TOYOTA RESEARCH INSTITUTE

Extracting Insights from Atomistic and Spectroscopic Materials Data

Steven Torrisi
Sr. Research Scientist
7/10/25, NIST

Talk Outline

1. TRI + AMDD Background
2. Challenges in AI-guided materials design
3. Characterization & bridging experiment & theory

Toyota Research Institute

Energy & Materials

Human Centered AI

Human Interactive Driving

Robotics


TOYOTA
LEXUS
Accelerated Materials Design & Discovery
Energy & Materials
Carbon Neutrality Strategy

Accelerated Materials Design & Discovery

Leadership


Brian Storey


Joey Montoya


Linda Hung


Jens Bakander

Highlighted in this Talk


Steven Torrisi


Weike Ye

AMDD


Hisatugu Yamasaki


Leena Sansguiri


Daniel Schweigert


Jith Subramanian


Amalie Trewartha


Kevin Tran


Santosh Suram


Koki Nakano

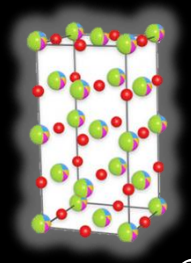

Michaela Burke-Stevens


Amanda Volk

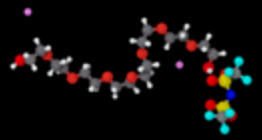
Materials on all length scales

Atomistic | **Molecular** | **Periodic (Spectra)** | **Device-Level**

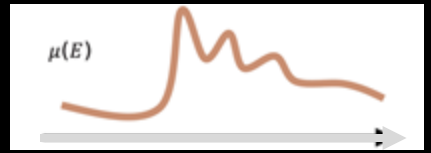
Disordered Rock-Salt Structures

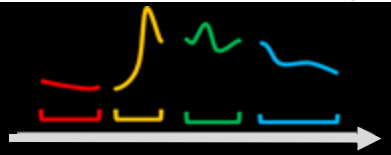


Transition Paths



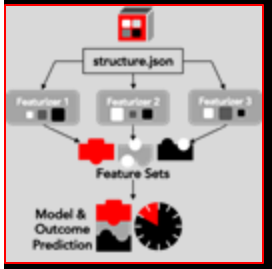
Polymer Trajectories





XANES Spectra

Featurization & Inverse Modeling



Battery Charge & Discharge Features

[1]Liu… **Torrisi***, Wolverton* *et al, Submitted 2025, arXiv*

*[2] Sheriff, Freitas, Trewartha, **Torrisi**, NeurIPS AI4Mat 2024*

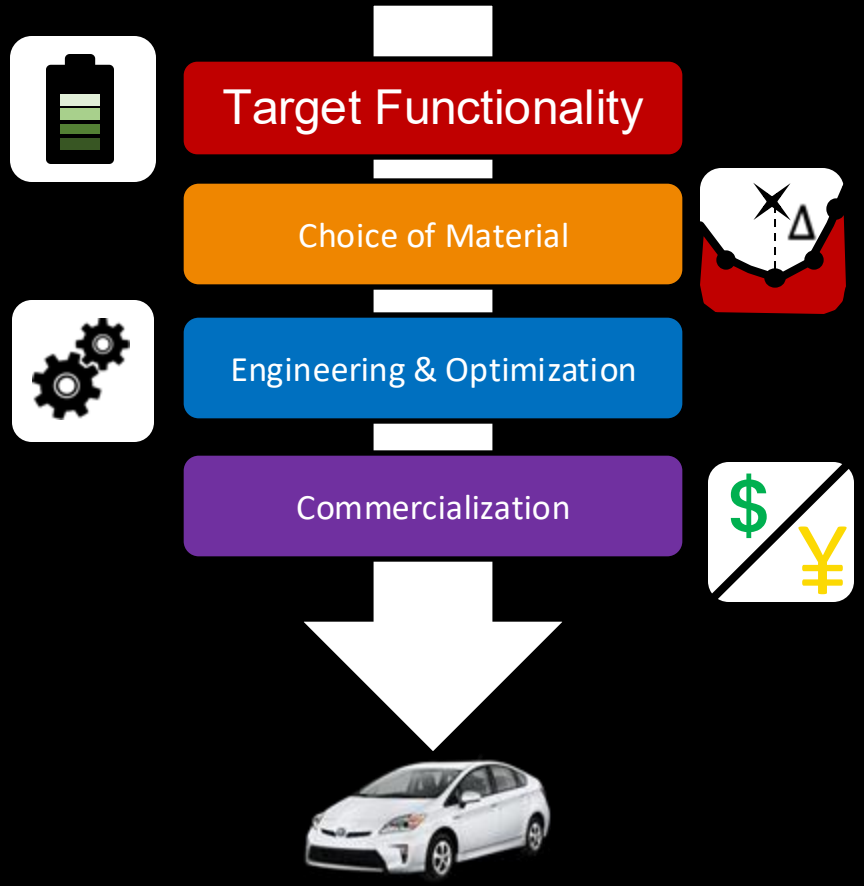
[3] Khajeh, Schweigert, **Torrisi** *et al.* Macromolecules (2023)

[4] **Torrisi** *et al.* NPJ Computational Materials, 2020

[5] Montoya, Aykol… **Torrisi**, Trewartha, Storey, Appl. Phys. Rev 2022

[6] Ansari, **Torrisi**, Trewartha, Sun, J. Energy Storage 2024

Materials Discovery in Context



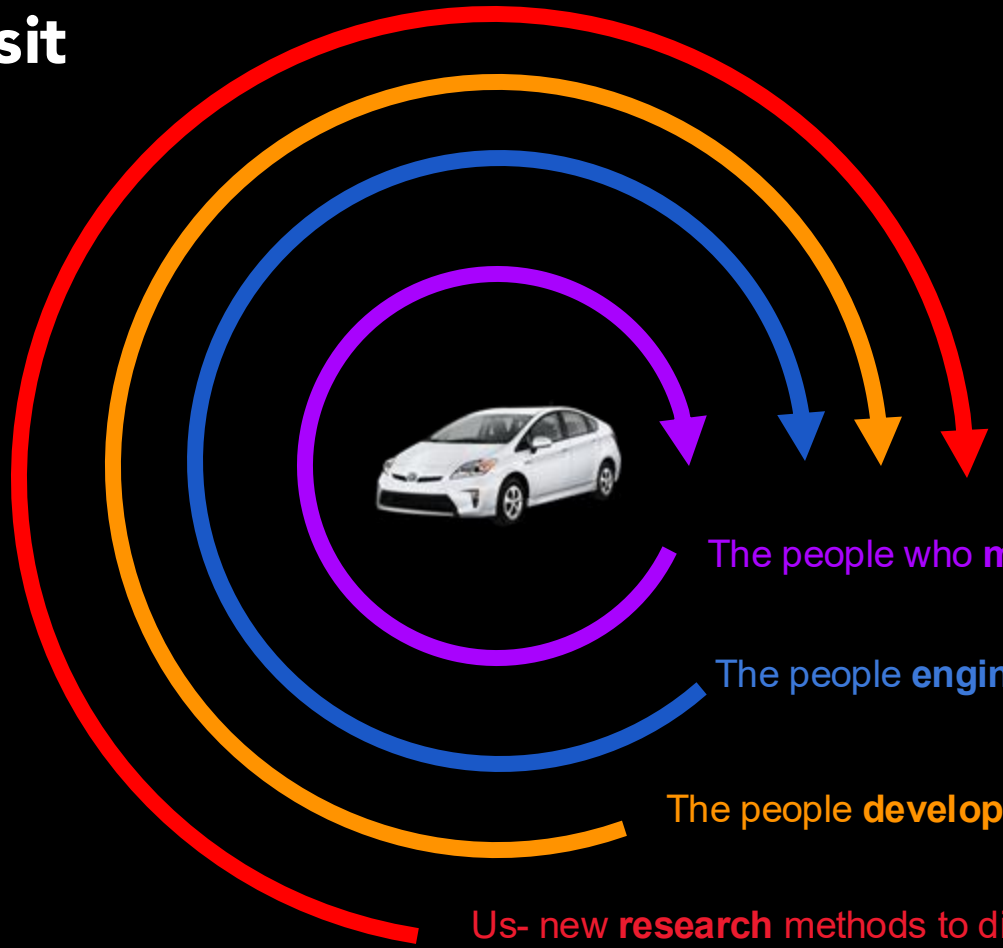
Where we sit

Target Functionality

Choice of Material

Engineering & Optimization

Commercialization



The people who **manufacture** the cars

The people **engineering** materials for the car

The people **developing** the next-gen materials

Us- new **research** methods to discover next-gen materials

Talk Outline

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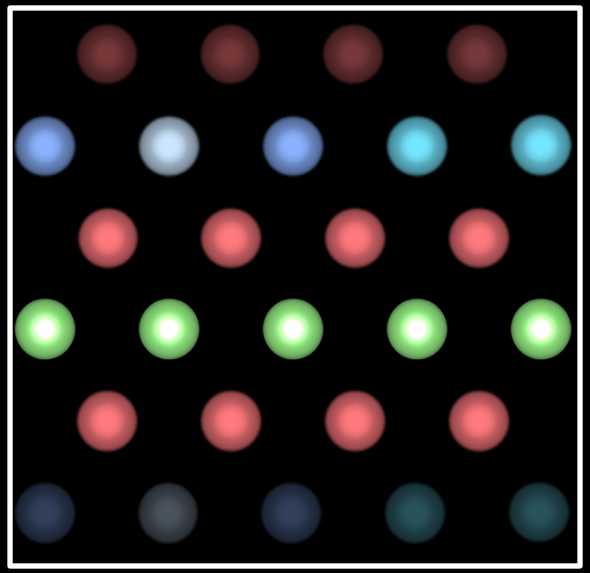
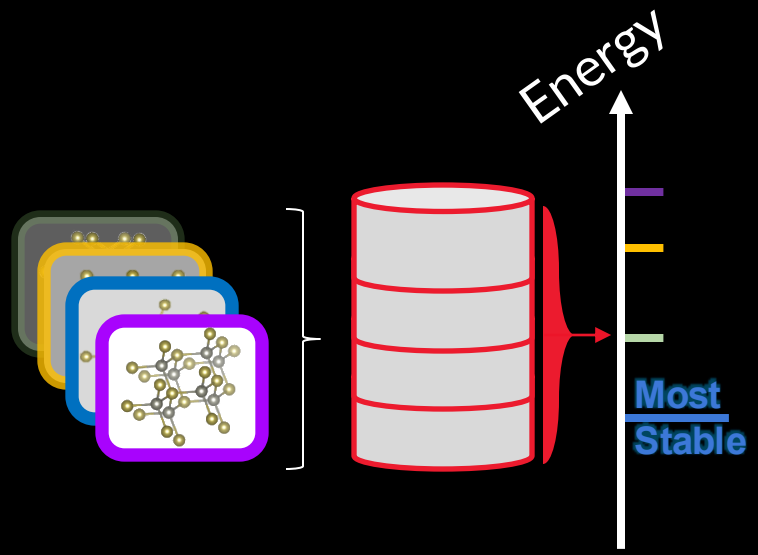
What goes into computational materials discovery?



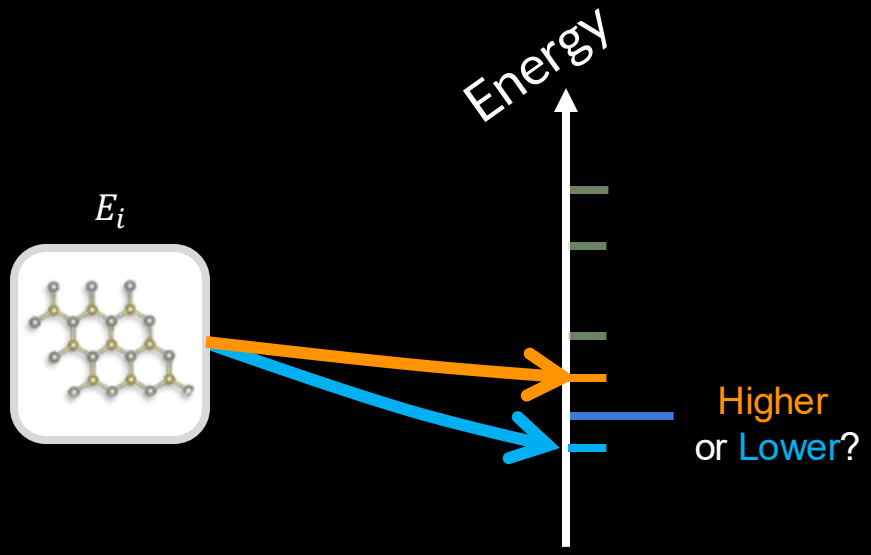
The Current Paradigm of

(inorganic, crystalline)

Computational Materials Discovery



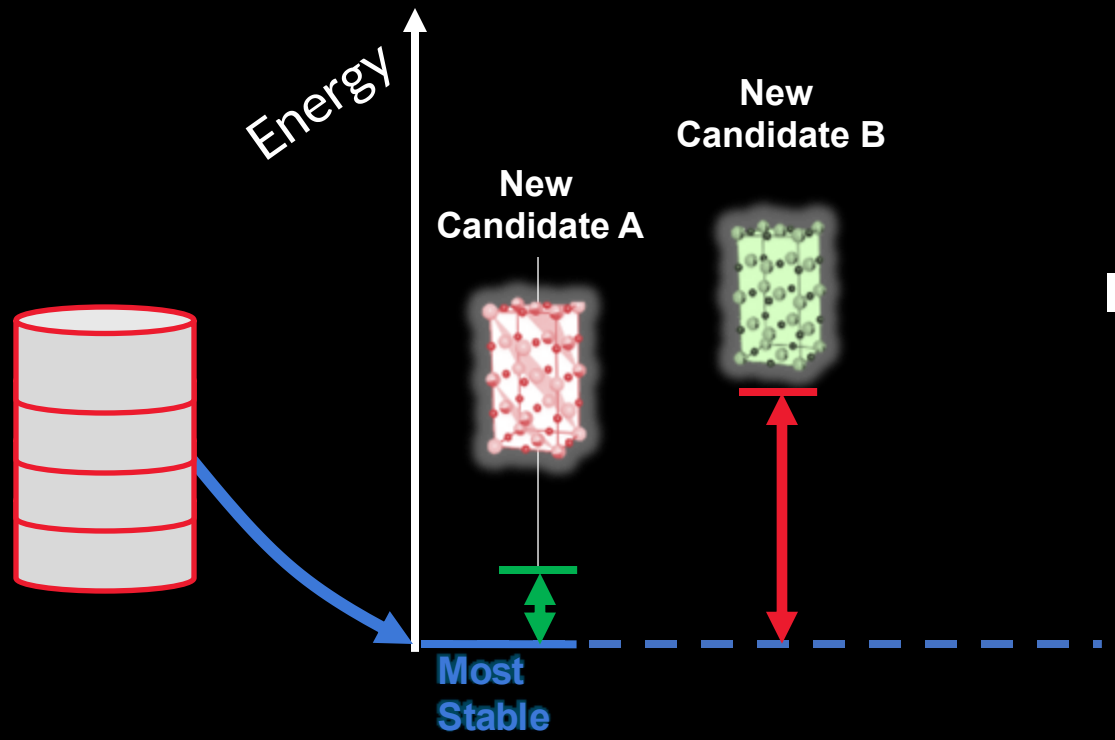
1. Rank Energies of Known Structures



2. Predict new compound & structure, compute energy

3. Compare Against Database

How we use energy-ranking



In general: The lower the energy difference, the better

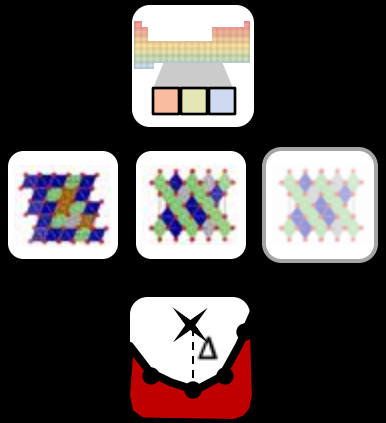
CAMD (2020, TRI)

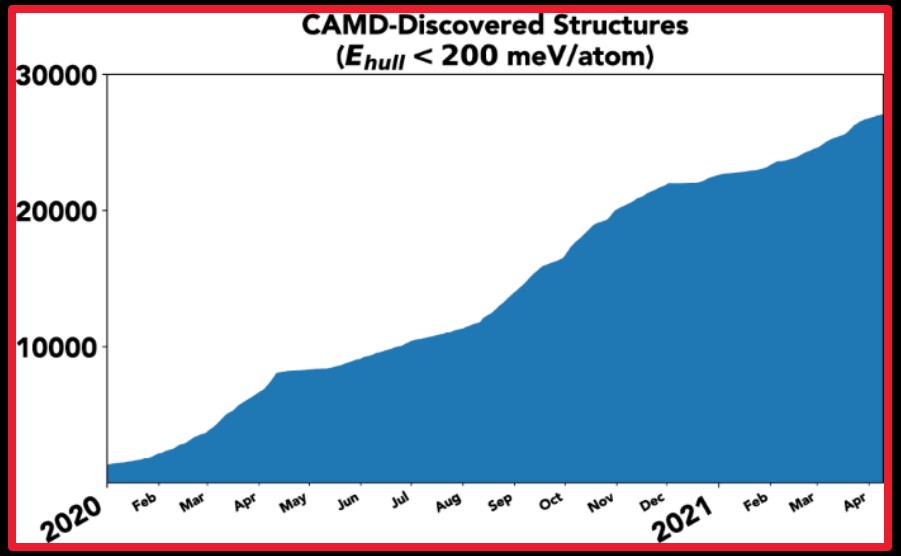
Choice of Material

Choice of Chemical System

Candidate Phases

Feasibility Screening (e.g. Thermodynamics)





Weike Ye, Ray Lei,
Joseph Montoya, Murat Aykol

Choice of Material

Choice of Chemical System

Candidate Phases

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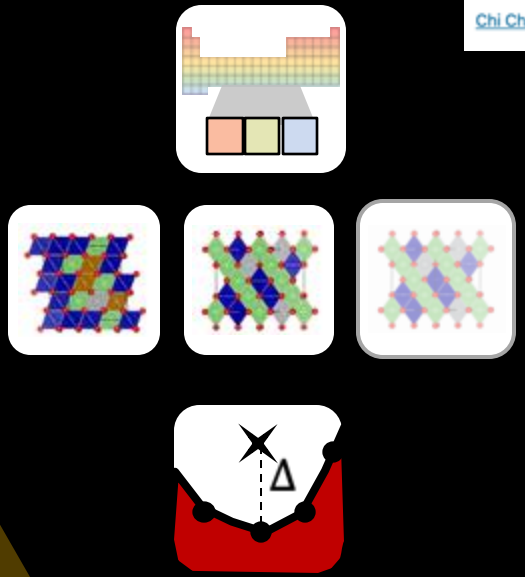


nature computational science

Article | Published: 28 November 2022

A universal graph deep learning interatomic potential for the periodic table

Chi Chen & Shyue Ping Ong

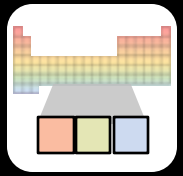
"About **1.8 million materials** were identified from a screening of 31 million hypothetical crystal structures to be potentially stable against existing Materials Project crystals based on M3GNet energies. "

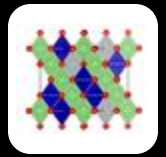
Choice of Material

Choice of Chemical System

Candidate Phases

Feasibility Screening (e.g. Thermodynamics)





Article

Scaling deep learning for materials discovery

https://doi.org/10.1038/s41586-023-06735-9
Received: 8 May 2023
Accepted: 10 October 2023
Published online: 29 November 2023

Amil Merchant[1,3], Simon Batzner[1,3], Samuel S. Schoenholz[1,3], Muratahan Aykol[1], Gowoon Cheon[2] & Ekin Dogus Cubuk[1,3]

Novel functional materials enable fundamental breakthroughs across technological applications from clean energy to information processing[1–11]. From microchips to

"2.2 million structures below the current convex hull…"

From the perspective:

*"Systems **such as GNoME can make many more computational predictions than even an autonomous lab can keep up with,** says Andy Cooper, …. **"What we really need is computation that tells us what to make,"** Cooper says. For that, AI systems will have to accurately calculate a lot more of the predicted materials' chemical and physical properties."*

Finding enthalpically stable ordered structures is now well trailblazed!

Choice of Material

Choice of Chemical Prototype

Candidate Phases

Feasibility Screening (e.g. Thermodynamics)

Article

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Novel functional materials enable fundamental breakthroughs across technological ... to information processing[1–11]. From microchips to

...le crystals identified in ... improved efficiency ...f **2.2 million** ...urrent convex hull…"

From the perspective:
"Still, **it's clear that systems such as GNoME can make many more computational predictions than even an autonomous lab can keep up with,** says Andy Cooper, academic director of the Materials Innovation Factory at the University of Liverpool, UK. **"What we really need is computation that tells us what to make,"** Cooper says. For that, AI systems will have to accurately calculate a lot more of the predicted materials' chemical and physical properties."

Choice of Material

Choice
Chemical S

Candidate

Feasibility Scre
(e.g. Thermody

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...GNoME can make many
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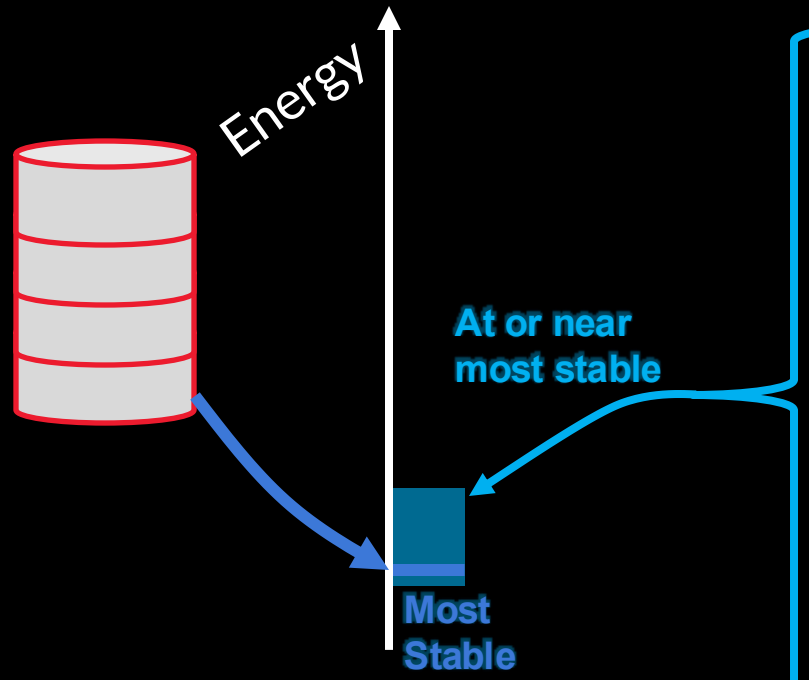
systems will have to accurately calculate a lot more of the predicted materials' chemical and physical properties."

But, enthalpically stable structures are *not the end of the story.*

There's some fine print…

Previous work highlighted synthesis challenges



12 Attempted Syntheses based on Energy Metric

Ca-Ag-O	$CaAg_3O_4$
	Ca_3AgO_4
Li-Ag-O	$LiAg_3O_4$
	$LiAgO_2$
Ca-Pd-O	$CaPd_3O_6$
	$CaPdO_3$
Mg-Ru-O	$MgRu_2O_6$
	$MgRuO_4$
Ca-Ru-O	$CaRuO_4$
	Ca_3RuO_6
Li-Ru-O	Li_4RuO_5
	Li_5RuO_5

Montya… **Torrisi**… Sun et al, Chem. Sci. 2024

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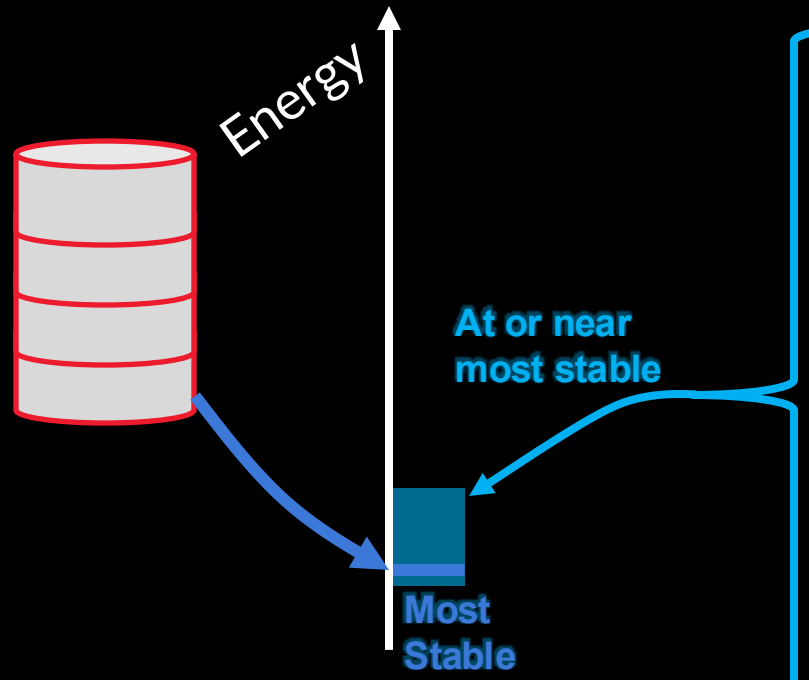

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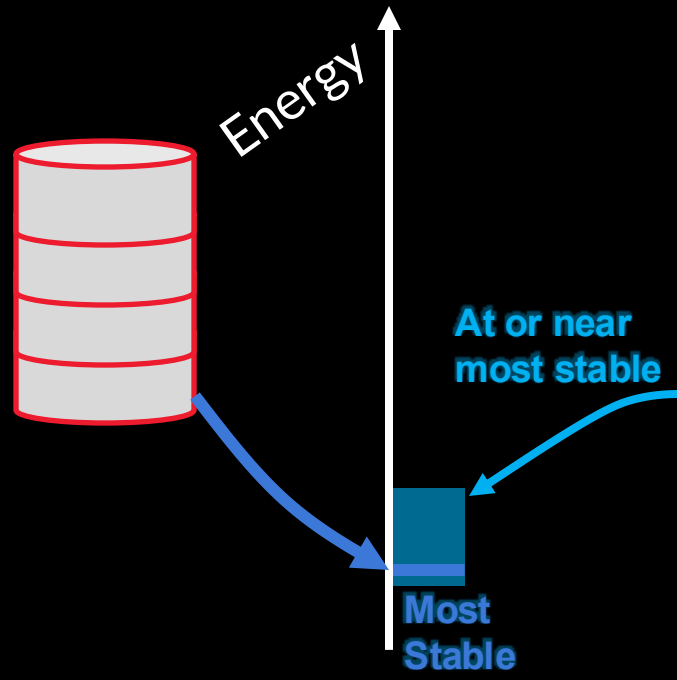

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Ca-Ru-O	$CaRuO_4$
	Ca_3RuO_6 → Kind of.
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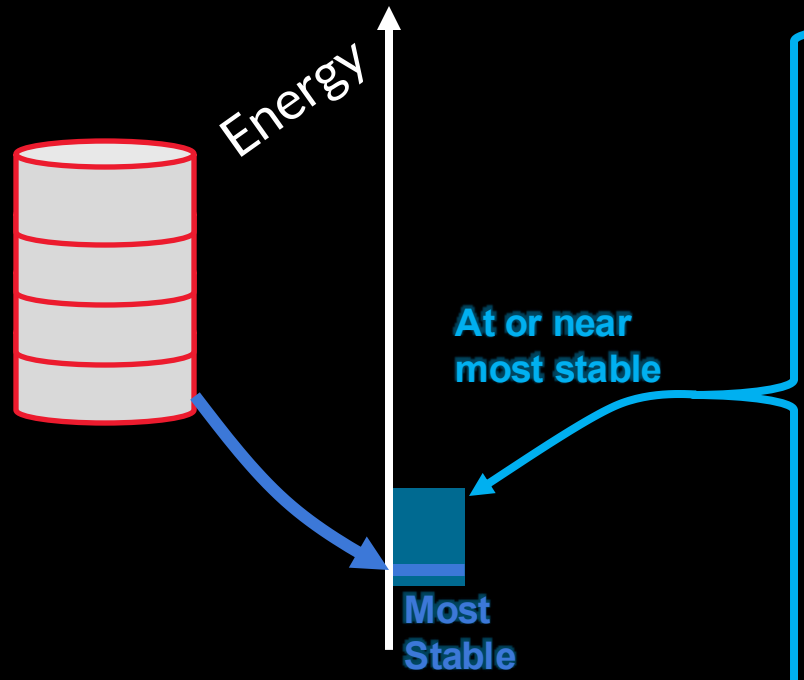

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→ Kind of.

… and it took 2 years.

Montya… **Torrisi**… Sun et al, Chem. Sci. 2024

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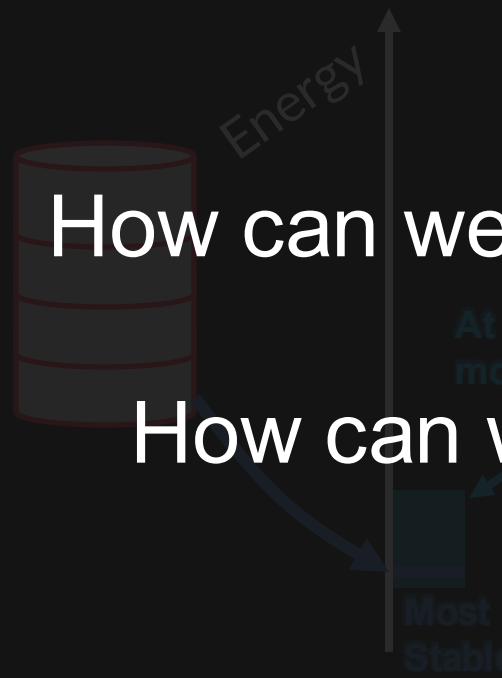

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Kind of.

… and it took 2 years.

How can we improve our synthesis rates?

How can we identify materials faster?

Montoya et al, Chem. Sci. 2024

3 challenges for our team

We don’t know how to make new candidates.

Identifying materials is hard & involves diverse data.

We have ∞ candidates.

3 challenges for our team

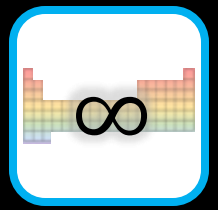
We don’t know how to make new candidates.

Develop theories of inorganic synthesis

Identifying materials is hard & involves diverse data.

Tools that make it easier to interface with experiment

We have ∞ candidates.



Tools that accelerate atomistic modeling

Talk Outline

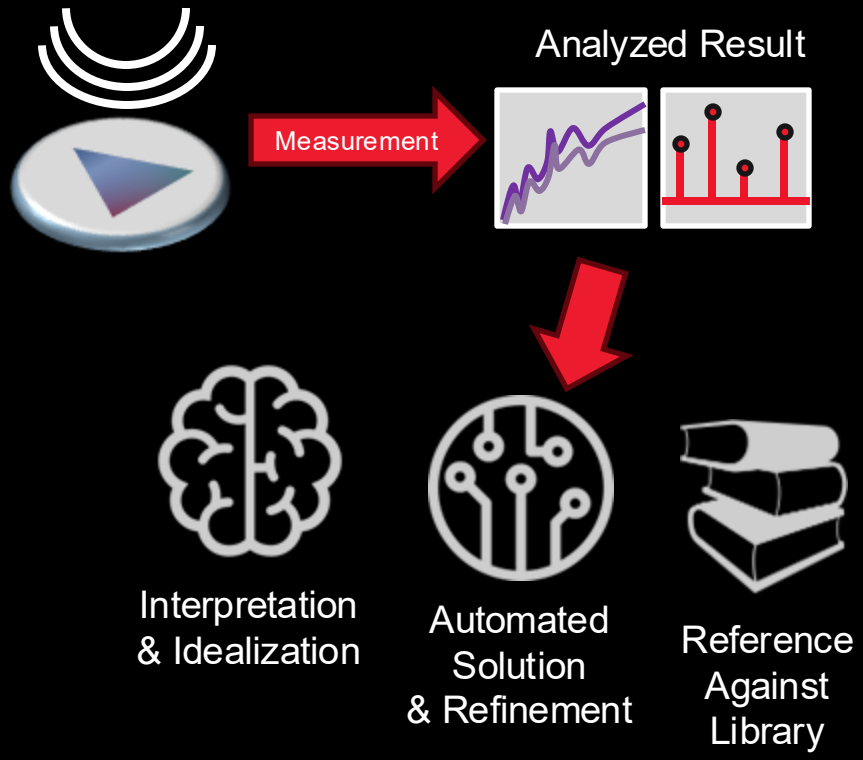
1. TRI Background & Challenges in AI-guided materials design
2. Challenges in AI-guided materials design
3. Characterization & bridging experiment & theory

Working with Spectral Data

Multi-modal Analysis & Spectra-scope

Characterization is a Bottleneck for High Throughput Materials Discovery

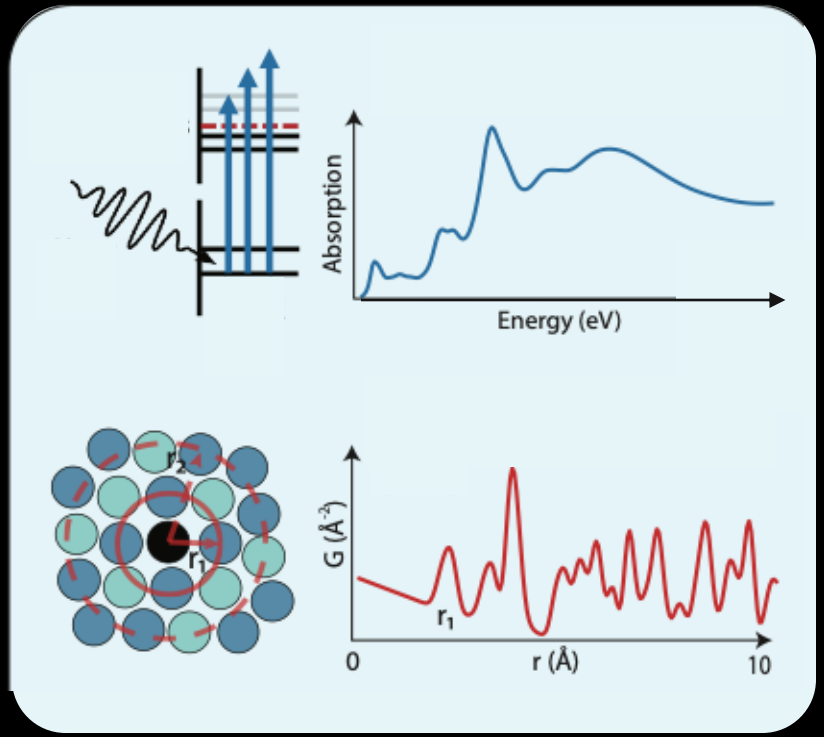
- Low-dimensional forms of characterization (e.g. XRD) can be accelerated
  - but may still require human verification
- Our research program assumes that humans will remain in the loop for the near future
- **Goal is to study interoperability & interpretability of spectra**



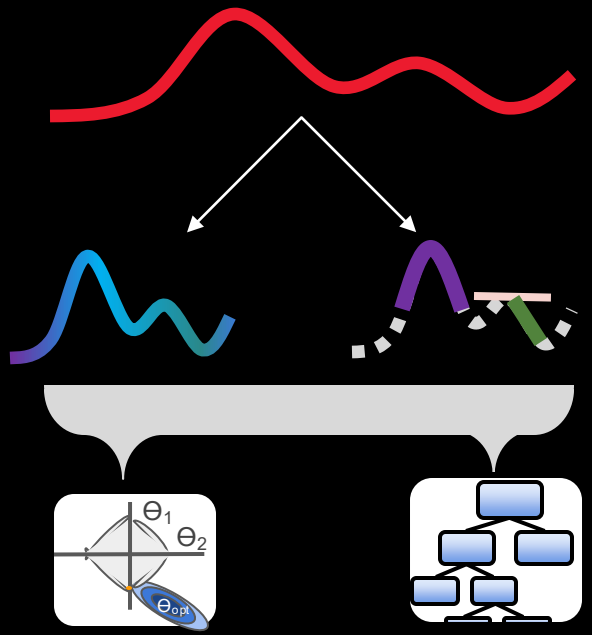
Guiding Questions

- How can we make it easier to utilize and combine diverse modes of spectra?
- How can we make it easier to use ML/statistical methods in the limited-data regime?
- How can extant databases of materials & spectra be utilized for optimal design of experiments?

Multimodal Studies of XANES vs. PDFs



Spectra-scope: A tool for feature discovery & downselection of spectrum-property relationships



Multimodal Studies of XANES vs. PDFs

Featuring work with Columbia University

Zoe Zachko

Dr. Tina Na Narong

Prof. Simon Billinge

NPJ Computational Materials, 2025
Na Narong, Zachko, **Torrisi***, Billinge*

Spectra-scope: A tool for feature discovery & downselection of spectrum-property relationships

And with TRI intern + scientist

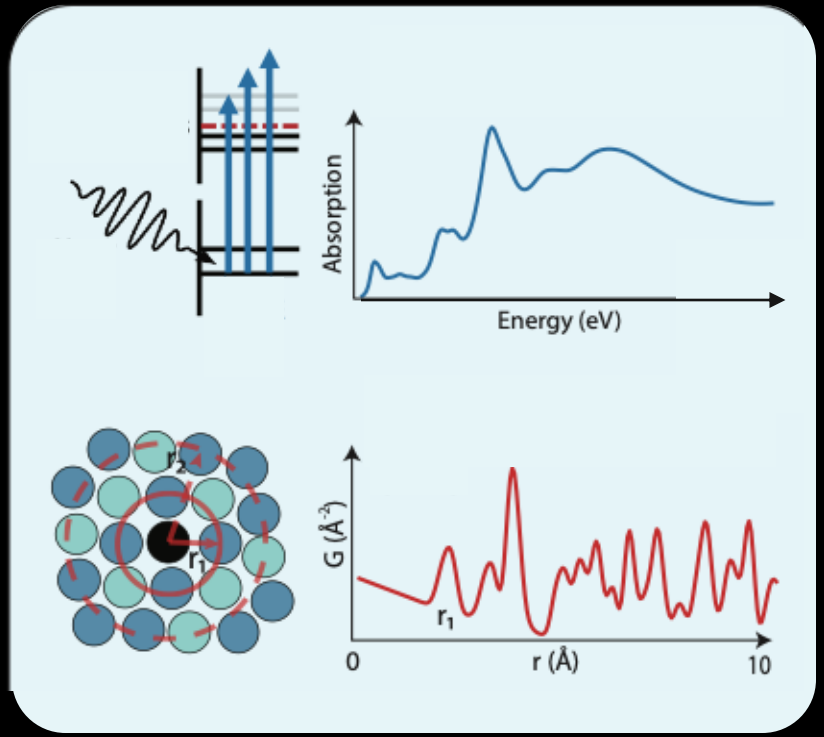
Amalya Johnson (Stanford)

Dr. Weike Ye

Leena Sansguiri

In prep. Johnson, Ye, **Torrisi**

Multimodal Studies of XANES vs. PDF



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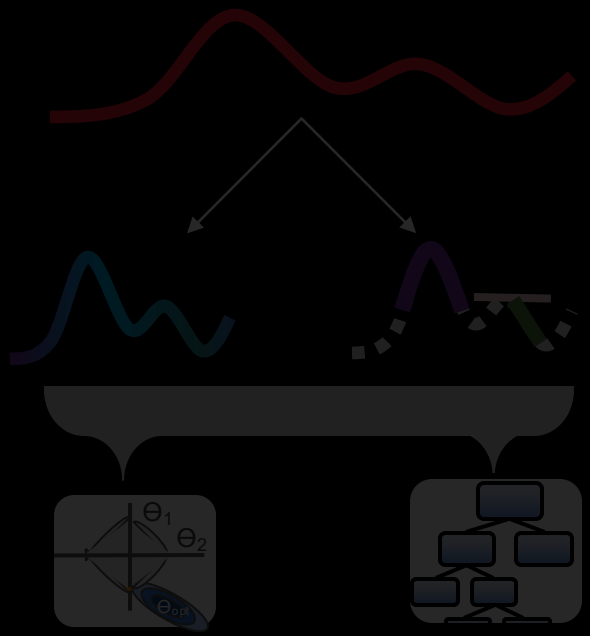
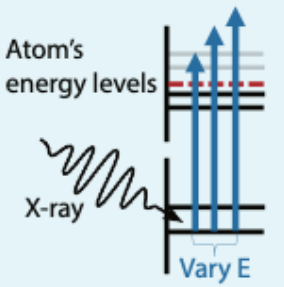
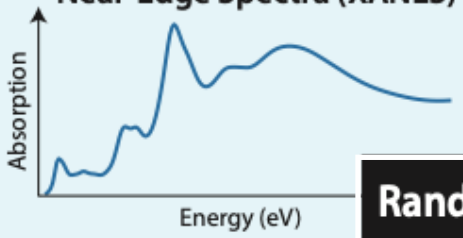
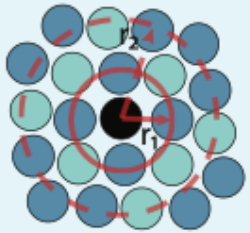
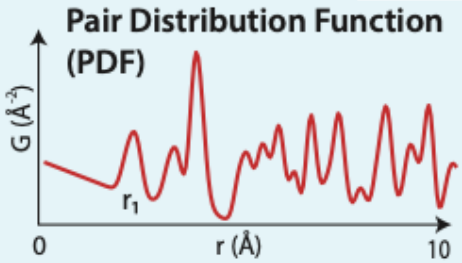


Data









Structures: Transition metal oxides
from Materials Project database

Ti Mn Fe Cu + O

Random Forest Models

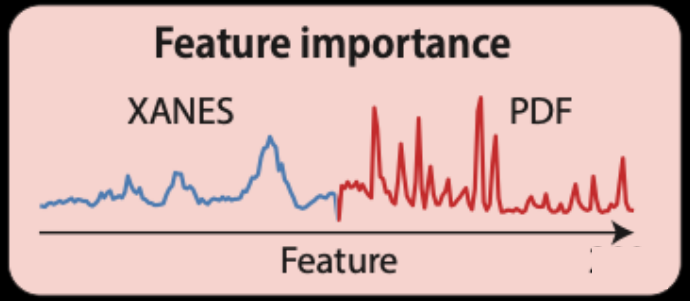
Models

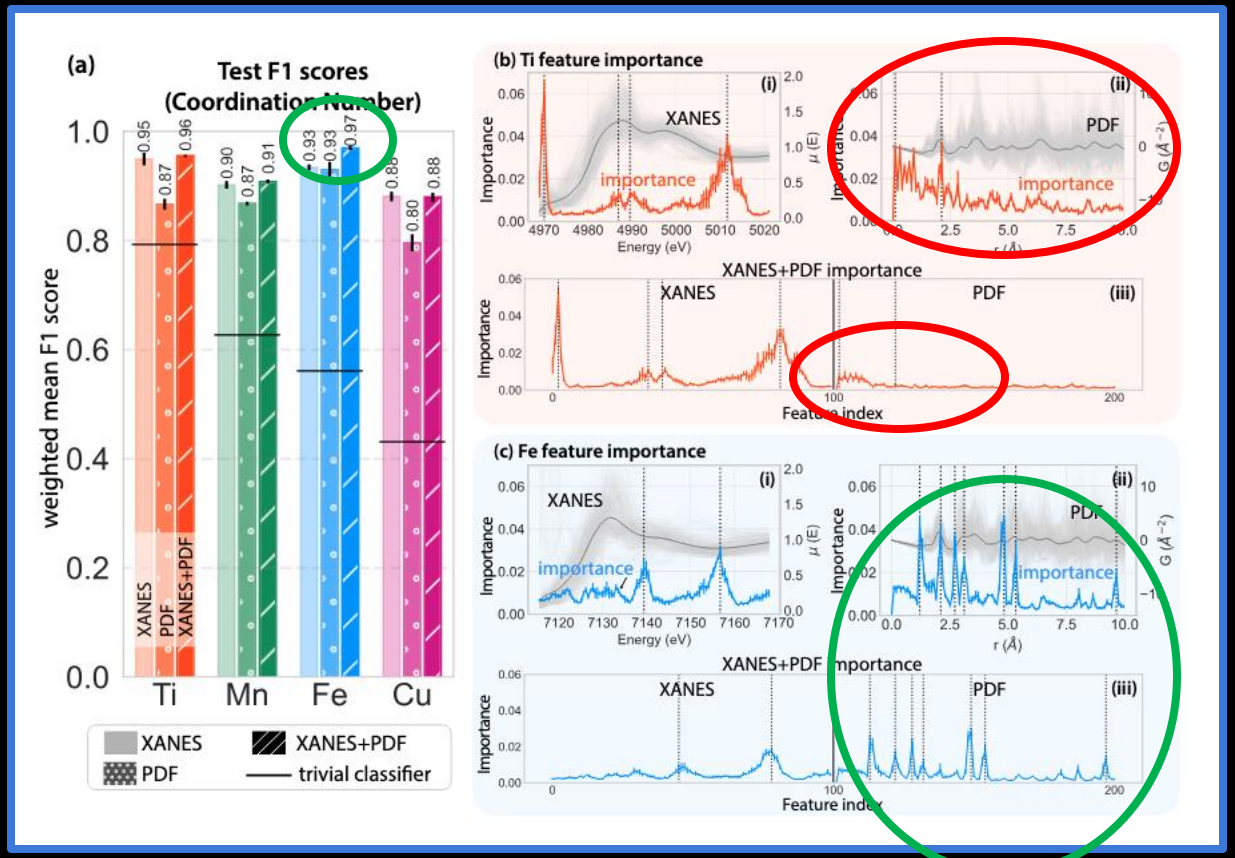
Prediction targets:
Metal's local atomic environments

Charge (oxidation) state
Ti, Mn, Fe: 2+ / 3+ / 4+
Cu: 1+/2+/3+

Coordination Number
4/5/6

Mean Bond Length
(metal to nearest neighbors)

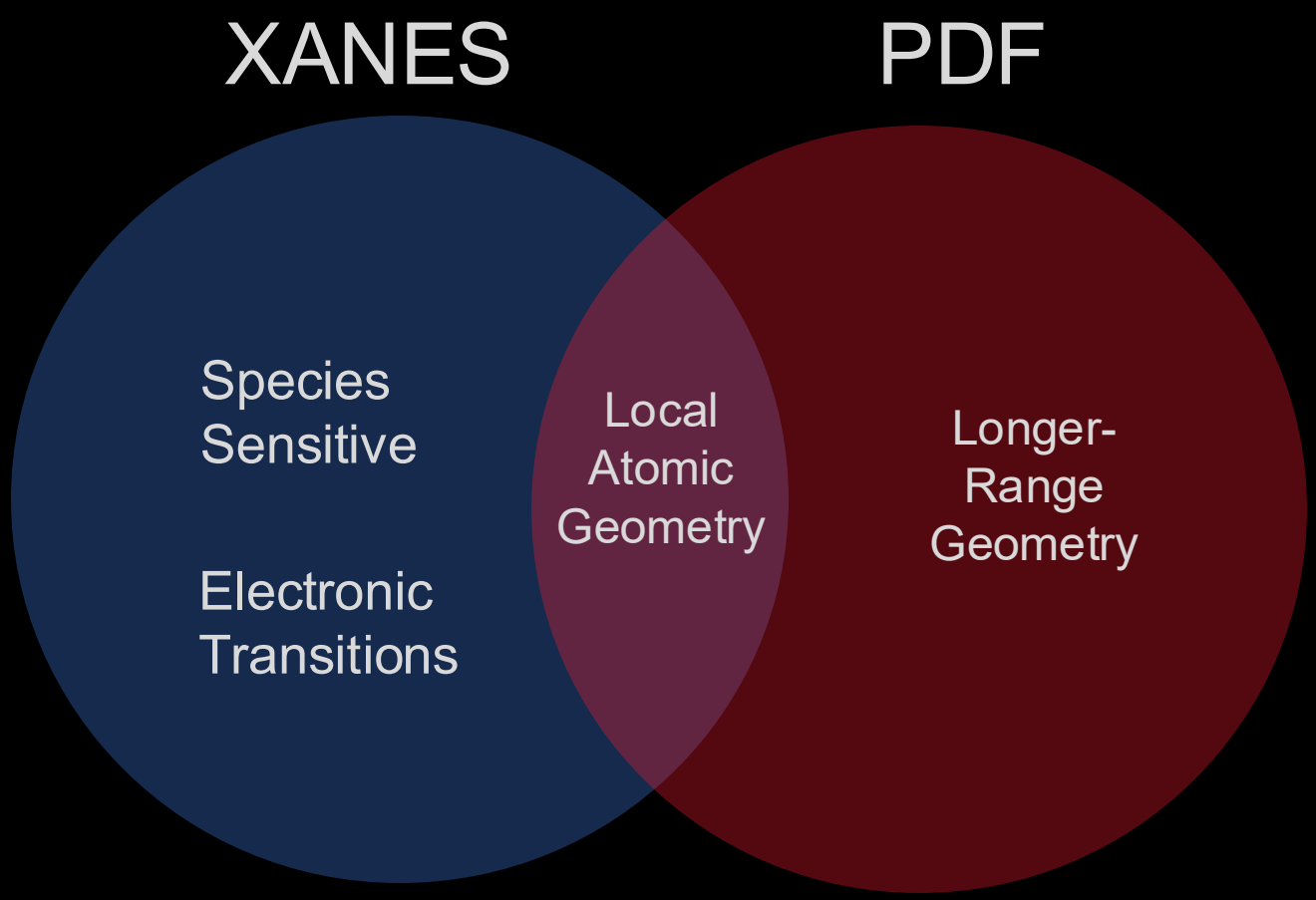


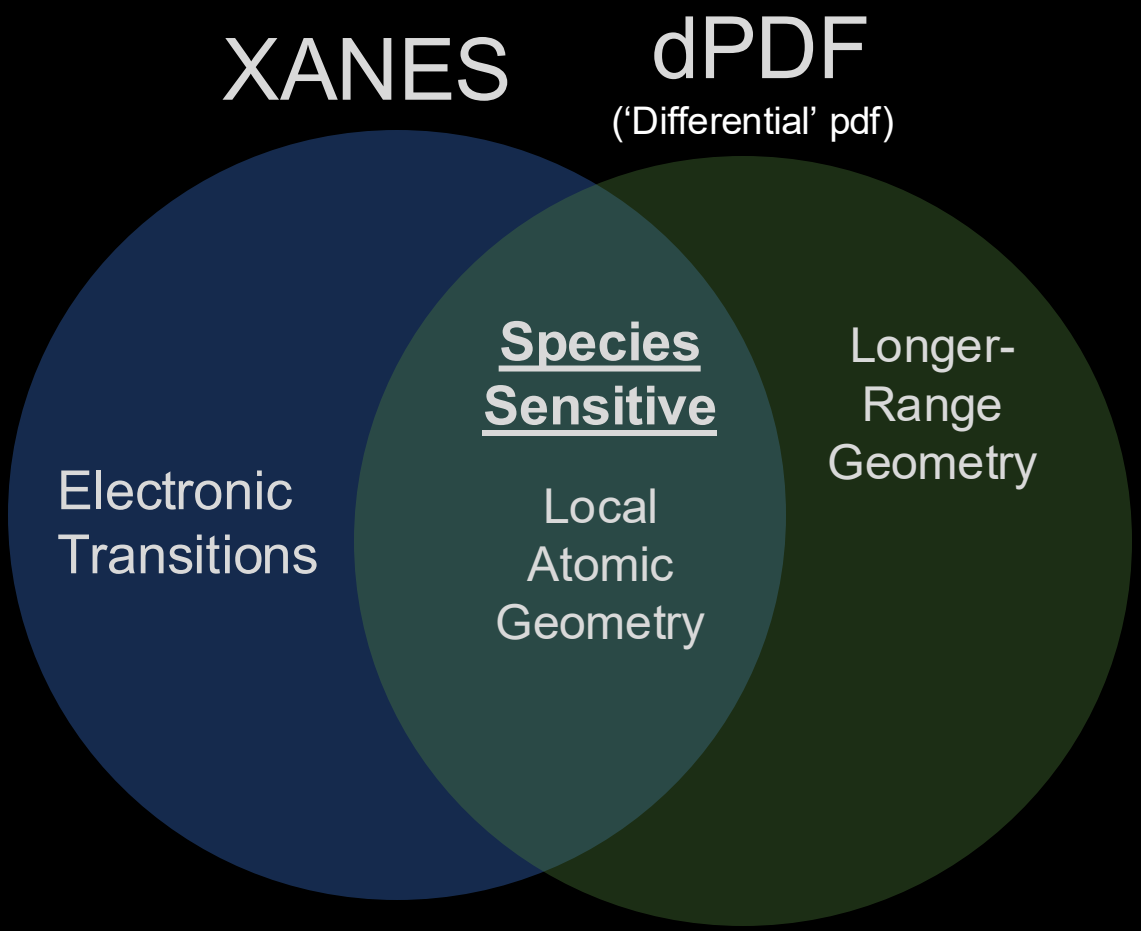


PDF doesn't contribute
When XANES + PDF present
For Titanium

But XANES + PDF improves
performance for Iron

Contributions are system & (data-set) specific, but can be measured

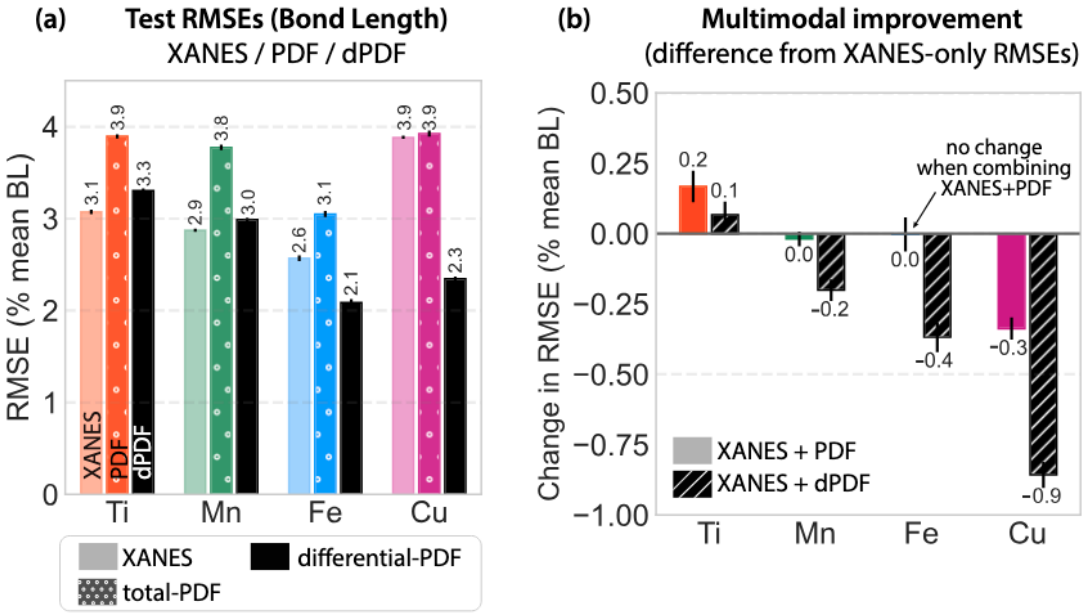


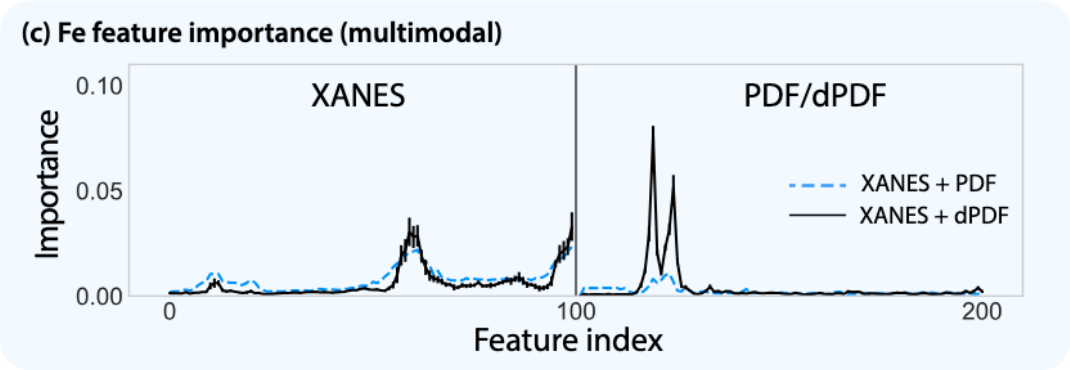


dPDF reduces error significantly;

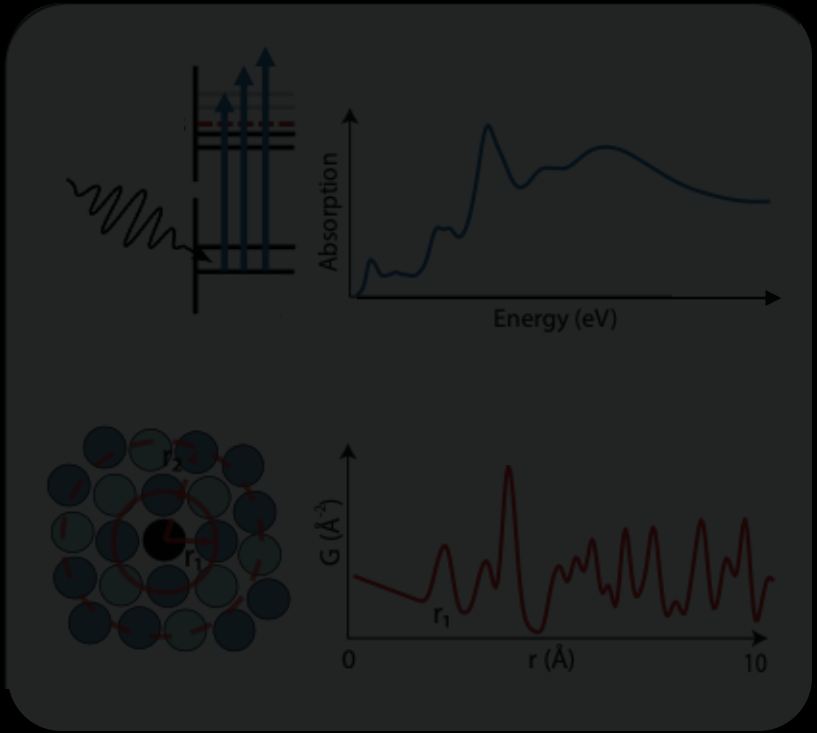
Closes the gap between XANES and PDF-only models

A database approach can help us understand the relative information of different modalities

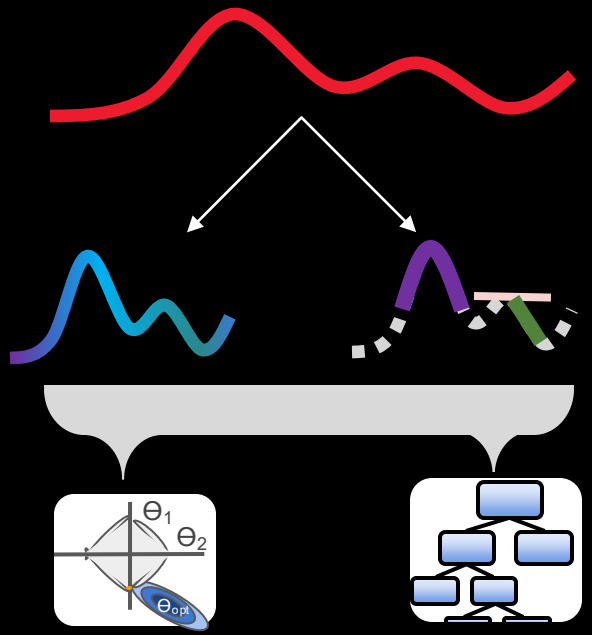




Multimodal Studies of XANES vs. PDF Spectra



Spectra-scope: A tool for feature discovery & downselection of spectrum-property relationships



SpectraScope

Hypotheses:

1. ’Raw’ spectra may be suboptimal representations, especially when using linear models.
2. Simpler models are easier for humans to interpret.
3. Interpretable models are easier for humans to trust.

SpectraScope

Input Data

$$\hat{y} = f(x)$$

Prediction Variable

ML Model

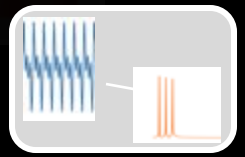
SpectraScope

Featurization

$$\hat{y} = f(x')$$

Prediction Variable

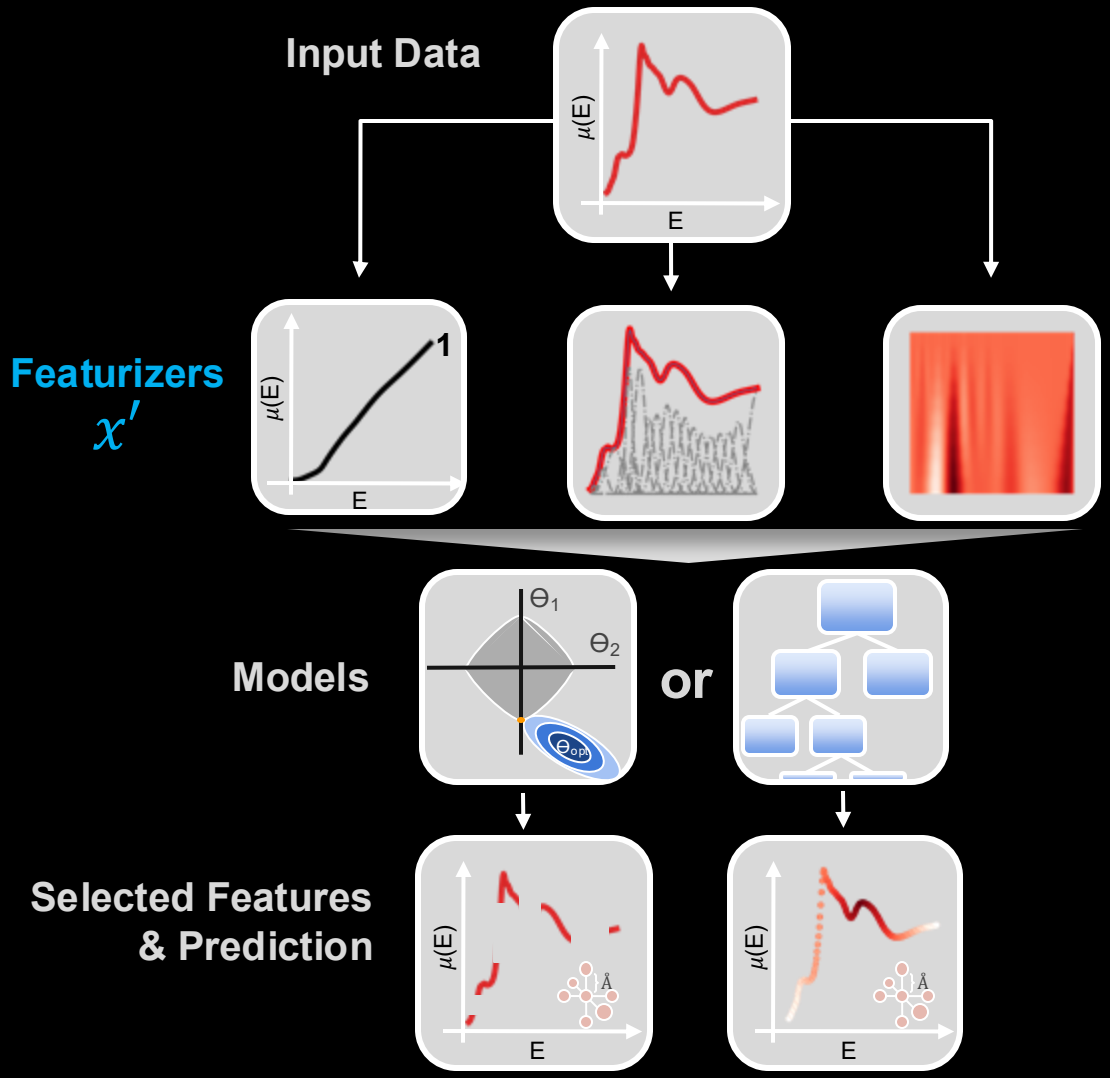
ML Model



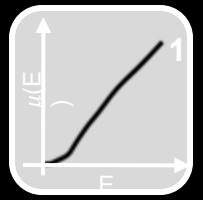
Why featurize?

- Improve performance
- Reduce overfitting

SpectraScope



Interpretable & Parsimonious Models

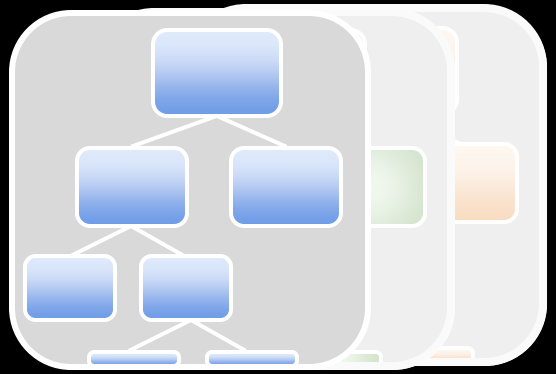


Lasso-Clip-Elastic Net

Models

or

Random Forests



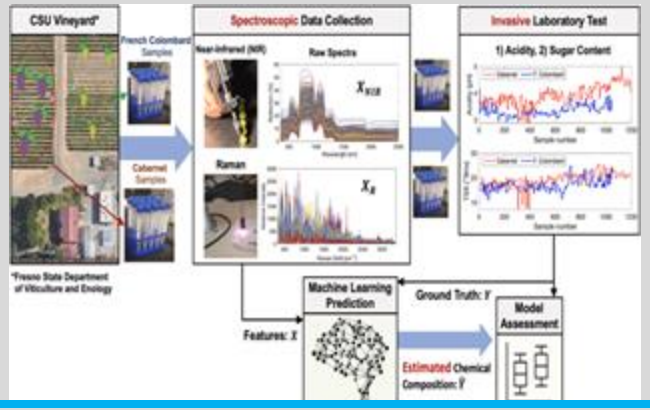
1. **Lasso Regression**
2. **Clip: coefficients < cutoff = 0**
3. **Elastic Net Regression**
4. **Clip**

Seber, P. & Braatz, R. D. https://arxiv.org/abs/2402.17120 (2024).

Predicting sugar content in wine grapes

Dataset

- X: Vis-NIR + Raman
- y: pH, TSS (°Brix)

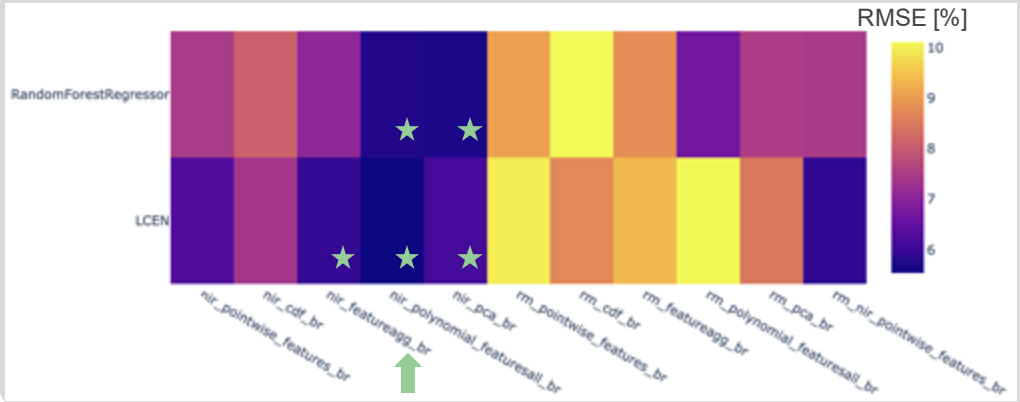


Predicting TSS with Vis-NIR Spectra: RMSE 5~7% Reported

Ebrahimi, I. et al. *Journal of Agriculture and Food Research* **16**, 101085 (2024).

SpectraScope

Comparing transformations & models



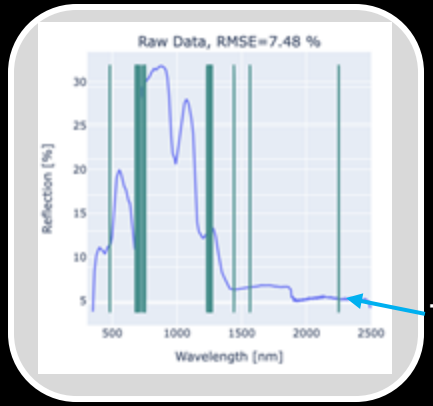
Well performing transformations

Comparable errors: RMSE 5~7%

Predicting sugar content in wine grapes

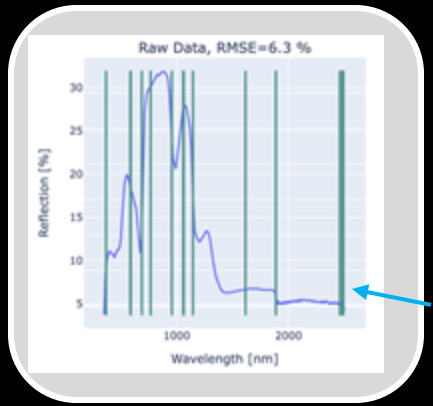
Raw Data

Random Forest



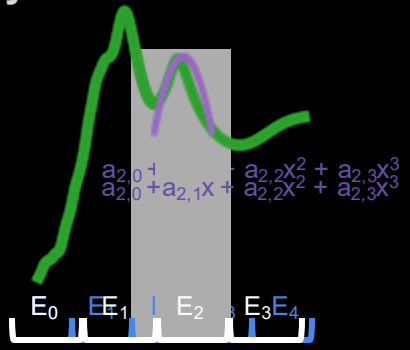
Top features

LCEN

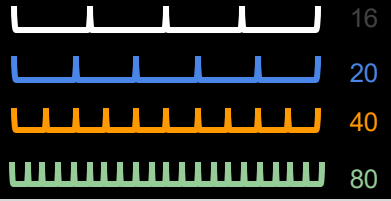


Top features

Polynomial Coefficients



$\vec{a}_4 = [a_{00}, a_{01}, a_{10}, a_{11} \ldots, a_{20} \ldots, a_{33}]$

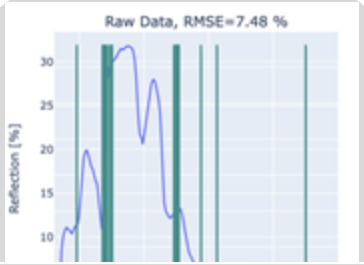


New feature vector: all fit coefficients (156)

Predicting sugar content in wine grapes

Raw Data | **Polynomial Coefficients**

Random Forest

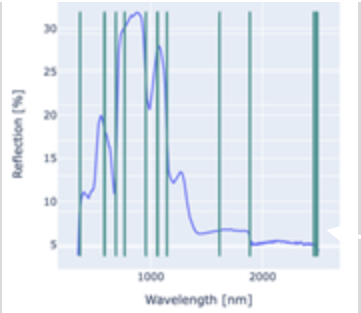


a_0

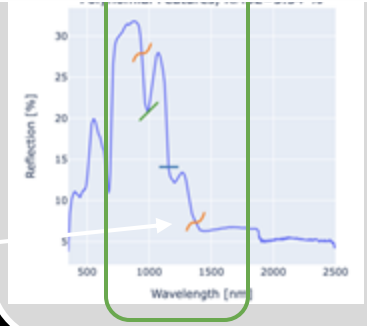
1. Transformations can yield better prediction than the raw data
2. Feature selection can highlight individual important parts of spectra

a_3

LCEN



Top features



We are turning Spectra-Scope into an app

home_page

localhost:8502

Relaunch to update

Deploy

home page

visualizing

Spectrascope Home

SpectraScope

1. Load data

Done! (using st.cache_data)

Show Full Dataframe

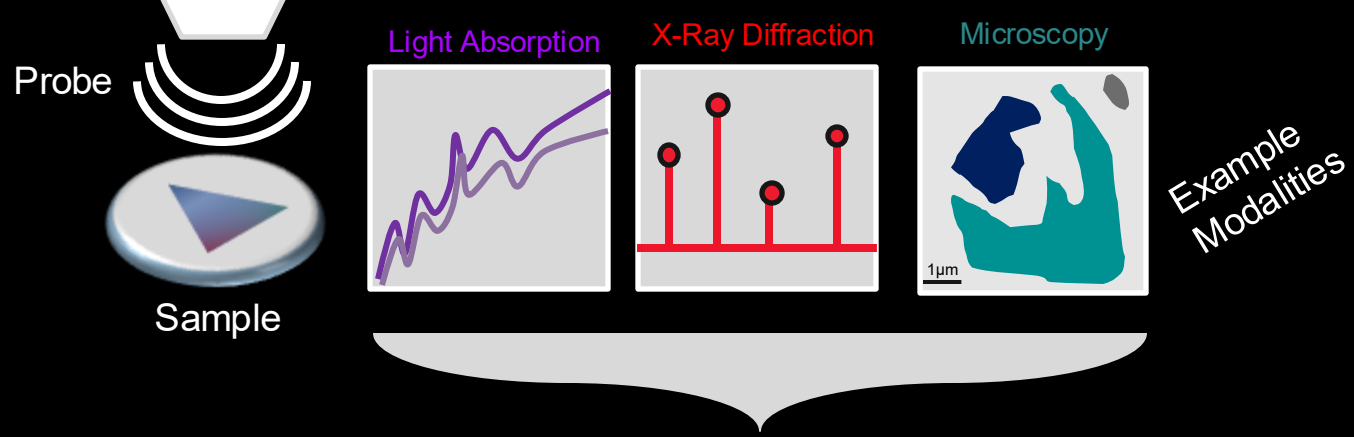
	mp_id	structure	xanes
0	mp-1041683	{"@class":"Structure","@module":"pymatgen.core.structure","charge":0,"lattice":{"a"	0.16897
1	mp-556341	{"@class":"Structure","@module":"pymatgen.core.structure","charge":0,"lattice":{"a"	0.12421
3	mp-769525	{"@class":"Structure","@module":"pymatgen.core.structure","charge":0,"lattice":{"a"	0.09676
4	mp-677246	{"@class":"Structure","@module":"pymatgen.core.structure","charge":0,"lattice":{"a"	0.33554
5	mp-5020	{"@class":"Structure","@module":"pymatgen.core.structure","charge":0,"lattice":{"a"	0.03973

Discussion & Caveats

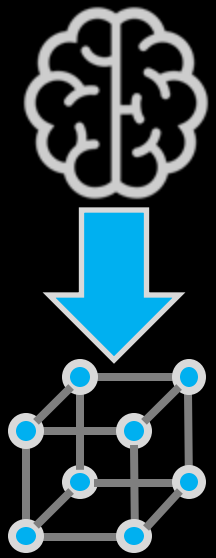
- These methods rely on data being available, or easily generated
  - Accelerated forward-modeling of complex spectra e.g. XANES may make it easier to assemble libraries of data
  - Same for other more demanding spectra
- Intended to be a guide for practitioners- not to replace them
  - Accelerate signal extraction from data
  - Highlight to practitioners relevant spectral components
- Possible applications may exist within manufacturing, process control

Other
Related TRI Work

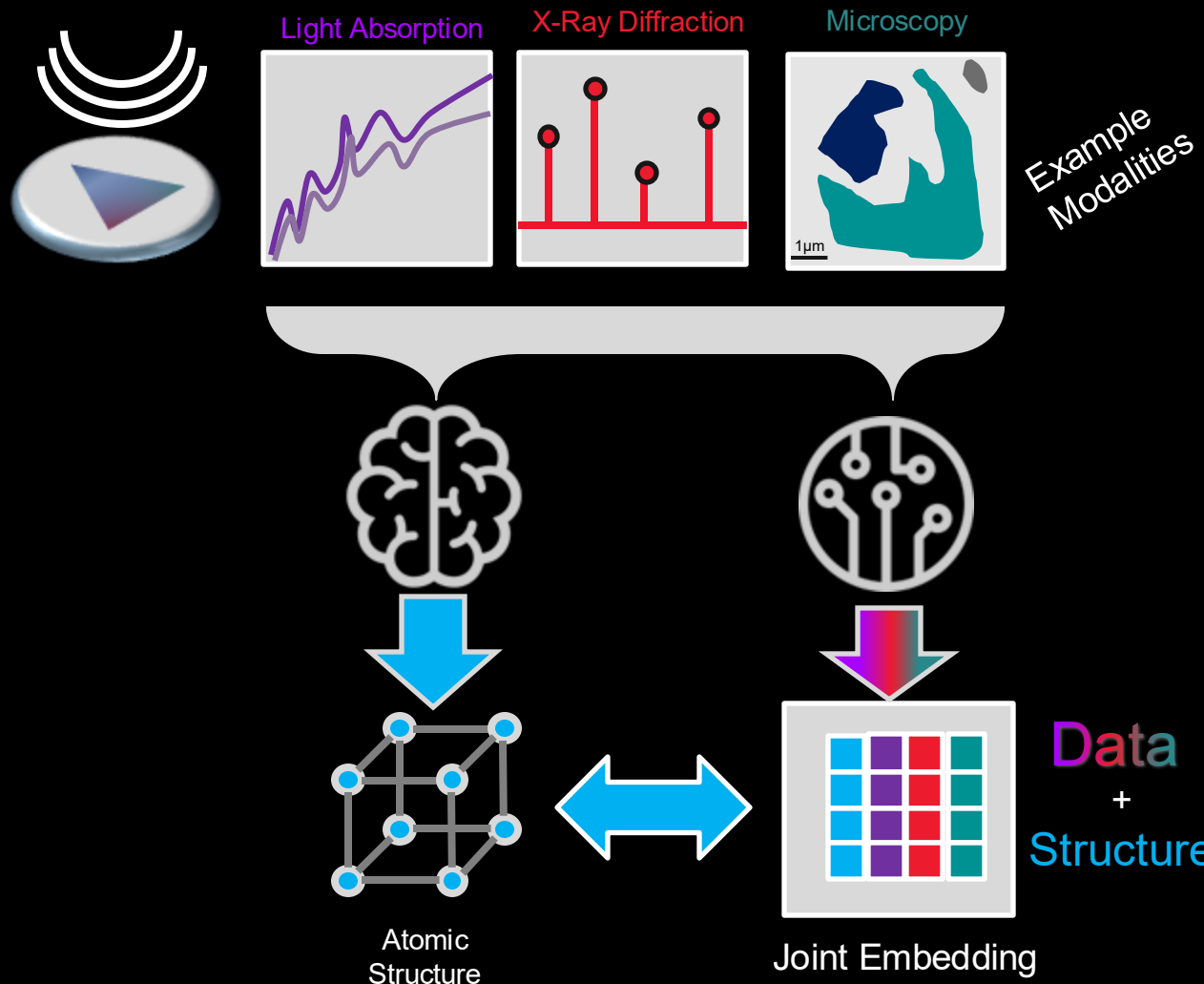
Experimental Data



Congruent Idealizations



Experimental Data

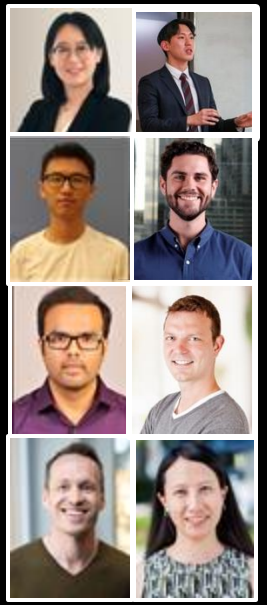


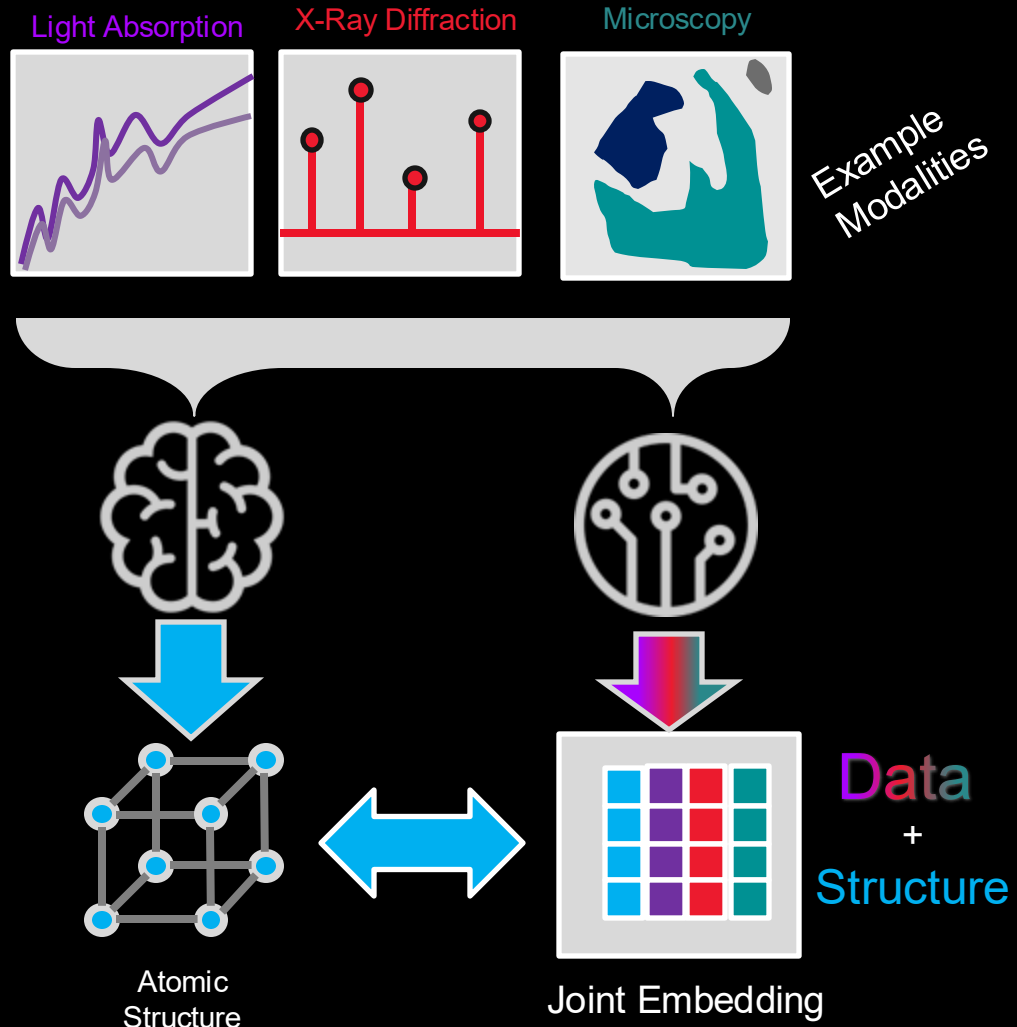
Congruent Idealizations

≈

Aligned Embeddings

Materials Multimodality (4M)

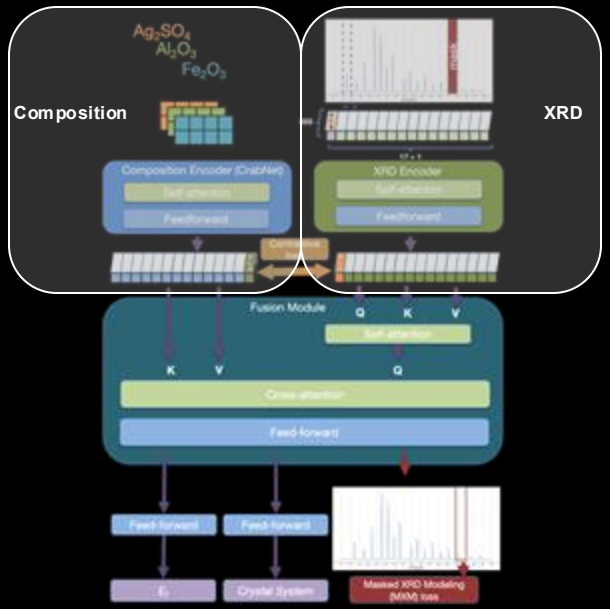




Seeing without crystal structure: structure agnostic multimodal learning for materials science

A strong bias in AI for materials: atomic structure as the core input representation of materials

alexandria 5M structures



XRD x-attention Composition Transformer-NN (**XxaCT-NN**)

- Cross-attention based multi-modal model based on composition + XRD
- Unsupervised pre-training: up to 4.2× speedup for task convergence
  - Contrastive loss
  - Masked XRD Modeling loss

Bimodal (XRD + Comp.) ~ Unimodal Structure > Unimodal (XRD/Comp.)

- Larger datasets favor multimodal models

		E_f (MAE, meV/atom)	Crystal System (e.g. cubic, tetragonal, etc. acc. %)
Unimodal	Composition	132	67.8
	XRD	421	92.3
	Structure	***16[Schmidt et al., 2024]***	*-*
Bimodal	Composition-XRD	***27.1***	***97.2***

Read the preprint!
Subramanian, Hung, Schweigert, Suram, Ye

Conclusions on Spectroscopy

i. A database approach can help us understand contributions of different spectral modes

ii. Feature generation and downselection can help reveal spectrum-property trends

iii. These might be combined for future optimal experiment planning & design

Talk Outline

1. TRI + AMDD Background
2. Challenges in AI-guided materials design
3. Characterization & bridging experiment & theory

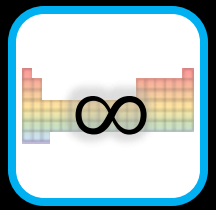
Conclusions

I

Conventional metrics for materials discovery may be limited in their applicability

II

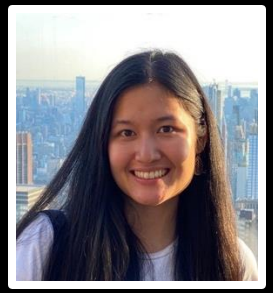
We should focus on ways to improve synthesis success rates



III

Interpretable ML may help practitioners make more trustworthy models

Zoe Zachko



Dr. Tina Na Narong

Amalya Johnson
(Stanford)

Weike Ye

Leena
Sansguiri

Joey
Montoya

Prof. Simon Billinge

Thank you very much to the organizers, and to you for your attention!

Sabina Mohan,
NIST Conference Services

Daniel Wines
Kamal Choudhary
Francesca Tavazza
Brian DeCost
… and others!

Thank You

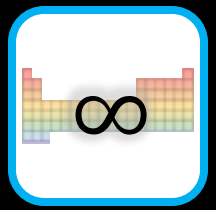
Questions?

I

Conventional metrics for materials discovery are limited in their applicability

II

We should focus on ways to improve synthesis success rates



III

Interpretable ML can help practitioners make more trustworthy models

steven.torrisi@tri.global

What success rates might we see?

Attempted Syntheses based on Energy Metric

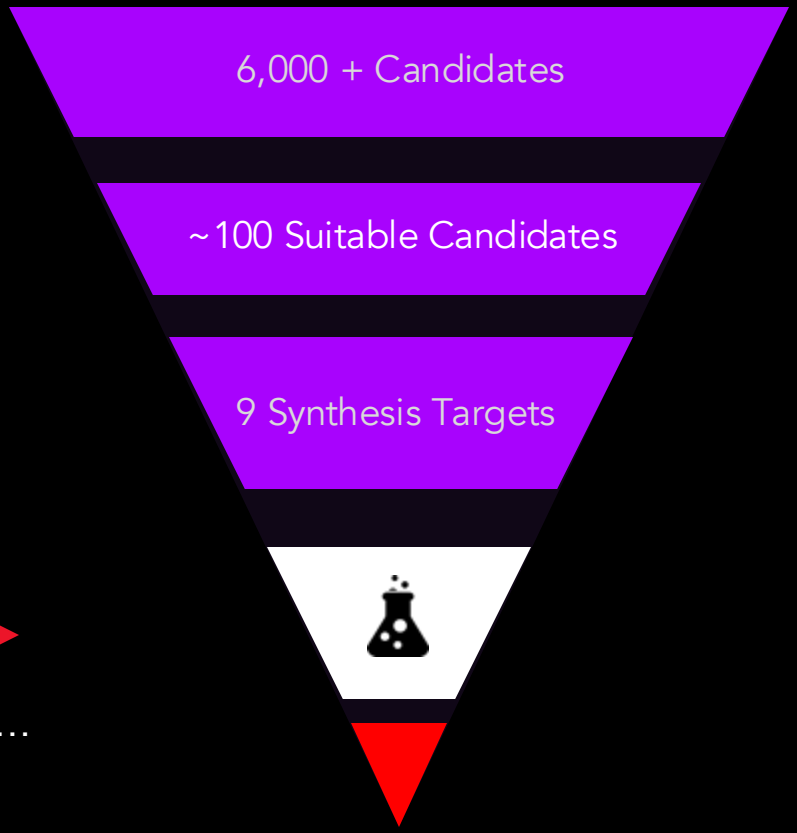
Ca-Ag-O	$CaAg_3O_4$
	Ca_3AgO_4
Li-Ag-O	$LiAg_3O_4$
	$LiAgO_2$
Ca-Pd-O	$CaPd_3O_6$
	$CaPdO_3$
Mg-Ru-O	$MgRu_2O_6$
	$MgRuO_4$
Ca-Ru-O	$CaRuO_4$
	Ca_3RuO_6
Li-Ru-O	Li_4RuO_5
	Li_5RuO_5

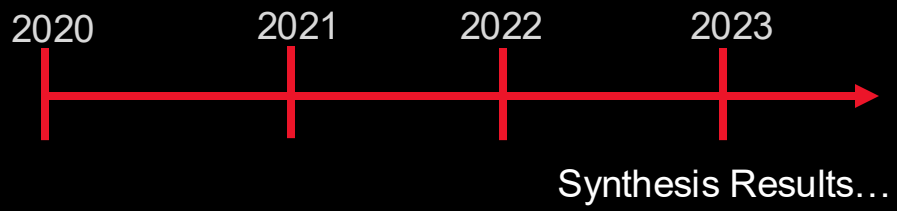
9 Target Candidates

- $Li_4CrFeNi_2O_8$
- $Li_4CrFe_2NiO_8$
- $Li_4TiCrNi_2O_8$
- $Li_4Cr_2FeNiO_8$
- $Li_4Cr_2FeCuO_8$
- Li_2CrCuO_4
- $Li_4Cr_2GaFeO_8$
- $Li_4Cr_3FeO_8$
- $Li_4TiCr_2CuO_8$

Computer-to-Lab Pipeline

- $Li_4Cr_3FeO_8$
- $Li_4CrFeNi_2O_8$
- $Li_4CrFe_2NiO_8$
- $Li_4TiCrNi_2O_8$
- $Li_4Cr_2FeNiO_8$
- $Li_4Cr_2FeCuO_8$
- Li_2CrCuO_4
- $Li_4Cr_2GaFeO_8$
- $Li_4TiCr_2CuO_8$

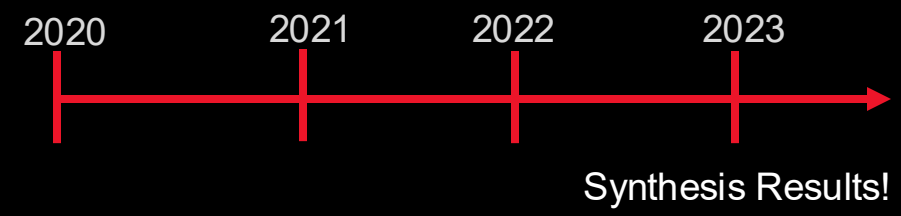


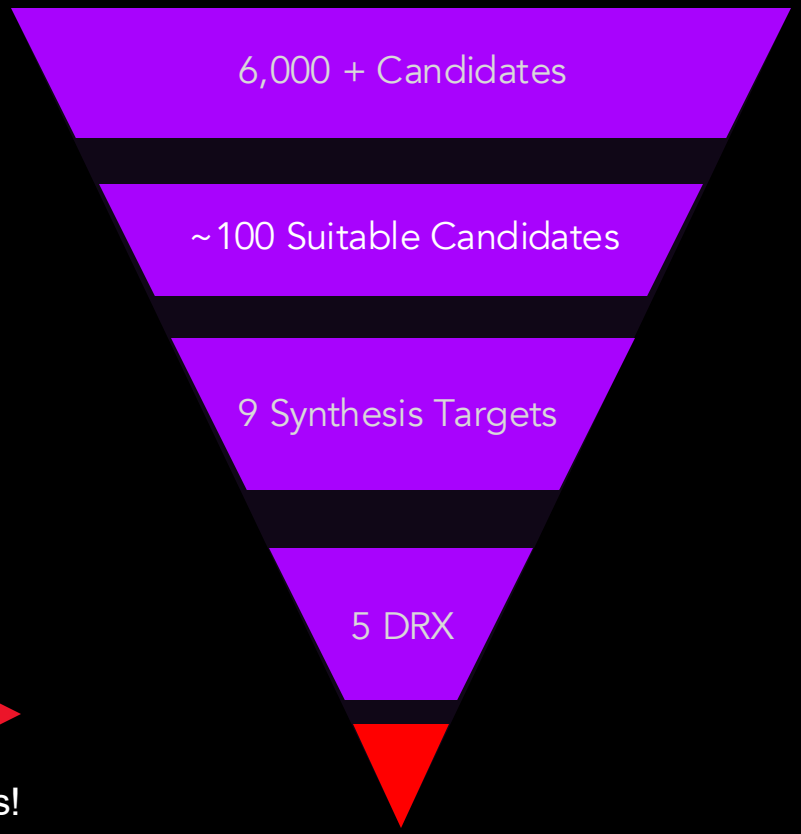


Computer-to-Lab Pipeline

DRX	Layered
$Li_4Cr_3FeO_8$	$Li_4Cr_2FeCuO_8$
$Li_4CrFeNi_2O_8$	Li_2CrCuO_4
$Li_4CrFe_2NiO_8$	$Li_4Cr_2GaFeO_8$
$Li_4TiCrNi_2O_8$	$Li_4TiCr_2CuO_8$
$Li_4Cr_2FeNiO_8$	

5/9 in DRX!





Further problems for the field for discussion

Do we suffer from a 'computability bias' towards ordered unit cells?

Streetlight effect

Article Talk

From Wikipedia, the free encyclopedia

Not to be confused with Street light interference phenomenon.

The **streetlight effect**, or the **drunkard's search** principle, is a type of observational bias that occurs when people only search for something where it is easiest to look.[1] Both names refer to a well-known joke:

Further problems for the field for discussion

Do many theorists suffer from a ‘computability bias’ towards ordered unit cells?

MP, OQMD, OCP etc are all wonderful resources and have come to shape a generation of scientific work-

But do they implicitly limit theorists’ picture of what constitutes a material?

Speaking as someone with a DFT background: is it an issue that we focus so heavily on materials that ‘fit through the keyhole’ of DFT?

Further problems for the field for discussion

Things sometimes left out when working at the 10,000 ft level (and the combinatorics of these will be challenging to contend with!):

- Surfaces
- Interfaces
- Defects
- Finite temperature effects, dynamic disorder
- Long length & time scale events (e.g. reconstruction)
- Interaction with liquids, atmospheres
- Functionalization processes
- Micro-scale phenomena (e.g. grain boundaries)