Accelerating the Design of Battery Materials by High-Throughput ab initio Calculations and Machine Learning

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Gian-Marco Rignanese

M ERA NET 3: international matchmaking event on battery materials
28 April 2021

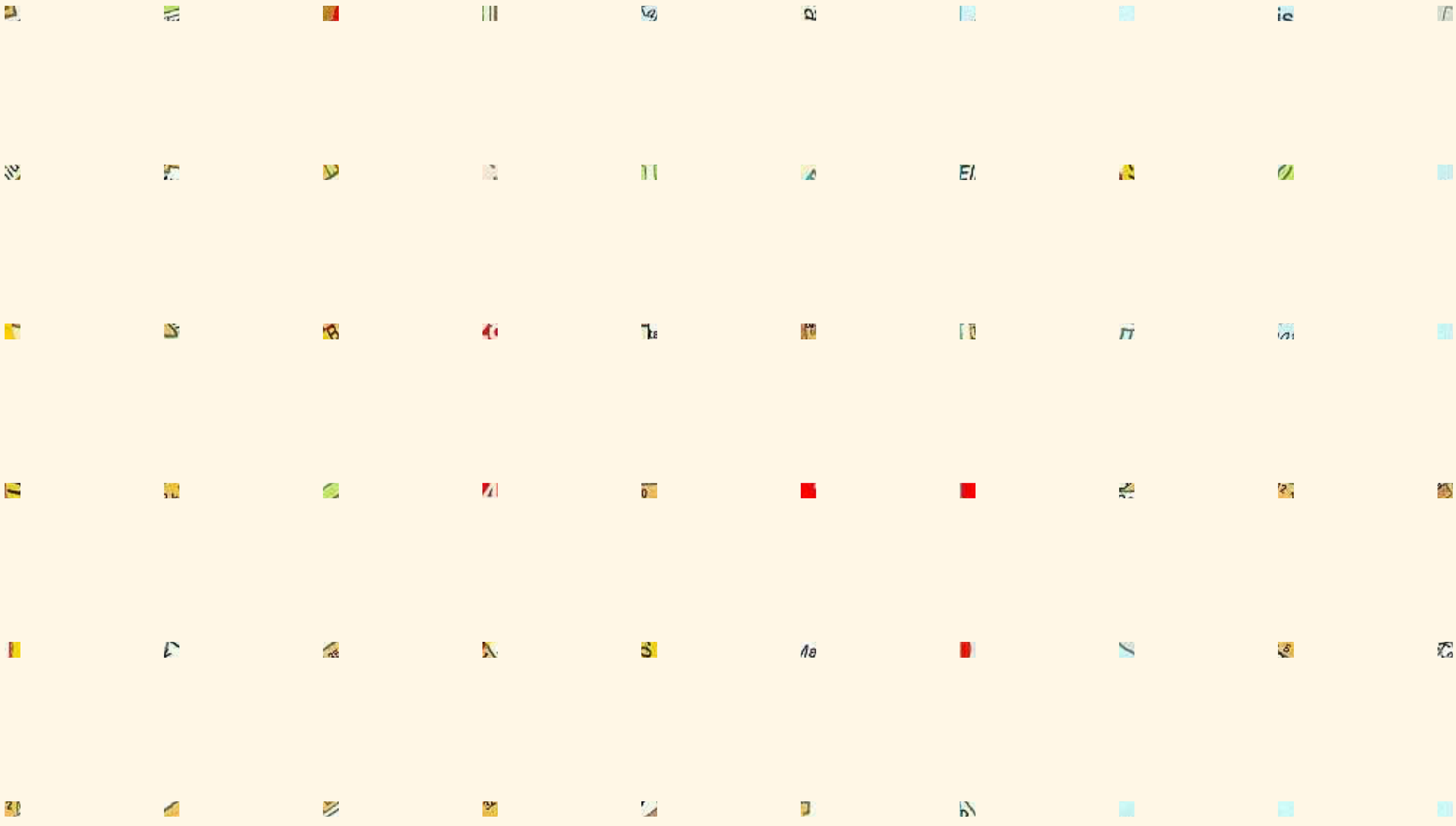
How can one find materials with targeted properties in the information age?

Google

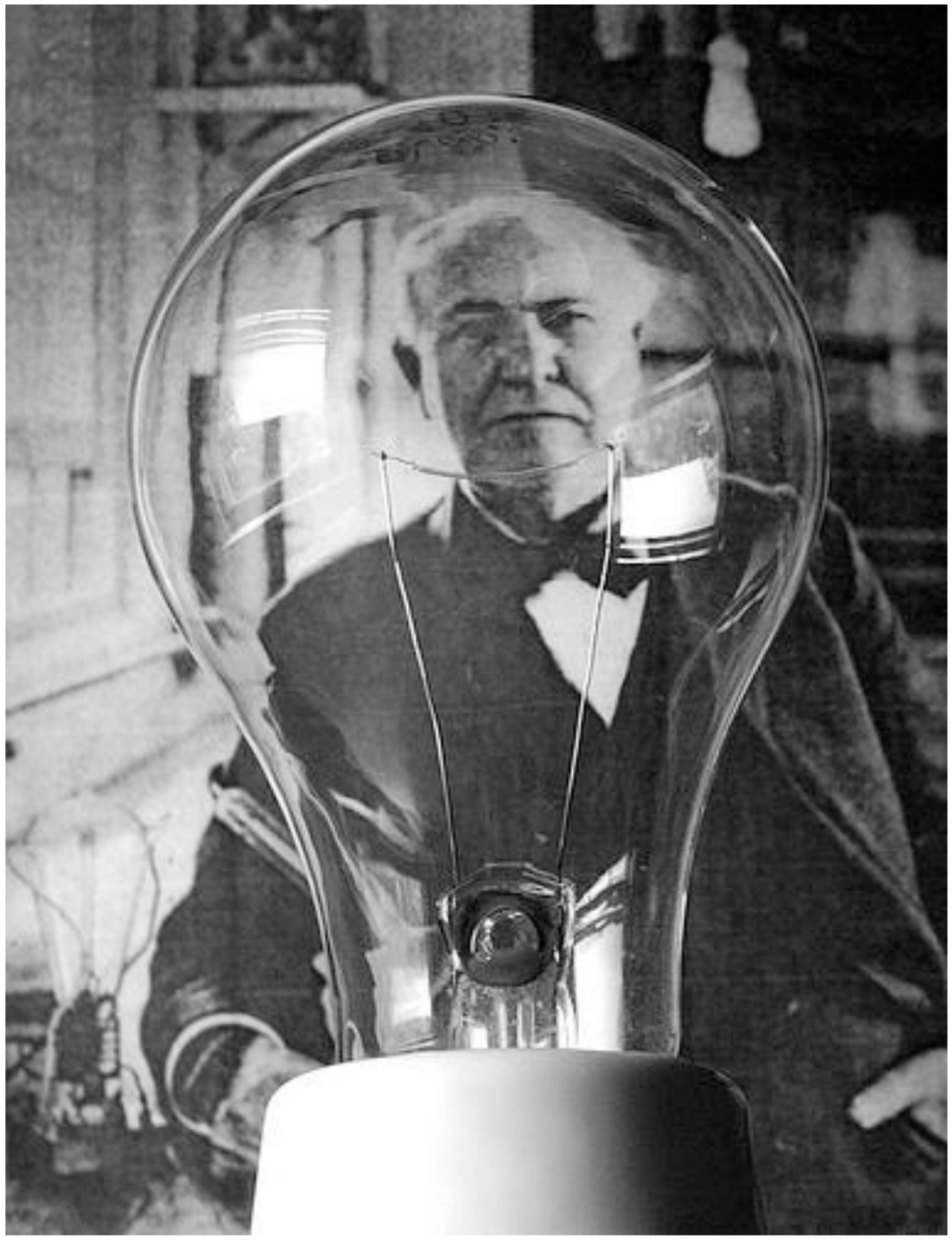
good battery material

Google Search | I'm Feeling Lucky

Materials properties are not known very well...
The typical coverage is below 1 %

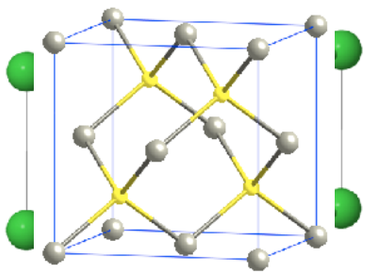


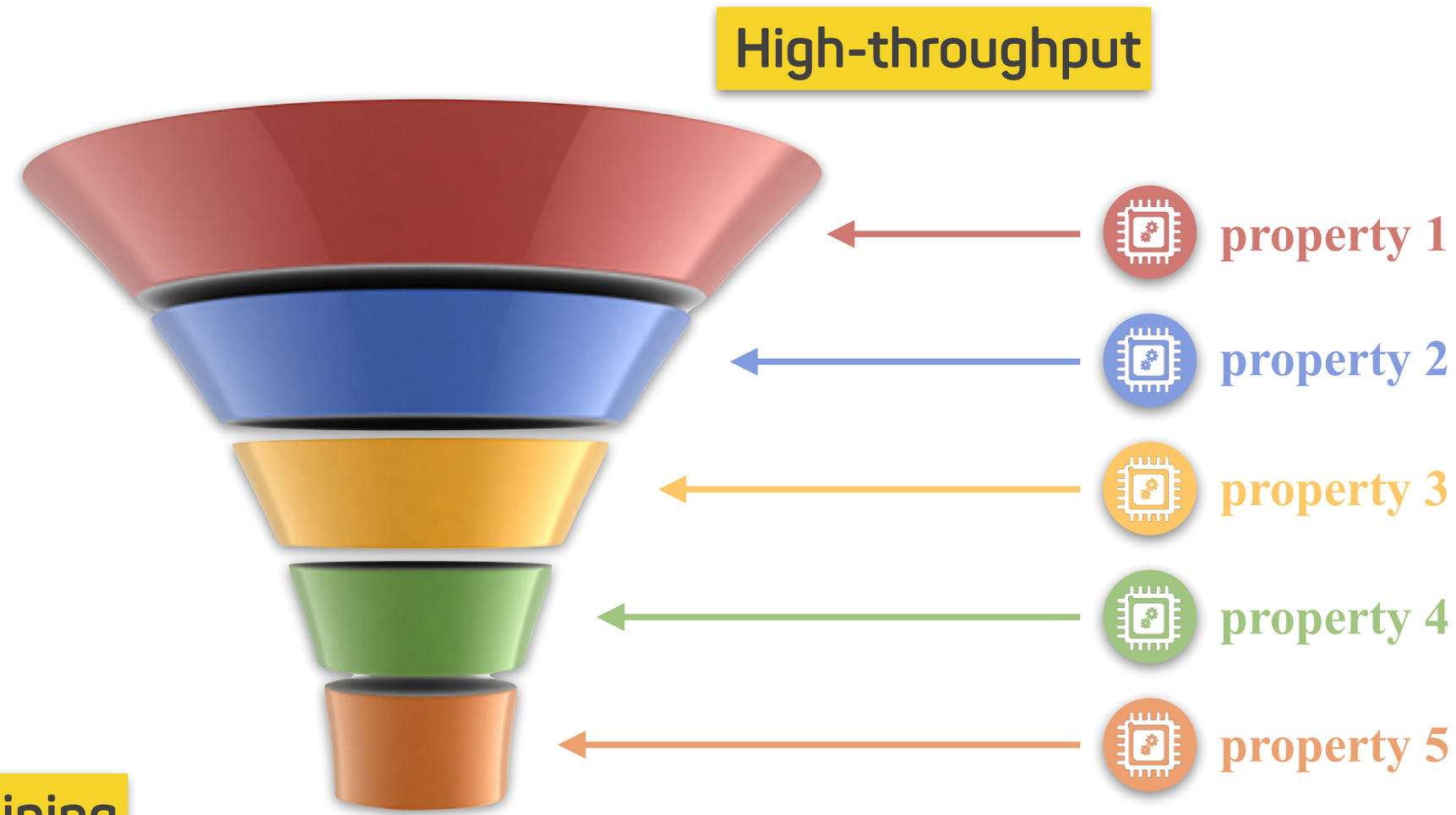
Experimental materials design often proceeds by trial and error



High-throughput ab initio materials design

Consider as many compounds as possible, typically O (10^3) → O (10^5)

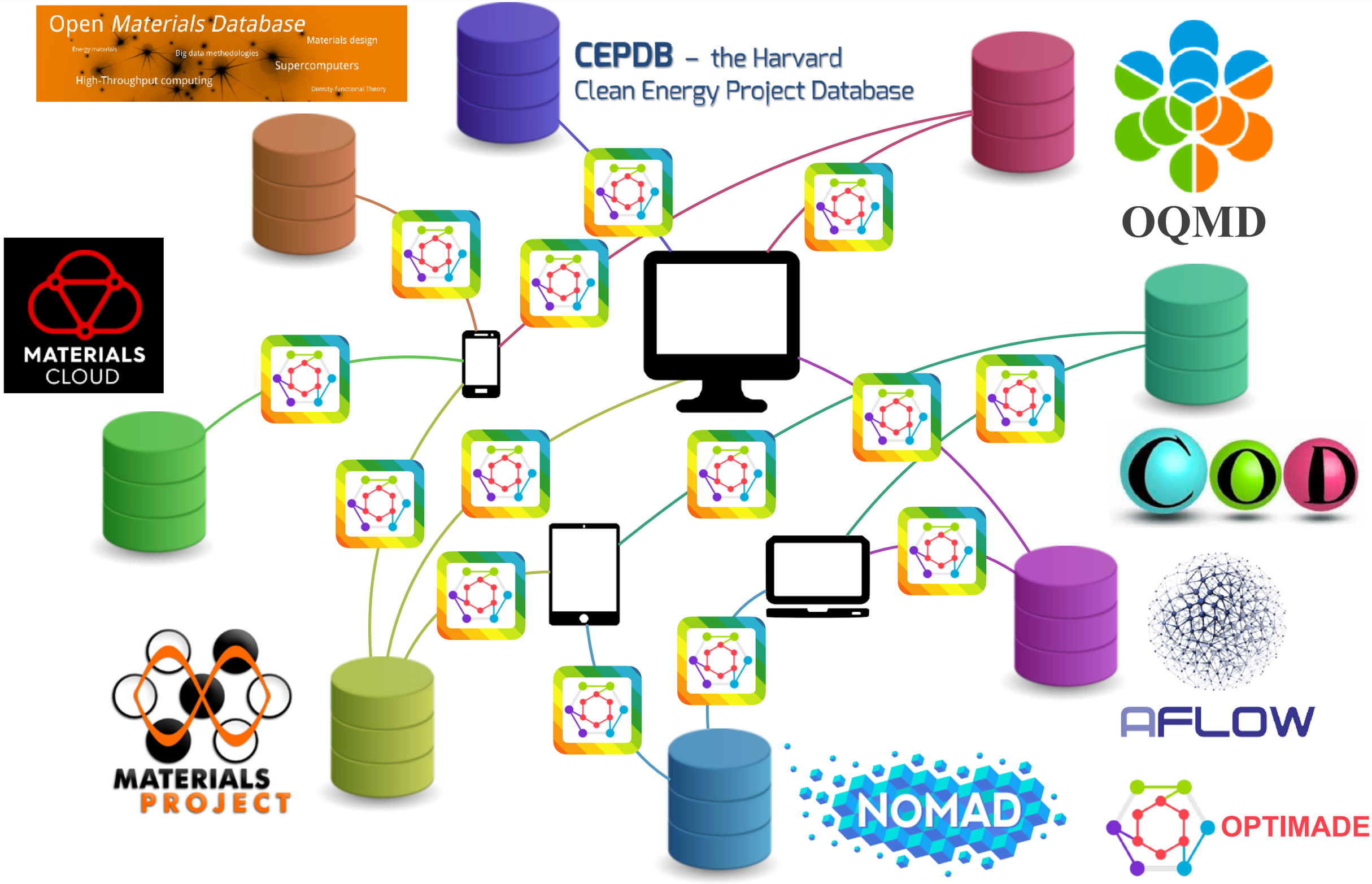




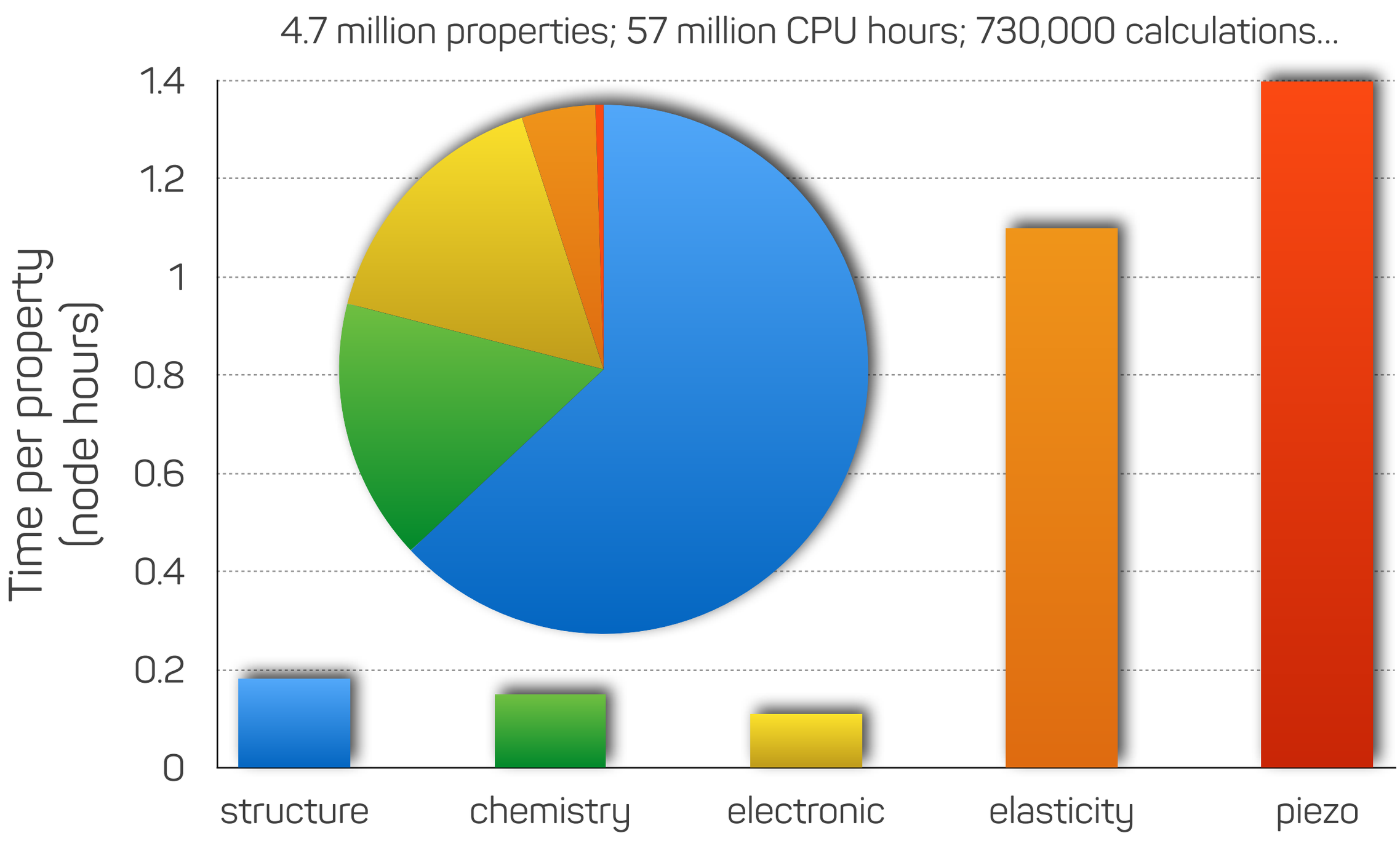
Data-Mining

O (10^1) → O (10^2) compounds

Many materials DBs have become available online which can be queried with the same API



Predicting different properties requires very different computing time



This is where the power of machine learning has become very handy

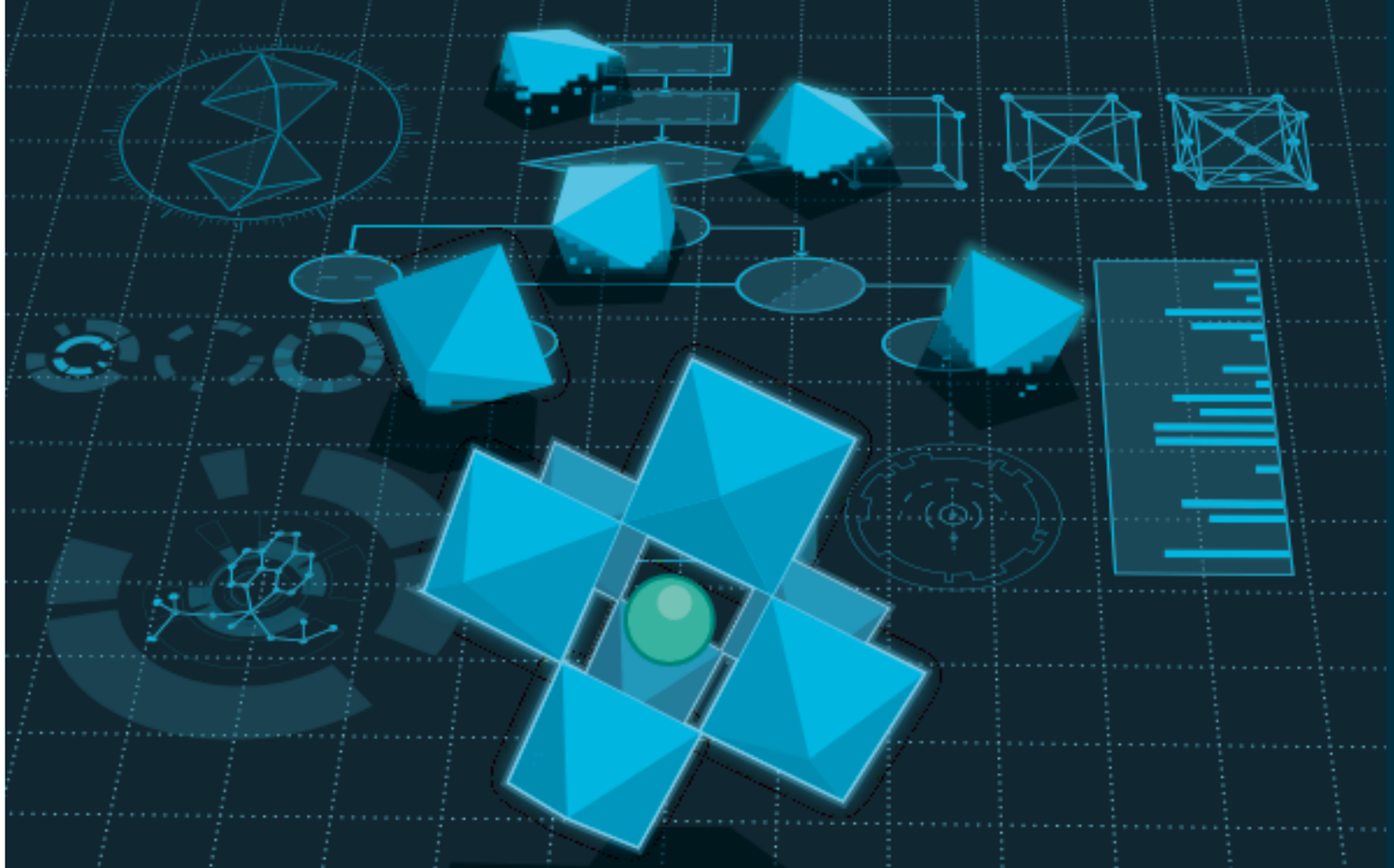
NEWS FEATURE

[N. Nosengo, Nature **566,** 475 (2016)]

THE MATERIAL CODE

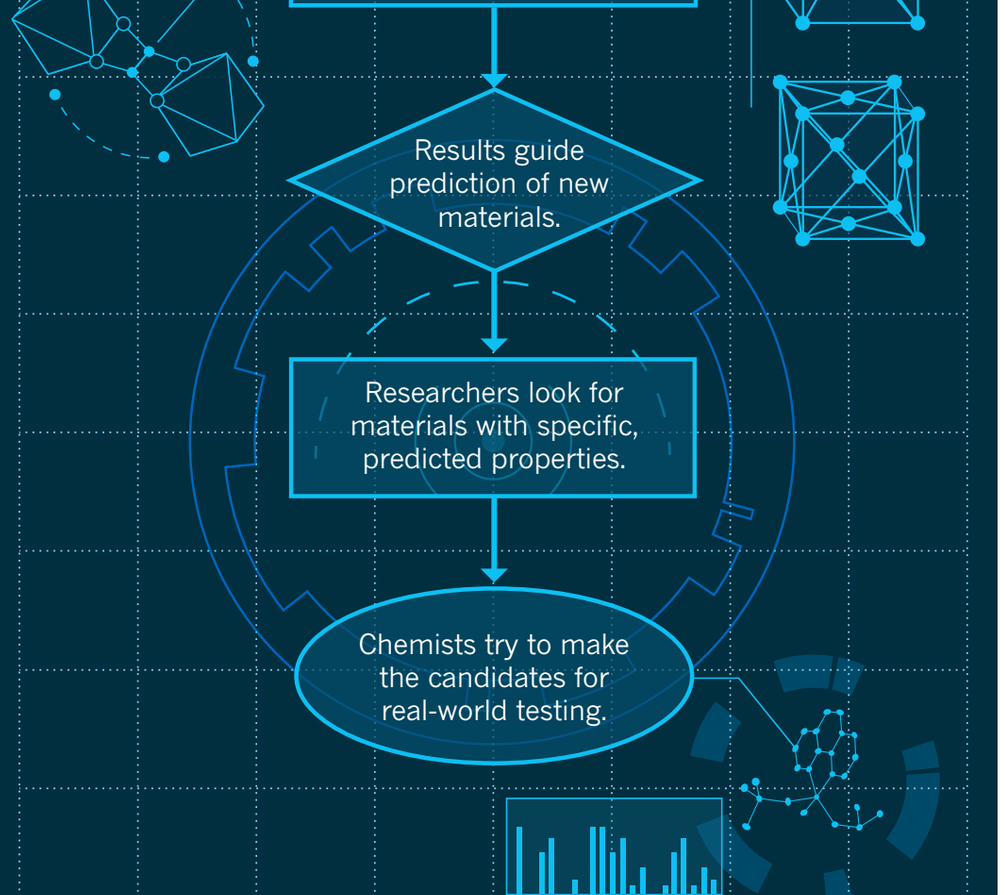
Machine-learning techniques could revolutionize how materials science is done.

BY NICOLA NOSENGO



INTELLIGENT SEARCH

Artificial intelligence can help researchers to comb through vast numbers of materials to find just the ones they need for the application at hand.

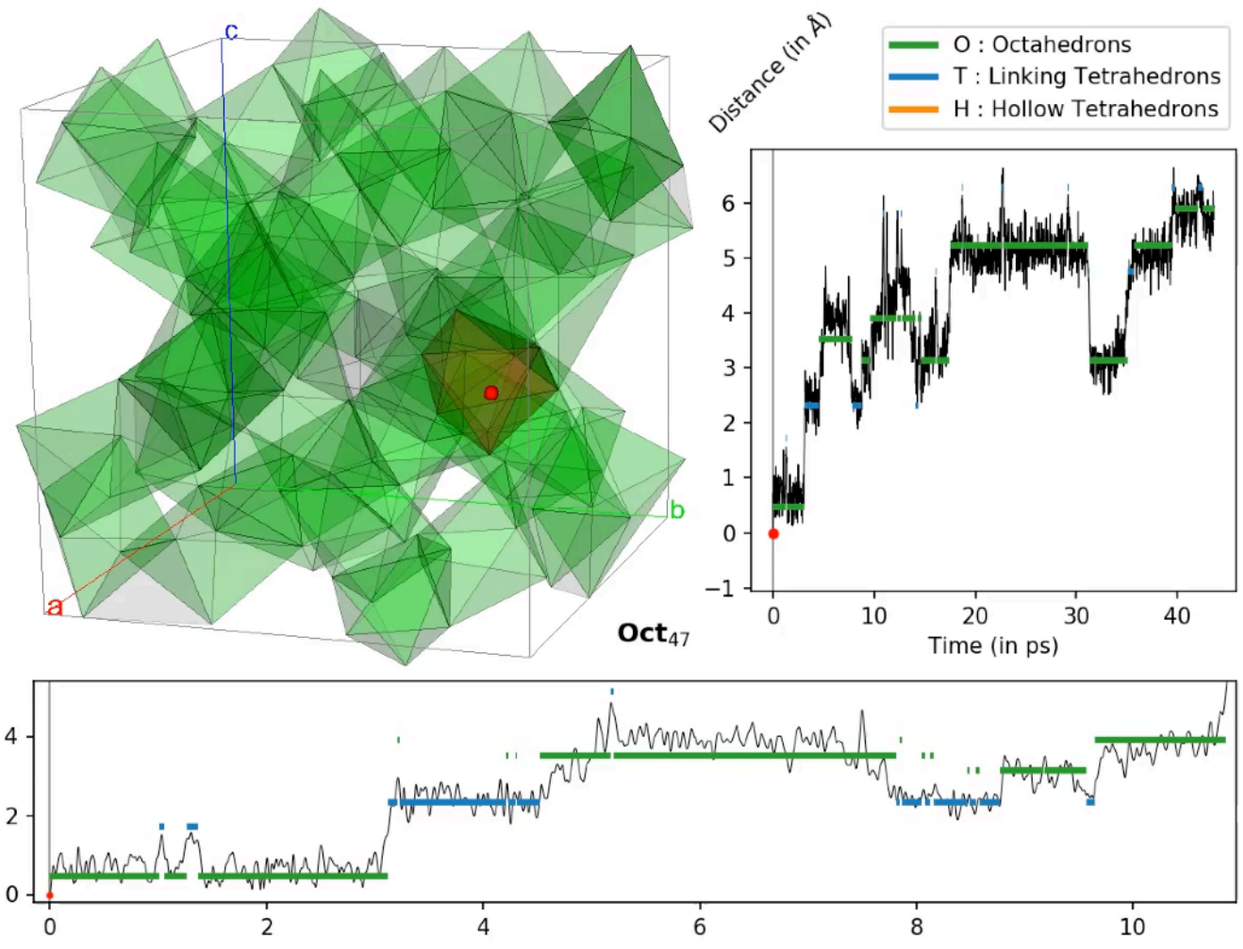


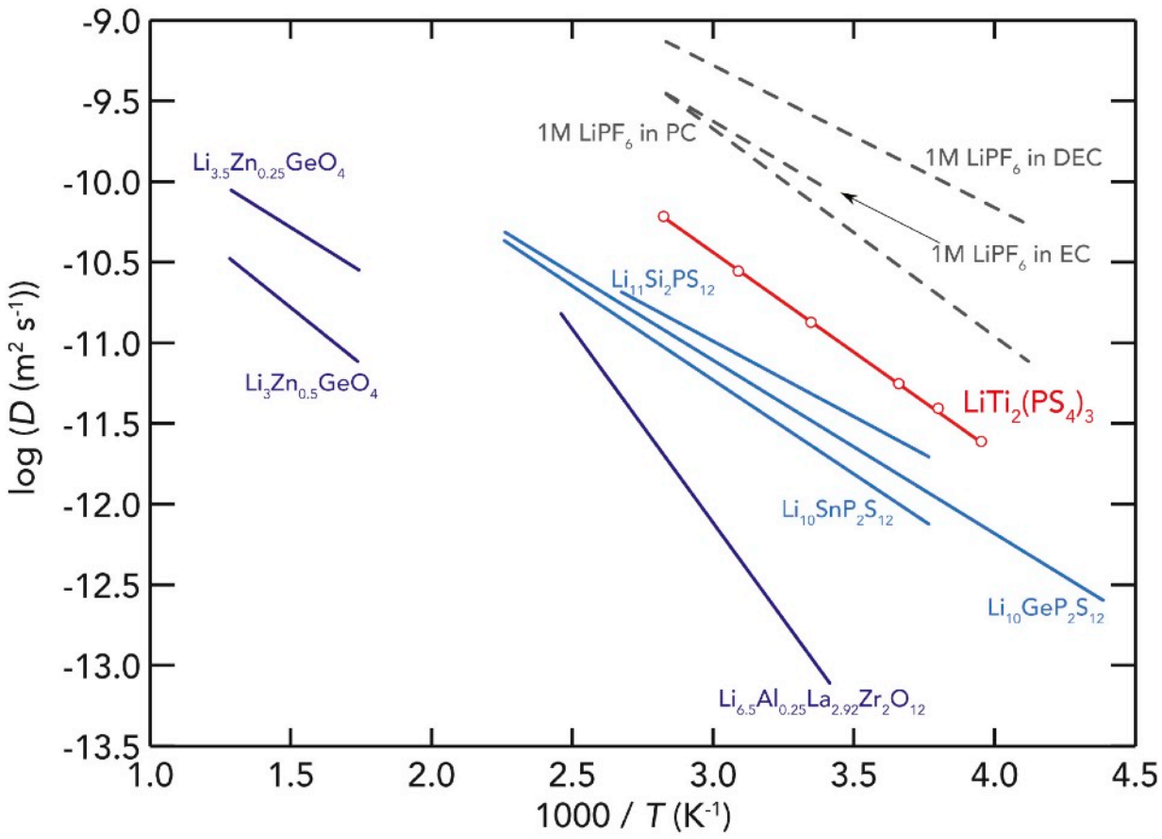
Modelling battery materials:

The example of solid-state electrolytes

Ab initio molecular dynamics can be used to study the diffusion of Li in the bulk

Mean squared displacement and diffusion coefficient $D = \frac{\Delta \mathrm{MSD}}{6\Delta t}$





New high-conductive battery material predicted and then synthesized.

G. Hautier and co-workers, Chem, **5**, 2450 (2019).

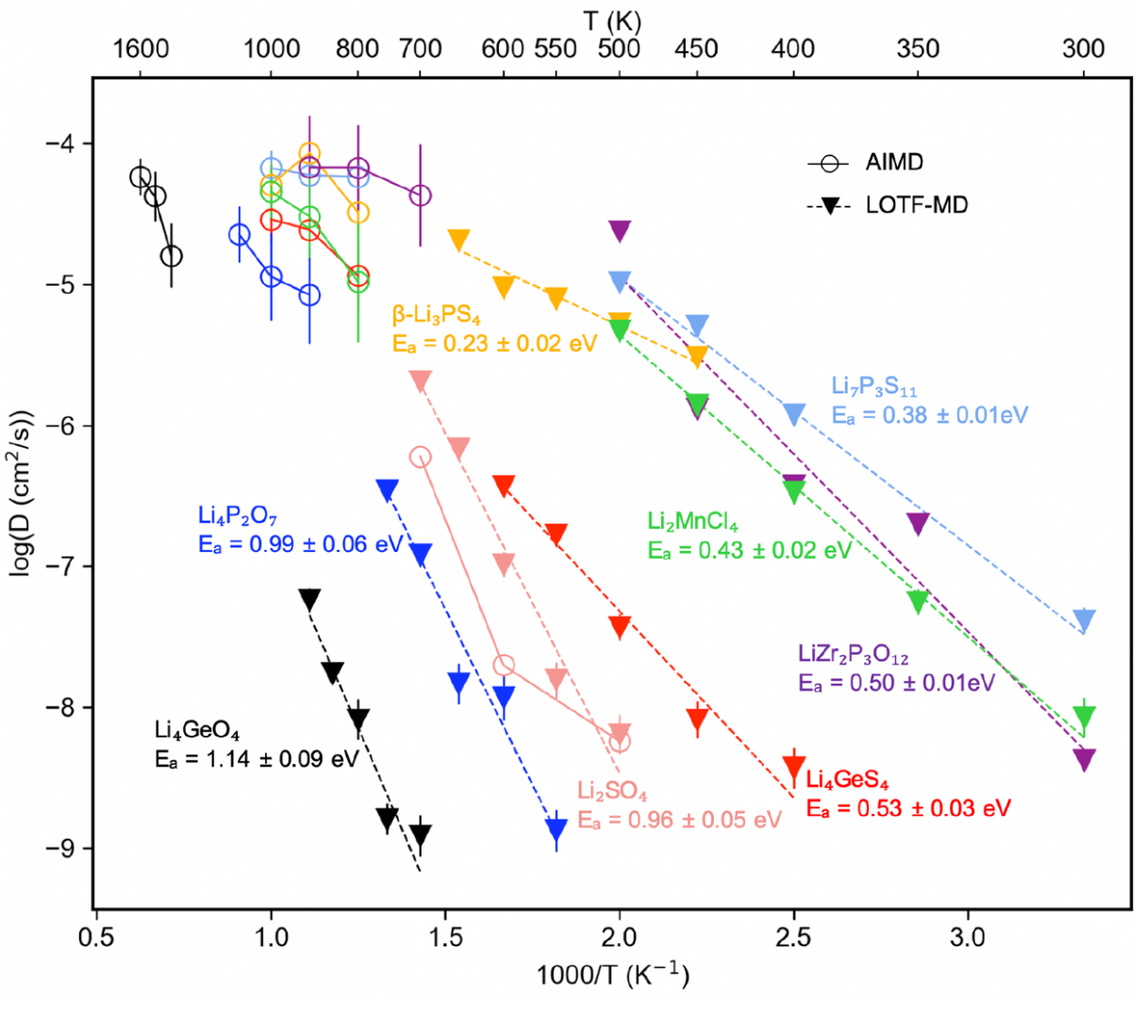
Machine-learned potentials make it possible to simulate much more realistic and complex systems

CHEMISTRY OF MATERIALS

Lithium Ion Conduction in Cathode Coating Materials from On-the-Fly Machine Learning

Chuhong Wang, Koutarou Aoyagi, Pandu Wisesa, and Tim Mueller*

Cite This: *Chem. Mater.* 2020, 32, 3741−3752 Read Online



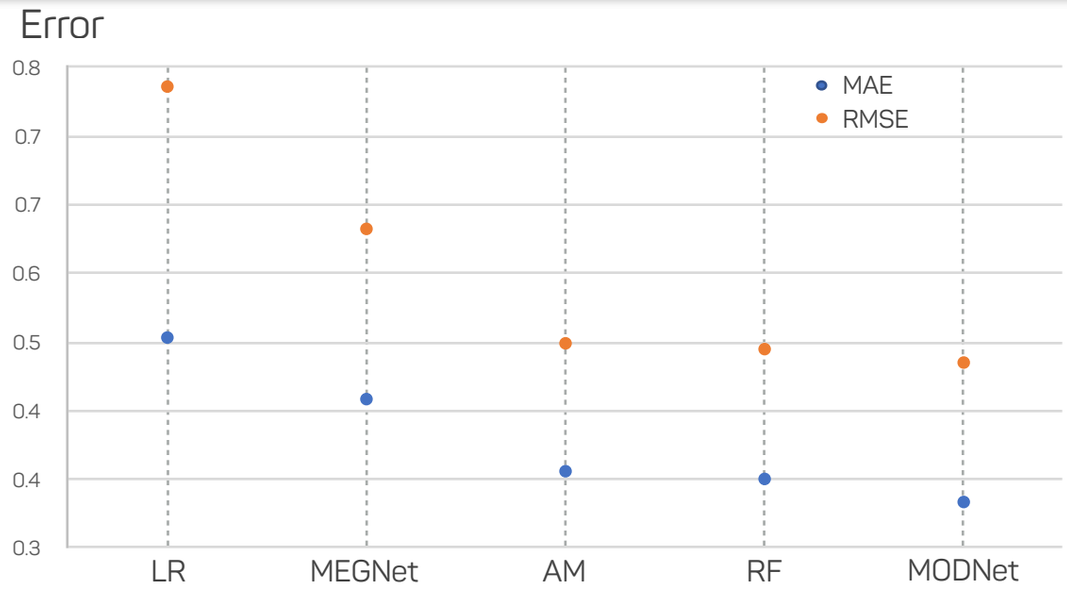
method	total CPU hours	MD time (ns)	production/cost (ns/CPU hour)
AIMD	2 3291	3.75×10^{-4}	1.61×10^{-8}
LOTF - MD	7186	1388	1.88×10^{-1}

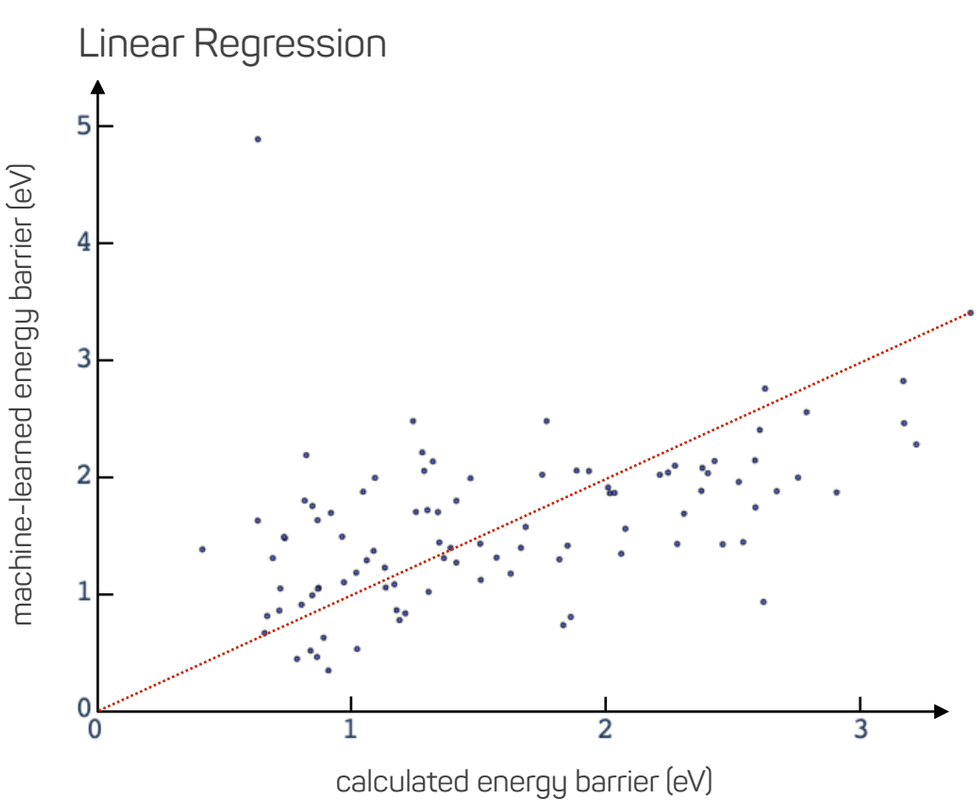
		experimental	high-T AIMD			
MP entry id	composition	E_a (eV)	T (K)	R^2	$E_a \pm$ stderr (eV)	ΔE_a
mp-10499	$LiZr_2P_3O_{12}$	0.59[72]	700−900	0.81	0.13 ± 0.32	−0.46
mp-30249	Li_3GeS_4	0.52[73]	800−1000	0.92	0.31 ± 0.23	−0.21

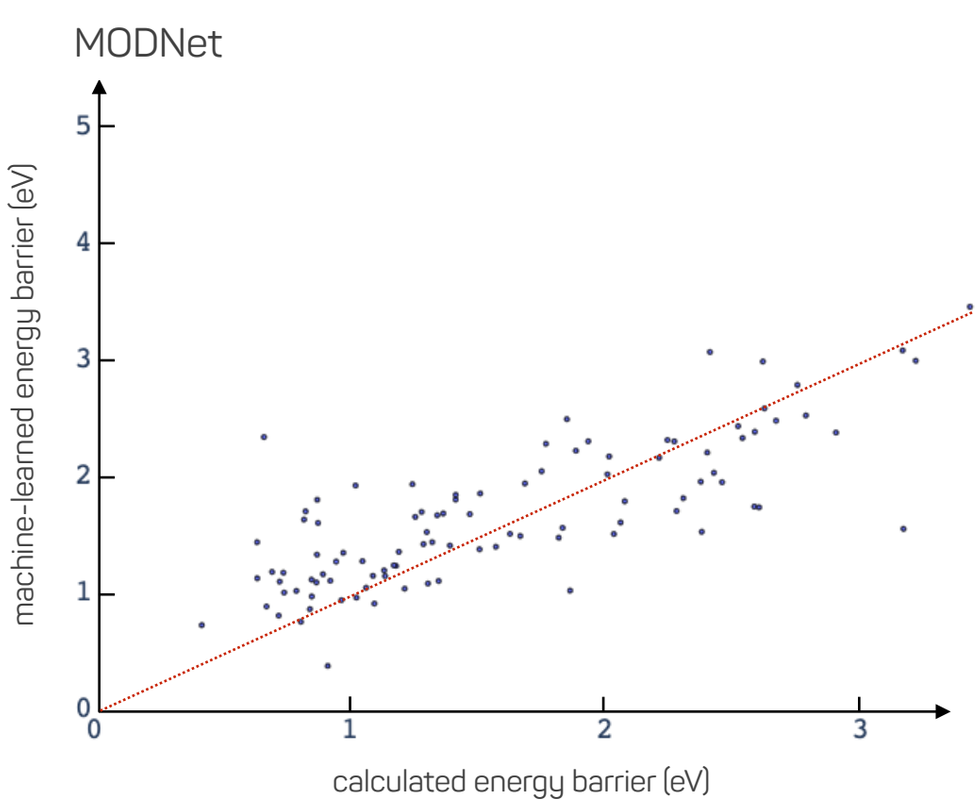
		experimental	LOTF − MD			
MP entry id	composition	E_a (eV)	T (K)	R^2	$E_a \pm$ stderr (eV)	ΔE_a
mp-10499	$LiZr_2P_3O_{12}$	0.59[72]	300−500	0.94	0.50 ± 0.01	−0.09
mp-30249	Li_3GeS_4	0.52[73]	400−600	0.97	0.53 ± 0.03	−0.01

Machine learning can also be used to predict diffusion energy barriers directly

- Linear Regression
- Random Forest
- MEGNet
- MODNet
- Automatminer

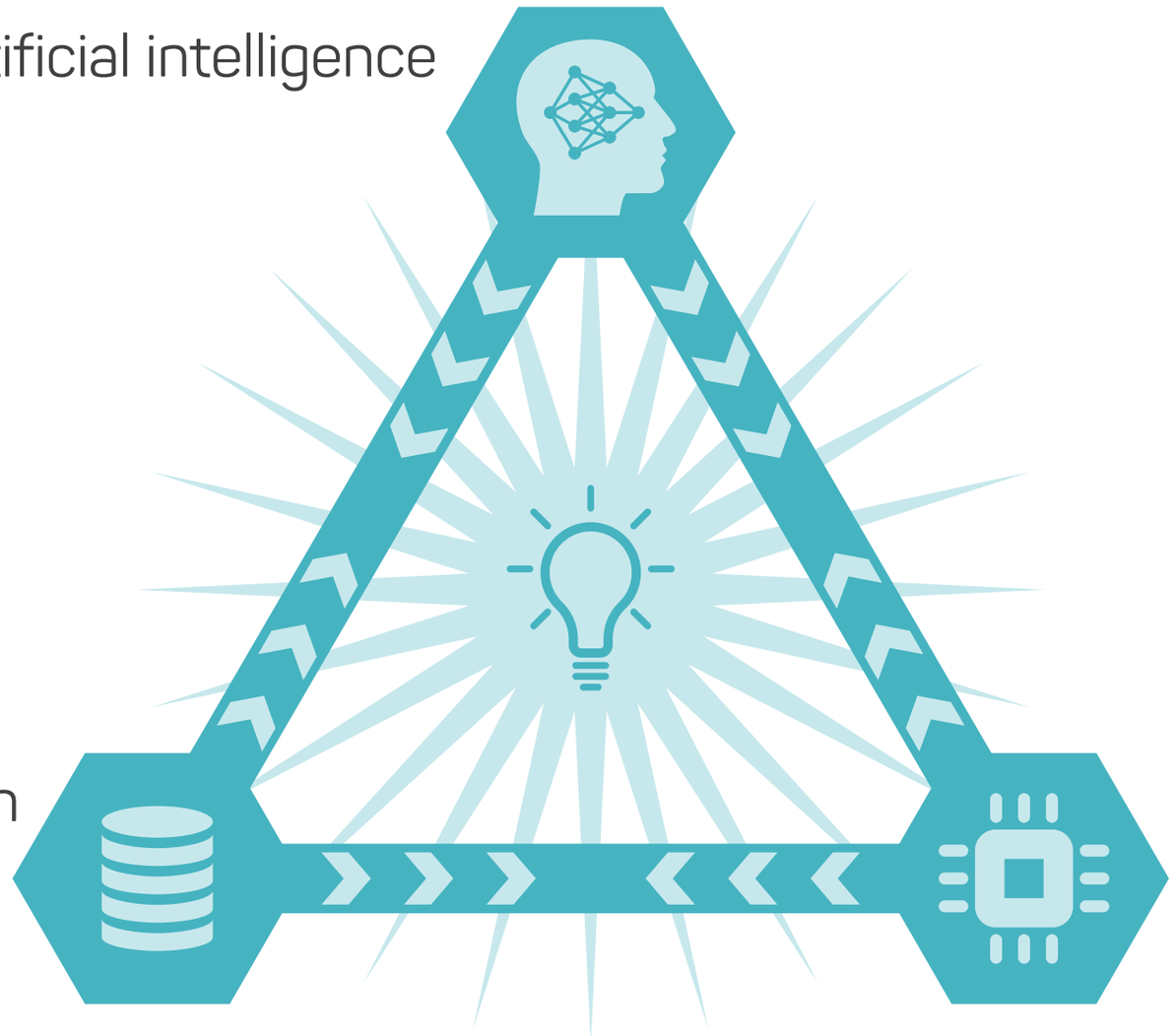






HT ab initio computing and ML can help discover battery materials with specific properties

- Artificial intelligence



- Data consolidation
- High-Throughput simulations

A few references

BASF
We create chemistry

TOYOTA

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