The Open Quantum Materials Database (OQMD): Features and Applications

(paradigms of materials discovery using prototypes and machine learning)

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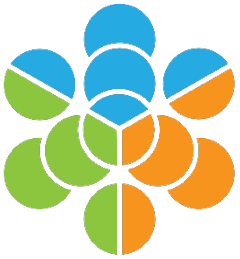
May 2, 2016

NORTHWESTERN
UNIVERSITY



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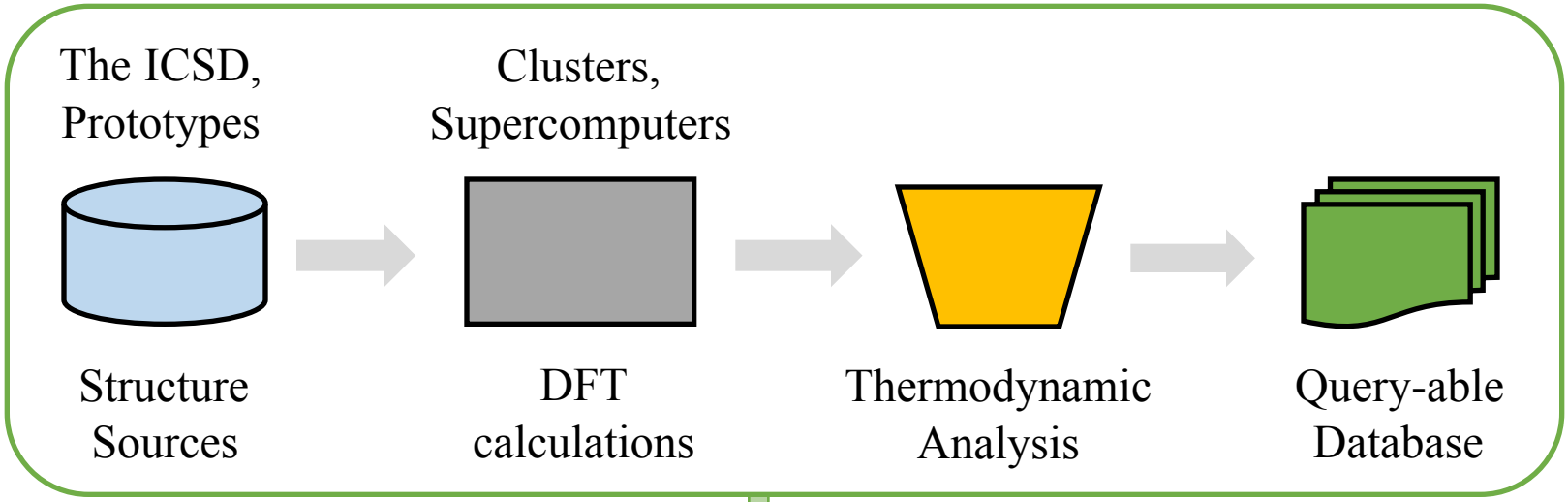
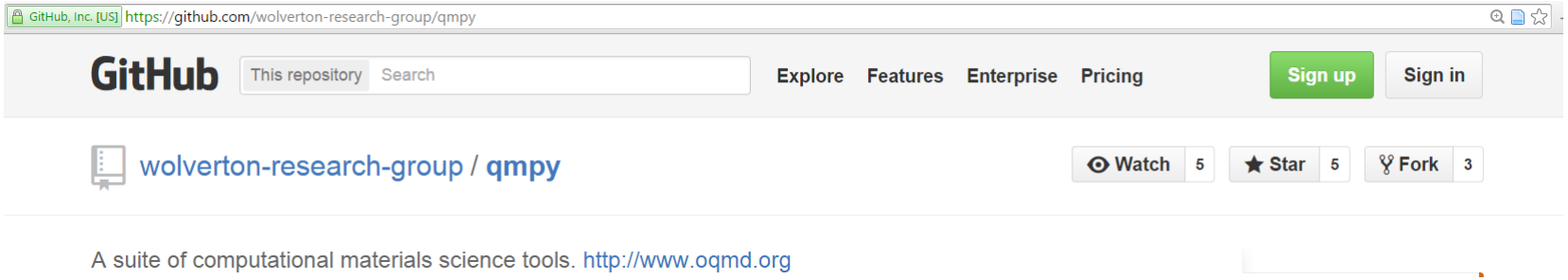
The OQMD: a HT DFT database

- A "high-throughput DFT" database of materials

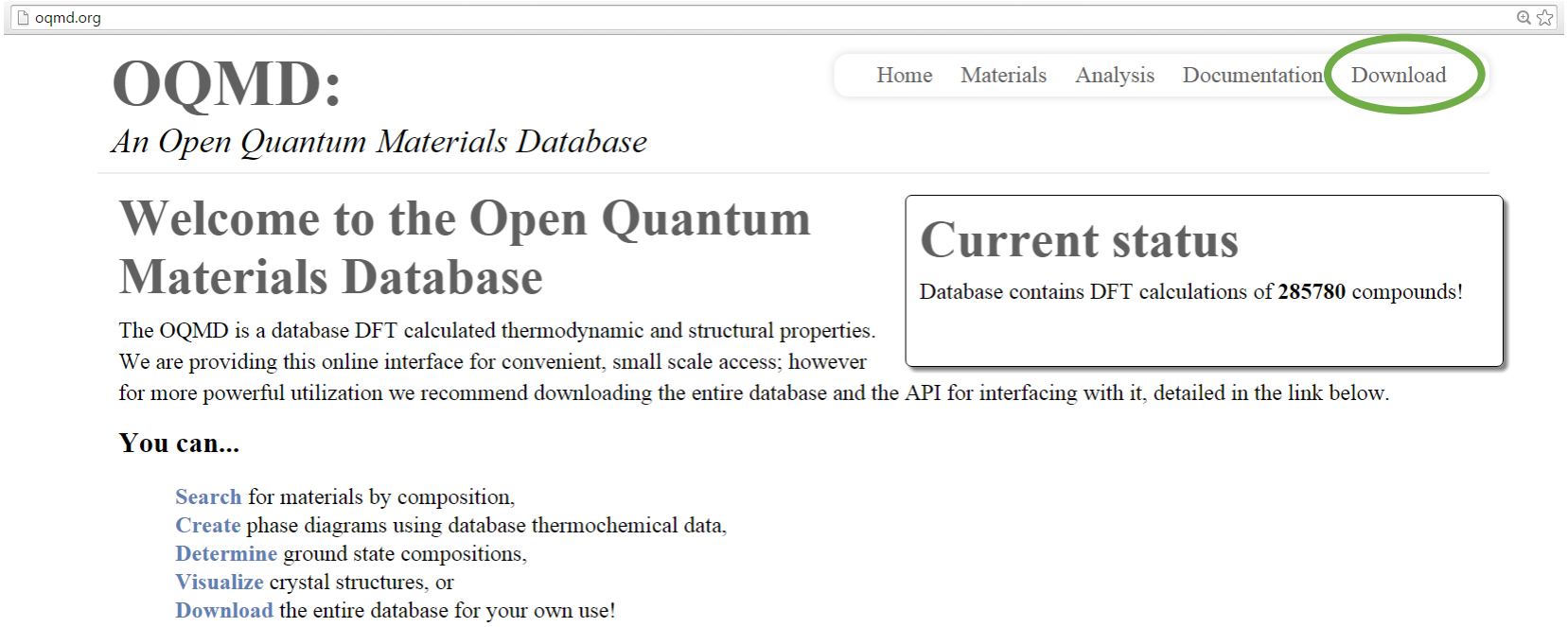


The *qmpy* framework



The **Open** QMD

- Entire database accessible at www.oqmd.org



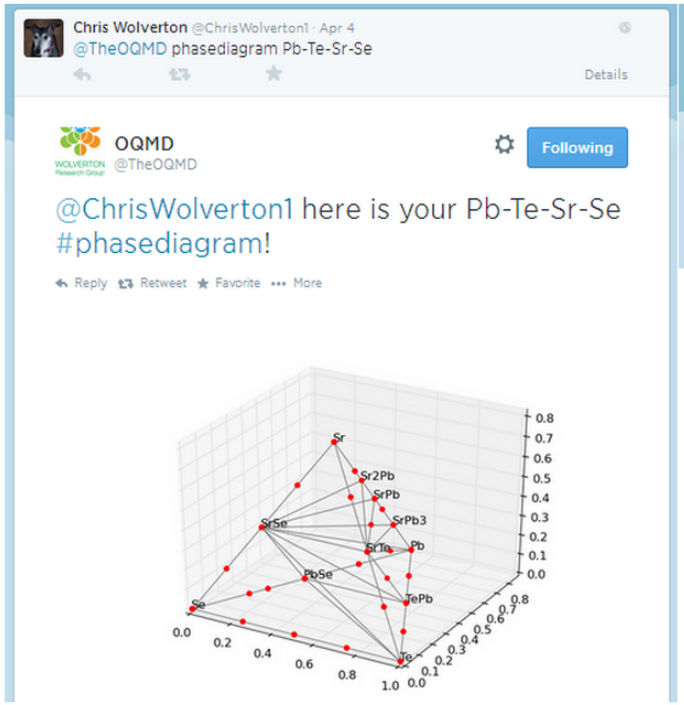
[[a convenient online interface for querying the database]]

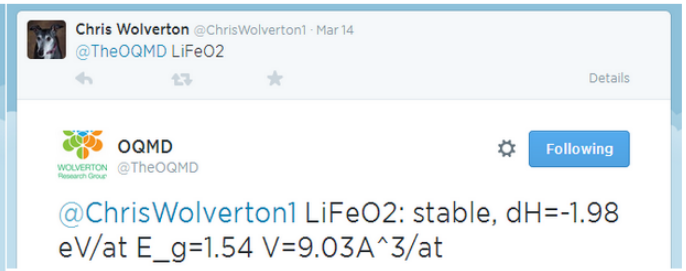
- The entire database can be downloaded, along with *qmpy*!

The **Open** QMD

- If you are so inclined, you can even tweet at it!

Tweet @TheOQMD to ask what is stable at a composition, or to get a simple phase diagram!





The OQMD was created in Chris Wolverton's group at Northwestern University.

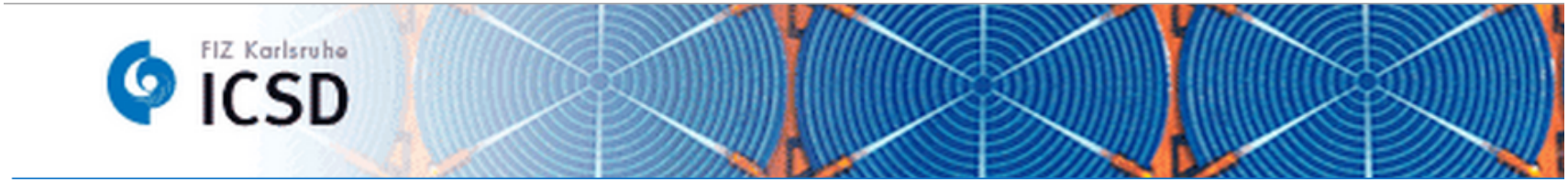
Contact us by e-mail

If you are using any results from this website, please reference this work as shown here

What data does the OQMD contain?

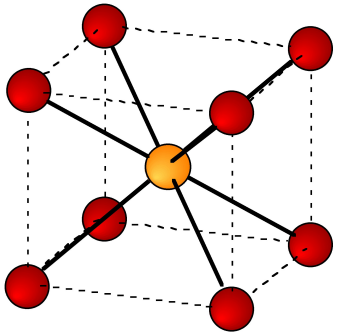
Structure sources:

- The Inorganic Crystal Structure Database (ICSD)



[[40,000+ compounds with (currently) <40 atoms per unit cell]]

- Decorations of known prototype crystal structures



B2 (CsCl) structure

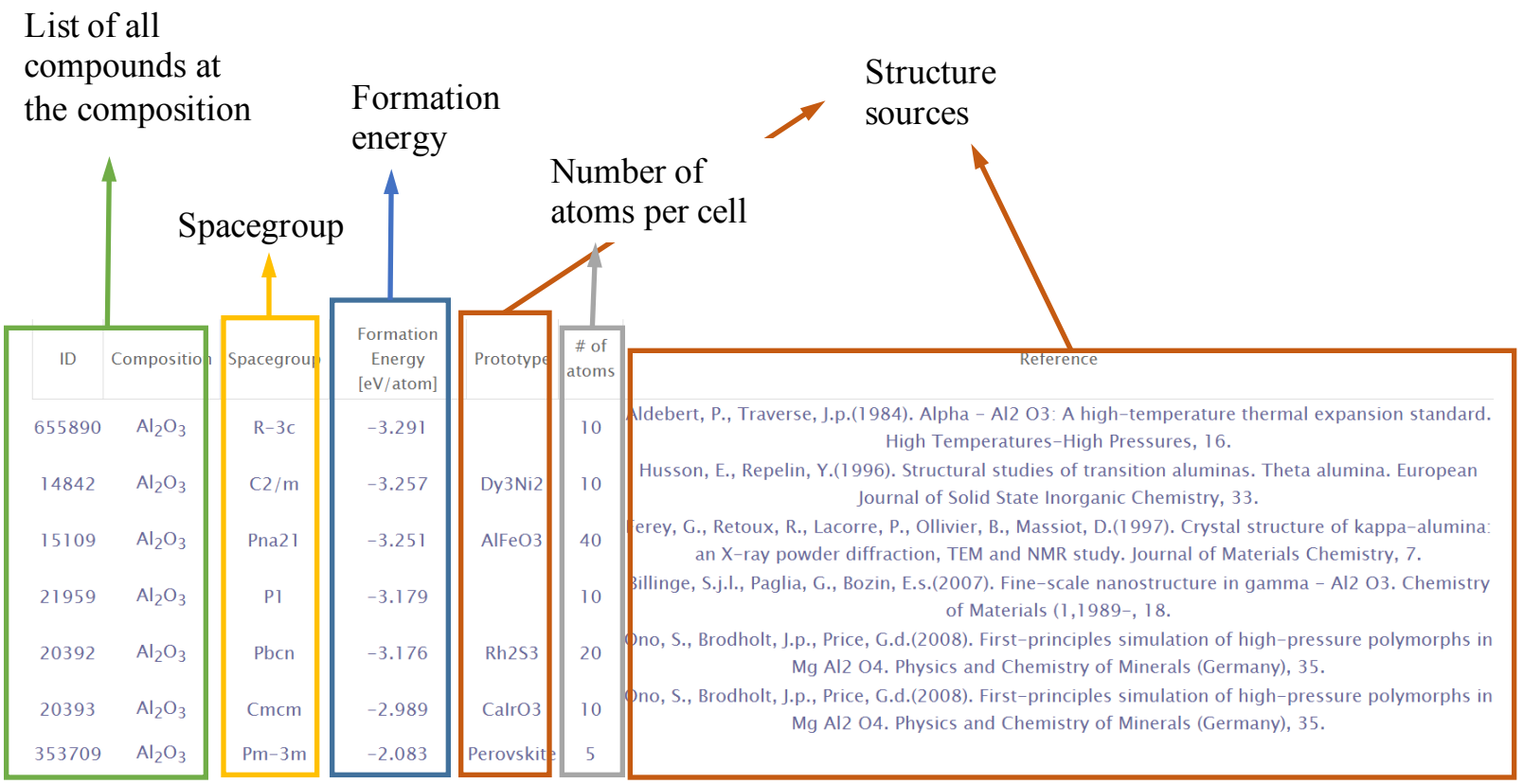
→ combinatorial replacement with all elements in the periodic table

[[400,000+ compounds from elemental, binary, ternary prototypes]]

The number of compounds is constantly growing!

What properties are calculated?

- At a given composition:



ID	Composition	Spacegroup	Formation Energy [eV/atom]	Prototype	# of atoms	Reference
655890	Al_2O_3	R-3c	-3.291		10	Aldebert, P., Traverse, J.p.(1984). Alpha - Al2 O3: A high-temperature thermal expansion standard. High Temperatures-High Pressures, 16.
14842	Al_2O_3	C2/m	-3.257	Dy3Ni2	10	Husson, E., Repelin, Y.(1996). Structural studies of transition aluminas. Theta alumina. European Journal of Solid State Inorganic Chemistry, 33.
15109	Al_2O_3	Pna21	-3.251	AlFeO3	40	Terey, G., Retoux, R., Lacorre, P., Ollivier, B., Massiot, D.(1997). Crystal structure of kappa-alumina: an X-ray powder diffraction, TEM and NMR study. Journal of Materials Chemistry, 7.
21959	Al_2O_3	P1	-3.179		10	Billinge, S.j.l., Paglia, G., Bozin, E.s.(2007). Fine-scale nanostructure in gamma - Al2 O3. Chemistry of Materials (1,1989-, 18.
20392	Al_2O_3	Pbcn	-3.176	Rh2S3	20	Ono, S., Brodholt, J.p., Price, G.d.(2008). First-principles simulation of high-pressure polymorphs in Mg Al2 O4. Physics and Chemistry of Minerals (Germany), 35.
20393	Al_2O_3	Cmcm	-2.989	CaIrO3	10	Ono, S., Brodholt, J.p., Price, G.d.(2008). First-principles simulation of high-pressure polymorphs in Mg Al2 O4. Physics and Chemistry of Minerals (Germany), 35.
353709	Al_2O_3	Pm-3m	-2.083	Perovskite	5	

What properties are calculated?

- For a each compound in the database:

Total energy, volume, magnetic moment, band gap calculated using DFT

Quantity	Value
Energy [eV/atom]	−7.379
Volume [Å^3/atom]	13.623
Net magnetic moment [μ_b/atom]	0.250
Band Gap [eV]	0

Input Structure

Lattice Vectors [Å]

$$\begin{bmatrix} 0 & 3.009 & 3.009 \\ 3.009 & 0 & 3.009 \\ 3.009 & 3.009 & 0 \end{bmatrix}$$

Stresses [kbar]

N/A

Output Structure

Lattice Vectors [Å]

$$\begin{bmatrix} 0 & 3.009 & 3.009 \\ 3.009 & 0 & 3.009 \\ 3.009 & 3.009 & 0 \end{bmatrix}$$

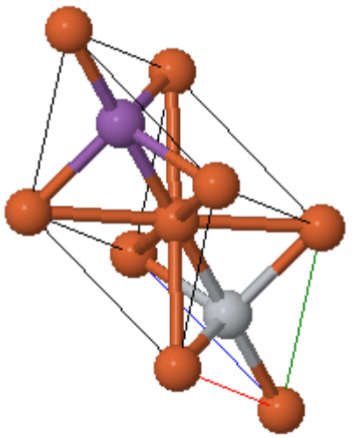
Stresses [kbar]

$$\begin{bmatrix} 0.742 & 0.002 & 0.002 \\ 0.002 & 0.742 & 0.002 \\ 0.002 & 0.002 & 0.742 \end{bmatrix}$$

Visualization

Crystal structure

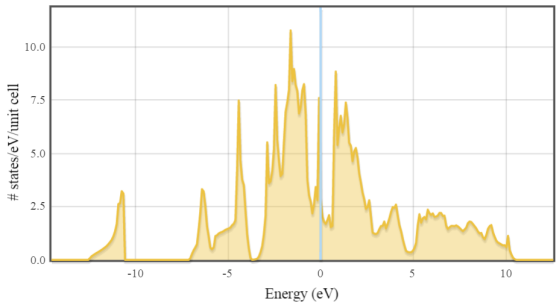
HM:Fm−3m
a=4.255Å
b=4.255Å
c=4.255Å
α=60.000°
β=60.000°
γ=60.000°



JSmol

Primitive Cell Conventional Cell
Download primitive or conventional cells (VASP format).

Density of electronic states



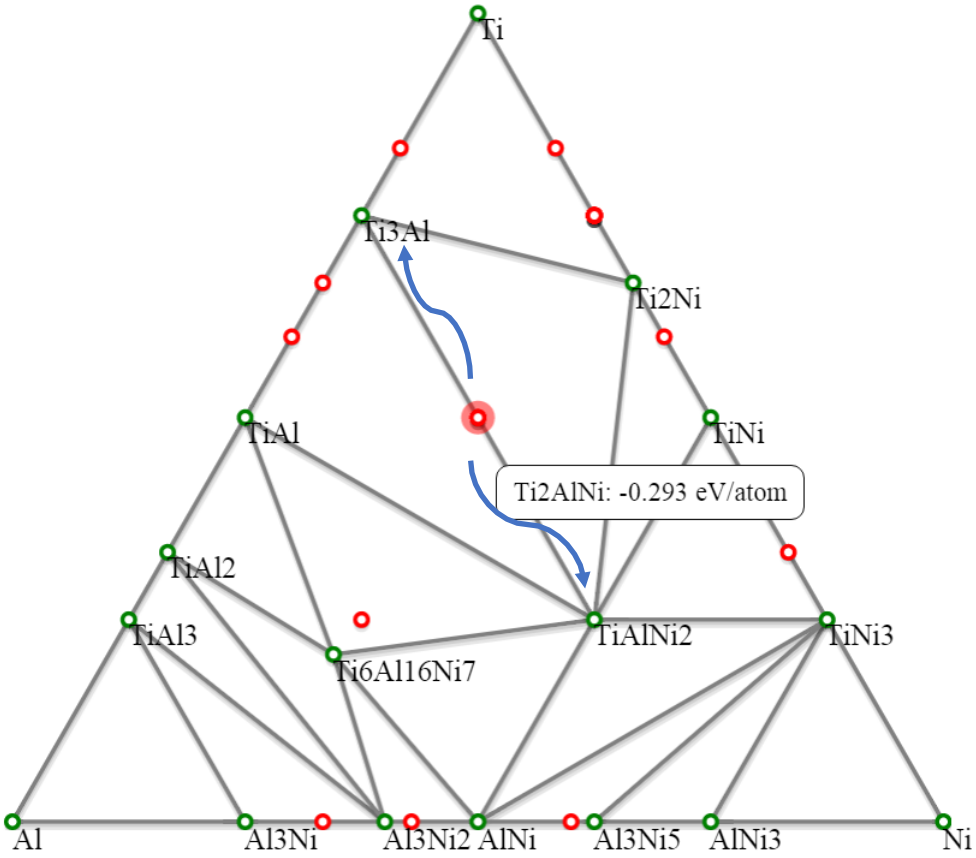
Fully (DFT) relaxed structure, available for download

What properties are calculated?

- For a given chemical system, the convex hull (0 K phase diagram):

e.g., Ti-Al-Ni

green = stable
red = unstable

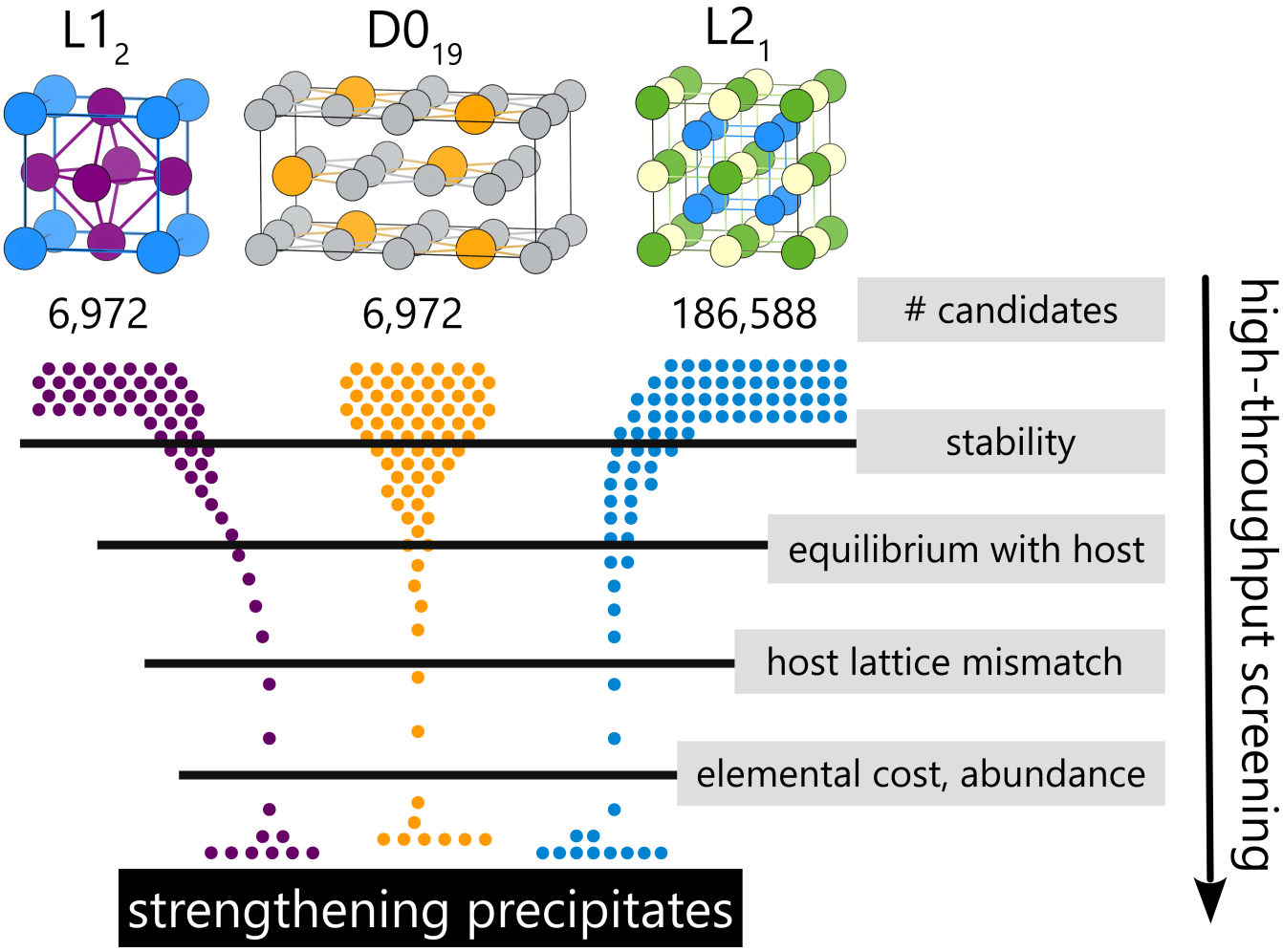


For example, Ti_2AlNi is predicted to decompose into $TiAlNi_2$ and Ti_3Al

qmpy: automating HT-DFT, thermodynamic analyses

- Symmetry analysis (interfaced with python-based `spglib`)
- Calculation of/plotting reaction voltages
- Chemical potentials to estimate synthesis conditions
- Multistep screening of prototypes for discovering materials, e.g.,
  - How many stable, tetragonal compounds of the form X_2YZ, with a bandgap between 0.5 eV and 1.5 eV, made of elements not heavier than Pb, and with lattice constant (a) close to that of Si, that have been synthesized experimentally are there in the OQMD?
  - Applications include searching for
    1. new cathode materials for batteries,
    2. new materials for thermochemical water splitting,
    3. new solar cell materials,
    4. new **strengthening precipitates in alloys**, and others…

An example of prototype screening: new strengthening precipitates in alloys!



Kirklin, S., Saal, J. E., Hegde, V. I., & Wolverton, C. "High-throughput computational search for strengthening precipitates in alloys", *Acta Materialia*, *102*, 125-135.

Machine Learning & OQMD

Motivation: The Prototype Search

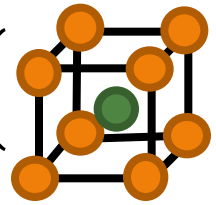
Common Method: Prototype Search

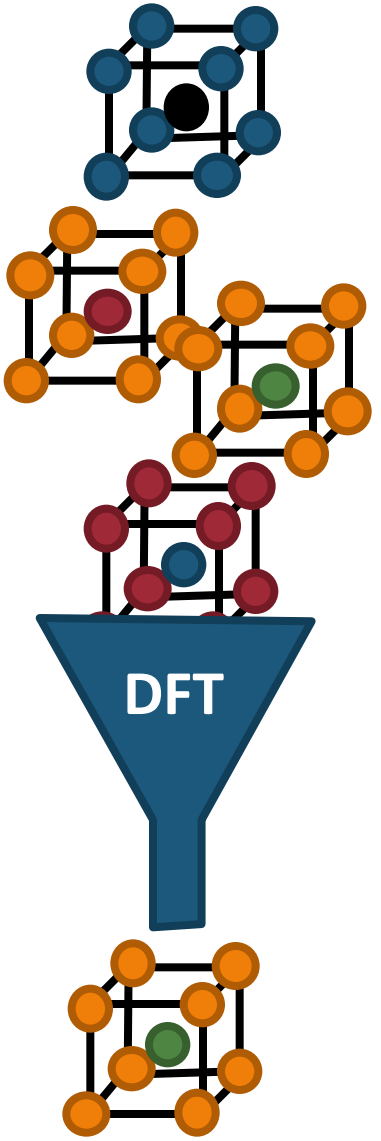
1. Select a crystal structure
2. Evaluate **all** possibilities with DFT
3. Select only stable ones

Challenge: Computational cost

Possible Solution: Guide with ML

$$\Delta H_f = f\left(\quad\right)$$



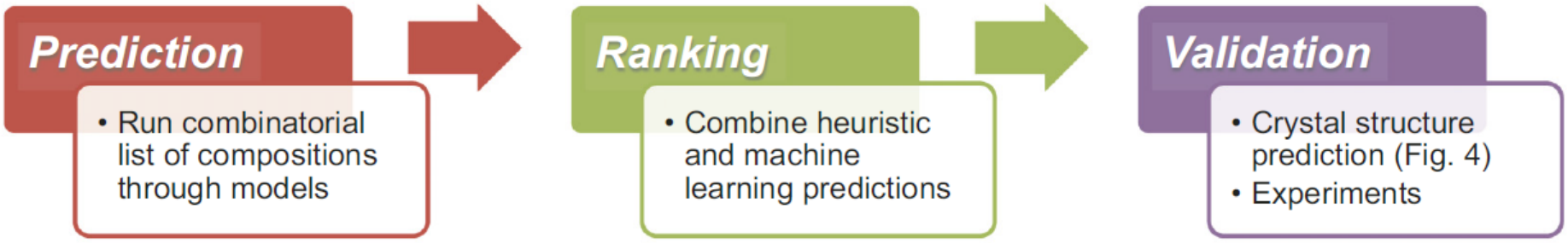


Route #1: Composition-Based Models

Goal: Find compositions of undiscovered phases

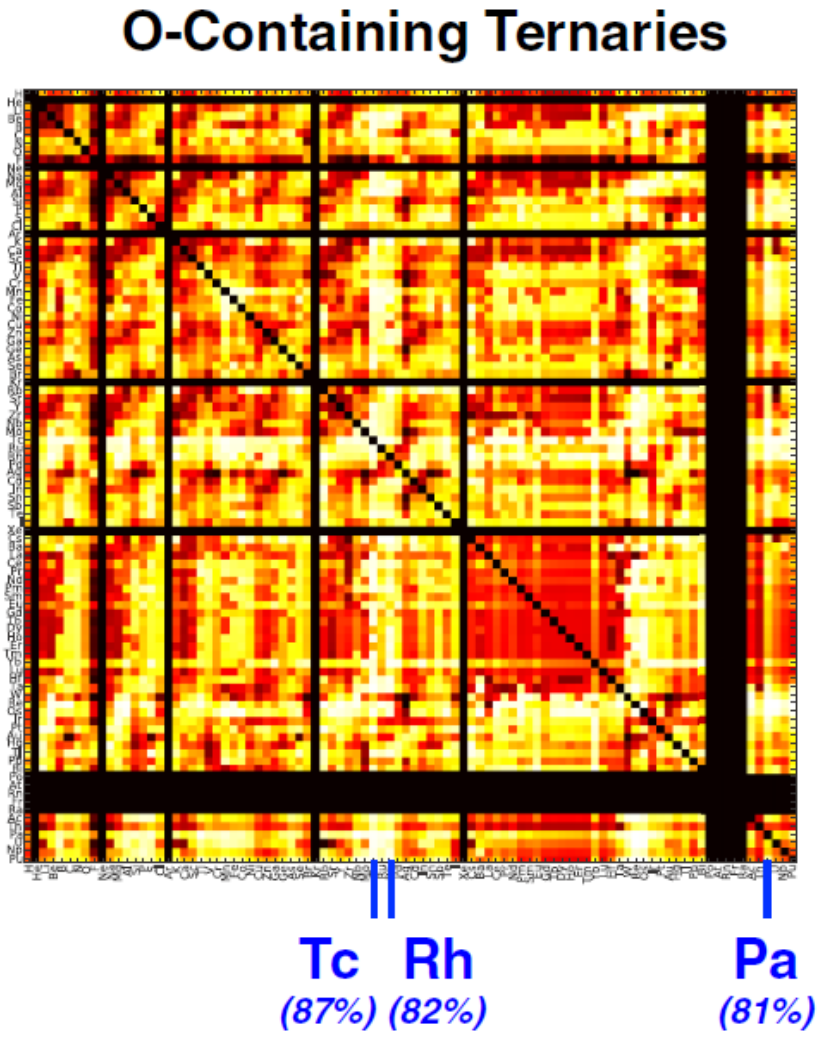
Method:

1. Train ML, heuristic model on OQMD data
2. Rank unseen compounds based on stability
3. Predict crystal structures of best entries



Ref: Meredig *et al.* PRB. (2014) 094104

Route #1: Predicted Compounds

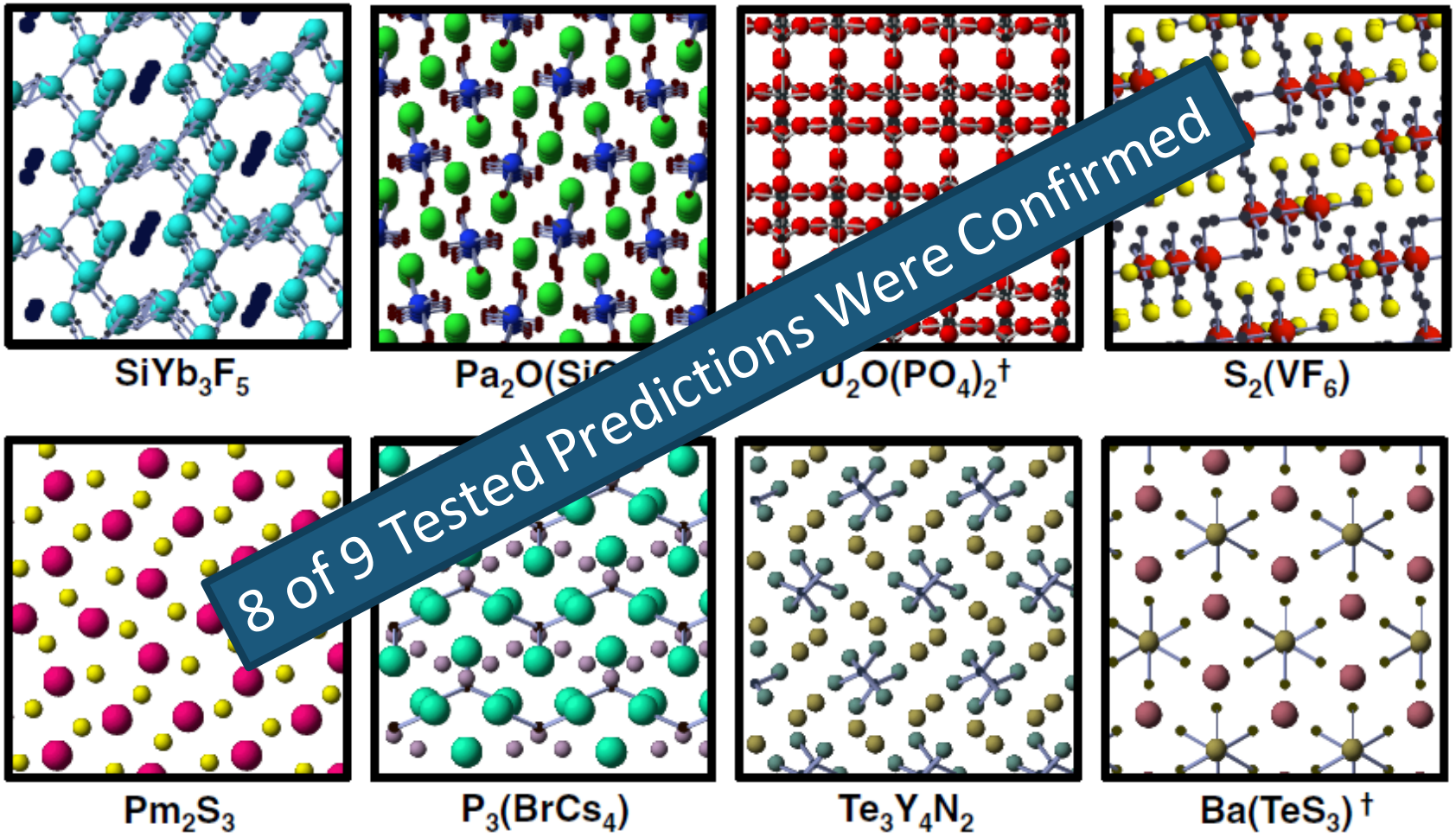


Brighter regions:
More likely to have undiscovered compounds

In total: >4500 Predicted materials

Ref: Meredig *et al.* PRB. (2014) 094104

Route #1: Validated Predictions



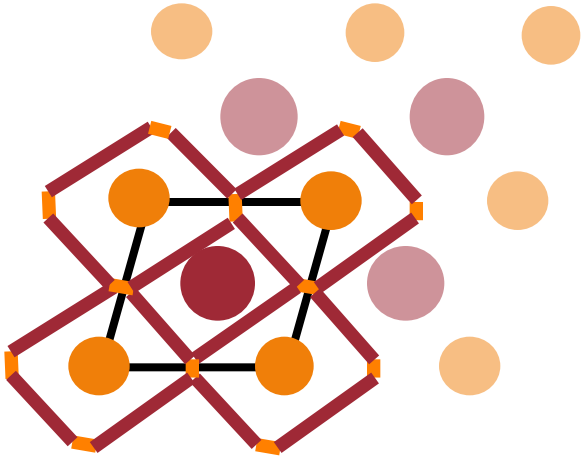
Ref: Meredig *et al.* PRB. (2014) 094104

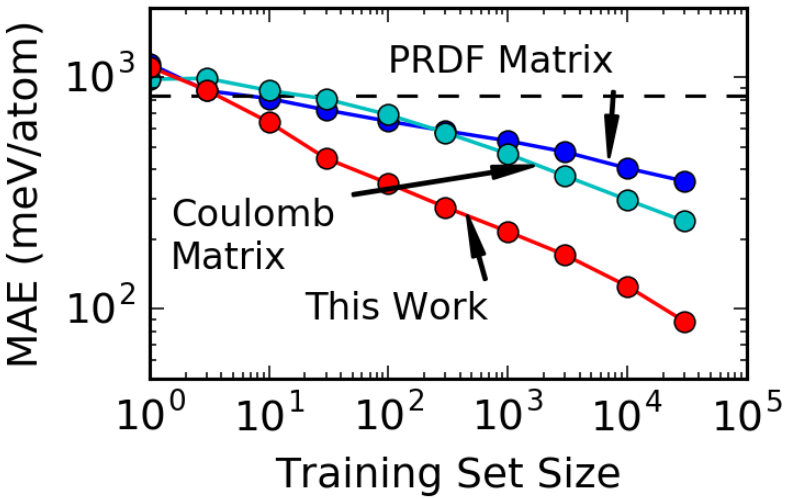
Route #2: Structure-Based Models

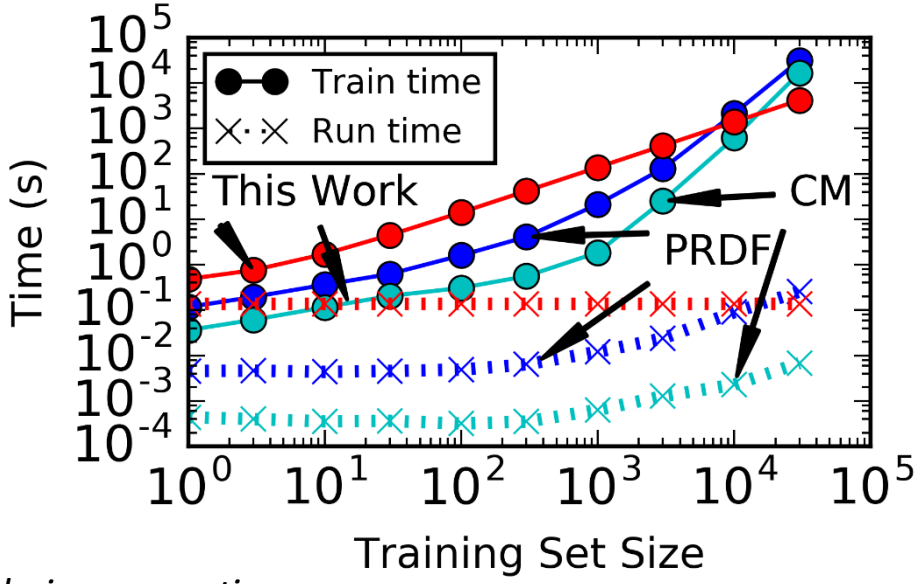
Goal: Predict composition *and* structure

Approach:

1. Compute Voronoi tessellation
2. Assess atomic environments
3. Link to ΔH_f with ML



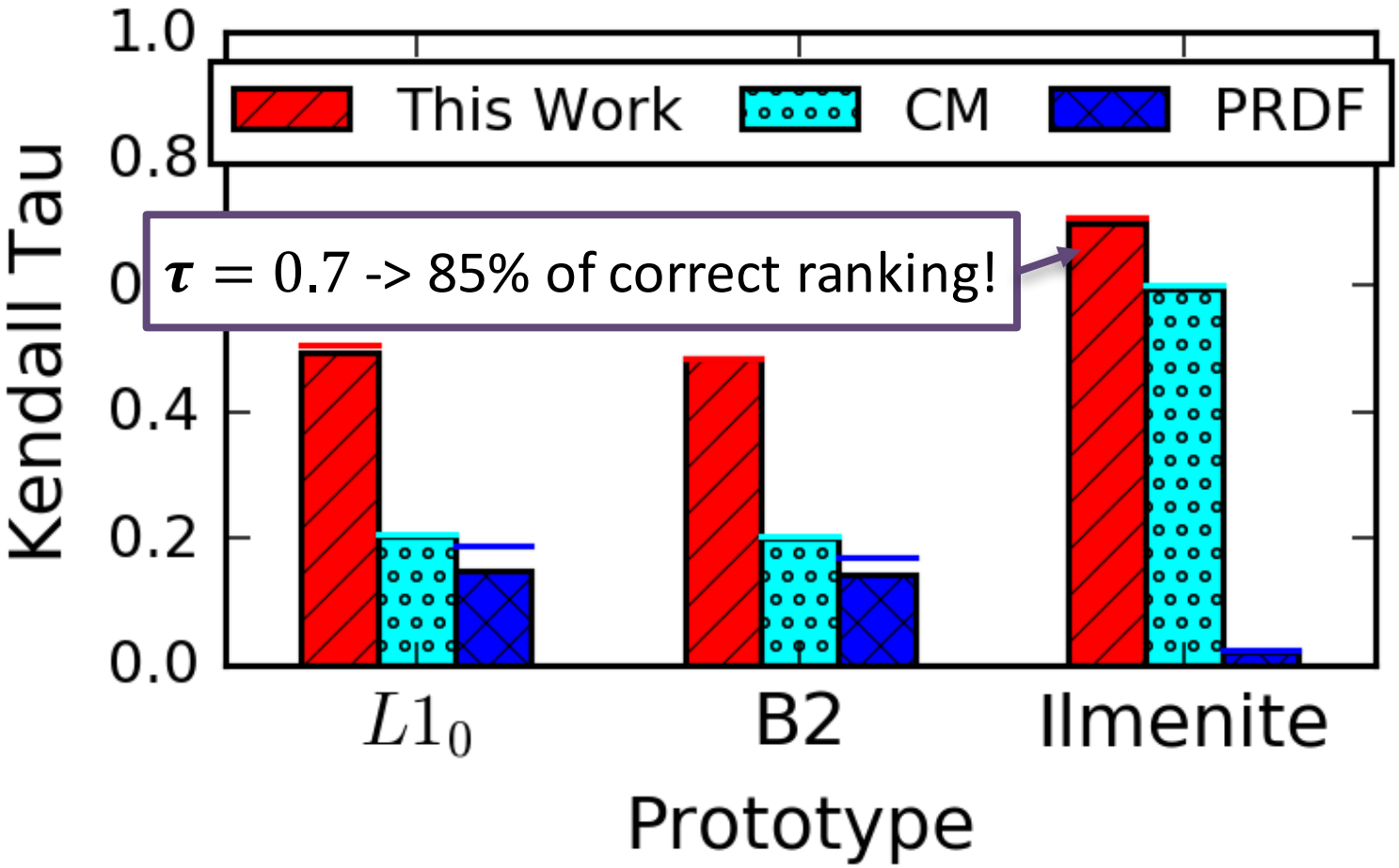




Ref: Ward *et al.*, *in preparation*

Route #2: Ranking Unseen Compounds

Test: Train on ICSD, rank prototypes by ΔH_f



Summary

- The OQMD: a high-throughput DFT database of materials
- Open access at www.oqmd.org; *qmpy* available on `GitHub`
- Discover new materials by screening prototypes and using ML
- ML tools for materials science: Magpie (https://bitbucket.org/wolverton/magpie)
- Materials property predictor (http://oqmd.org/static/analytics/composition.html)

→ **platform for accelerated materials discovery and design!**

For more details about OQMD:

J. E. Saal et al., *JOM* **65**, 1501-1509 (2013)
[featured on JOM cover!]

S. Kirklin et al., *npj Computational Materials* **1**, 15010 (2015)
[featured on the website!]