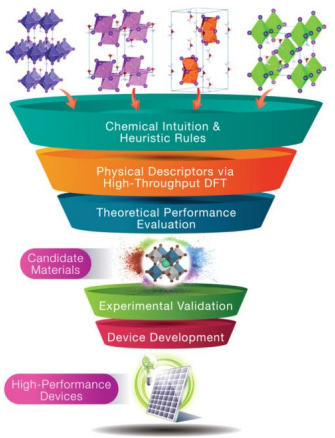
How can atomistic simulations contribute to the energy and climate transition ?

Chris Erik Mohn
UiO



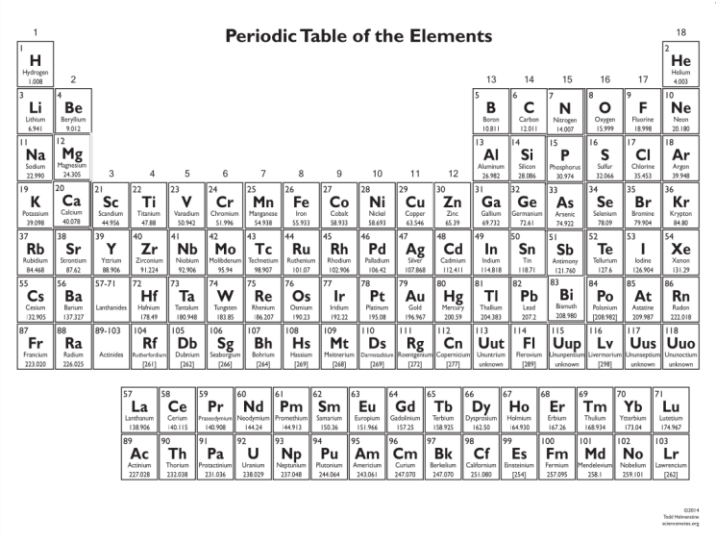




Discovery and **E**xploration of **N**ovel materials for **T**andem solar cells

UiO:Energy and Environment

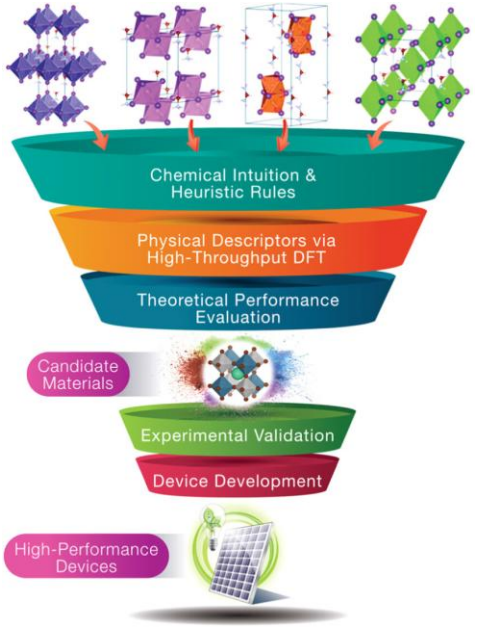
Chemical space



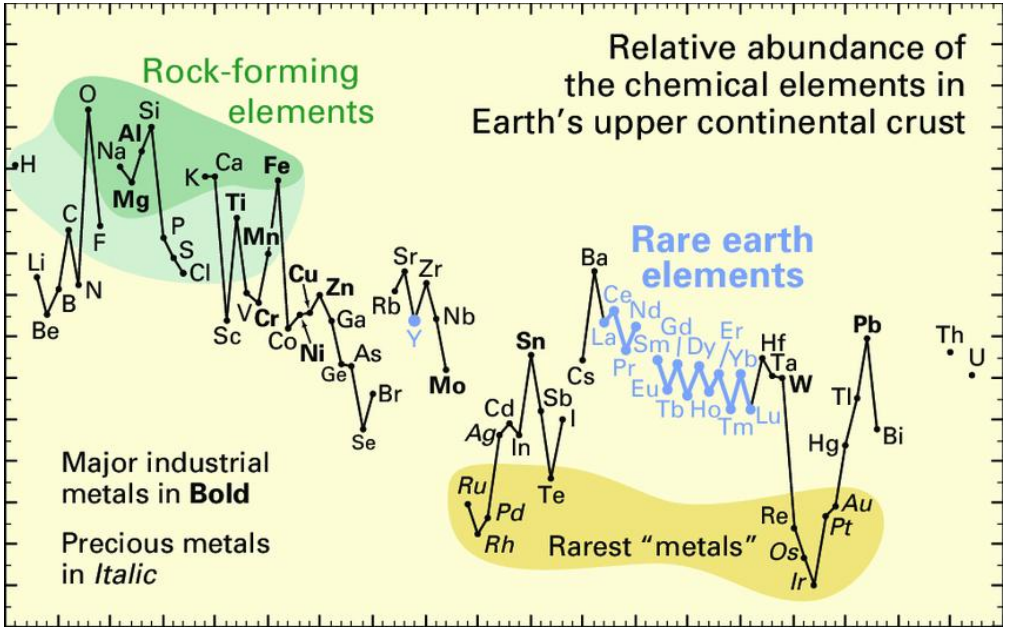
$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

n choose k

The number of ways to choose k elements from a set of n elements



Chemical space





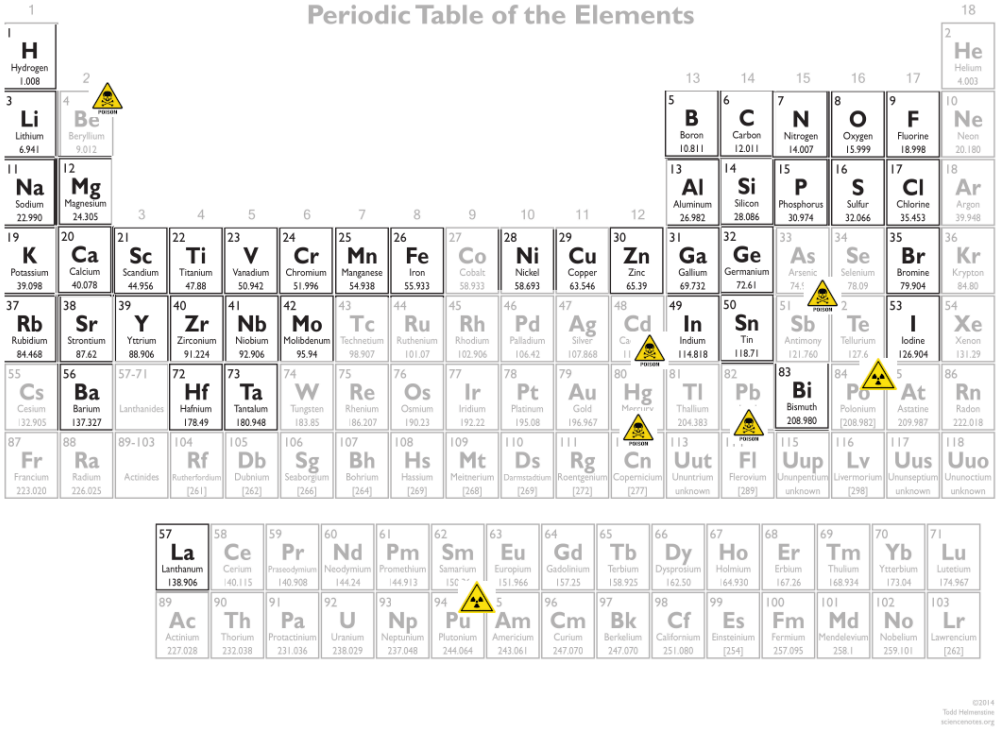








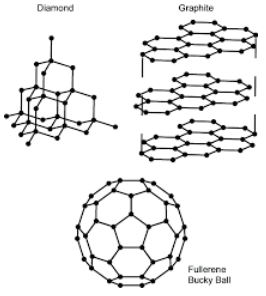
Chemical space



$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

n choose k

The number of ways to choose k elements from a set of n elements

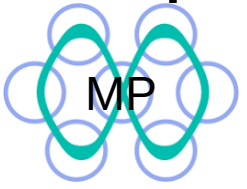


Strategies to predict new materials

(e.g. solar cells or batteries)

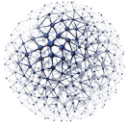
- Scan databases/literature to find candidates
- Use databases to predict new compounds







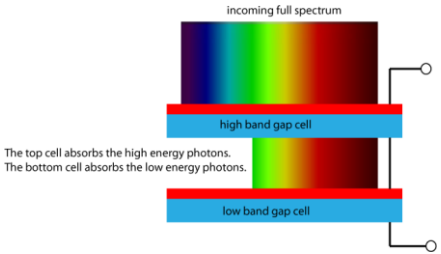
OPTIMADE
Open Databases Integration
for Materials Design



AFLOW
Automatic - FLOW for Materials Discovery



High throughput material screening
(nitrides for tandem solar cells)

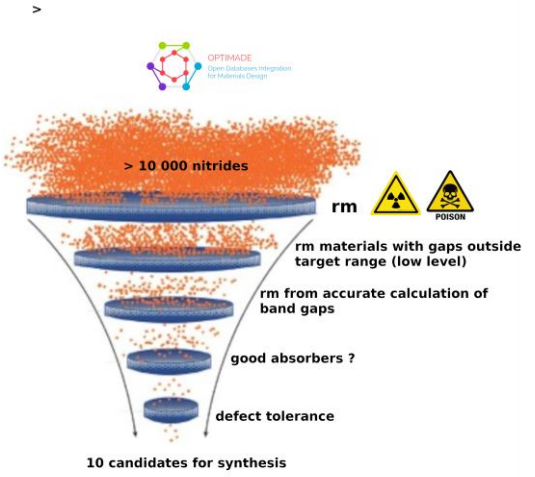


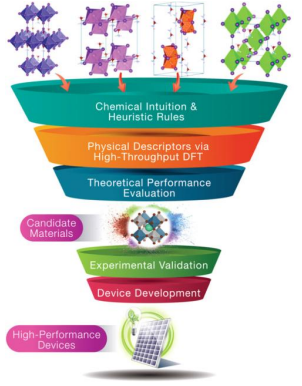


Selection Metric

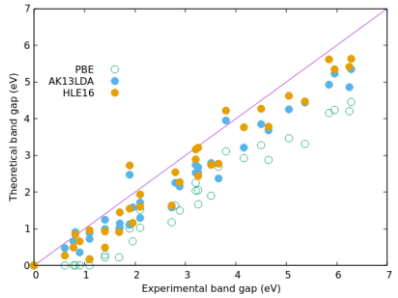
1. Band gap ~ 1.7 eV
2. Good flow of el./holes
3. Good abs. of sunlight
4. Defect tolerant

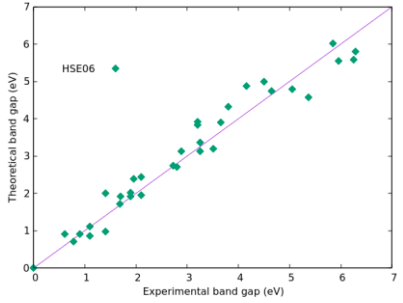
etc.

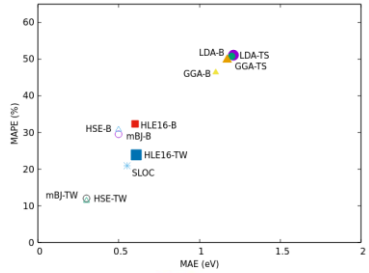


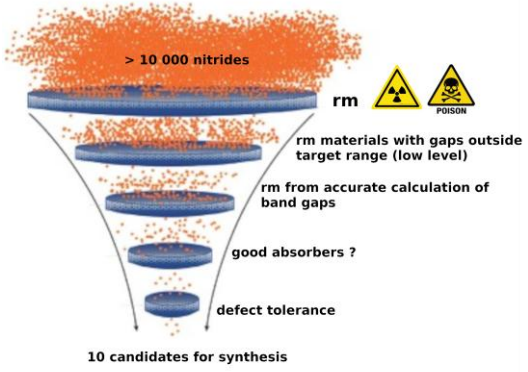


Database quality (low level DFT)

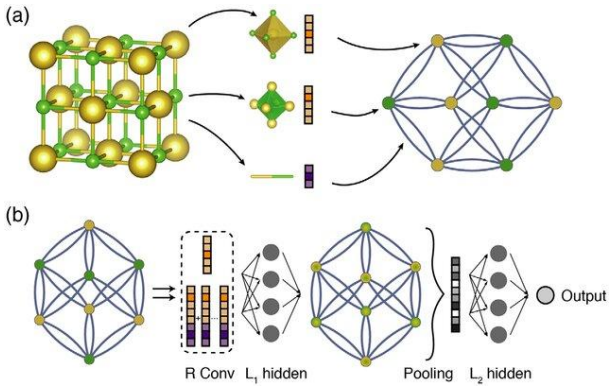








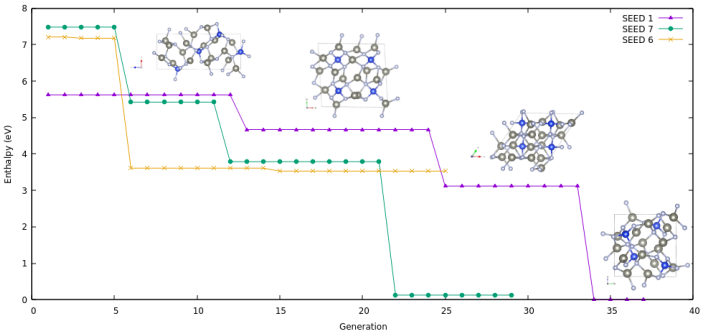
Predict entirely new candidates using NN and GA



Crystal graph convolutional neural network

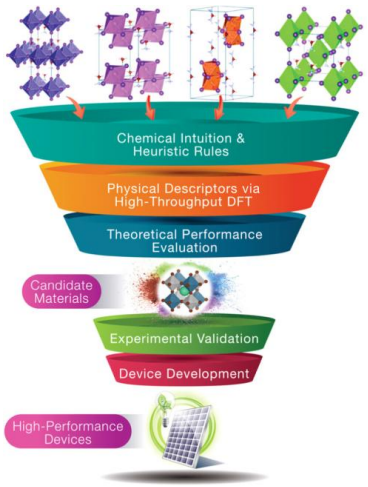
Xie and Grossman, PRL, 120, 145301 (2018)

GA to predict the structure of Zn_4SiN_4

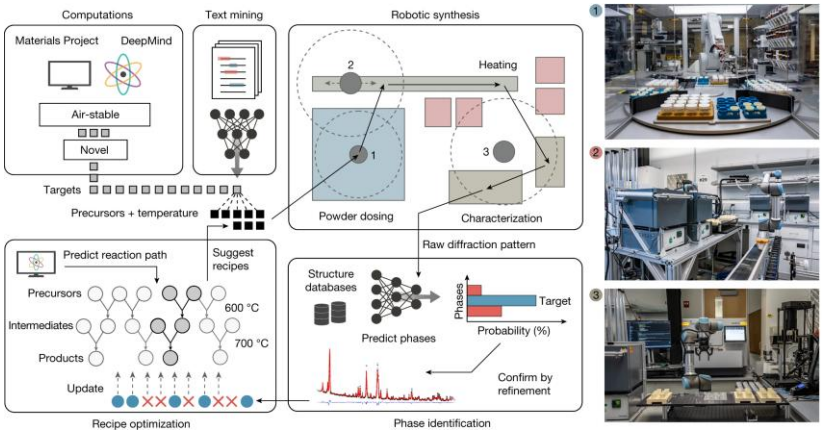


DENT work in progress

Bottlenecks in material developments



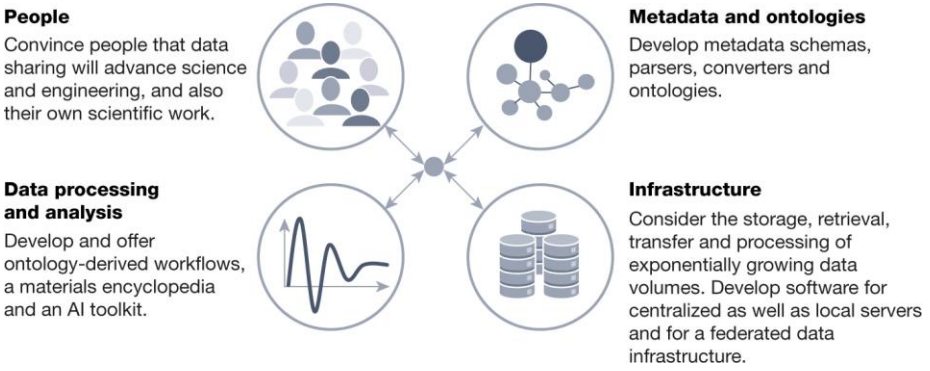
The A-lab (Berkely lab): An autonomous laboratory for the solid-state synthesis of inorganic powders



N.J.Szymanski *et al.* Nature, **624**, 86-91 (2023)

Bottleneck in FAIR data enabling

- FAIR (Findable, Accessible, Interoperable, Reusable)
- FAIR (Findable and AI ready)



M.Scheffler *et al.* Nature, **604**, (2022)

CoC

- Code of conduct to ensure transparency in supply chain and ethical standards



Thank you!



