



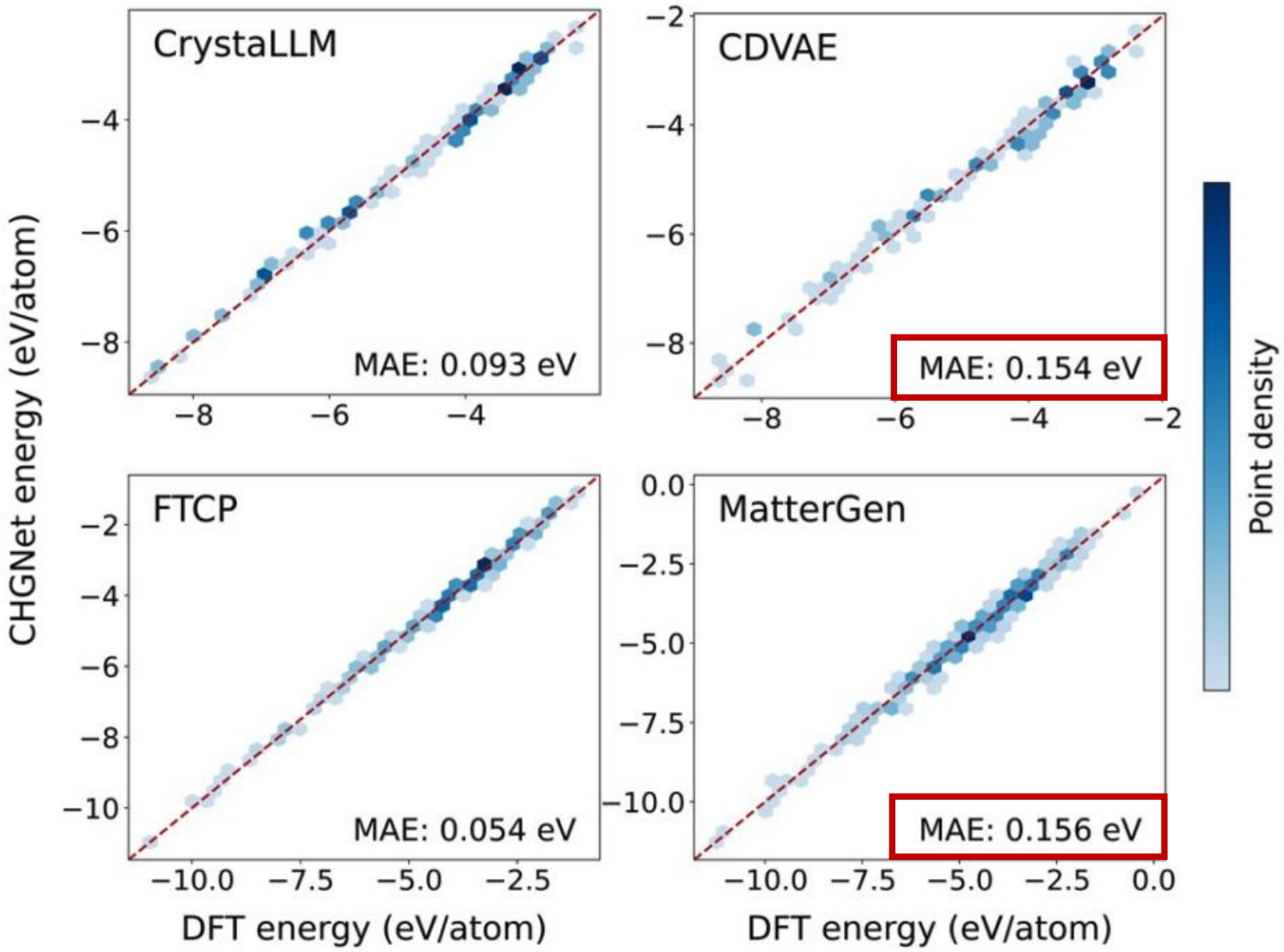

CHGNet

**DFT-confirmed stability rates up to 22%**

**Yet still…**
**None of the *new* prototypes are stable**

B. Deng *et al.*, *Nat. Mach. Intell.* (2023).

# Need better predictions on out-of-distribution structures




MLIP errors are largest on the models with higher novelty rates (CDVAE and MatterGen)

**Future directions:**

1. Better universal MLIPs

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2. Active learning

Generate new structures ⇄ Fine-tune MLIP

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Chris Bartel at the University of Minnesota

MD² LAB
MATERIALS DESIGN THROUGH DYNAMICS

**Paper:** Szymanski & Bartel, *Materials Horizons* 12 (2025).

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