Google DeepMind

Scaling up materials discovery via deep learning

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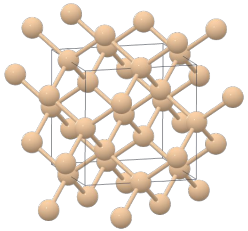
SEMI Conference, San Jose, California, 2024

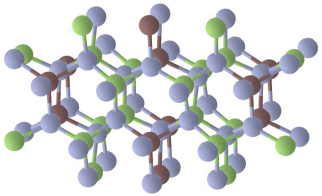
Technological advances hinge on materials

Compute



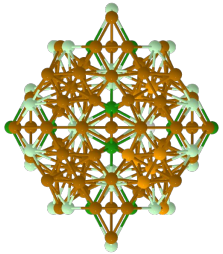
Si (Fd3m)

See



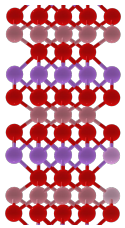
$InGa_2N_3$ ($Cmc2_1$)

Hear

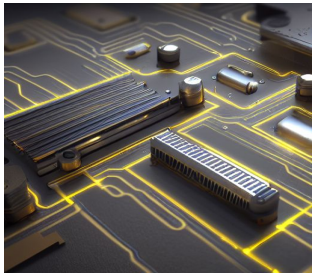


$Nd_2Fe_{14}B$ ($P4_2/mnm$)

Power



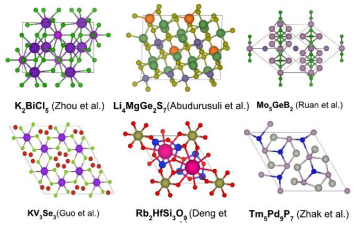
$LiCoO_2$ ($R3m$)



Areas of Big AI Impact in Materials Science

Foundation Models

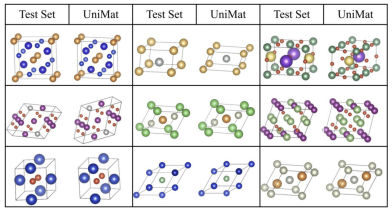
High accuracy with ML for all materials in atomistic simulations



E.g. Merchant et al. Nature, 624, 80 (2024)

Generative Models

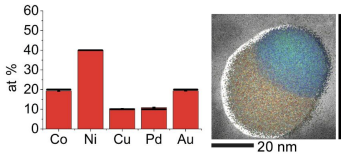
Crystals generated algorithmically (e.g. diffusion models)



E.g. Yang et al. ICLR (2024)

Optimization

Closed-loop optimization to improve materials, models, systems



E.g. Wahl et al. Sci Adv (2021)

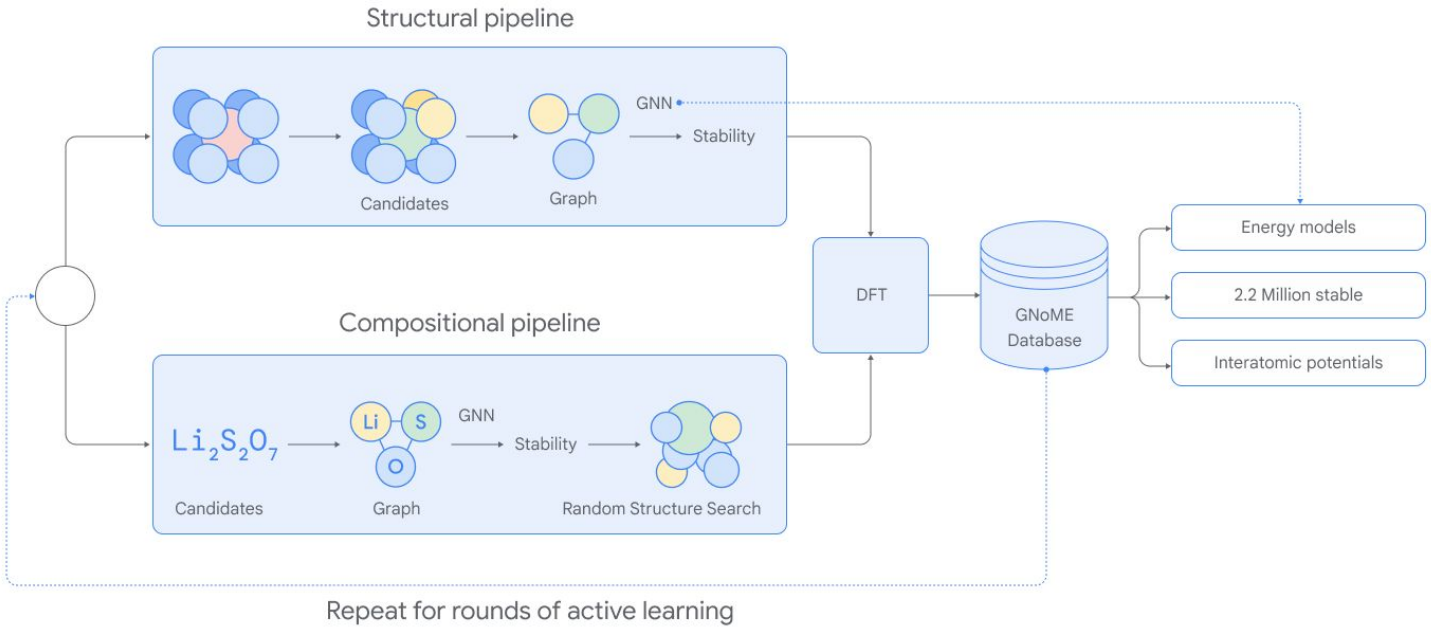
Graph Networks for Materials Exploration (GNoME)

nature *Merchant et al. Nature (2023).

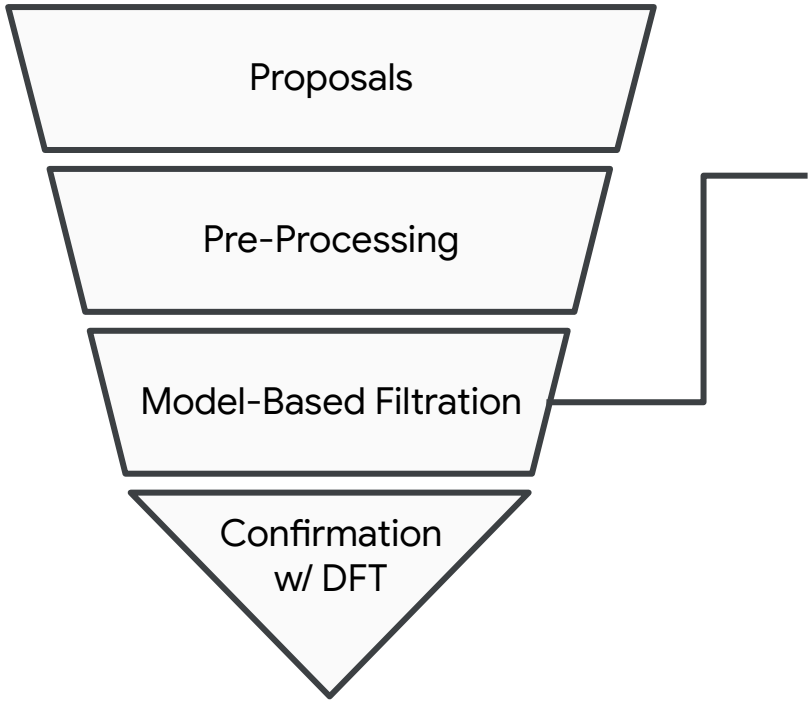
https://github.com/google-deepmind/materials_discovery

Google DeepMind

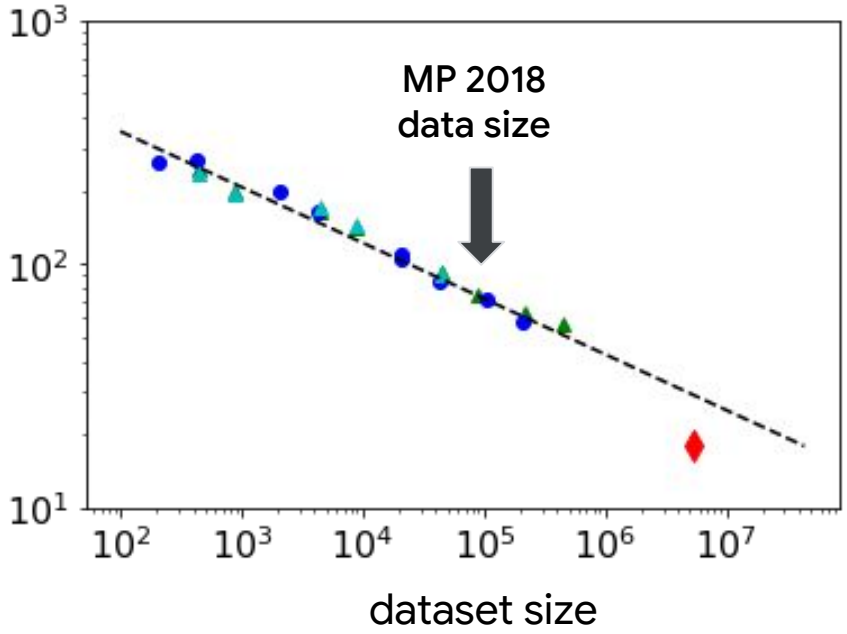
Computational Materials Discovery Pipeline



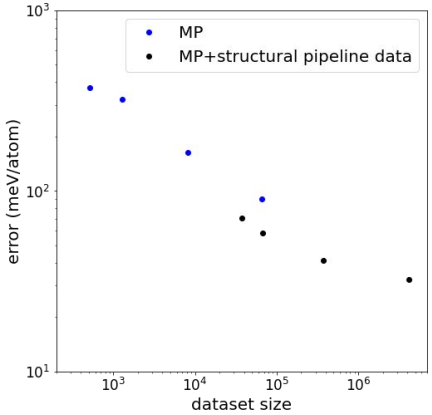
Computational Materials Discovery Pipeline

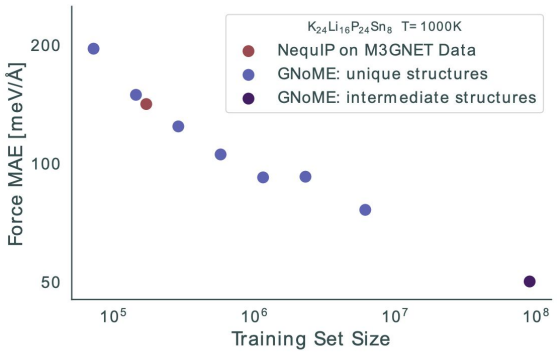


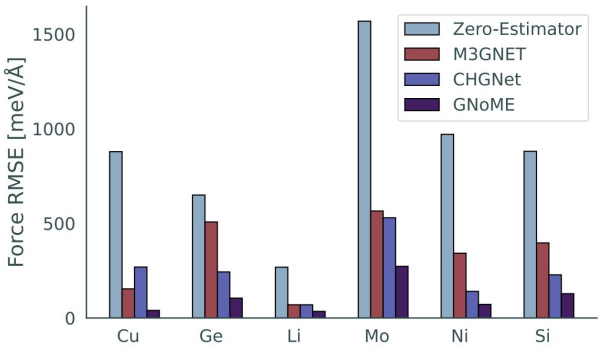
Out of Distribution Error (meV/atom)



GNoME: A Foundation Model for Materials Simulations







- Models approaching quantum mechanical accuracy
- Zero-shot generalization to new tasks
- Universal: works for the entire periodic table

*__GNoME:__ Merchant, Batzner et al. Nature (2023) 80.

What does this all mean for materials research?

Next Frontier

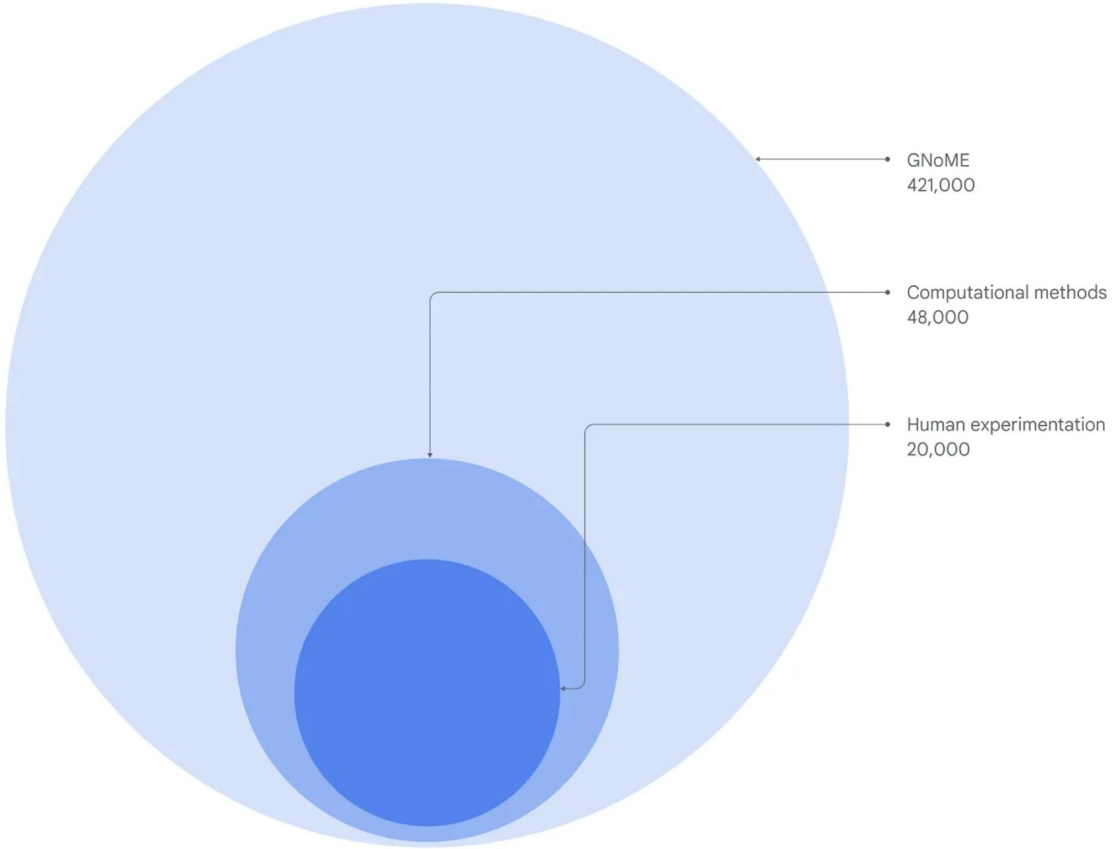
Machine learning potentials will bridge quantum mechanical accuracy to unprecedented scales

2.2 M

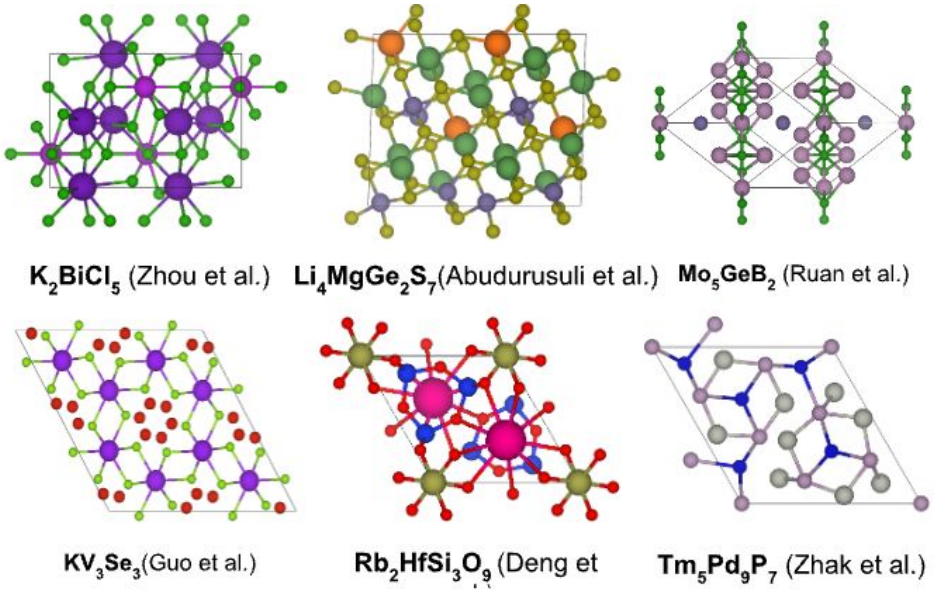
Stable with respect to Materials Project

>400,000

New stable inorganic materials

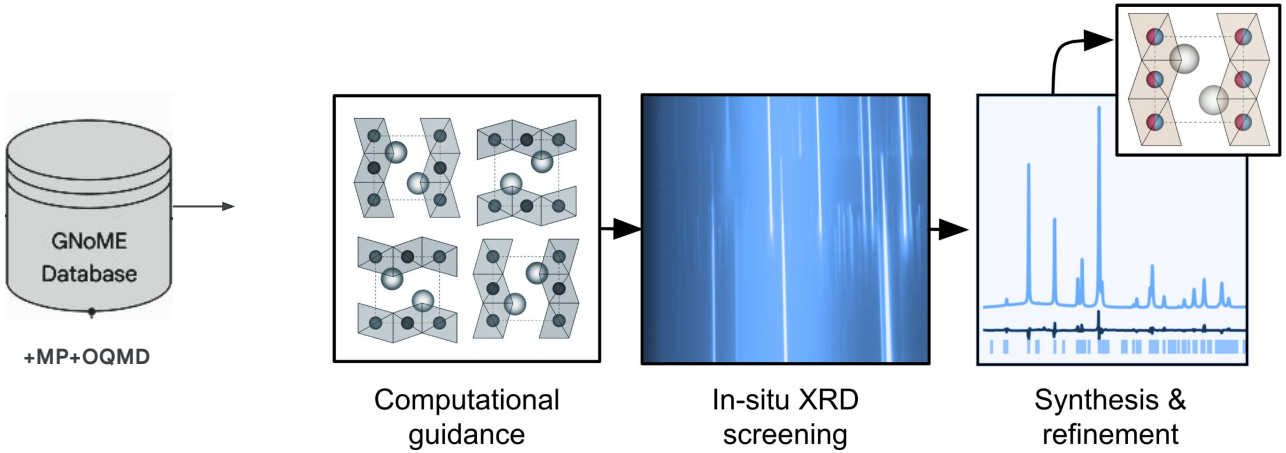

GNoME
421,000
Computational methods
48,000
Human experimentation
20,000

736 have already been made experimentally



1 Material discovery

GNoME Database Enables Efficient Synthesis of New Materials

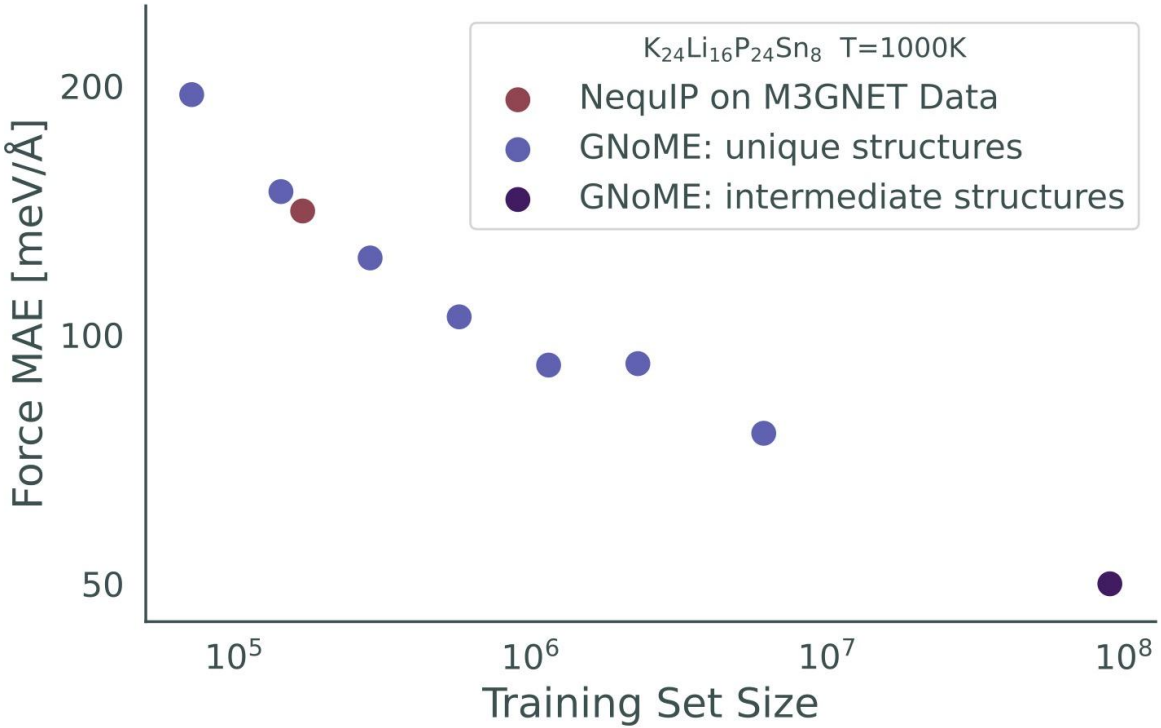


Synthesized new quaternary chlorides by driving in-situ experiments with GNoME-predicted stabilities

Miura et al. Journal of American Chemical Society (2024) in press

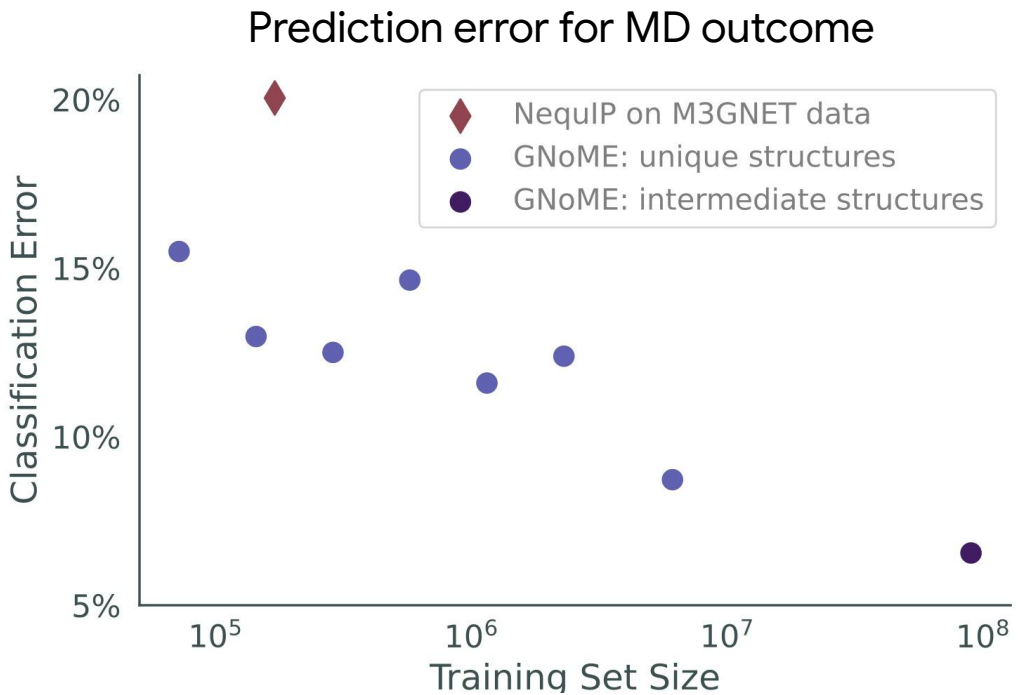
2 Li-ion Battery Materials

Accurate prediction of forces in molecular dynamics



Finding good Li-ion conductors for solid-state batteries

TASK: Given a crystal, predict if it will be a good Li-ion conductor.



Solid Lithium Ion Conductors

21

Materials Project

vs.

528

Novel candidates

Sendek et al. EES 2017

Li-Mn-{TM}-O Cathode Materials

9

Materials Project

Bartel et al. 2020

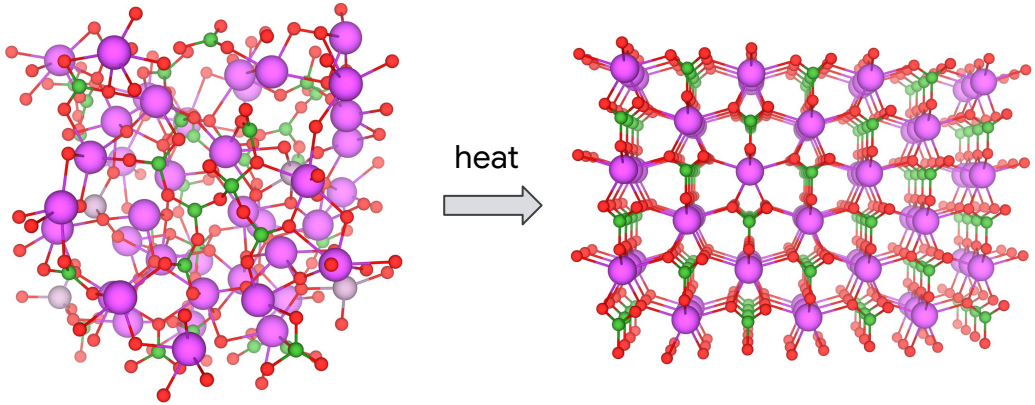
vs.

20

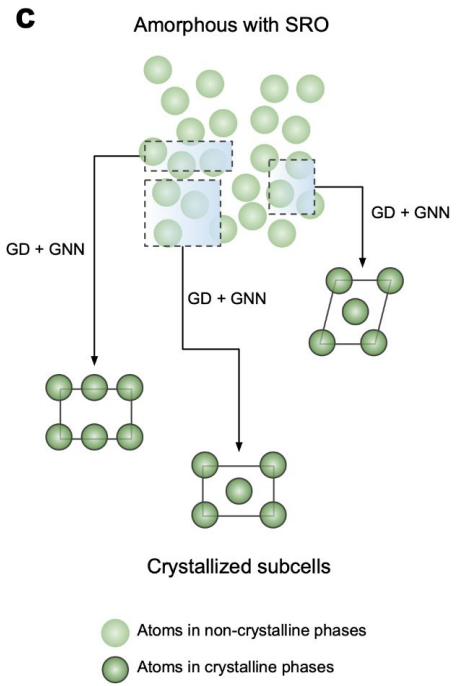
Novel candidates

3 Predictive synthesis

Predicting the crystallization products of amorphous phases

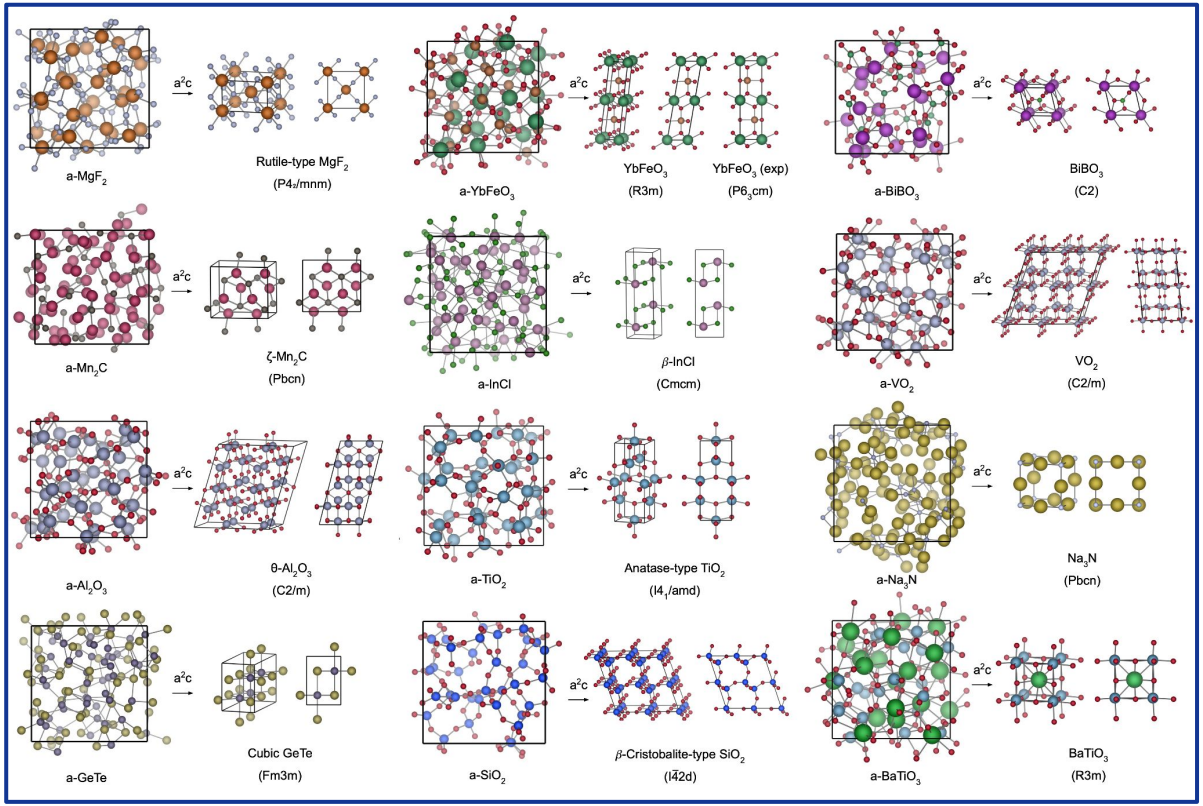


Predicting the crystallization products of amorphous phases



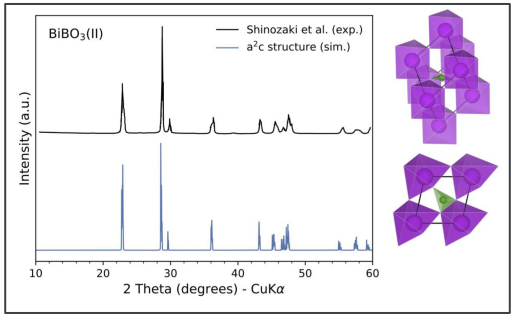
Predicting the crystallization products of amorphous phases

Highly-accurate structure prediction with GNoME + Molecular Simulations

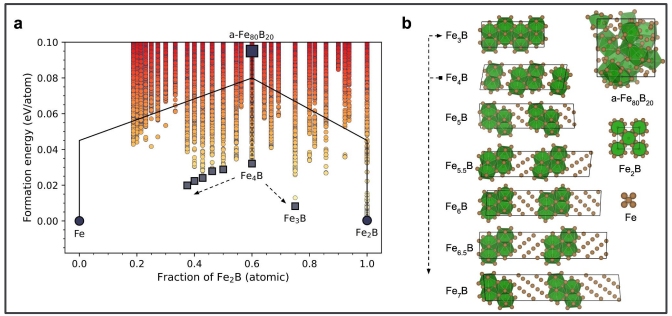


Predicting the crystallization products of amorphous phases

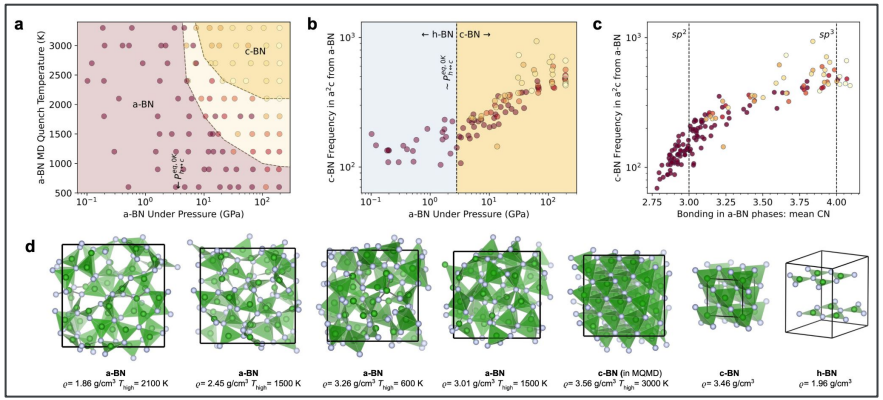
Bridges gaps in materials science using GNoME + Molecular Simulations



Solving structure from X-ray



Explaining crystallization path of a magnetic material



Phase selection for the ultra-hard BN materials

*PES image by Dellago and Bolhuis (2009) https://doi.org/10.1007/978-3-540-87706-6_3

Takeaways:

- Key Areas of AI Impact:
  - Foundation Models for Materials Simulations
  - Generative Modeling
  - AI driven optimization
- Foundation models can bridge the time & length scale gap in simulations between quantum mechanics and realistic systems.
- Compute & AI can shift a good fraction of the hypothesis testing to computers.
- GNoME enabled computational discovery of >400k new stable materials
- GNoME enabled synthesis of new compounds

Thank you.

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