Institut des Matériaux de Nantes Jean Rouxel (IMN)
UMR CNRS 6502

From *Crystal Structure Prediction* to Materials Discovery : the case of metastable (oxy)sulfide compounds

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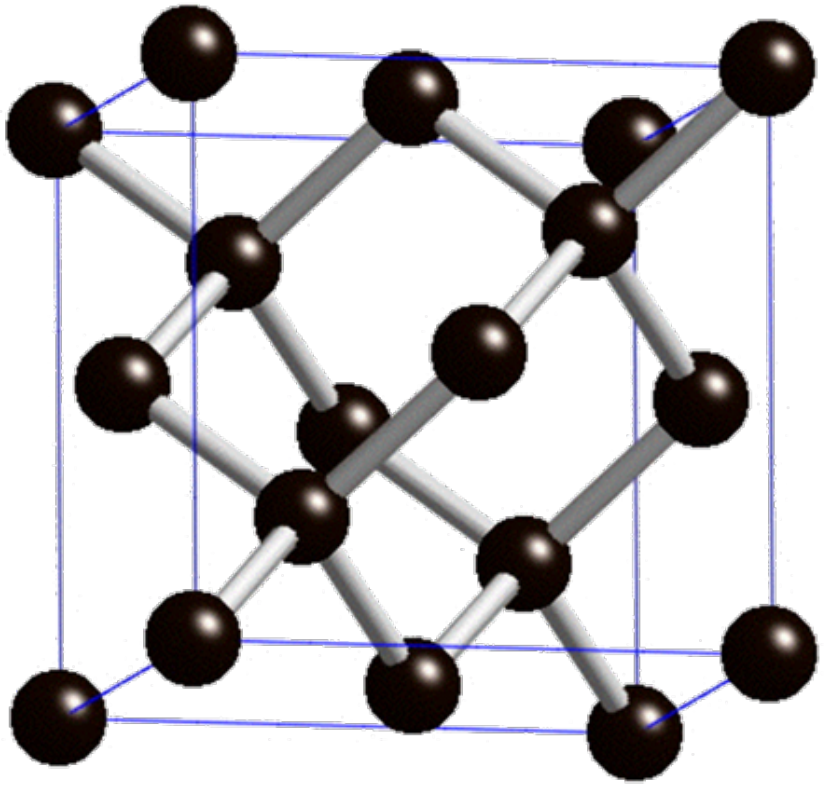
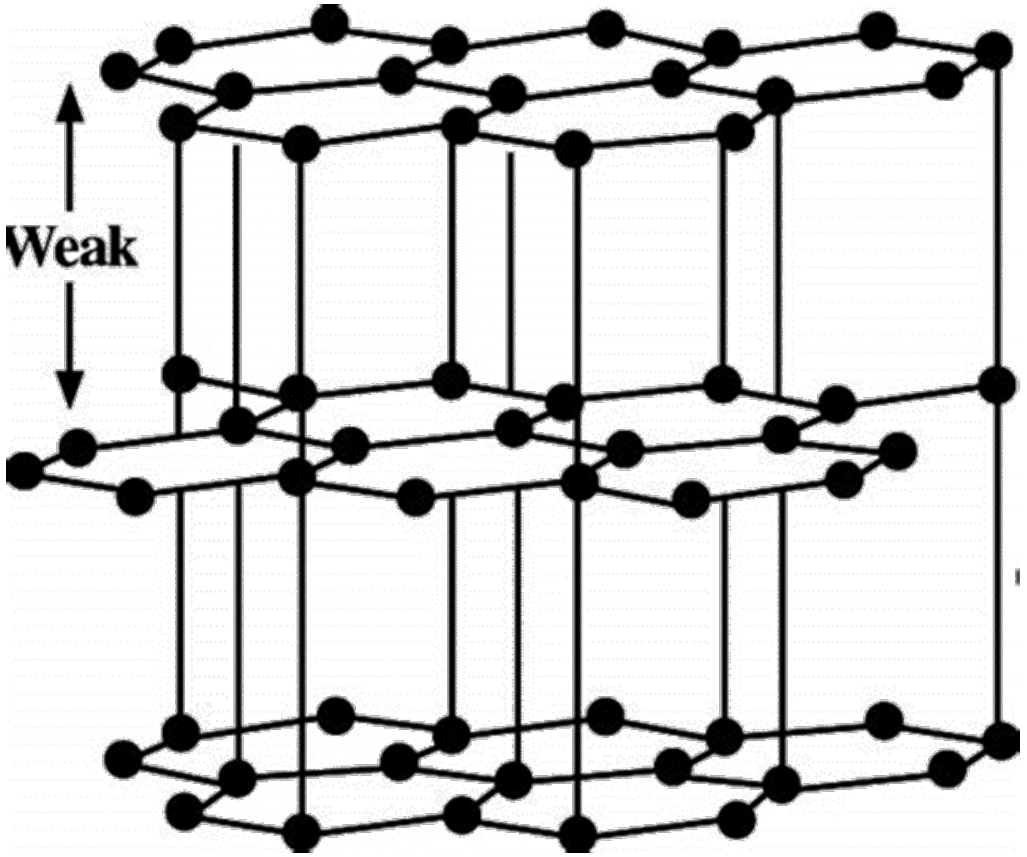
GDR MEETICC Conférence plénière 2023

Latresne - Bordeaux, 30 mai- 2 juin 2023

?

Crystal structure explains crystal properties

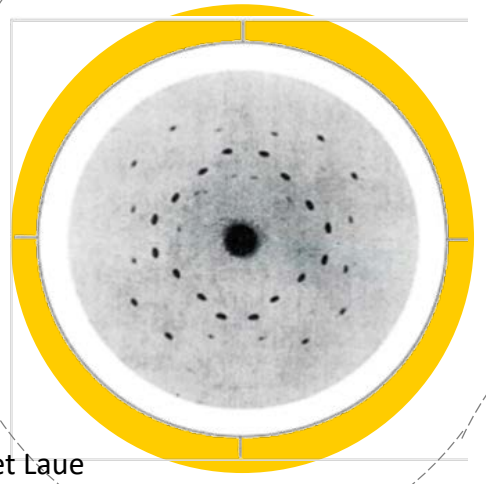




« Seeing is believing » V. Ramakrishnan (NP Chemistry, 2009)

The Nobel Prize in Physics 1914

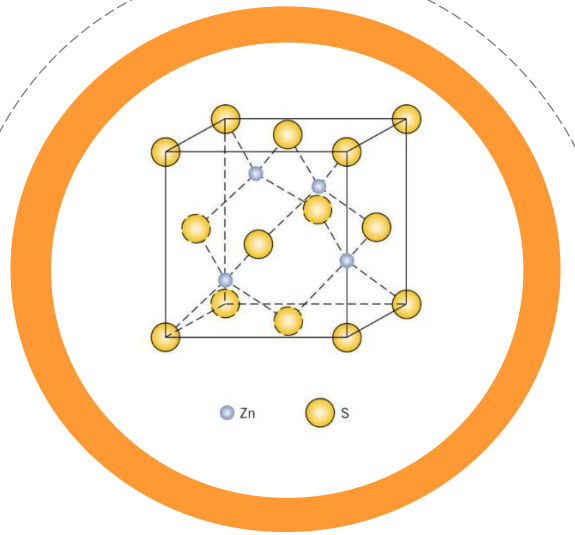
Max von Laue "for his discovery of the diffraction of X-rays by crystals"

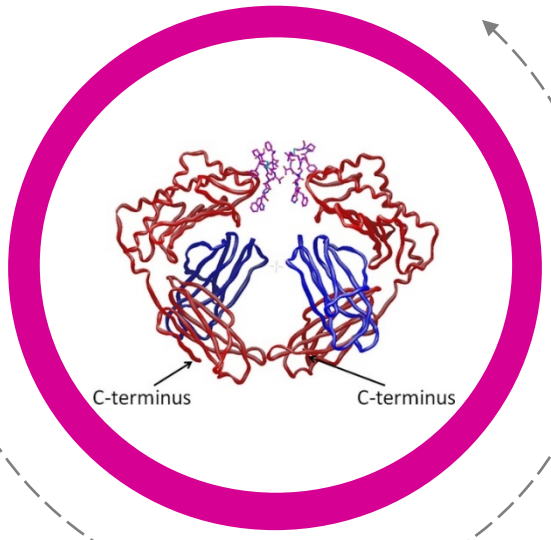


Friedrich, Knipping et Laue
Sitzungsberichte der Kgl. Bayer.
Akad. der Wiss. 1912

The Nobel Prize in Chemistry 2017

Jacques Dubochet, Joachim Frank and Richard Henderson "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution"





The Nobel Prize in Physics 1915

Sir William Henry Bragg and William Lawrence Bragg "for their services in the analysis of crystal structure by means of X-rays"

https://www.nobelprize.org/

?

Crystal Structure Prediction (CSP)

Predict the crystal structure based only on structural formula $A_xB_yC_z$

?

1925

Goldschmidt rules

geometrical restraints

1926

Hume-Rothery rules

1929

Pauling rules

Who would guess ?

Acc. Chem. Res. **1994,** *27,* 309−314

Are Crystal Structures Predictable?

ANGELO GAVEZZOTTI*

Dipartimento di Chimica Fisica ed Elettrochimica, Università di Milano, Milano, Italy

Received May 16, 1994

"No": by just writing down this concise statement, in what would be the first one-word paper in the chemical literature, one could safely summarize the

NATURE VOL. 335 15 SEPTEMBER 1988 NEWS AND VIEWS 201

Crystals from first principles

ONE of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition. Who, for example, would guess that

?

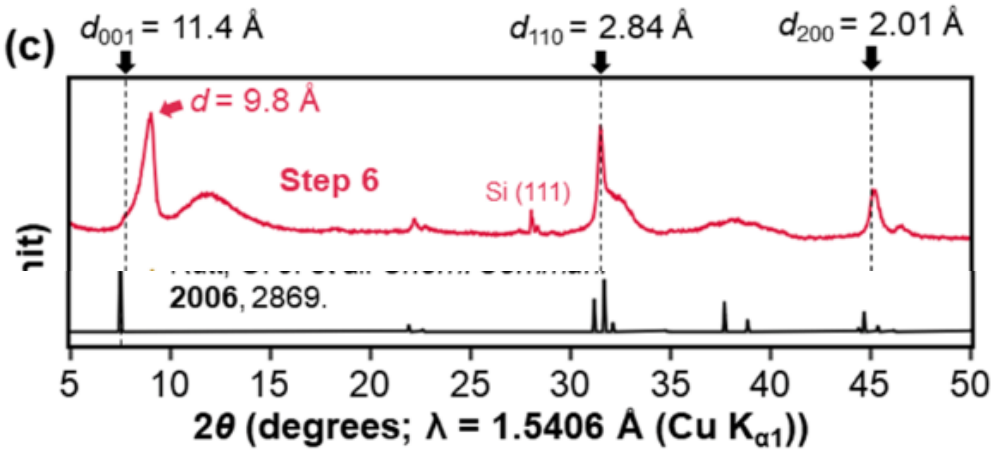
Computational material design to compress time…

"The process of material design and discovery is traditionally long and complex. ***It takes roughly 10 years and upwards of $10 to $100 million on average*** to discover one new material with specific properties.

A. Curioni (IBM Fellow, Vice President of IBM Europe & Africa and Director of the IBM Research Lab in Zurich, Switzerland)

Only about 72% of binary, 16% of ternary, 0.6% of quaternary, and less than 0.05% of more complex systems have ever been studied experimentally.

… key to help experimental structure characterization



https://research.ibm.com/topics/materials-discovery

?

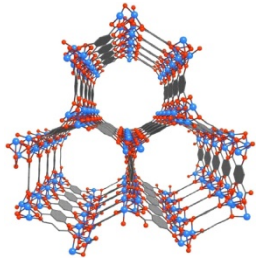
CSP ladder

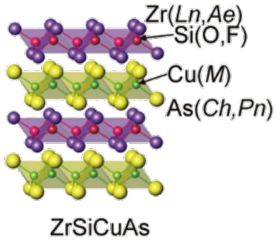
COMPUTING TIME

INVERSE METHODS

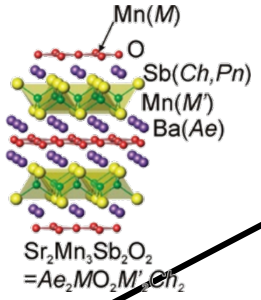
Global Optimisation
(2006)

Data Mining
(2003)





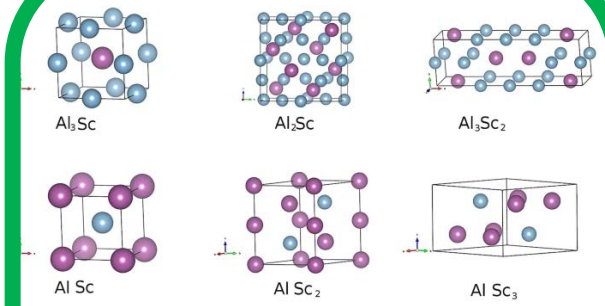
ZrSiCuAs

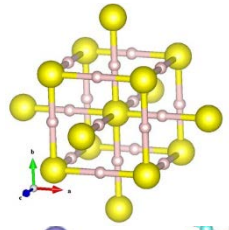


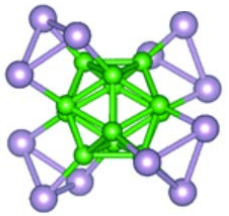
$Sr_2Mn_3Sb_2O_2$
$=Ae_2MO_2M'_2Ch_2$

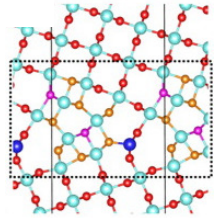
KNOWLEDGE-BASED
(DIRECT)

Assembling
Building units
(2000)





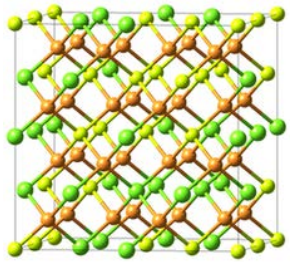




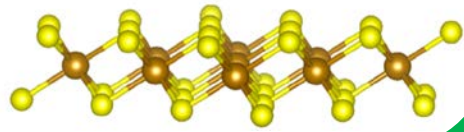
Chemical decoration
(1980)

PRIOR
KNOWLEDGE

Metals
Close-packed oxides

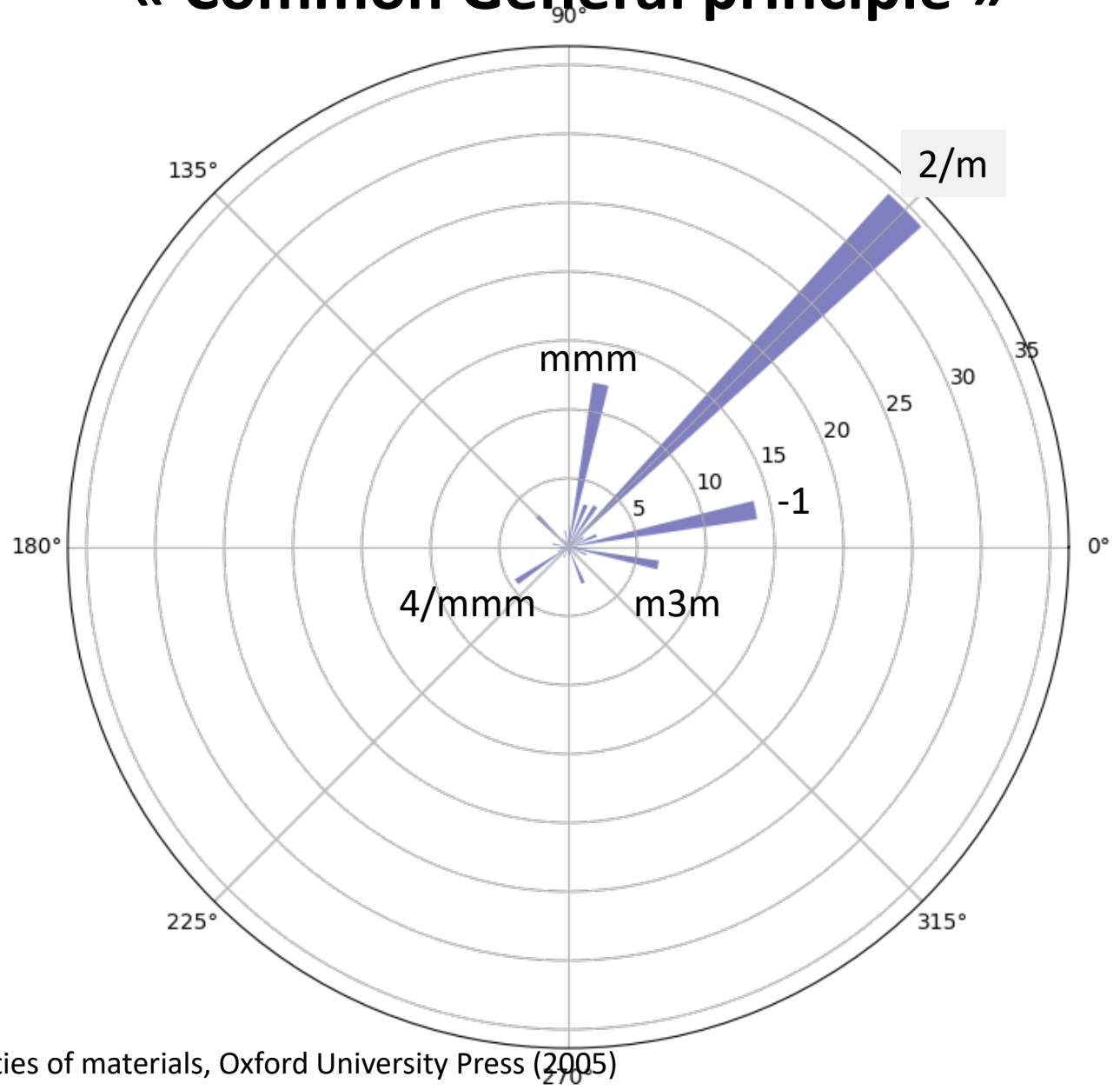


Unravel new structures



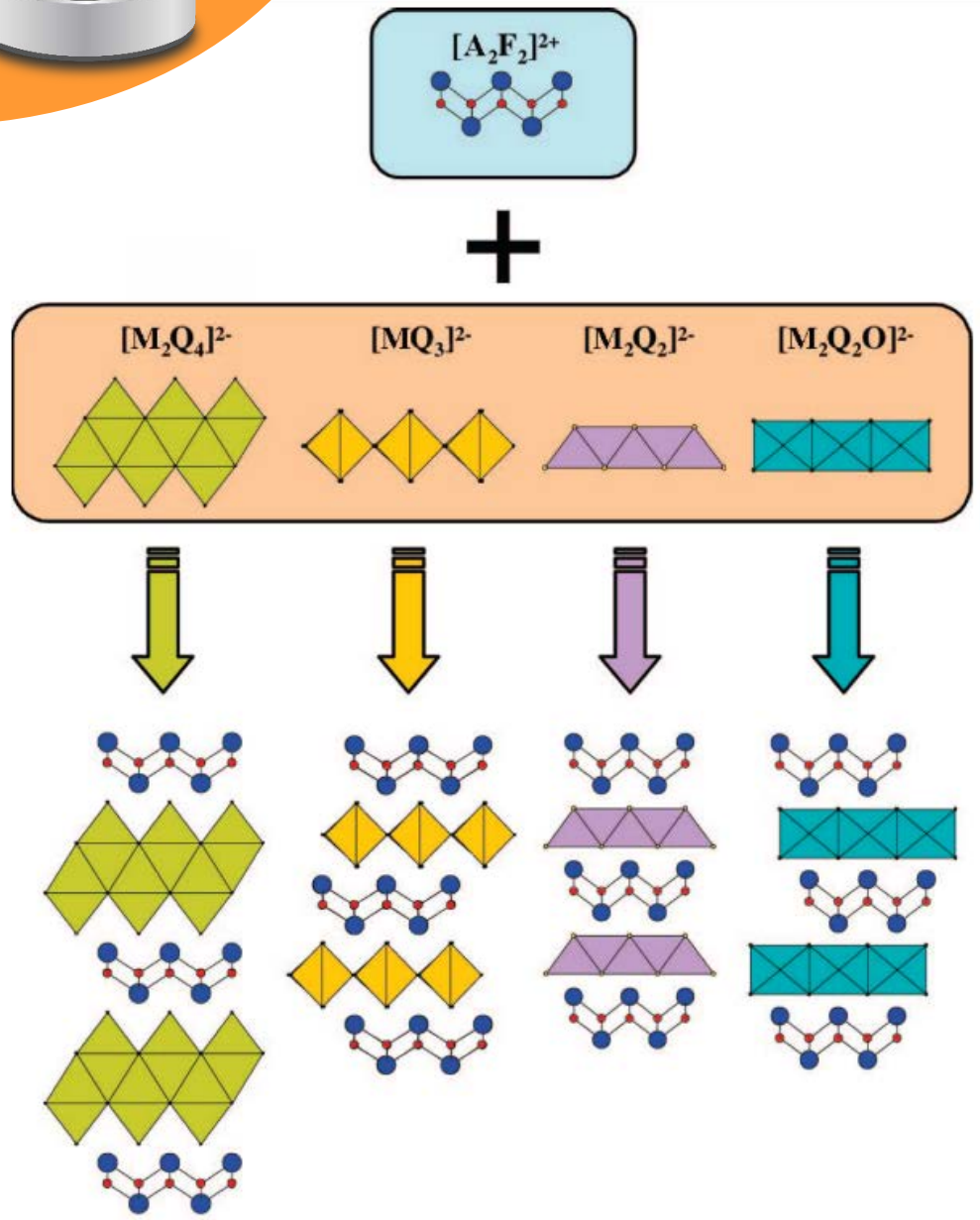
« Common General principle »

280 000
Inorganic
Chemical compounds



Adapted from Newnham, R.E. Properties of materials, Oxford University Press (2005)

Assembling building units

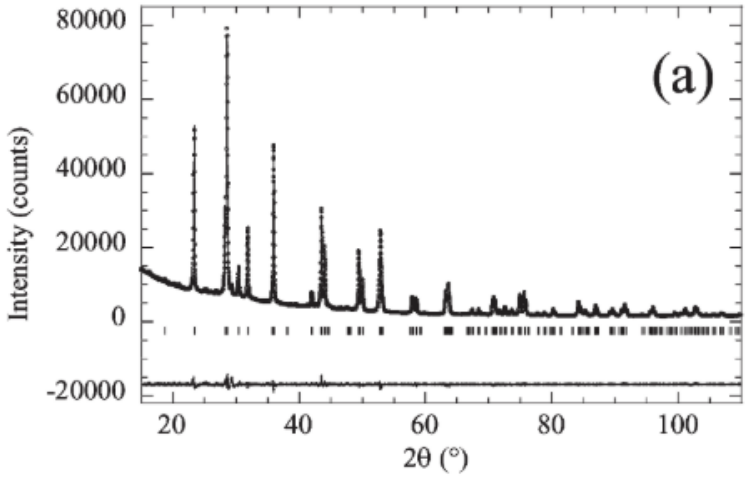


(a) Ferey, G. J. Sol. State Chem. 2000, 152, 37.
(b) Yaghi, O. M.; O'Keefe, M.; Ockwig, N. W.; Chae, H. K.; Eddaoudi, M.; Kim, J. Nature 2003, 423, 705.
(c) Mellot-Draznieks, C.; Ferey, G. Curr. Opin. Solid State Mater. Sci. 2003, 7, 13

H. Kabbour, E. Janod, B. Corraze, M. Danot, C. Lee, M. Whangbo, and L. Cario, JACS, 2008, 130, 8261–8270

L. Cario, H. Kabbour, A. Meerschaut, Chem Mater. 17,2005, 234-236

H Kabbour, L. Cario, S. Jobic and B. Corraze J. Mater. Chem., 2006, 16, 4165–4169 | 4165



BaFZnP

Direct method

$$BaFCl + NaZnP \xrightarrow{\Delta G<0} BaFZnP + NaF$$

Correlation-based Data Mining

« The best way to have a good idea is to have lots of ideas »
Linus Pauling

Large 3D databases (3 530 330 in AFLOWlib)

ICSD

The Materials Project

OQMD
The Open Quantum Materials Database

PAULING FILE

AFLOW
Automatic-FLOW for Materials Discovery

NOMAD
NOVEL MATERIALS DISCOVERY

MATERIALSCLOUD
LEARN WORK DISCOVER EXPLORE ARCHIVE

Small 2D DataBases (6351 materials, 2dmatpedia)

Materials Cloud two-dimensional crystals database (MC2D)

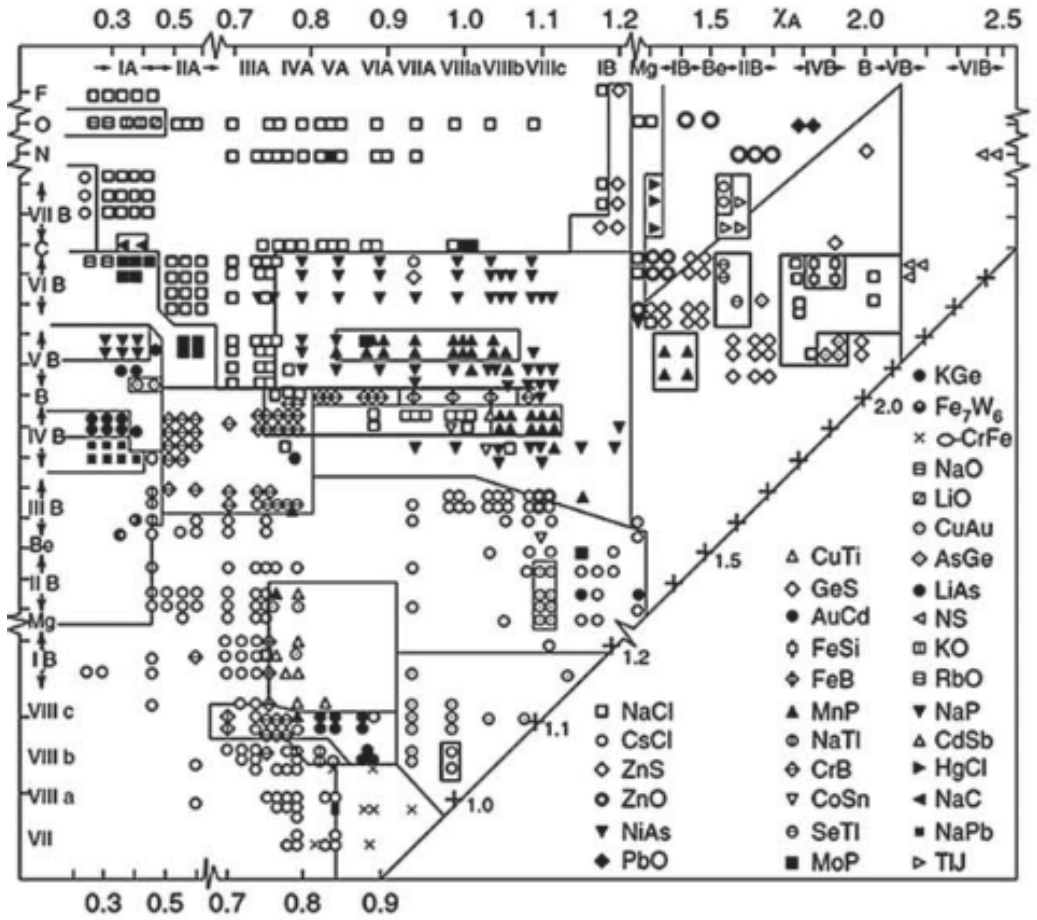
2D Materials Encyclopedia

Stanford ENGINEERING
Materials Science & Engineering

MAGICS
Materials Genome Innovation for Computational Software

MATDAT

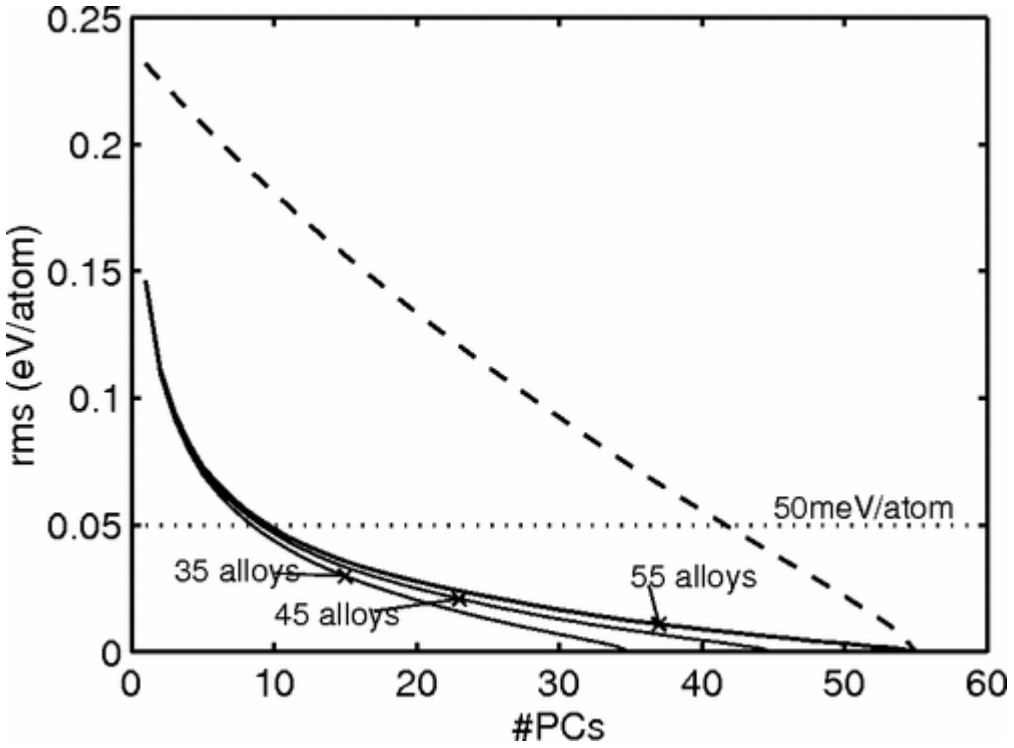
UNREAL ENGINE 5

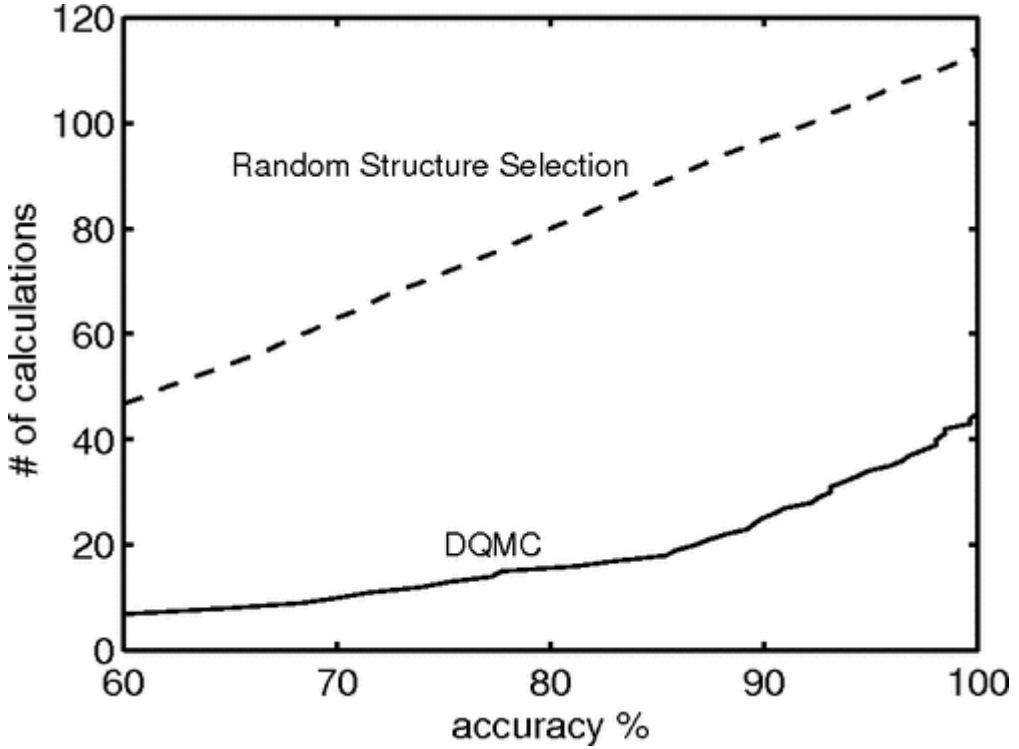


D. G. Pettifor, A chemical scale for crystal structure maps, *Solid State Commun.*, 1984, 51, 31–34.

Data Mining approaches

① **Virtual *computed*** prototypes: Principal component analysis: LiB



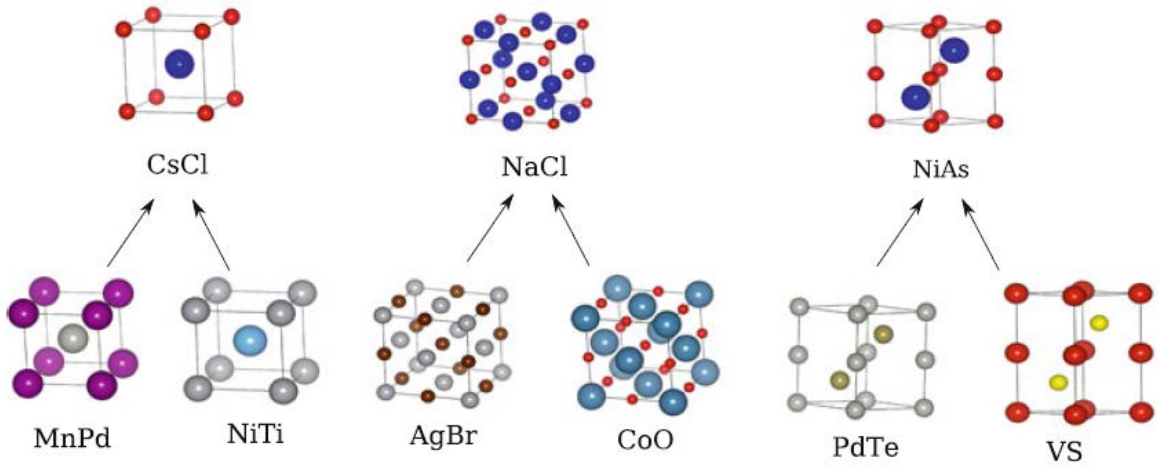


S. Curtarolo, D. Morgan, K. Persson, J. Rodgers, and G. Ceder, *Phys. Rev. Lett.* **91**, 135503

Data Mining approaches

① **Virtual *computed*** prototypes: Principal component analysis: LiB

② **Classification** based on **correlation** in in ICSD prototypes:



$LaMn_2O_5$:
- $PrMn_2O_5$
- $NdMn_2O_5$
- $EuMn_2O_5$
- $SmMn_2O_5$
- $GdMn_2O_5$

(see Materialsproject.org)

C. C. Fischer, K. J. Tibbets, D. Morgan and G. Ceder, *Nat. Mater*, **5**, 641 (2006)

Data Mining approaches

① **Virtual *computed*** prototypes: Principal component analysis : LiB

② **Classification** based on **correlation** in in ICSD prototypes

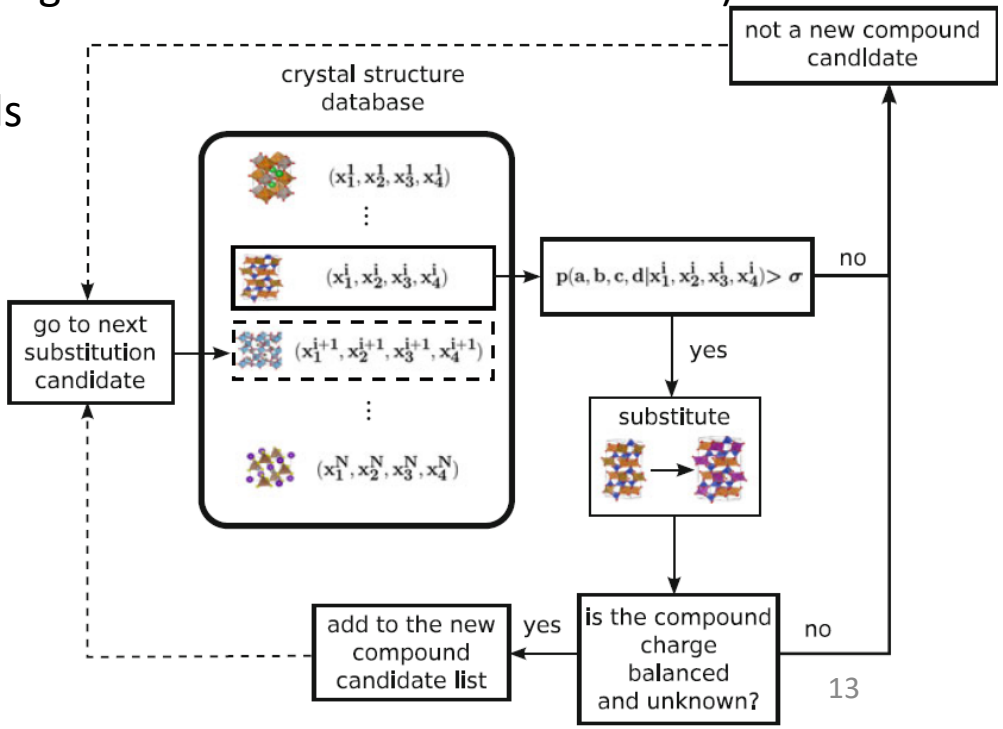
③ Data Mined Ionic **Substitution** Model: a probabilistic model (likelihood) that predicts ionic substitutions which keep the crystal structure of a compound unchanged: extension of Goldschmidt rule)

first superconducting pnictide oxide
$LaFeAsO_{1x}F_x$

→

Isostructural new compounds
$SmLaFeAsO_{1x}F_x$

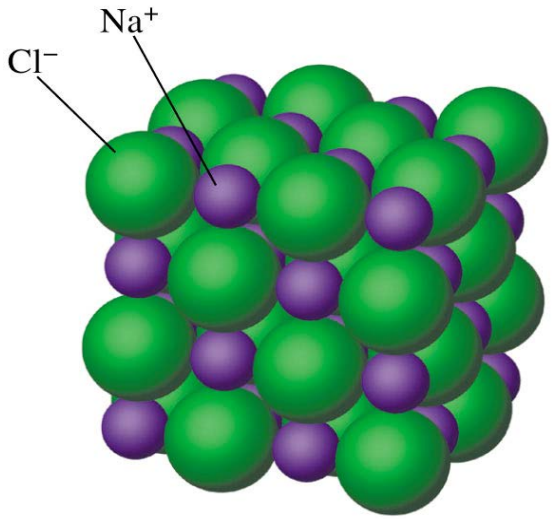
The Materials Project
materialsproject.org



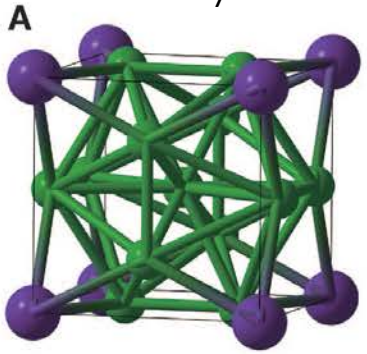
G Hautier, C. Fischer, V. Ehrlacher, A. Jain, and G. Ceder, *Inorg. Chem*. 2011, **50**, 656–663

What if the underlying lattice is not known?

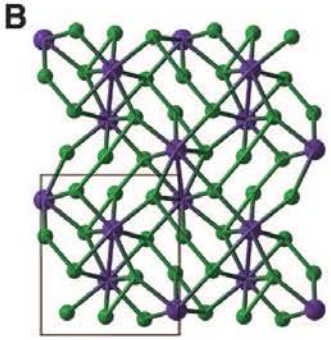
Pressure induced phases: computationally predicted and (some) later confirmed experimentally



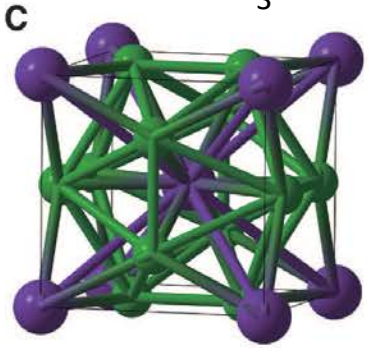
Pm3-$NaCl_7$.



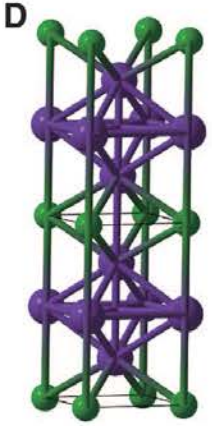
Pnma-$NaCl_3$



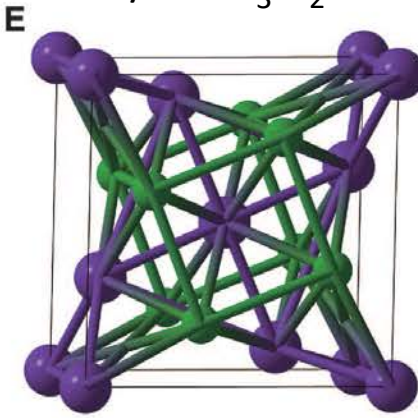
Pm3n-$NaCl_3$.

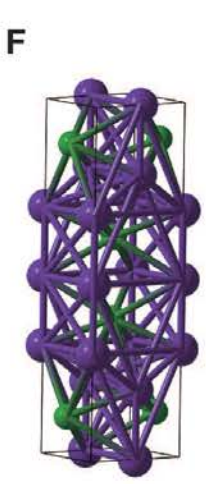


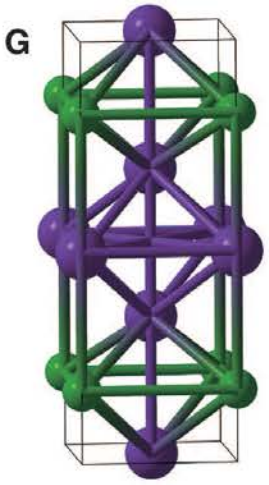
P4/mmm-Na_3Cl.

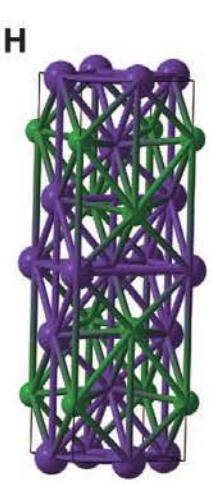


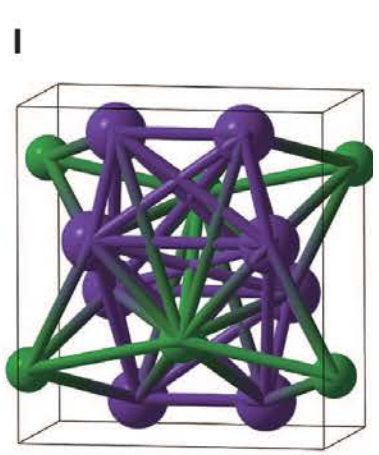
P4/m-Na_3Cl_2.



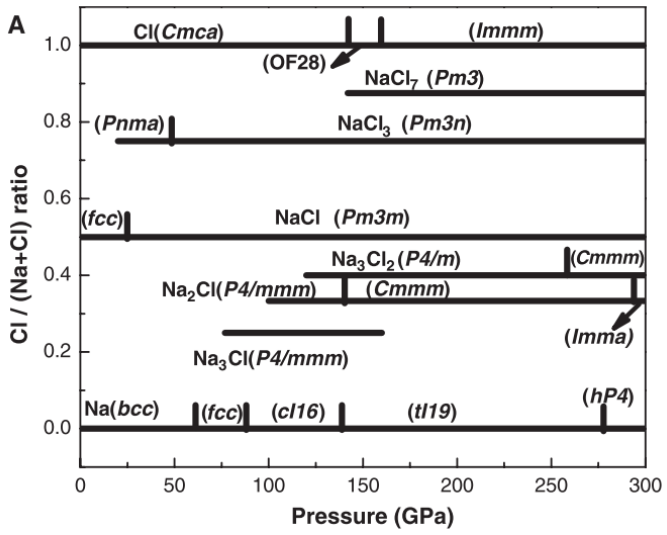








Imma-Na_2Cl



$Cmmm\text{-}Na_3Cl_2$. $P4/mmm\text{-}Na_2Cl$

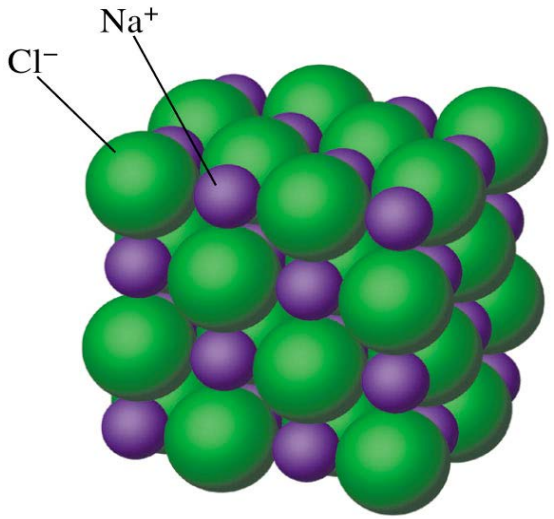
$Cmmm\text{-}Na_2Cl$.

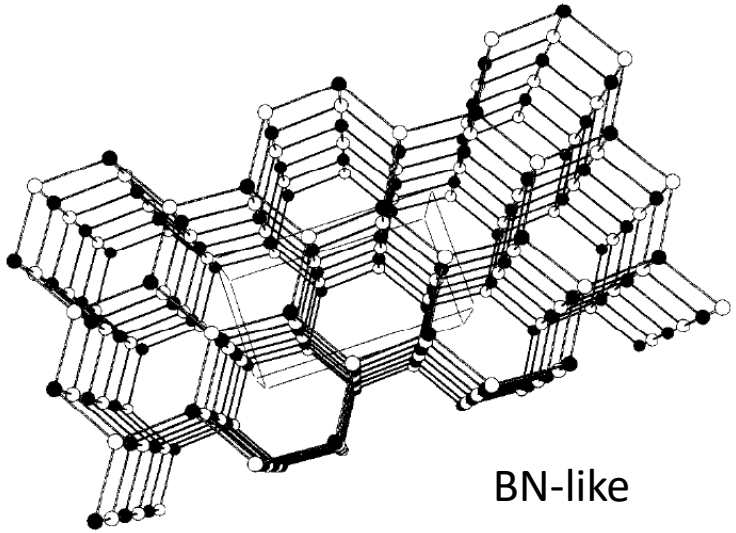
W Zhang,A. R. Oganov et a*l, Science*, 342 (2013)

What if the underlying lattice is not known?

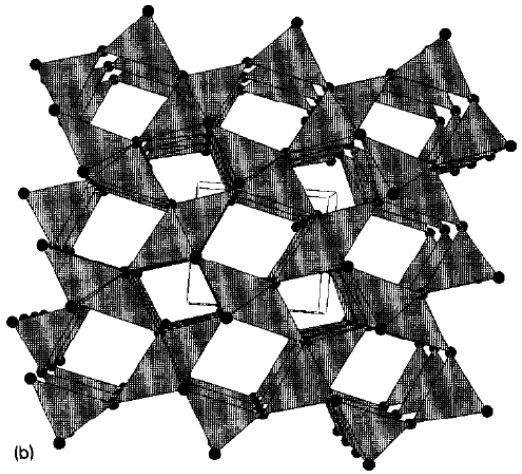
Metastable phases computationally predicted and (some) later confirmed experimentally

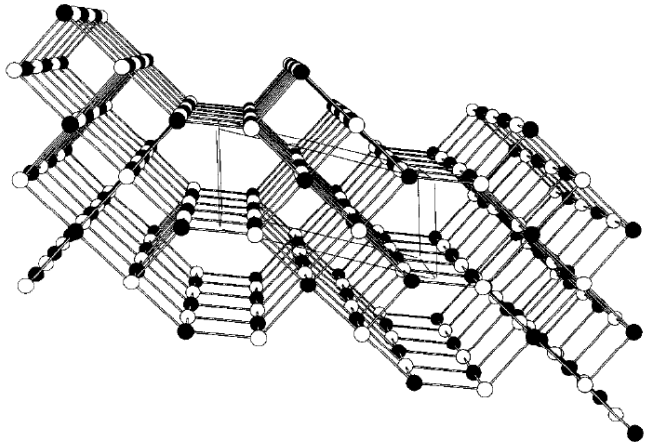
Metastable compounds

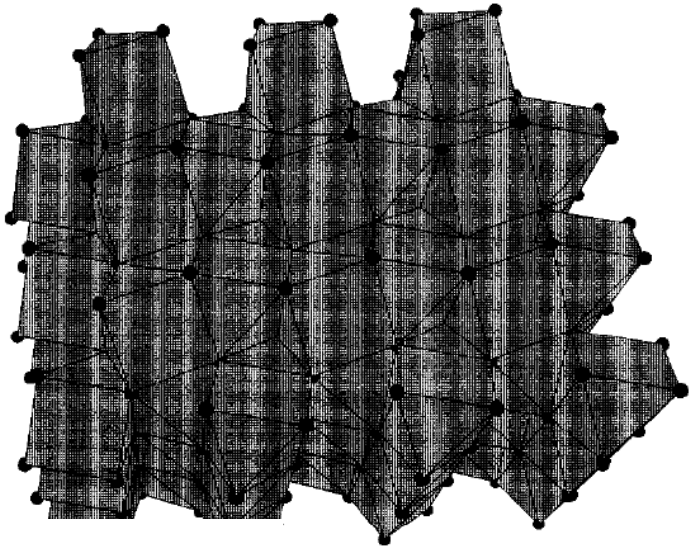




BN-like







Schön, JC, Jansen, M. *Comp. Mater. Sci* **4** (1995) 43-58

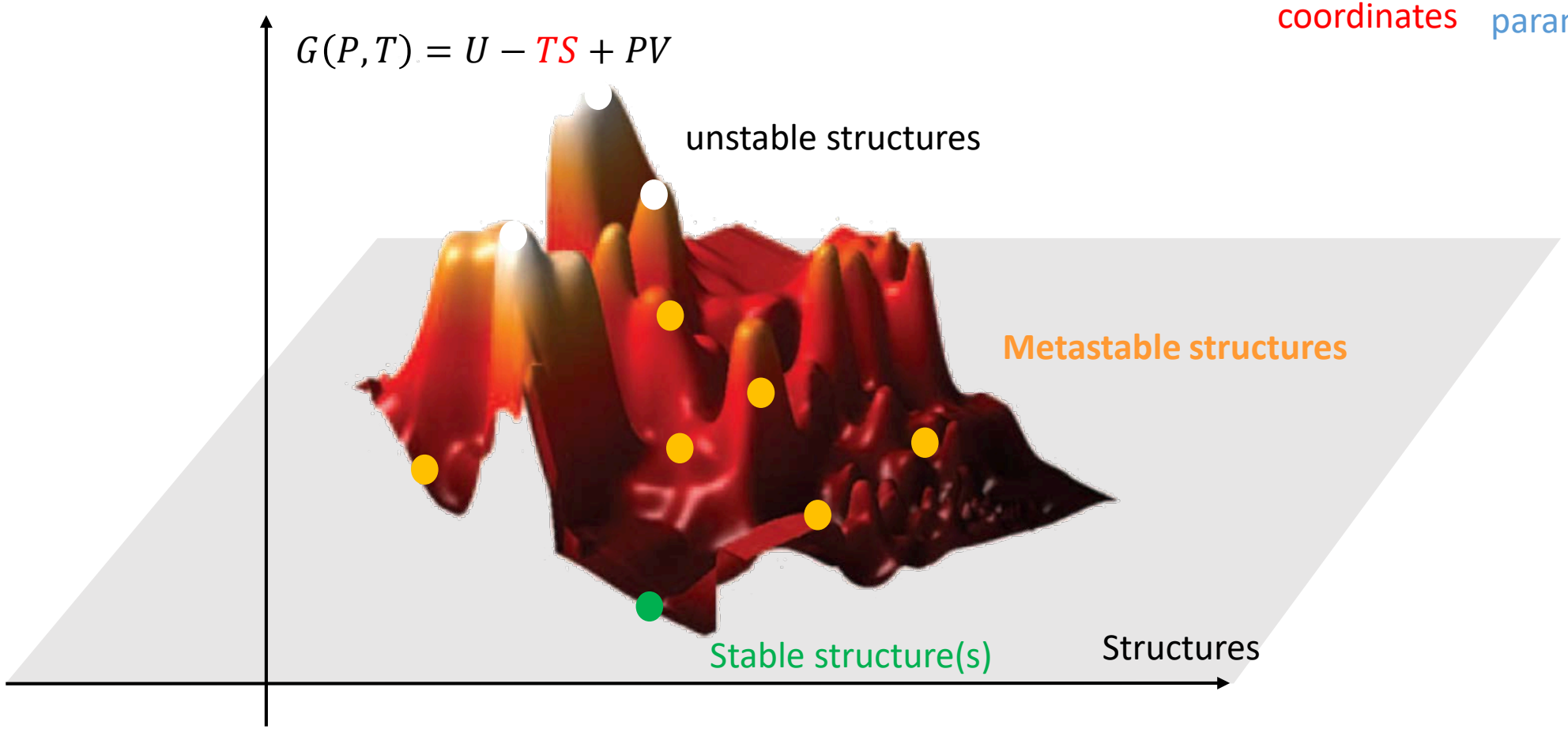
Requires a method functioning with **no prior knowledge** to allow unexpected discoveries

Exploration of the rugged Potential Energy Surface (PES)

$$d = 3N - 3 + 6$$

atom coordinates

Cell parameters



2D-projection of the reduced landscape of Au_8Pd_4 (Oganov, Modern Methods of CSP, Wiley, 2011)

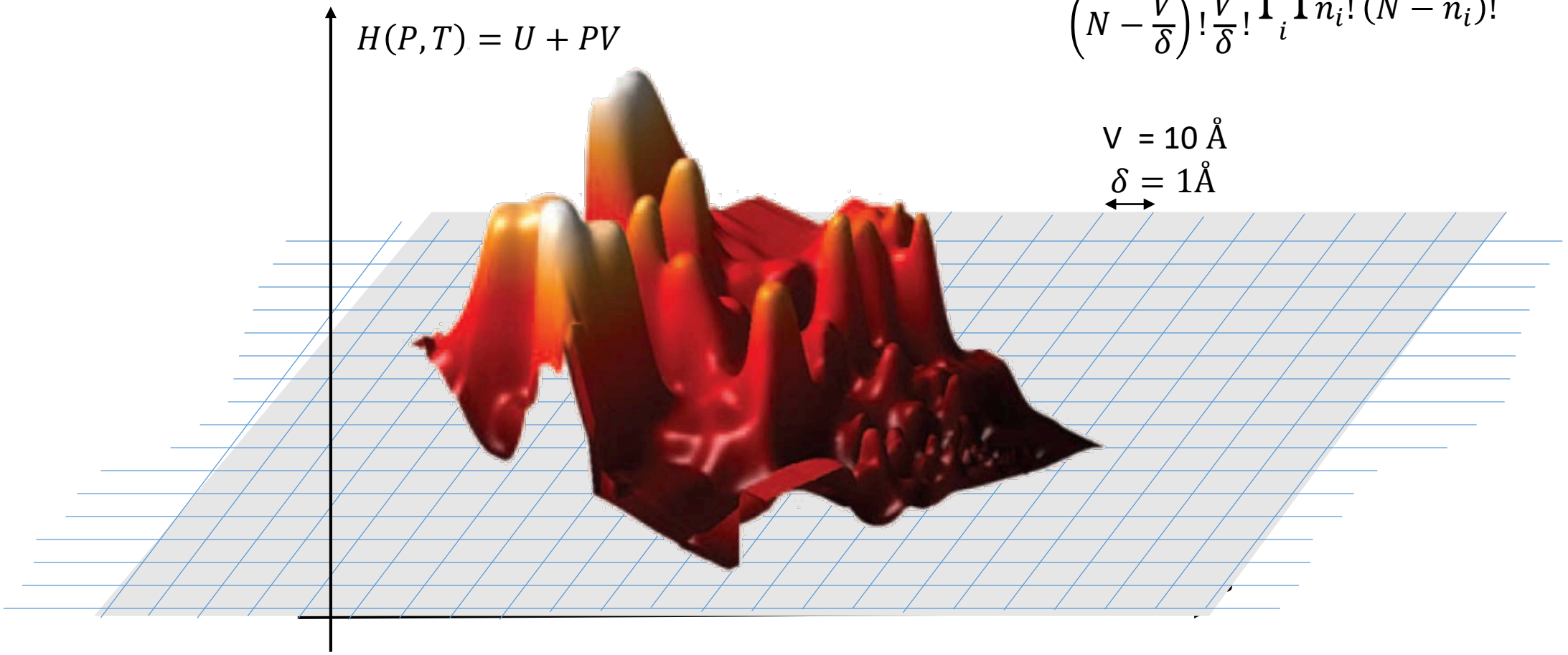
Exhaustive exploration is a NP-hard problem

$$C = \frac{N!}{\left(N - \frac{V}{\delta}\right)!\frac{V}{\delta}!}\prod_i \frac{N!}{n_i!\,(N - n_i)!} = 10^N$$

$H(P,T) = U + PV$

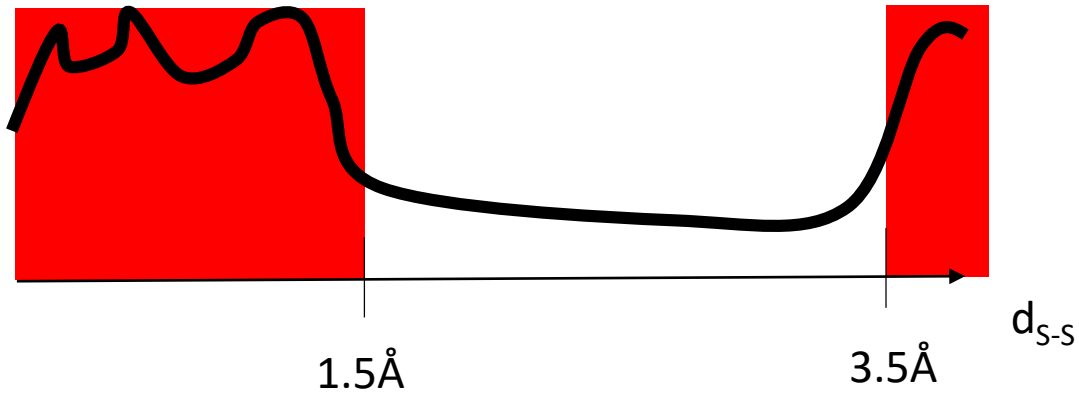
V = 10 Å

$\delta = 1$Å

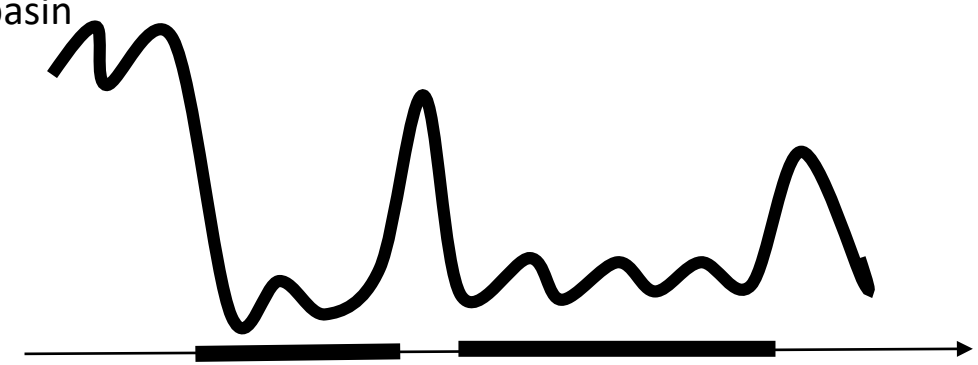


Why does it work ?

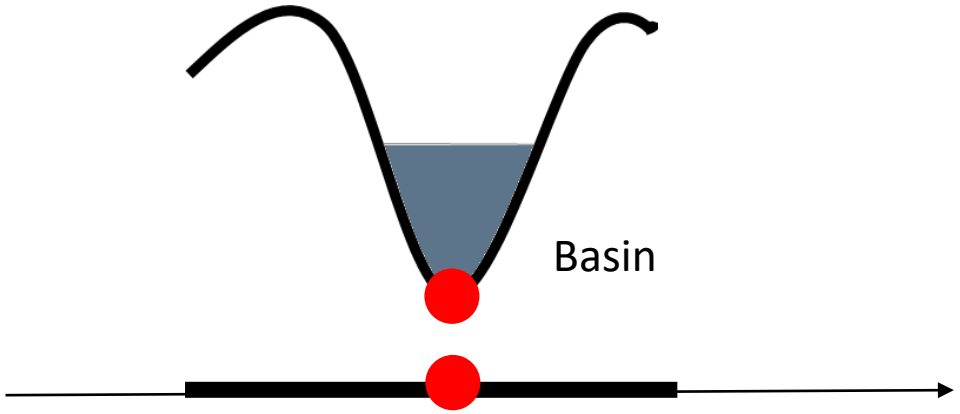
- Only certain regions of the PES are ***chemically relevant*** **(bond types, lengths..)**
  No need to explore chemically unreasonable regions.



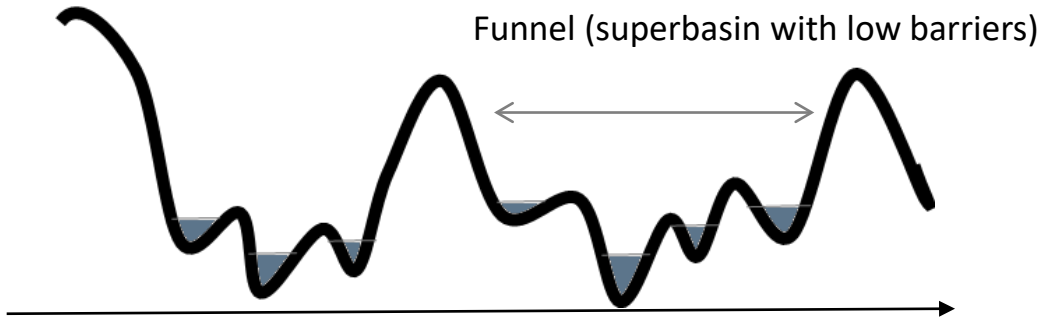
- Low-energy basins occupy ***the largest amount of*** the PES : a randomly generated structure has a high probability to fail in the basin



- ***Relaxation*** decreases the dimensionality of the PES

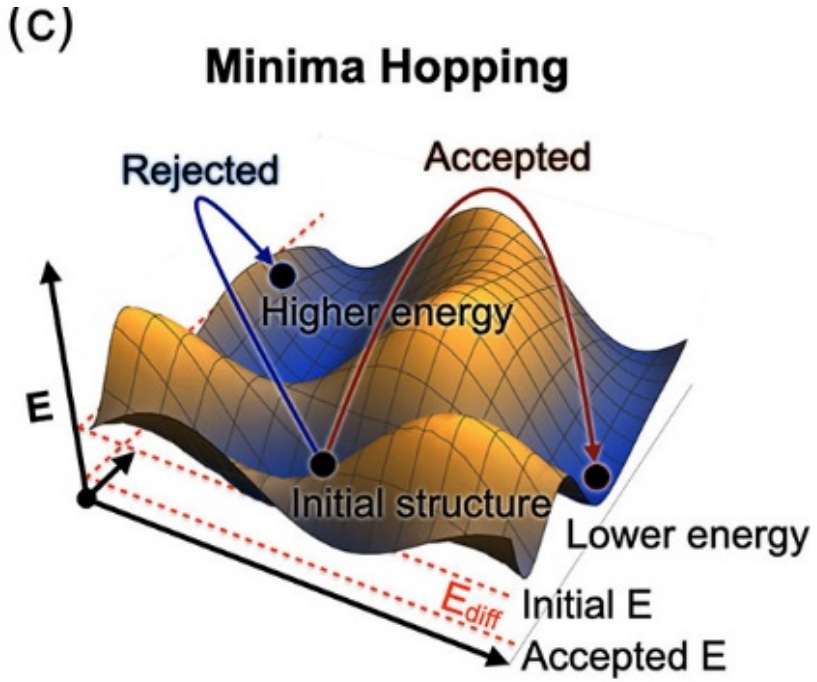


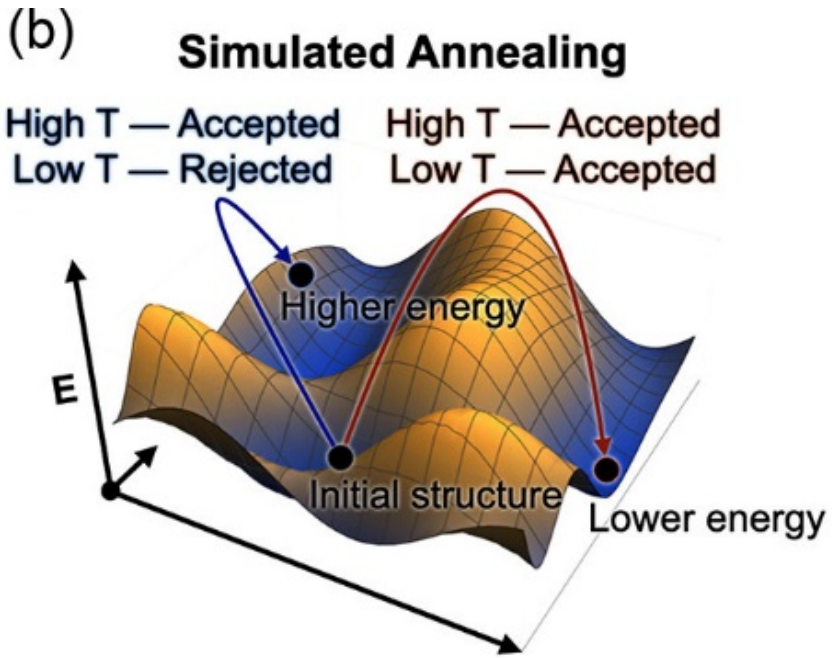
- ***Bell Evans Polanyi principle***: barriers between low-lying minima in a PES are expected to be small. Low-energy basins are likely to be close to one another.

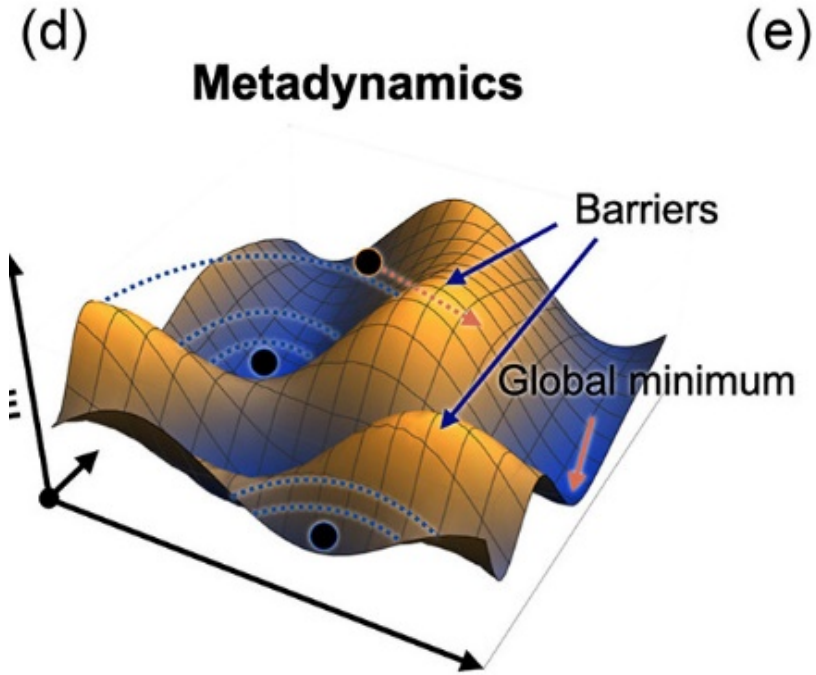


Global optimization techniques

When a good guess of the structure is known







superconducting $S_xSe_{(1-x)}H_3$ phases

metal pernitrides, BN, GeF_2

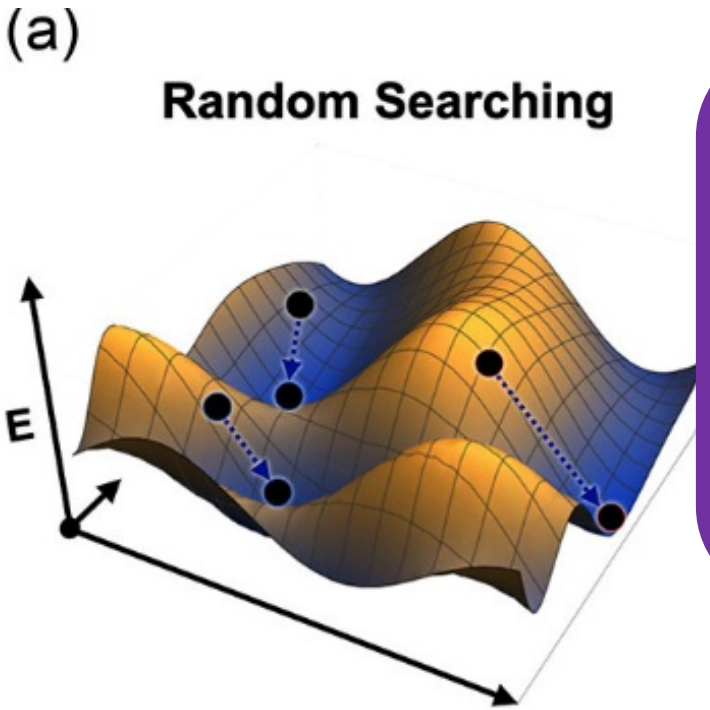
Carbon under pressure

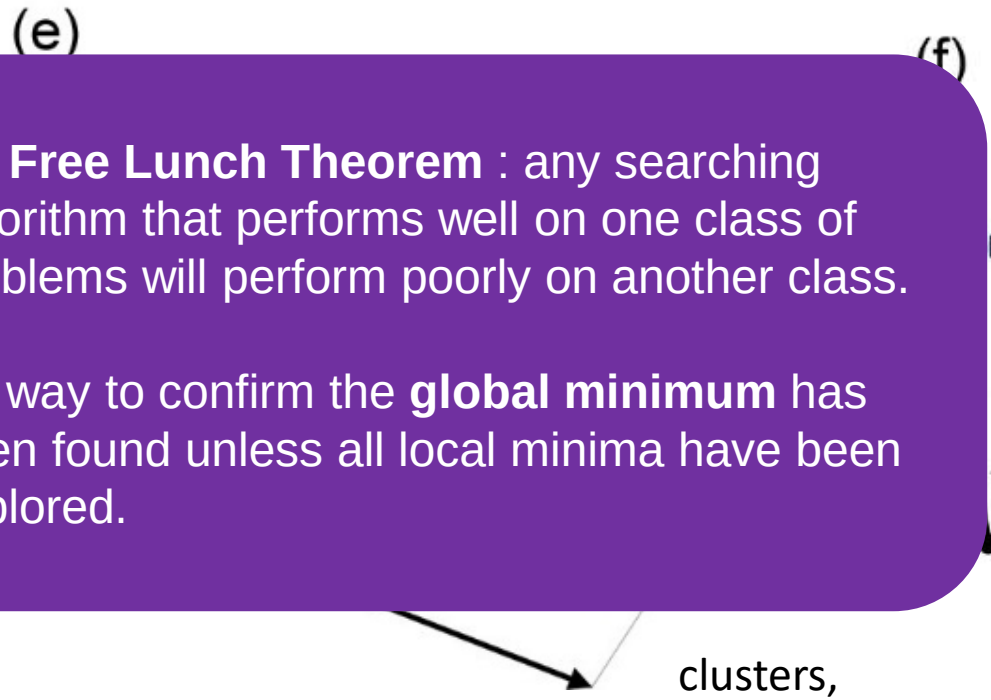
Mainly used as accelerating tools in current softwares

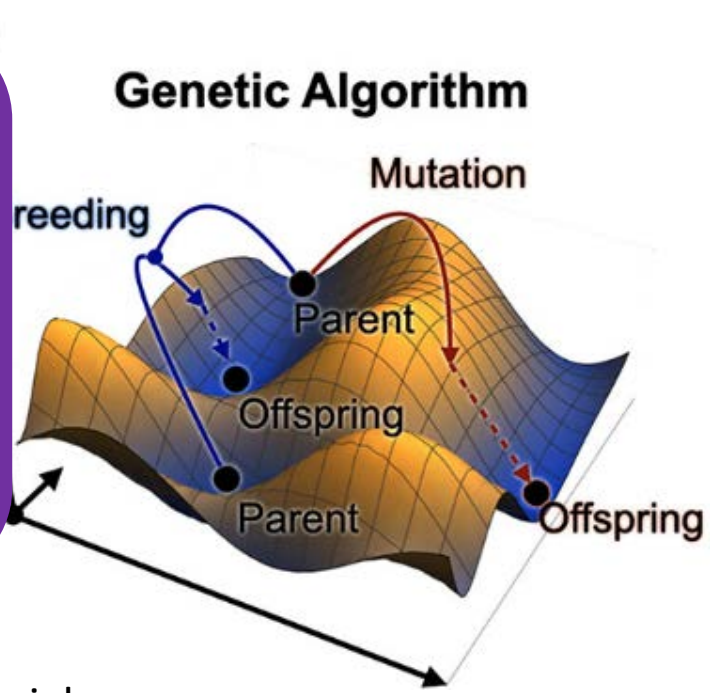
Z. Falls, P. Avery, X. Wang, K. P. Hilleke, and E. Zurek, J. Phys. Chem. C 2021, 125, 1601−1620

Global optimization techniques

When nothing or little about the structure is known







No Free Lunch Theorem : any searching algorithm that performs well on one class of problems will perform poorly on another class.

No way to confirm the **global minimum** has been found unless all local minima have been explored.

Battery materials

clusters,
2D layered materials,
solids, electrides
and superhard
compounds.

CALYPSO

USPEX Computational Materials Discovery

MUSE

XtalOpt Evolutionary Crystal Structure Prediction

gasp EVO

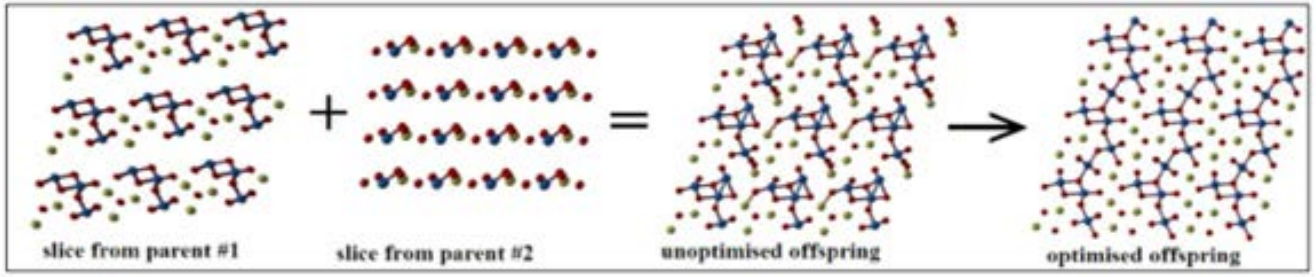
Z. Falls, P. Avery, X. Wang, K. P. Hilleke, and E. Zurek, J. Phys. Chem. C 2021, 125, 1601−1620

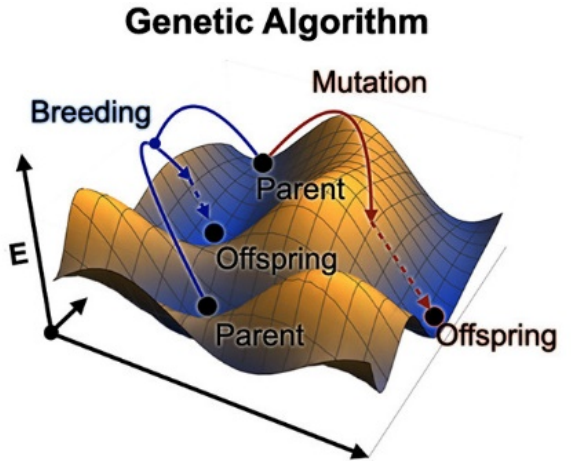
Evolutionary Algorithm Variation Operators

Generation of a **Diverse** Population of Structures

« Self-Learning » tool

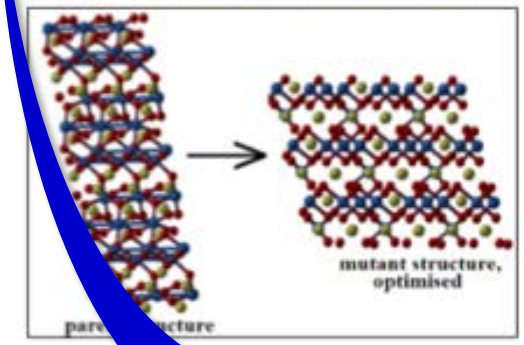
(1) Heredity (crossover)



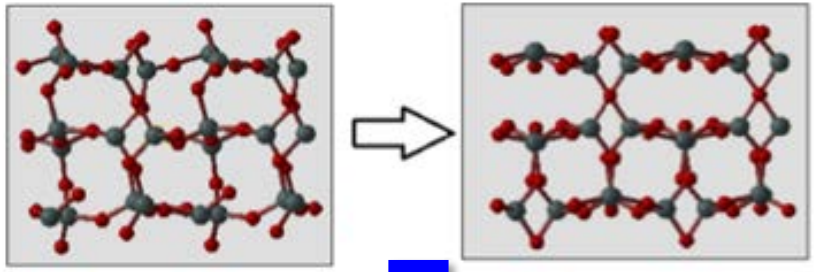


Mutation operators - Enhanced Search

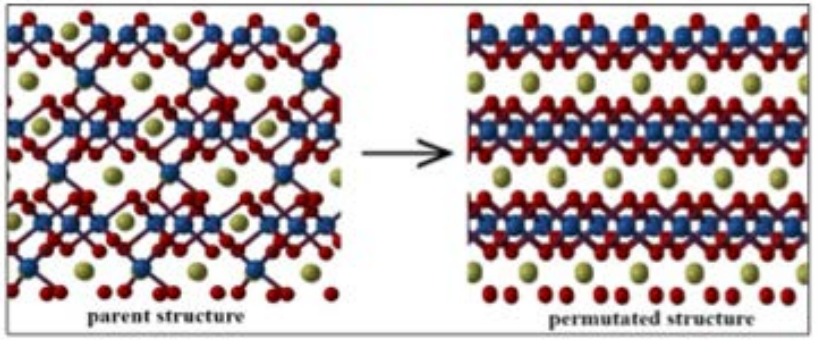
(2) Lattice mutation



(3) Softmutation



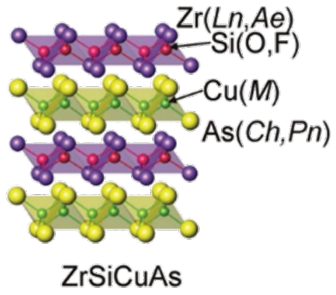
(4) Permutation

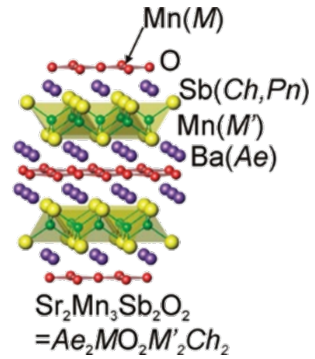


Eugenic selection of the fittest (survivors) and elimination of the others

Topochemical syntheses driven by redox-active (sulfide) anion

Pseudo-lamellar host lattice : $[LaO]^+$, $[Sr_2MnO_2]^{2+}$…



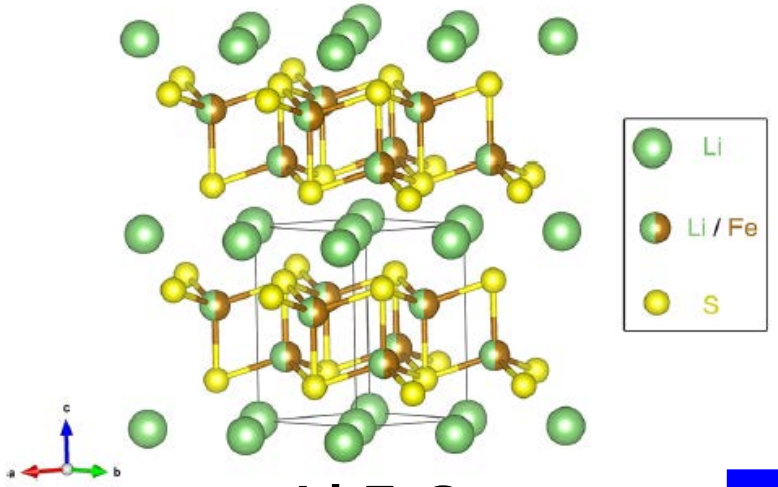


Extended array of sulfide dimers

S. Sasaki, M. Caldes, C. Guillot-Deudon, IB, G. Steciuk, L. Palatinus, E. Gautron, G. Frapper, E. Janod, B. Corraze, S. Jobic and L. Cario, *Nat. Commun.* 2021, *12*, 3605.

S. Sasaki, et al. *Angew. Chem. Int. Ed.* 2018, *57*, 13618.

Structure of twice-delithiated Li_2FeS_2 ?



Li_2FeS_2

-Li

Structure unknown for 30 years

$Fe^{3+}S^{2-}(S_2)^{2-}_{1/2}$

- ***IR spectroscopy :***
  - d(S–S)= 2.12 Å
- ***Mössbauer and EXAFS :***
  - Fe^{3+}HS ion in **tetrahedral sites**
  - d(Fe–S)=2.28 Å
  - **S^{2-}/S_2^{2-} = 2/1**
- **Lamellar structure** expected due to the stacking of $LiFeS_2$ and Li layers.

R. Brec et al. *J. Power. Sources.* **1989**, *26*, 325

Structure of twice-delithiated Li_2FeS_2 ?

3D

ICSD

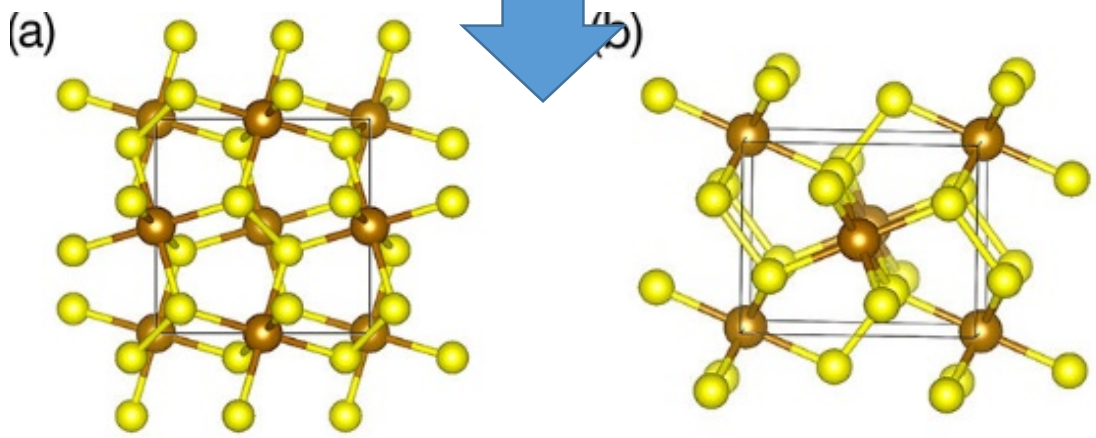
The Materials Project

OQMD
The Open Quantum Materials Database

AFLOW
Automatic-FLOW for Materials Discovery

NOMAD
NOVEL MATERIALS DISCOVERY

MATERIALSCLOUD
LEARN WORK DISCOVER EXPLORE ARCHIVE



NM Pyrite

NM Marcasite

2D

Materials Cloud two-dimensional crystals database (MC2D)

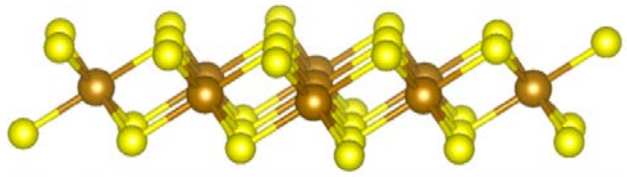
2D Materials Encyclopedia

MAGICS
Materials Genome Innovation for Computational Software

UNREAL ENGINE 5

Stanford ENGINEERING
Materials Science & Engineering

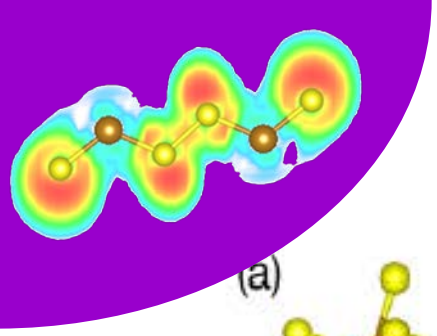
MATDAT



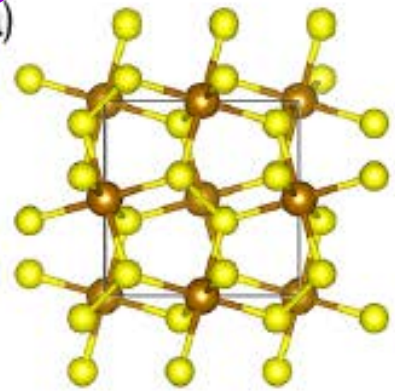
FM *P*-3*m*1 1T-2D

(MoS_2-like)

Crystal Structure Prediction of FeS_2



(a)

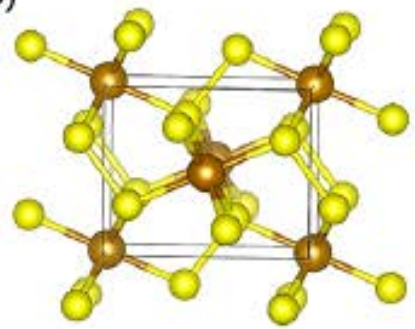


NM Pyrite

ΔE = 0.000 eV/f.u.

(Ground state)

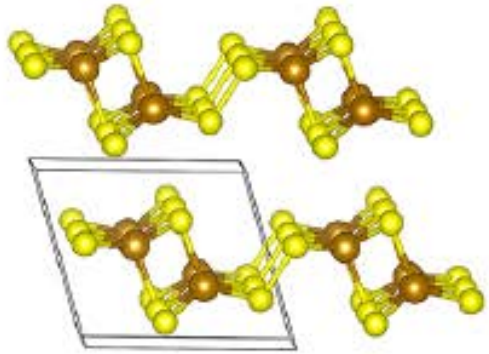
(b)



NM Marcasite

ΔE = 0.009 eV/f.u.

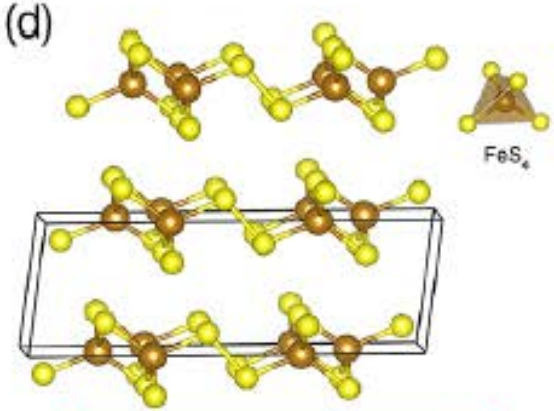
(c)



AFM *P*-1-3D

ΔE = 0.282 eV/f.u.

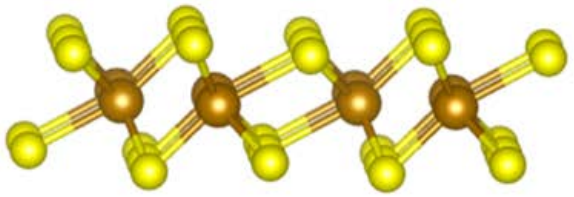
(d)



AFM *C*2/*m*-3D

ΔE = 0.425 eV/f.u.

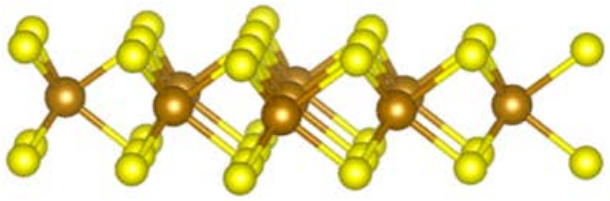
(c)



AFM $P2_1/m$ 1T'-2D

ΔE = 0.713 eV/f.u.

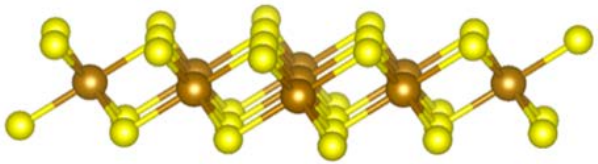
(d)



FM *P*-6*m*2 1H-2D

ΔE = 1.254 eV/f.u.

(e)



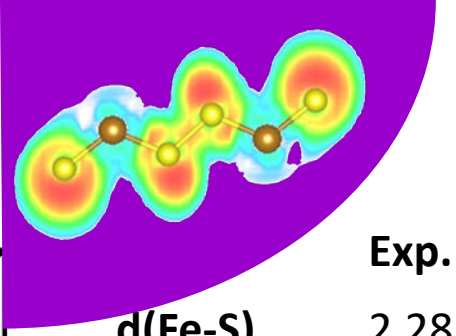
Dynamical unstable

FM *P*-3*m*1 1T-2D

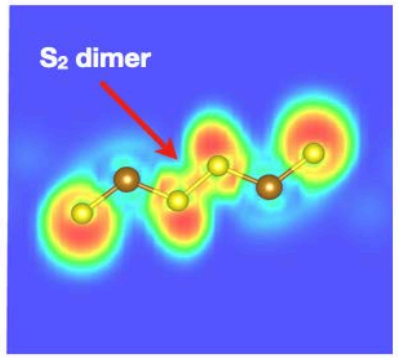
ΔE = 0.777 eV/f.u.

B. Wang, IB, S. Sasaki, G. Guegan, L. Cario, S. Jobic and G. Frapper, *J. Phys. Lett.* **2020**, *11*, 8861.

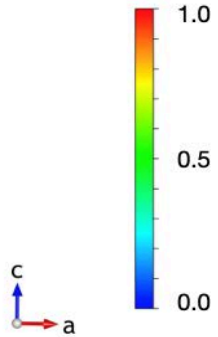
Crystal Structure Prediction of FeS_2

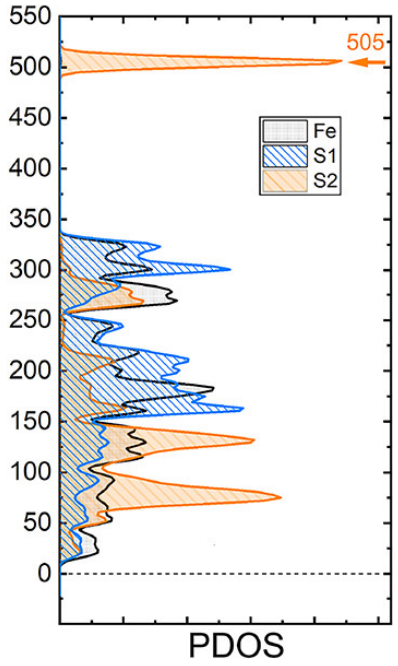


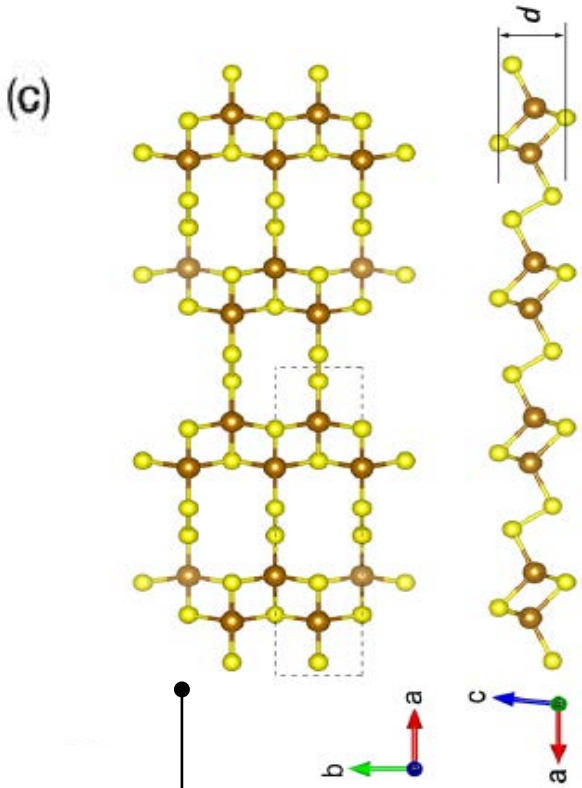
	Exp.	Predicted
d(Fe-S)	2.28	2.27
d(S-S)	2.12	2.03

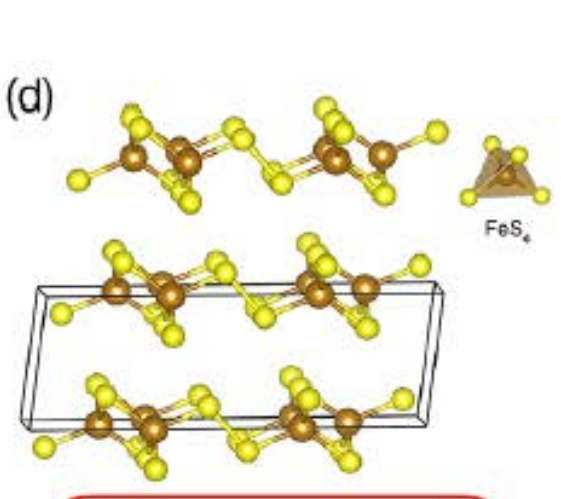


C2/m-2D FeS_2









AFM *C2/m*-3D
ΔE = 0.425 eV/f.u.

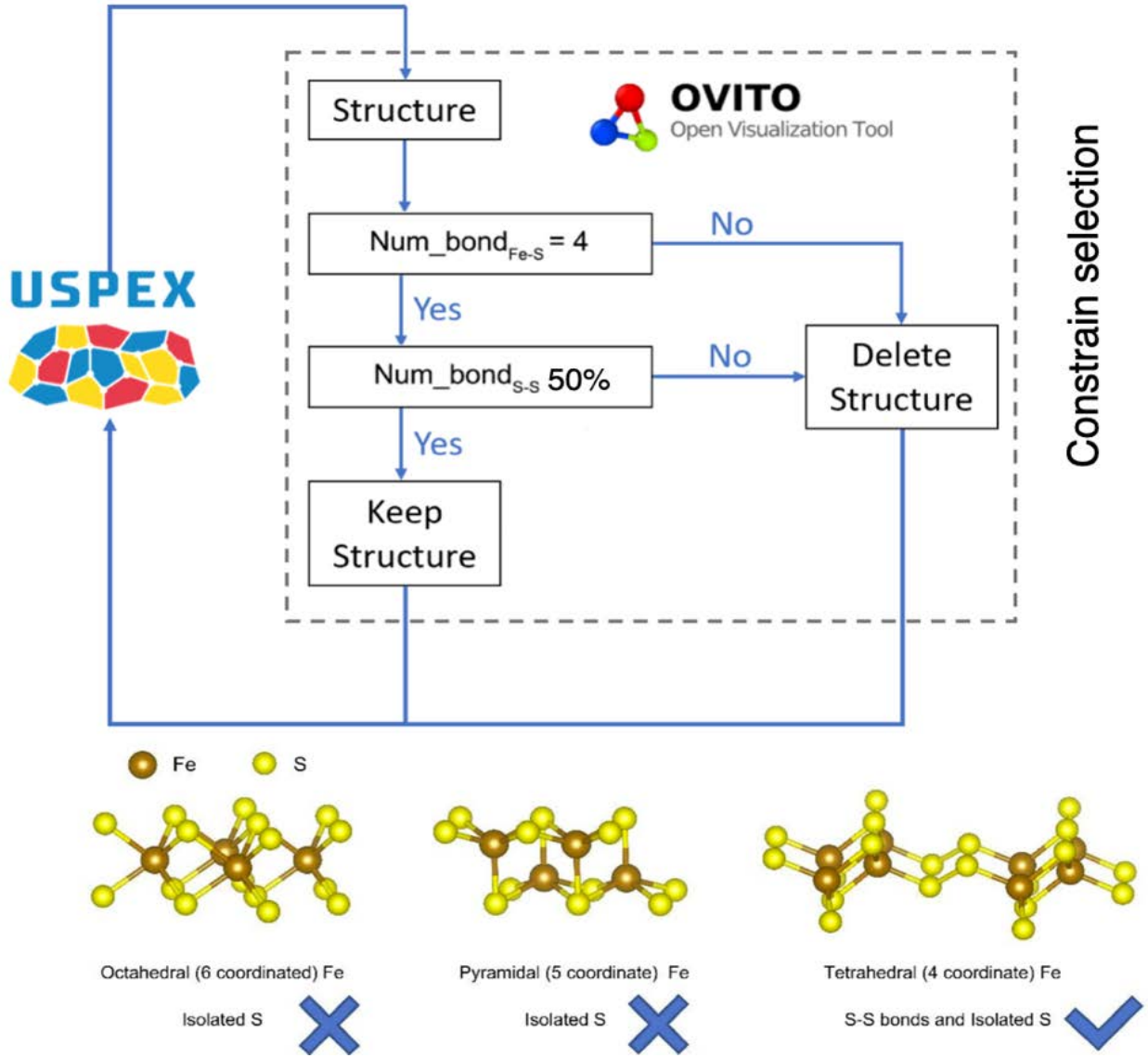
Corrugated $2/\infty[FeS_2]$ layer made of blocks linked to each other via S–S bonds

$1/\infty[Fe_2S_4]$ ribbons consisting of edge-sharing FeS_4 tetrahedra with zigzag iron rows

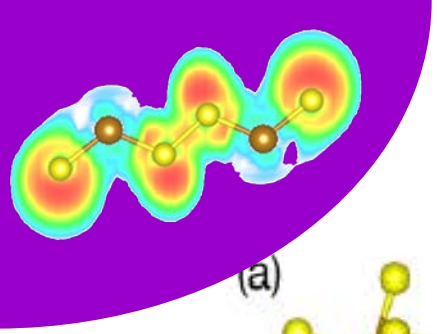
Strongly differs from classical MS_2 slabs !

B. Wang, IB, S. Sasaki, G. Guegan, L. Cario, S. Jobic and G. Frapper, *J. Phys. Lett.* **2020**, *11*, 8861.

Constrained Crystal Structure Prediction of FeS_2

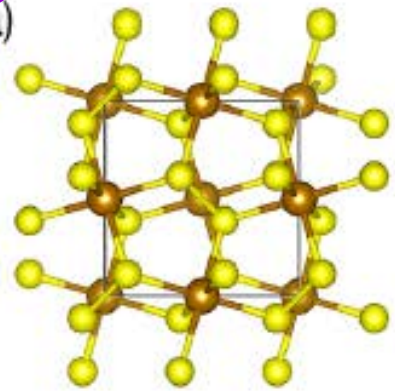


B. Wang, IB, S. Sasaki, G. Guegan, L. Cario, S. Jobic and G. Frapper, *J. Phys. Lett.* **2020**, *11*, 8861.



What about the newly unraveled and more stable FeS_2 phase ?

(a)

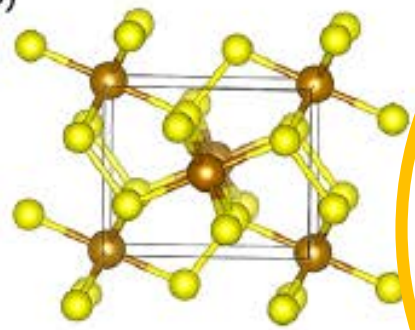


NM Pyrite

ΔE = 0.000 eV/f.u.

(Ground state)

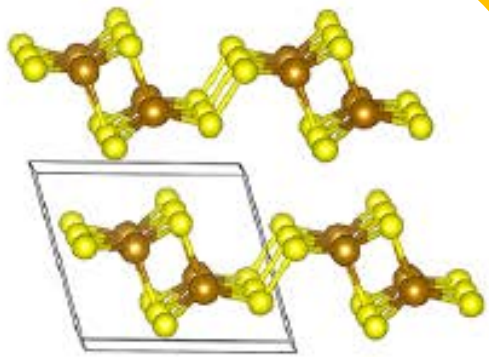
(b)



NM Marcasite

ΔE = 0.009 eV/f.u.

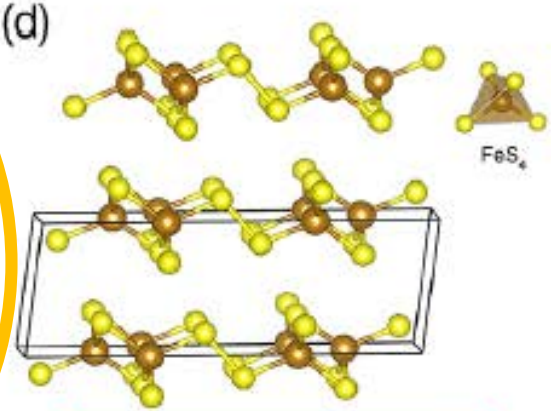
(c)



AFM *P*-1-3D

ΔE = 0.282 eV/f.u.

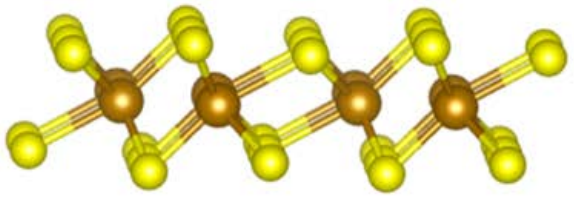
(d)



AFM *C*2/*m*-3D

ΔE = 0.425 eV/f.u.

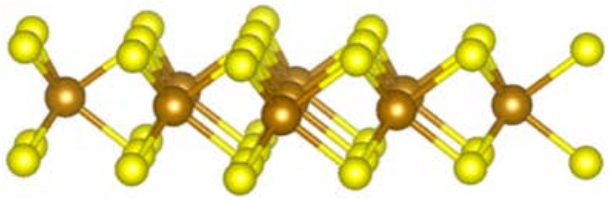
(c)



AFM $P2_1/m$ 1T'-2D

ΔE = 0.713 eV/f.u.

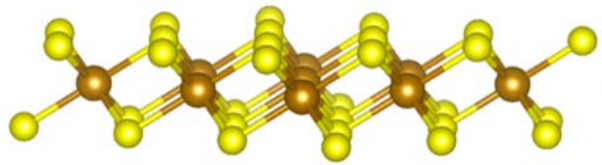
(d)



FM *P*-6*m*2 1H-2D

ΔE = 1.254 eV/f.u.

(e)

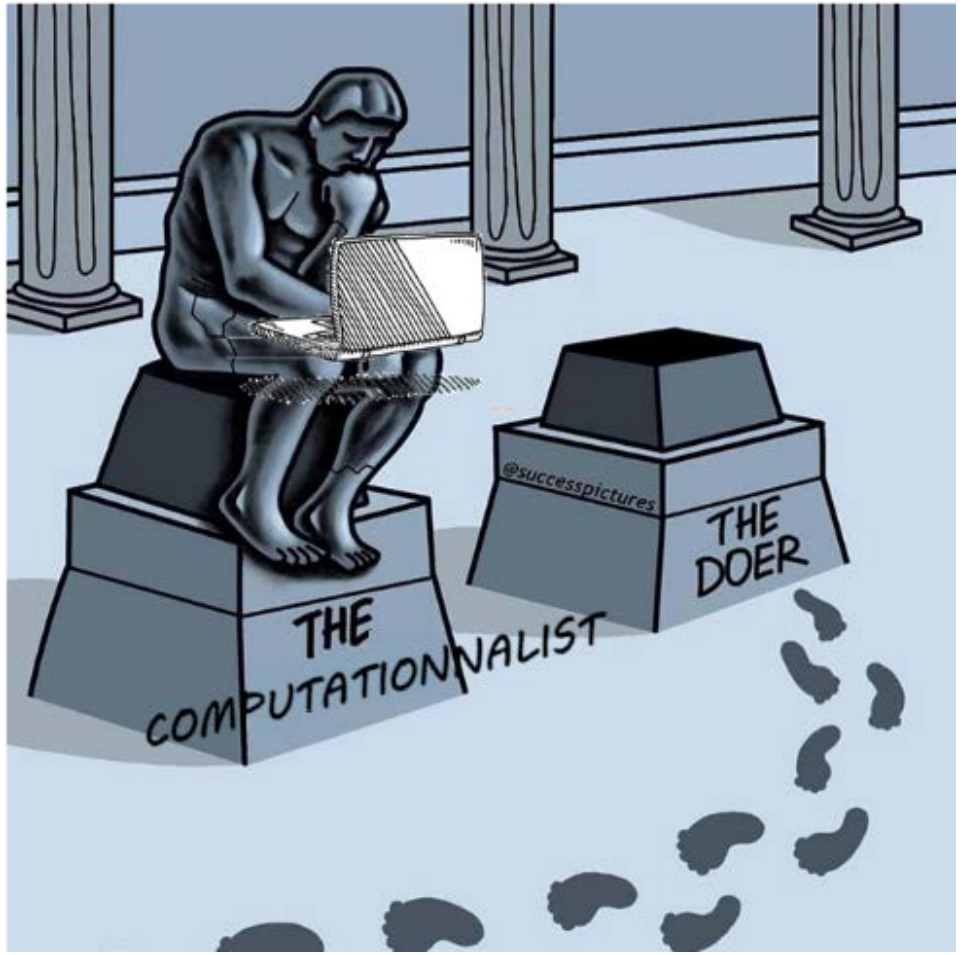


Dynamical unstable

FM *P*-3*m*1 1T-2D

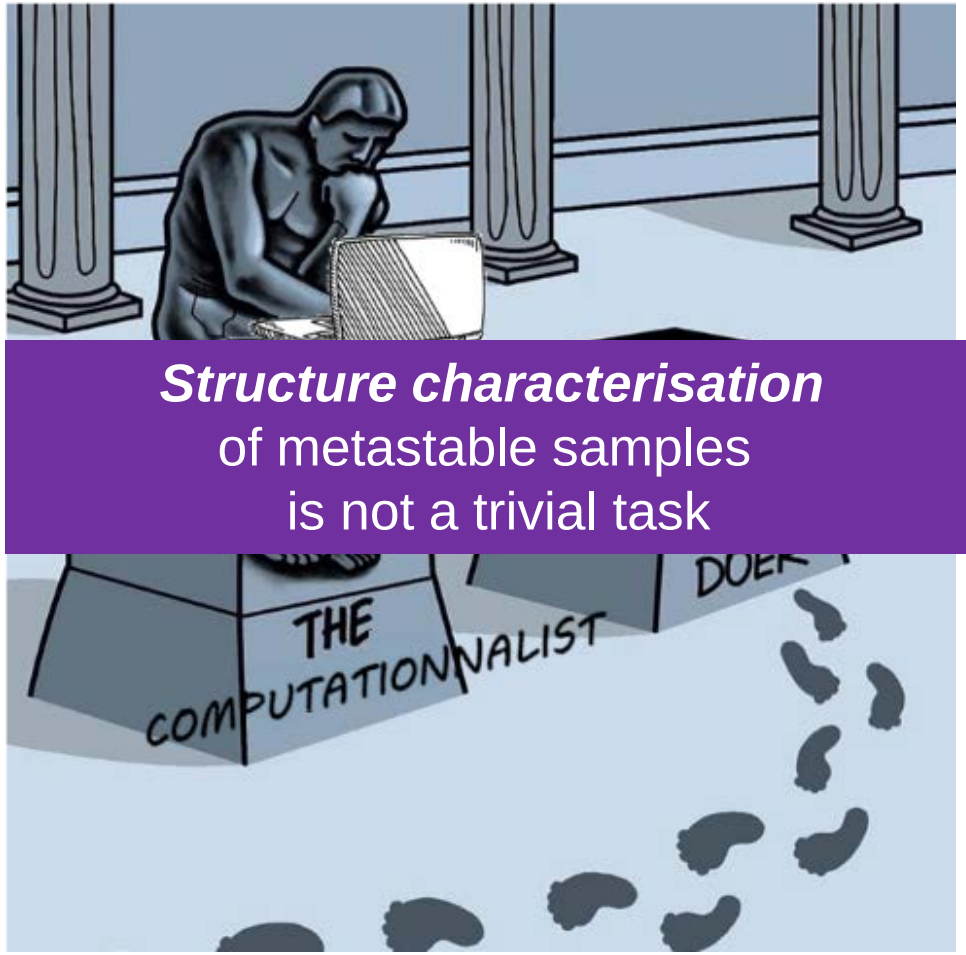
ΔE = 0.777 eV/f.u.

Is it really compressing time if there is no synthetisability criterion ?



Our approach : *coupling* advances in *computational* material and material *synthesis* design by selecting one synthesis route

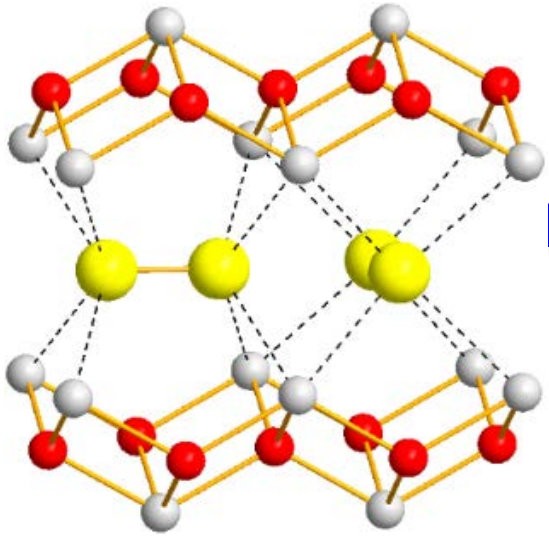
Still a need to predict ?



Structure characterisation
of metastable samples
is not a trivial task

Topochemical S (de)intercalation of $La_2O_2S_2$

$La_2O_2S_2$



CmCa*

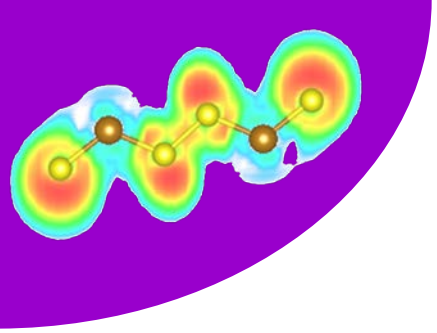
-1.0 S

Unknown metastable La_2O_2S phase

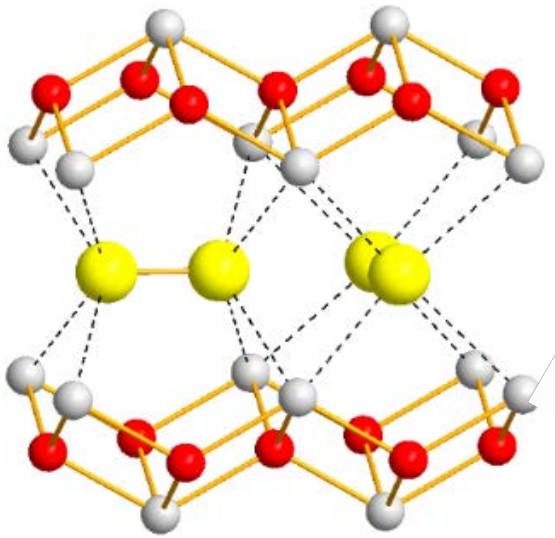
L-B Mvélé, S. Sasaki, C. Latouche, P. Deniard, E. Janod, IB, Stéphane Jobic and Laurent Cario, *Inorg. Chem.* **62**, 19, 7264–7272 (2023)

S. Sasaki, M. Caldes, C. Guillot-Deudon, IB, G. Steciuk, L. Palatinus, E. Gautron, G. Frapper, E. Janod, B. Corraze, S. Jobic and L. Cario, *Nat. Commun.* **12**, 3605, (2021)

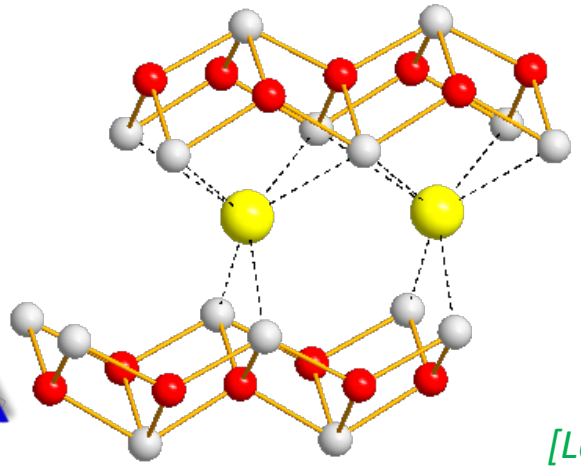
S (de)intercalation of $La_2O_2S_2$

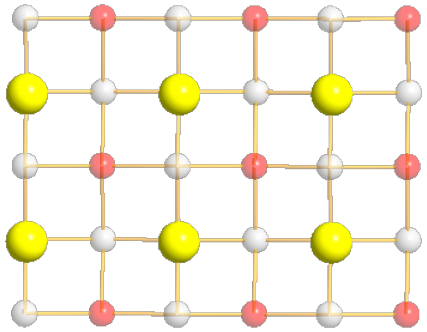


$La_2O_2S_2$



– 1.0 S

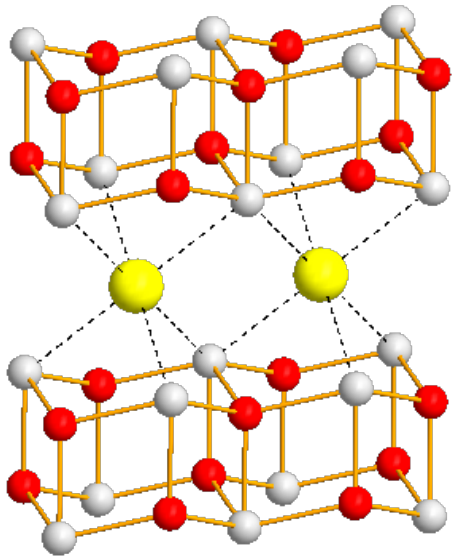


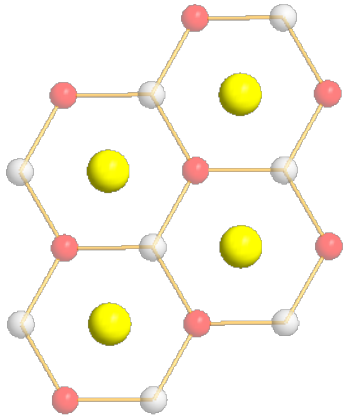


$[LaO_4S_2]$ and $[LaO_4S_4]$ polyhedra

Predicted Pattern
oA-La_2O_2S
Metastable
(SG: Amm2)

ΔE=72meV



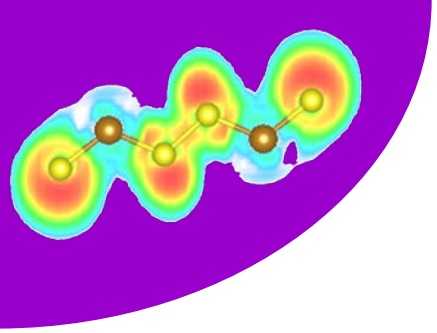


$[LaO_3S_3]$ polyhedra only

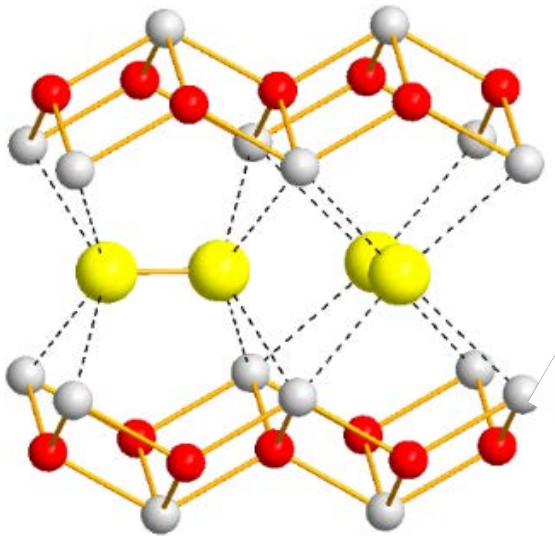
Morosin et al.
Acta Cryst. B
(1973)

Predicted Pattern
hp-La2O2S
Stable
(SG: $P\bar{3}m1$)

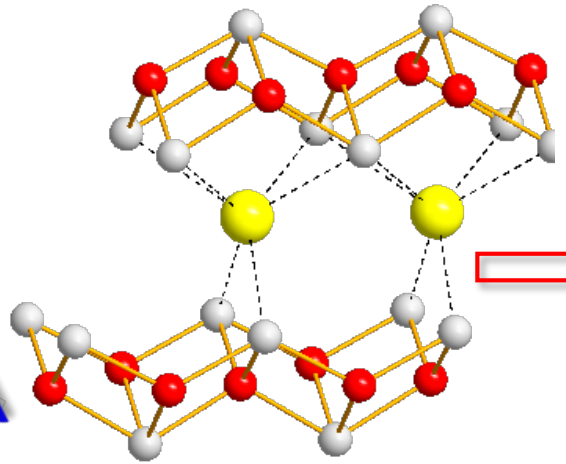
S (de)intercalation of $La_2O_2S_2$

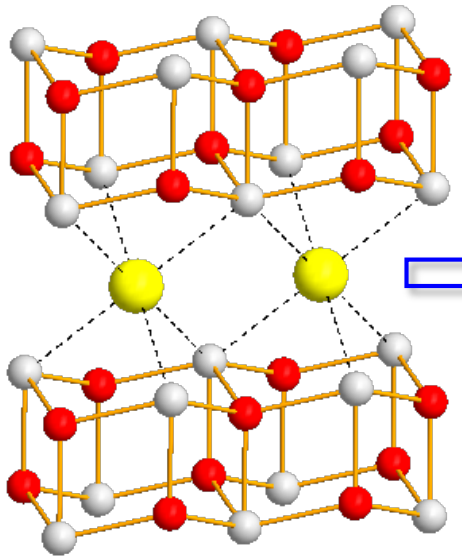


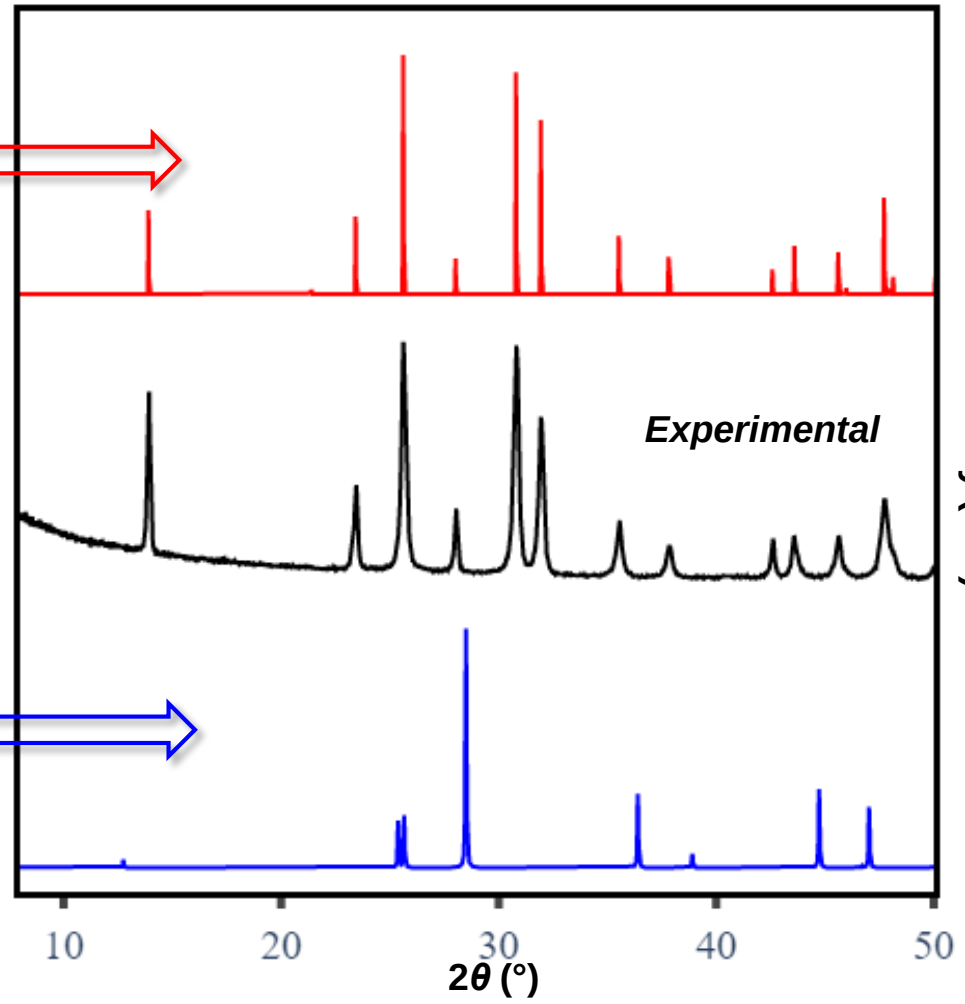
$La_2O_2S_2$



– 1.0 S

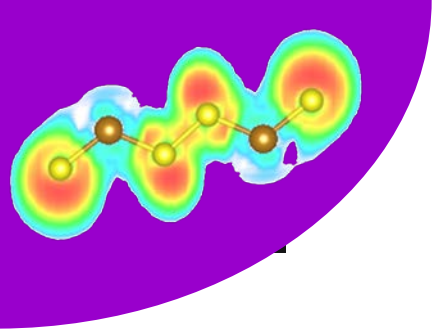




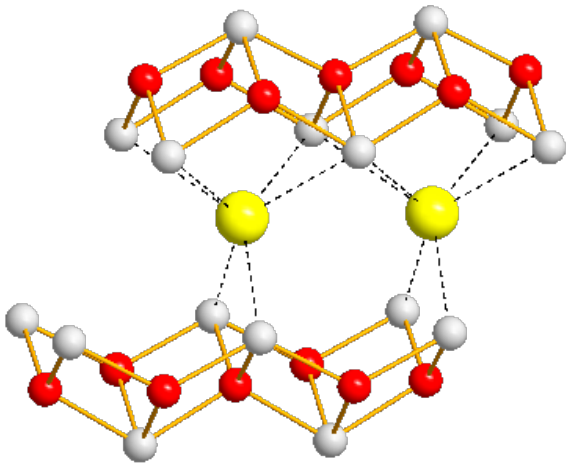


S. Sasaki, M. Caldes, C. Guillot-Deudon, IB, G. Steciuk, L. Palatinus, E. Gautron, G. Frapper, E. Janod, B. Corraze, S. Jobic and L. Cario, *Nat. Comm.* **12**, 3605 (2021)

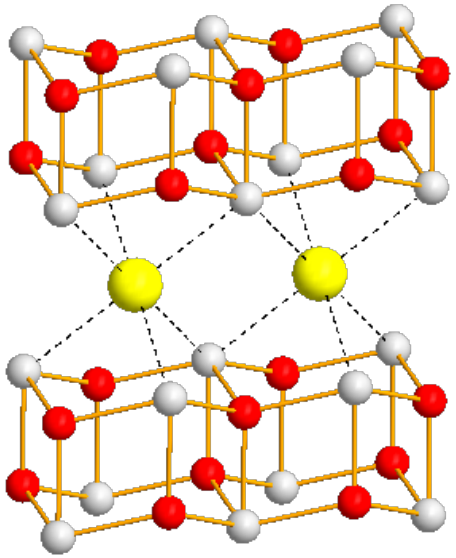
Structure-related luminescence properties



Predicted Pattern
oA-La_2O_2S
Metastable
(SG: Amm2)

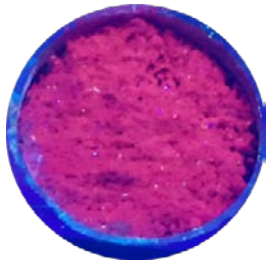


Predicted Pattern
hp-La2O2S
Stable
(SG: P$\bar{3}$m1)



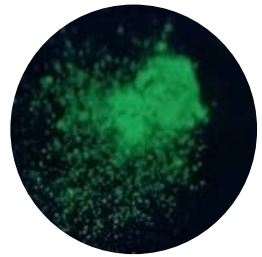
Eu^{3+} doping

Pr^{3+} doping



o*A*-La_2O_2S : Eu (1%)

o*A*-La_2O_2S : Pr (1%)



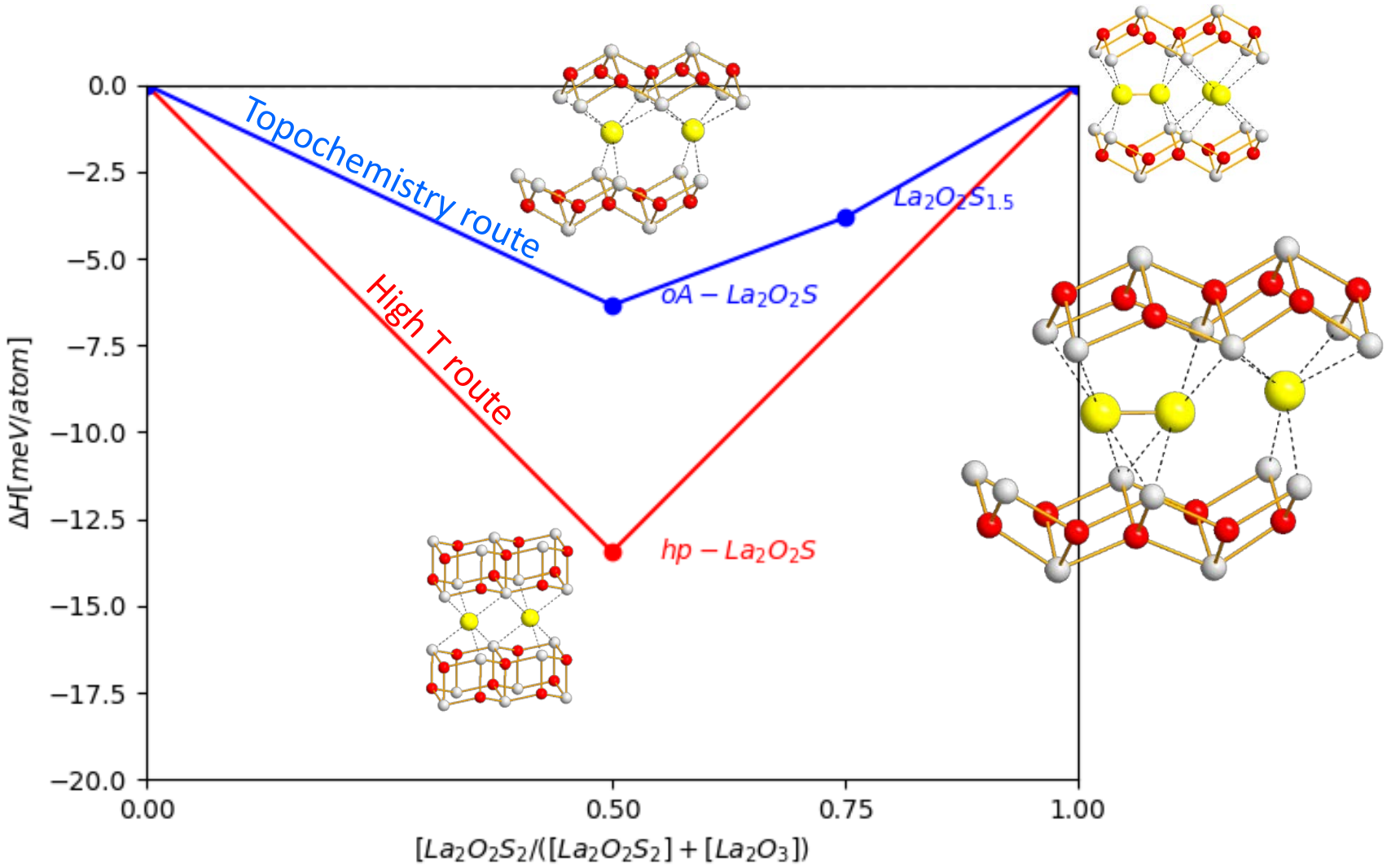
hP-La_2O_2S : Eu (1%)

hP-La_2O_2S : Pr (1%)

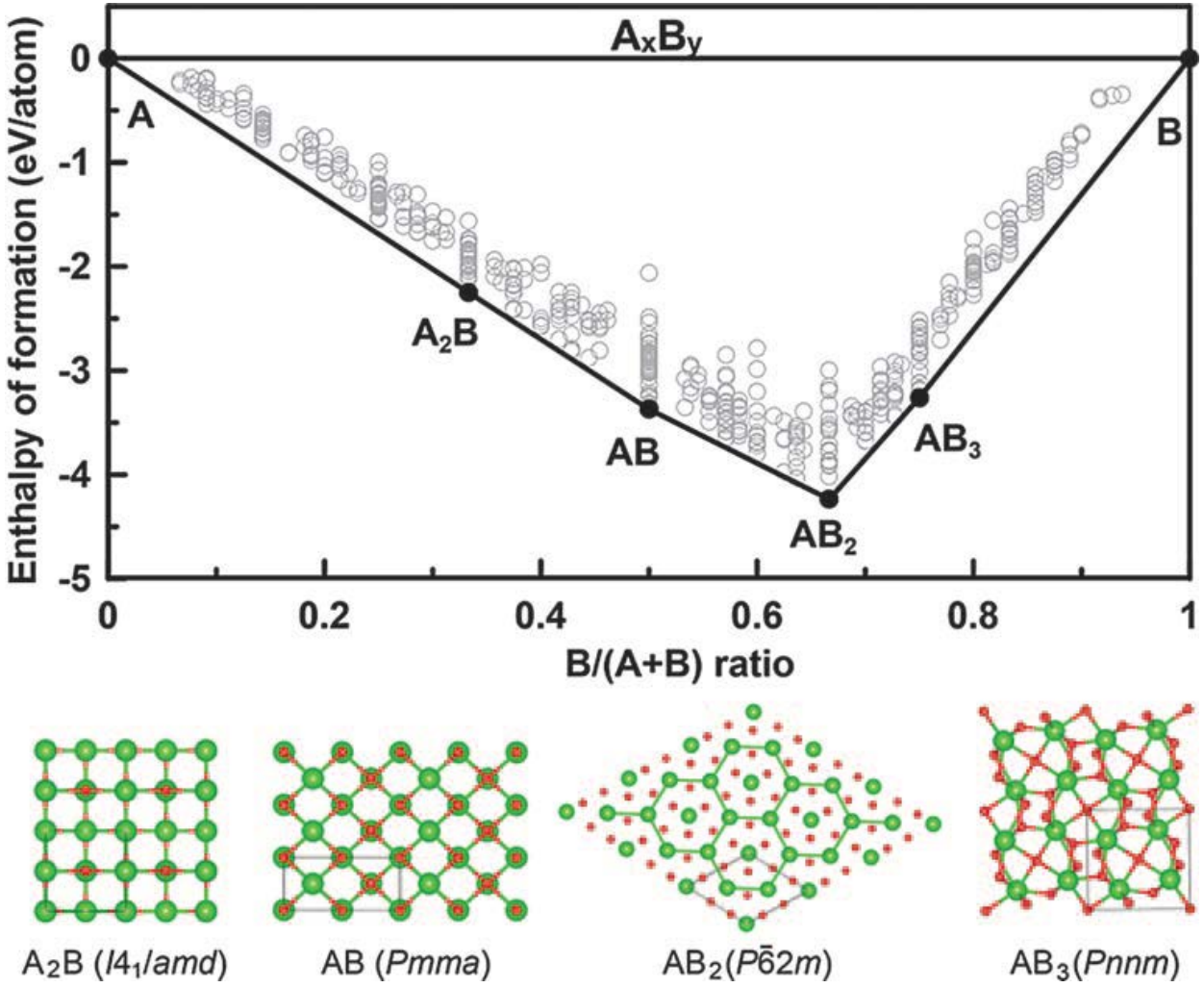
L. B. Mvélé, S. Sasaki, P. Deniard, Y. Tsujimoto, E. Janod, C. Guillot-Deudon, M Caldes, IB, B Corraze, S. Jobic, L. Cario, *Chem Mater, submitted*

Towards a phase diagram function of the synthesis route

Simple structural filiation with gliding of fluorine sheets



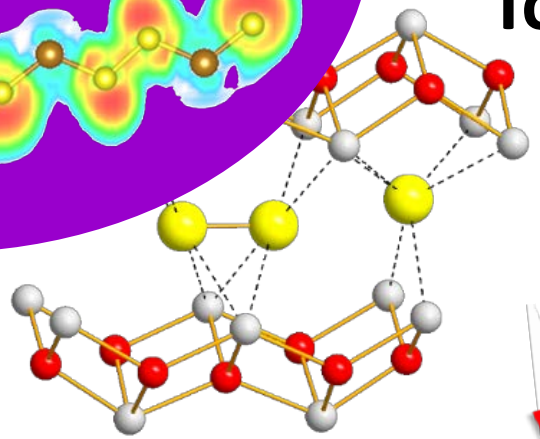
Convex hull when composition is unknown (stable compounds)



A.R.Oganov et al, Computational Materials Discovery

Topochemistry of Layered Polychalcogenides

Cation intercalation



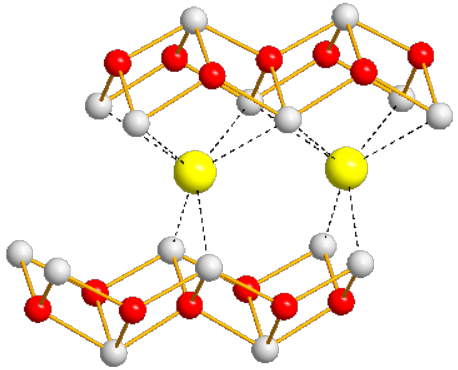
$oA - La_2O_2S_{1.5}$

+ 0.5 S

– 0.5 S

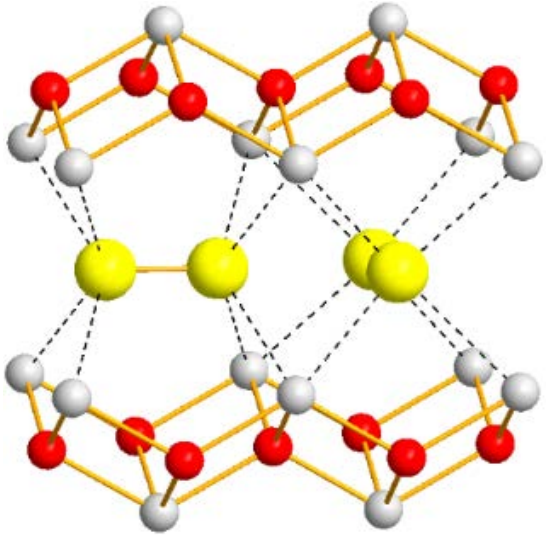
+ 0.5 S

Topochemistry of Sulfide Anion



$oA - La_2O_2S$

– 1.0 S

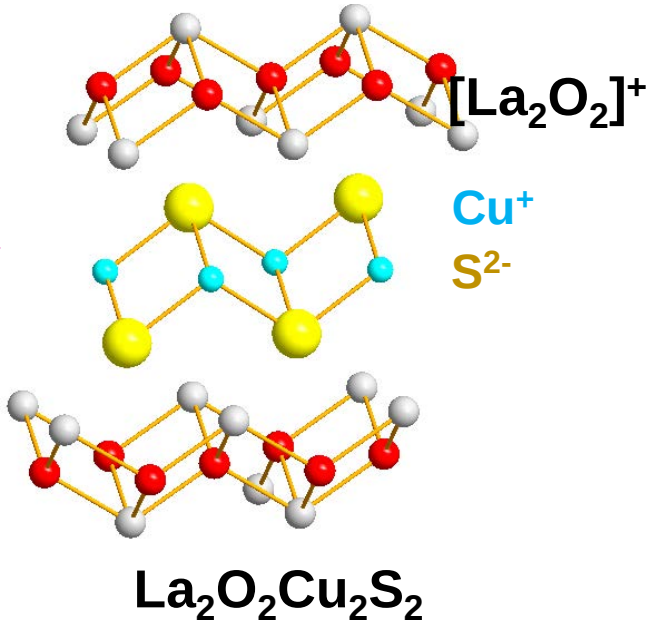


$La_2O_2S_2$

+ $2M^0$
(M = Cu, Fe, Co, Ni)

Topochemistry of Metal Cation

– M^0
(by Iodine)

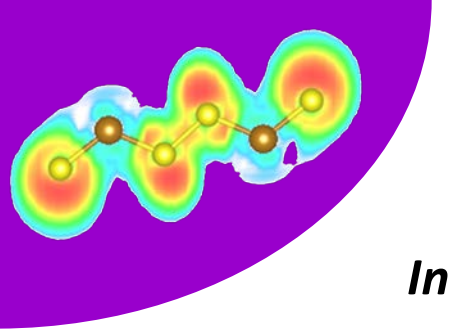


$[La_2O_2]^+$

Cu^+

S^{2-}

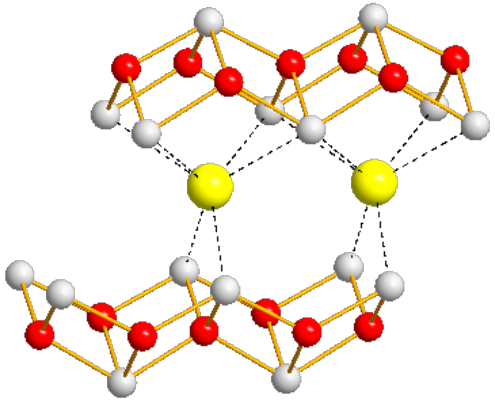
$La_2O_2Cu_2S_2$

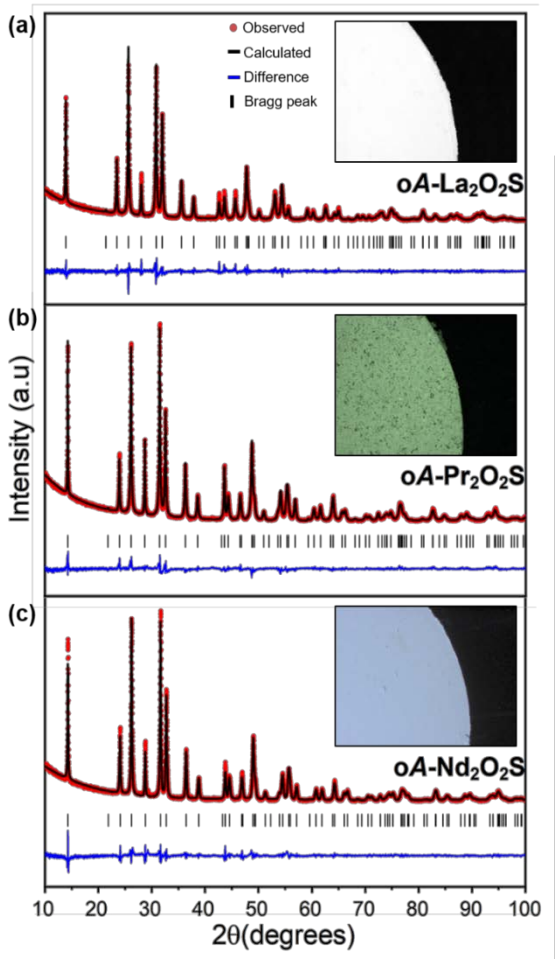


Rationalizing cation substitution

In the host lattice

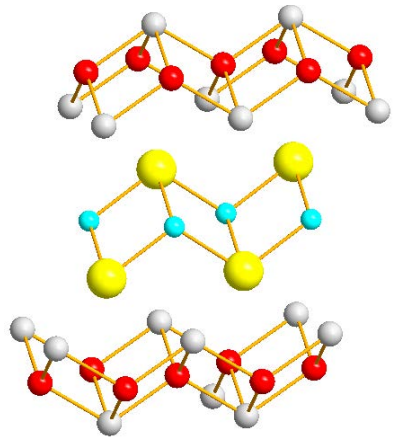
oA-Ln_2O_2S (Ln=La, Pr, Nd)





L-B.Mvélé, S. Sasaki, P. Deniard, Y. Tsujimoto, E. Janod, C. Guillot-Deudon, M Caldes, IB, B. Corraze, S. Jobic, L. Cario, *Chem Mater., submitted*

In the confined layer



$[La_2O_2]^+$

Cu^+

S^{2-}

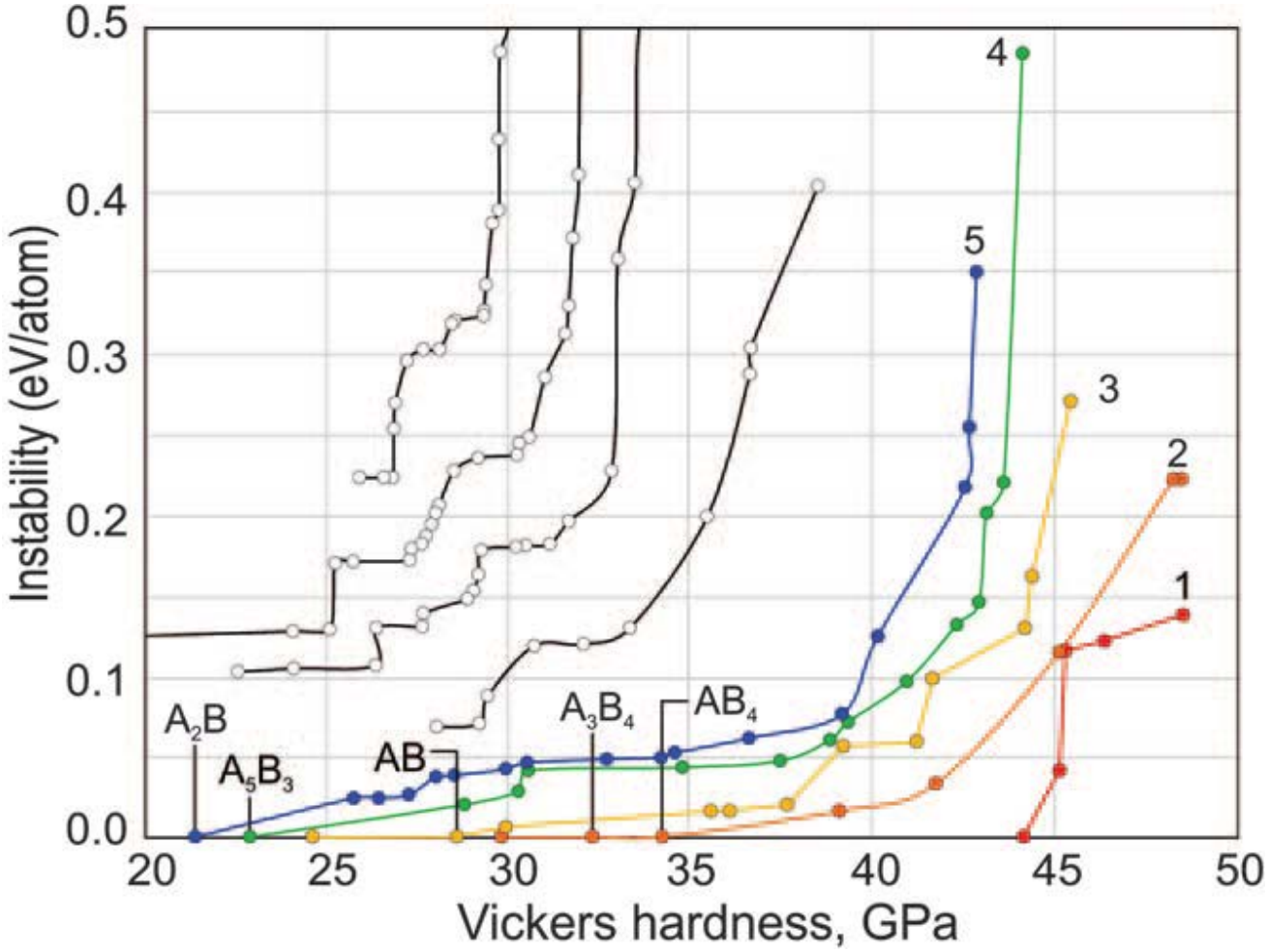
$La_2O_2Cu_2S_2$

S. Sasaki, IB et al, *in preparation*

IB, S. Sasaki, E. Janod, B. Corraze, S. Jobic, L. Cario, *in preparation*

Metastable with optimised desired property

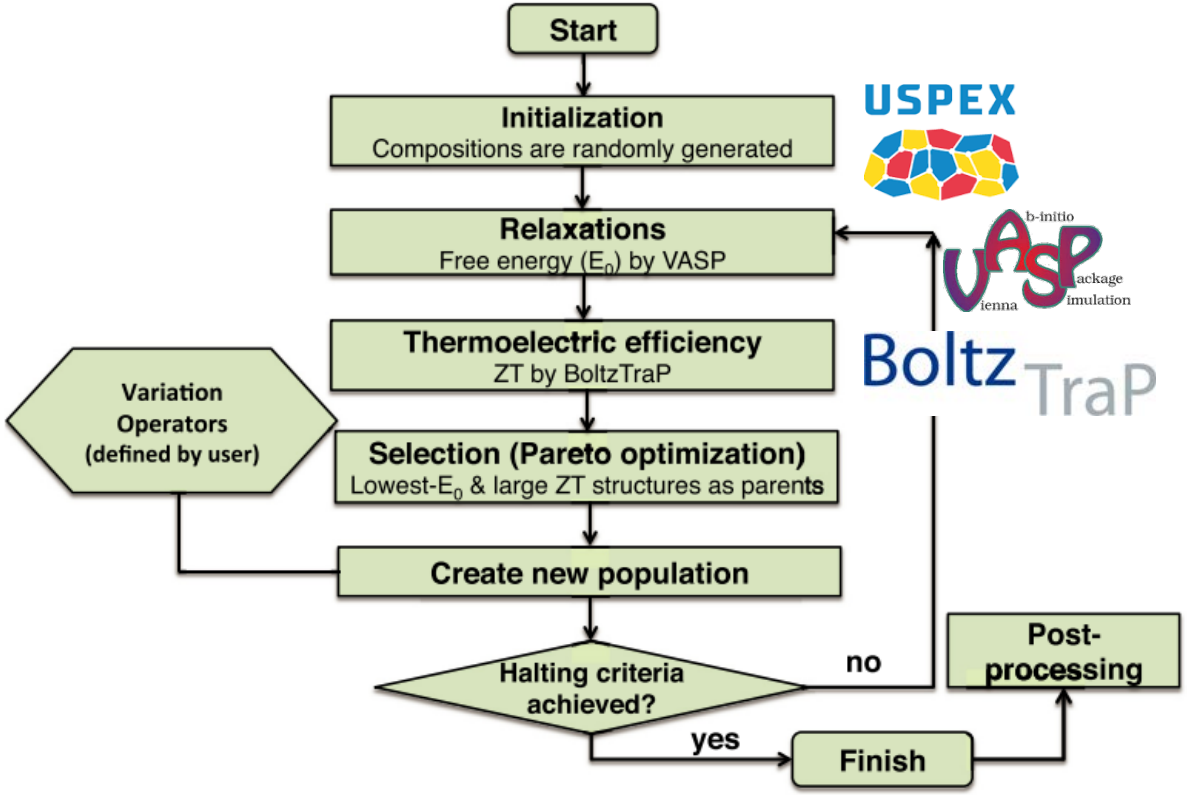
Multi-target optimization



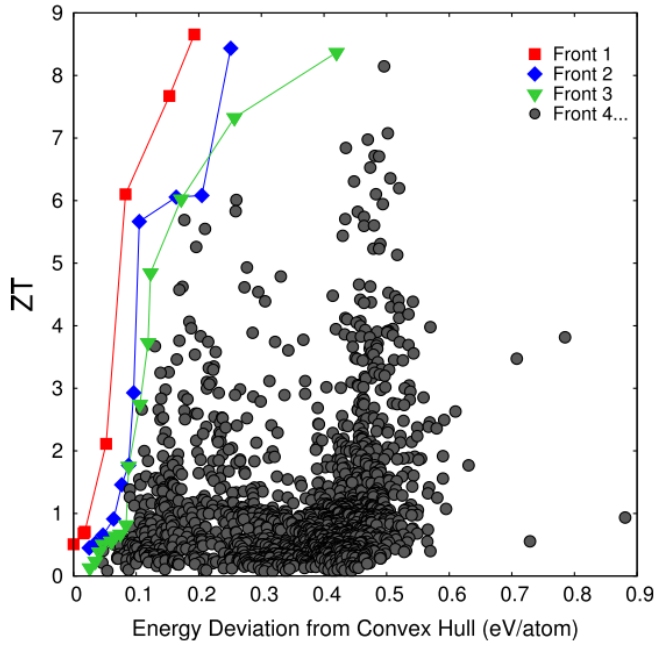
enthalpy
structure density
volume of system unit cell (for 3D)
Structure hardness
degree of order
structural quasientropy
Elastic bulk modulus calculated using ML model.
Elastic shear modulus calculated using ML model.
Elastic Young's modulus calculated using ML model.
Elastic Poisson's ratio calculated using ML model.
Elastic Pugh's modulus ratio calculated using ML model.
Elastic Vickers hardness calculated using ML model.
Elastic fracture toughness calculated using ML model.

Computational design of thermoelectric materials

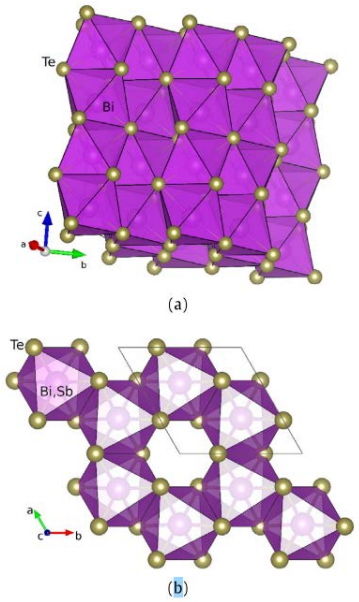
seek structures that are not only the most stable, but at the same time, possess a large figure of merit ZT



most optimal solutions



P63cm phases



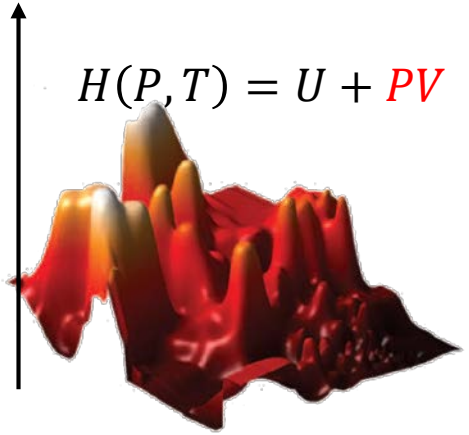
Bi_2Te_3-Sb_2Te_3

M. Núñez-Valdez, Z. Allahyari, T. Fan , AR Oganov, *Comp. Phys. Comm*, 222, 2018, 152-157

Superconductors

Pressure diagram for bulk compounds is nowadays routine

$$H(P,T) = U + PV$$



D. Duan, Y. Liu, F. Tian, D. Li, X. Huang, Z. Zhao, H. Yu, B. Liu, W. Tian & . Cui (2014). *Nat. Sci. Rep.* **4**, 6968.
D. Duan, X. Huang, F. Tian, D. Li, H. Yu, Y. Liu, Y. Ma, B. Liu, and T. Cui (2015). *Phys. Rev. B* **91(18)**, 180502.

Non-Fermi-Liquid Behavior of Superconducting SnH_4

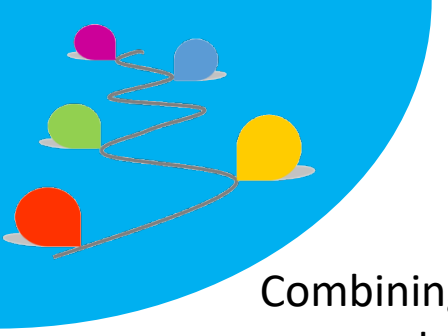
Ivan A. Troyan, Dmitrii V. Semenok, Anna G. Ivanova, Andrey V. Sadakov, Di Zhou, Alexander G. Kvashnin, Ivan A. Kruglov, Oleg A. Sobolevskiy, Marianna V. Lyubutina, Dmitry S. Perekalin, Toni Helm, Stanley W. Tozer, Maxim Bykov, Alexander F. Goncharov, Vladimir M. Pudalov, Igor S. Lyubutin

ADVANCED MATERIALS

Research Article | Full Access

Effect of Magnetic Impurities on Superconductivity in LaH_{10}

Dmitrii V. Semenok, Ivan A. Troyan, Andrey V. Sadakov, Di Zhou, Michele Galasso, Alexander G. Kvashnin, Anna G. Ivanova, Ivan A. Kruglov, Alexey A. Bykov ... See all authors



Take-home message

Combining structure prediction with diffraction or other experimental methods has provided a very successful approach to solving crystal structures of metastable compounds.

Win-win :

- **information on Z** greatly simplifies the searching.
- structure prediction could yield **better models for structural refinement**

Material discovery can tackle desired target, unknown stoechiometries and even **search through the periodic table**

"For most bulk materials synthesizing and processing procedures are reasonably well established. However, theoretical approaches have limited analytical power for predicting viable synthetic routes towards making entirely new materials. State-of-the-art in materials design needs to be complemented with substantial efforts in advancing the field of synthesis design.

To increase predictive ability of material synthesizability, it is necessary to ***define both equilibrium and out-of-equilibrium descriptors that control synthetic routes and outcomes***."

Kirstin Alberi et al 2019, The 2019 materials by design roadmap, *J. Phys. D: Appl. Phys*. 52 013001

Thank you for your attention !

Open to questions and collaborations