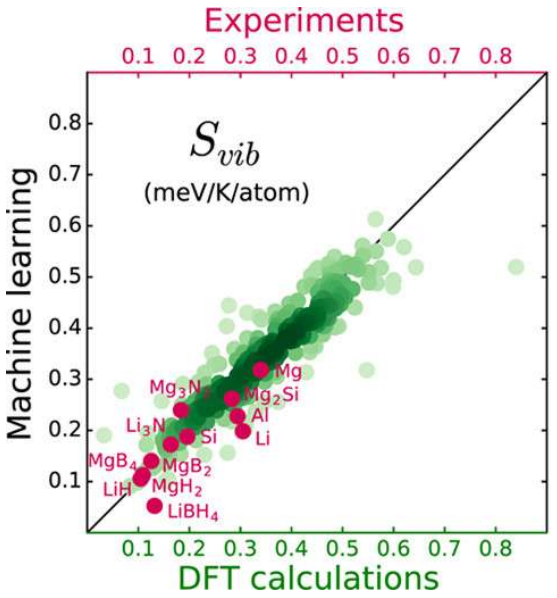
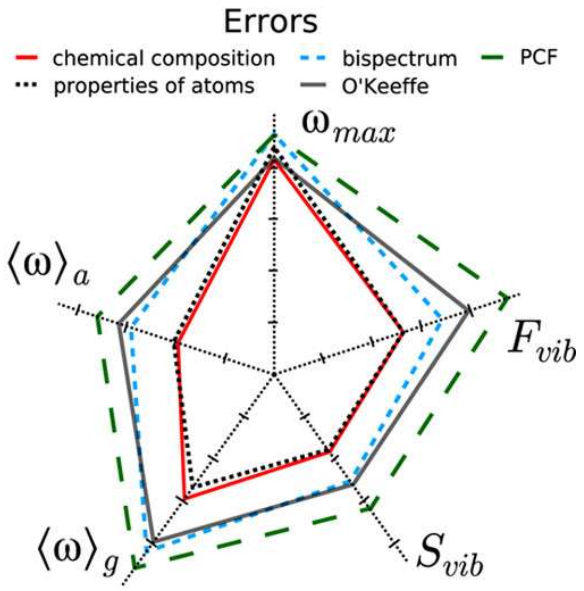
liten
cea tech



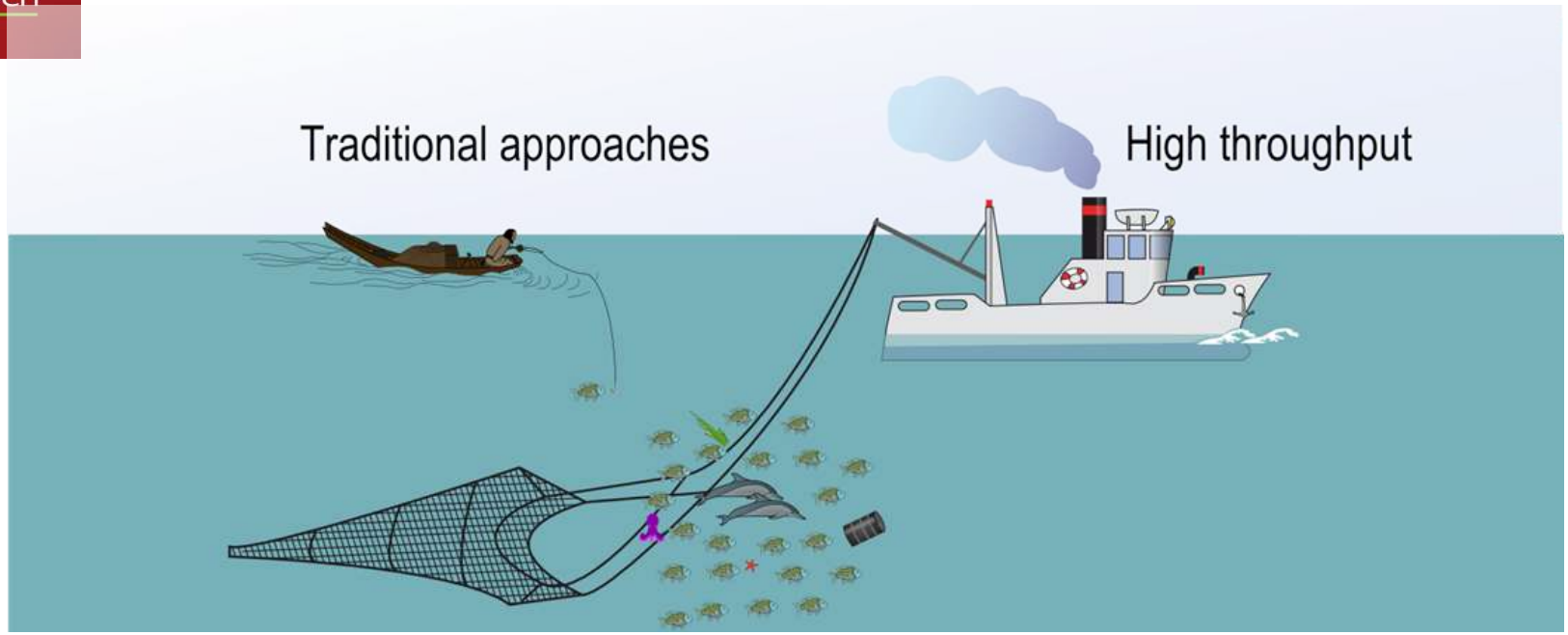


MACHINE LEARNING AND HIGH-THROUGHPUT COMPUTATIONAL SCREENING

L'intelligence artificielle pour la chimie des matériaux – ICMPE – Thiais – 25/09/2018

Ambroise van Roekeghem

HIGH-THROUGHPUT SCREENING



MATERIALS PROJECT

Energy & Environmental Science

RSC Publishing

PAPER

View Article Online
View Journal | View Issue

First principles high throughput screening of oxynitrides for water-splitting photocatalysts

Cite this: *Energy Environ. Sci.*, 2013, **6**, 157

Yabi Wu,[a] Predrag Lazic,[a] Geoffroy Hautier,†[a] Kristin Persson[b] and Gerbrand Ceder*[a]

AFLOW

Automatic - FLOW for Materials Discovery

nature materials

REVIEW ARTICLE

PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3568

The high-throughput highway to computational materials design

Stefano Curtarolo[1,2]*, Gus L. W. Hart[2,3], Marco Buongiorno Nardelli[2,4,5], Natalio Mingo[2,6], Stefano Sanvito[2,7] and Ohad Levy[1,2,8]

NOMAD

NREL

NATIONAL RENEWABLE ENERGY LABORATORY

High Performance Computing Center

Materials Database

ARTICLES

PUBLISHED ONLINE: 24 MARCH 2015 | DOI: 10.1038/NCHEM.2207

nature chemistry

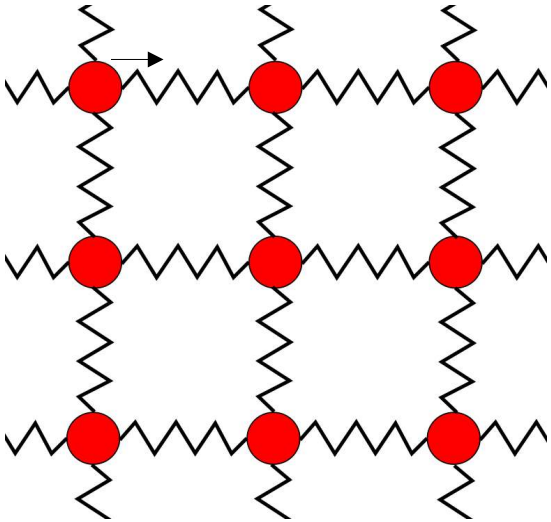
Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds

Romain Gautier[†], Xiuwen Zhang[2†], Linhua Hu[1], Liping Yu[2], Yuyuan Lin[1], Tor O. L. Sunde[1], Danbee Chon[1], Kenneth R. Poeppelmeier[1]* and Alex Zunger[2]*

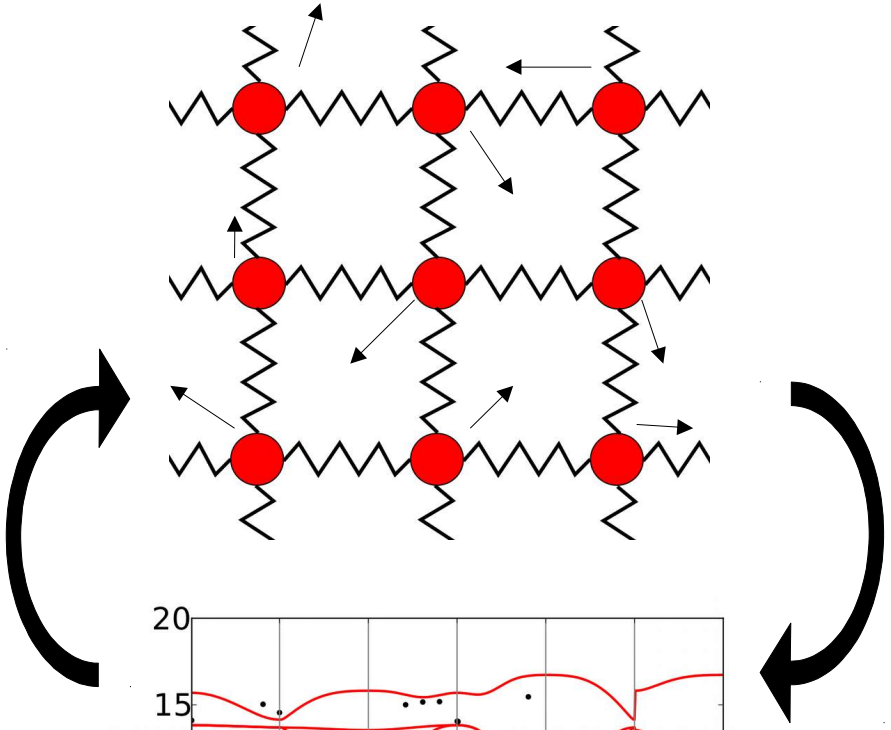
AiiDA

FINITE-TEMPERATURE PHONON CALCULATIONS

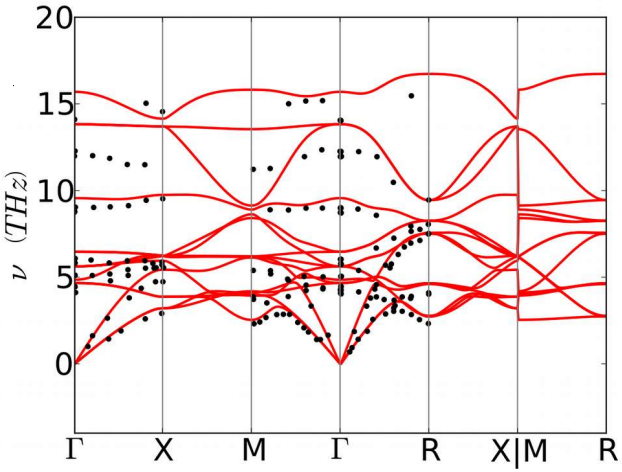
Small displacements



Quantum statistics, finite T



$$F_i^\alpha = \sum_{j\beta} \Phi_{ij}^{\alpha\beta} u_j^\beta + \frac{1}{2} \sum_{jk\beta\gamma} \Psi_{ijk}^{\alpha\beta\gamma} u_j^\beta u_k^\gamma$$



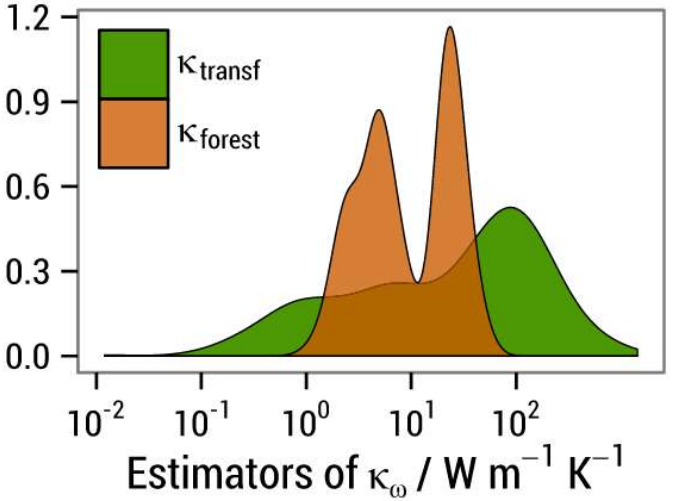
→ 2nd and 3rd order force constants

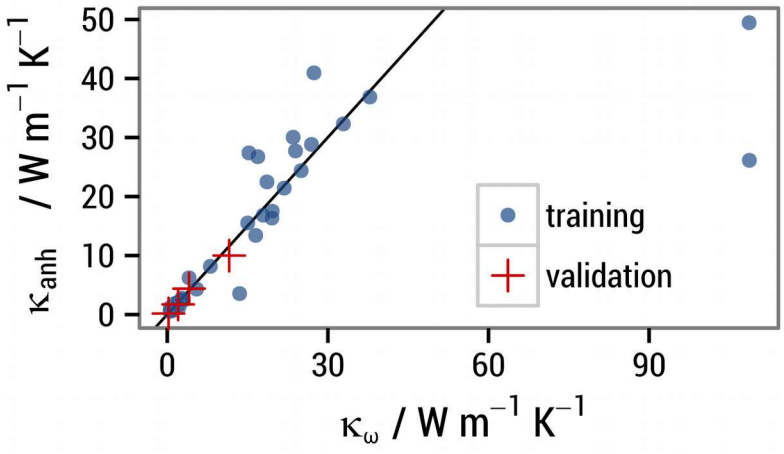
→ Thermal conductivity

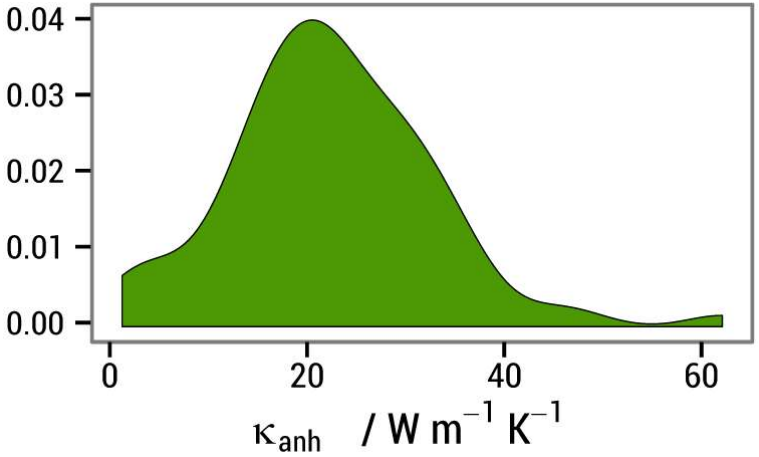
van Roekeghem et al., Physical Review B 94, 020303(R) (2016)

RANDOM FORESTS AND DIMENSIONALITY REDUCTION

Label	Definition
κ_ω	Lattice contribution to κ from the "full calculation"
κ_{transf}	Approximated κ_ω with anharmonic force constants from Mg_2Si
κ_{forest}	κ_ω obtained random-forest regression
κ_{anh}	κ_ω obtained with four exact anharmonic force constants and a linear model for the rest
κ_e	Electronic contribution to κ
$\tilde{\kappa}_{grain}$	Scaled nanograined limit κ_ω

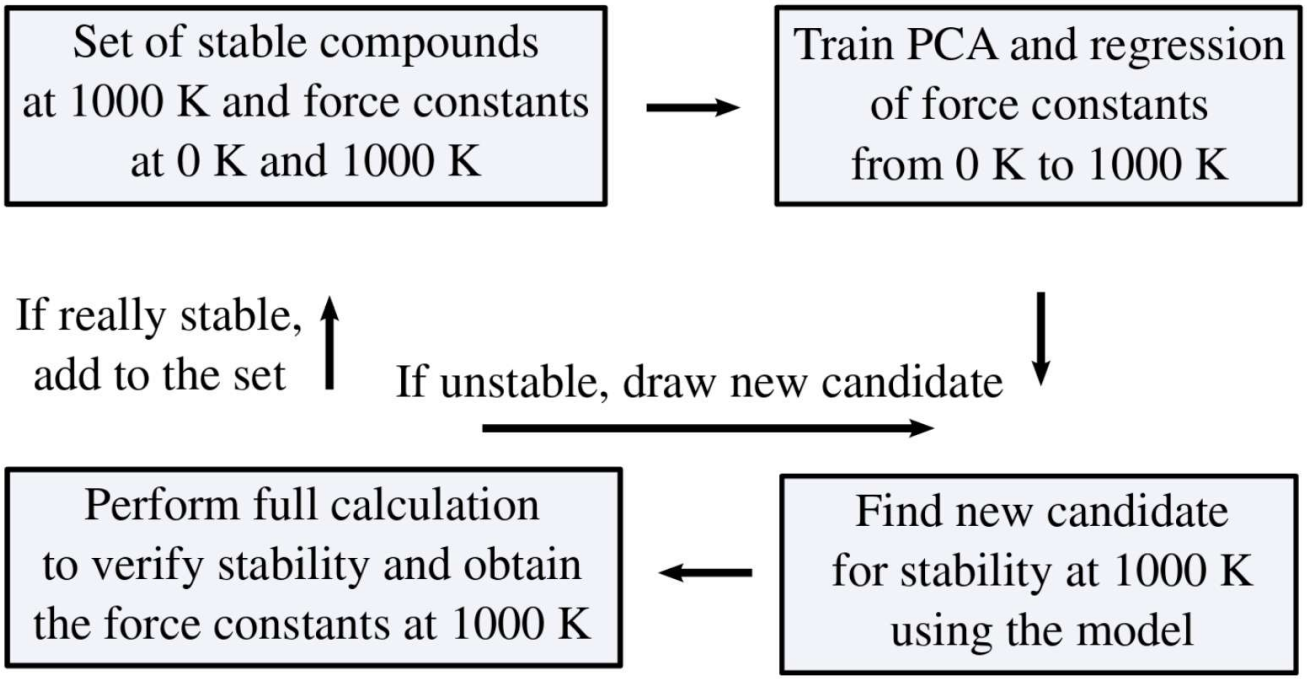






Carrete et al., Physical Review X 4, 011019 (2014)

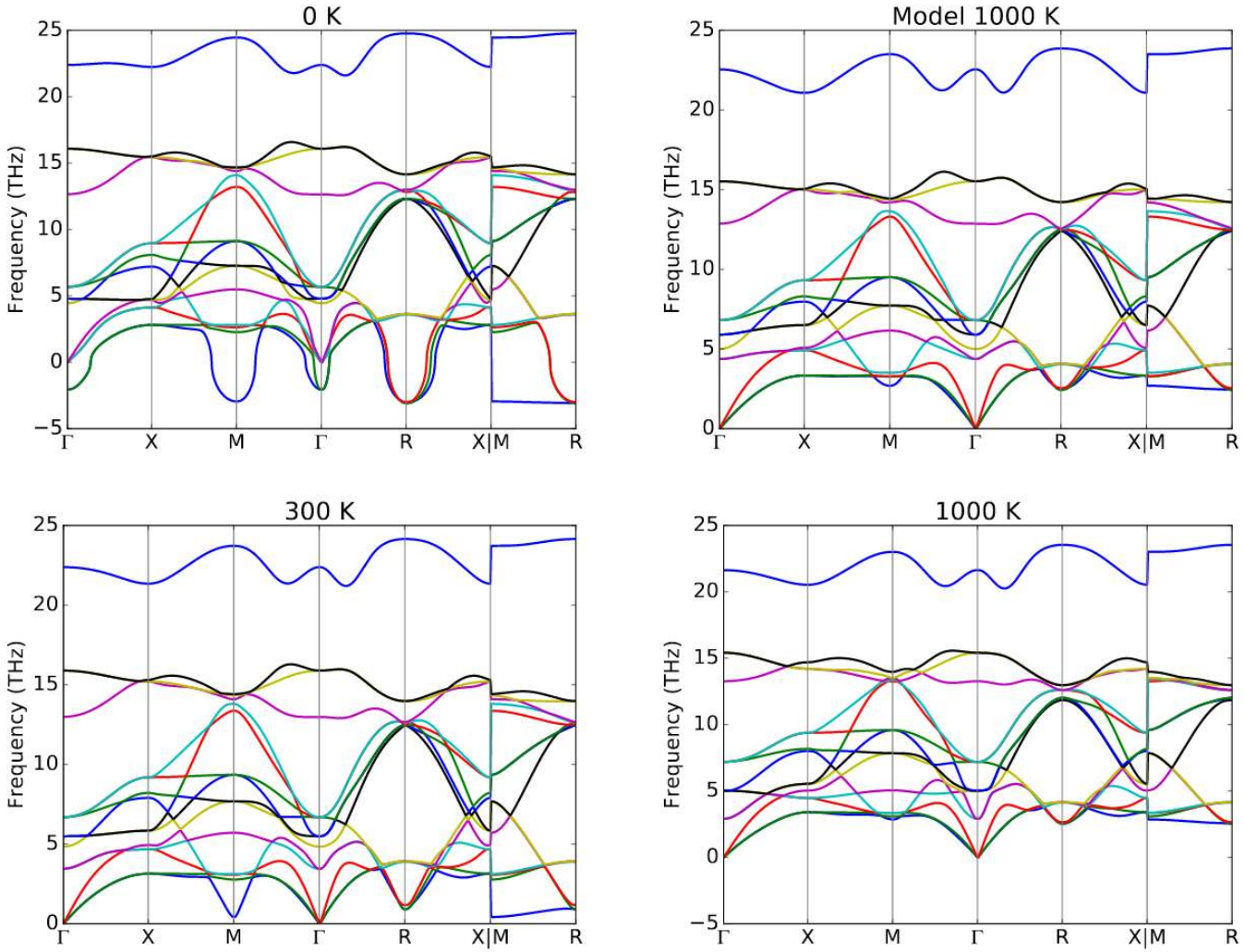
DIMENSIONALITY REDUCTION



79 candidates out of about 400 compounds
68 positives vs 92 for the brute force calculation

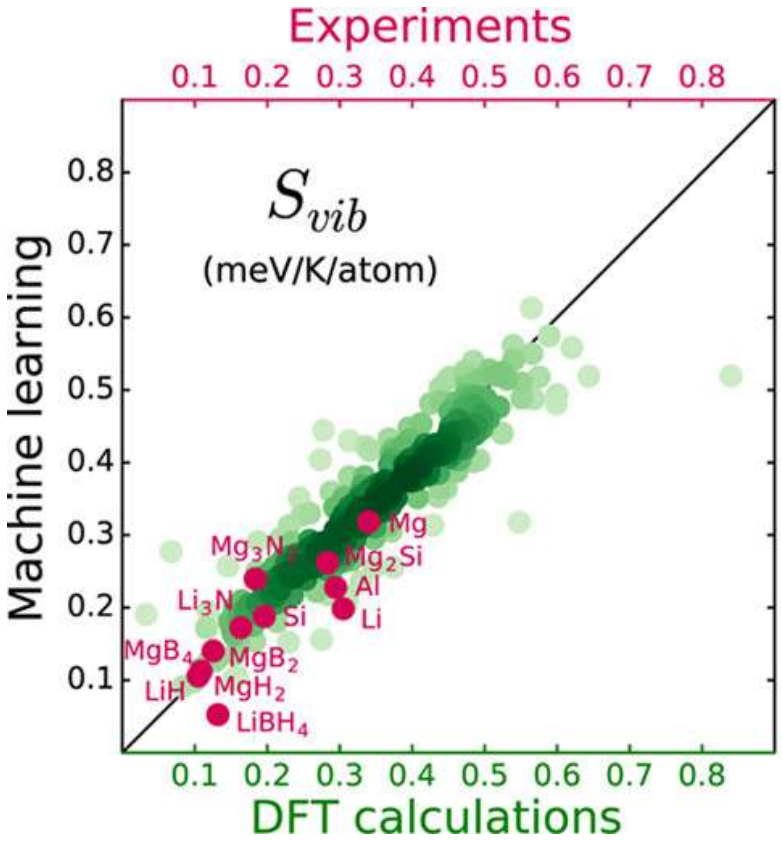
van Roekeghem et al., Physical Review X 6, 041061 (2016)

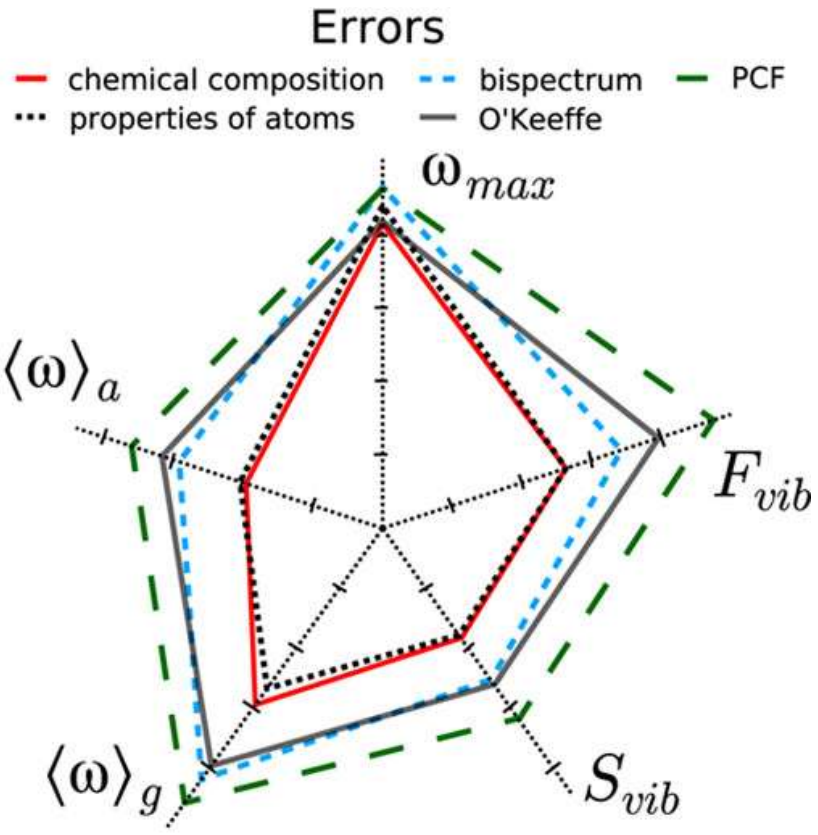
DIMENSIONALITY REDUCTION



van Roekeghem et al., Physical Review X 6, 041061 (2016)

CHEMICAL DESCRIPTORS





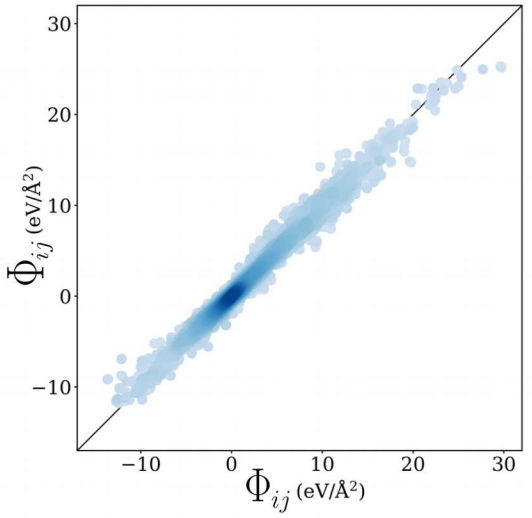
Legrain et al., Chemistry of Materials 29, 6220 (2017)

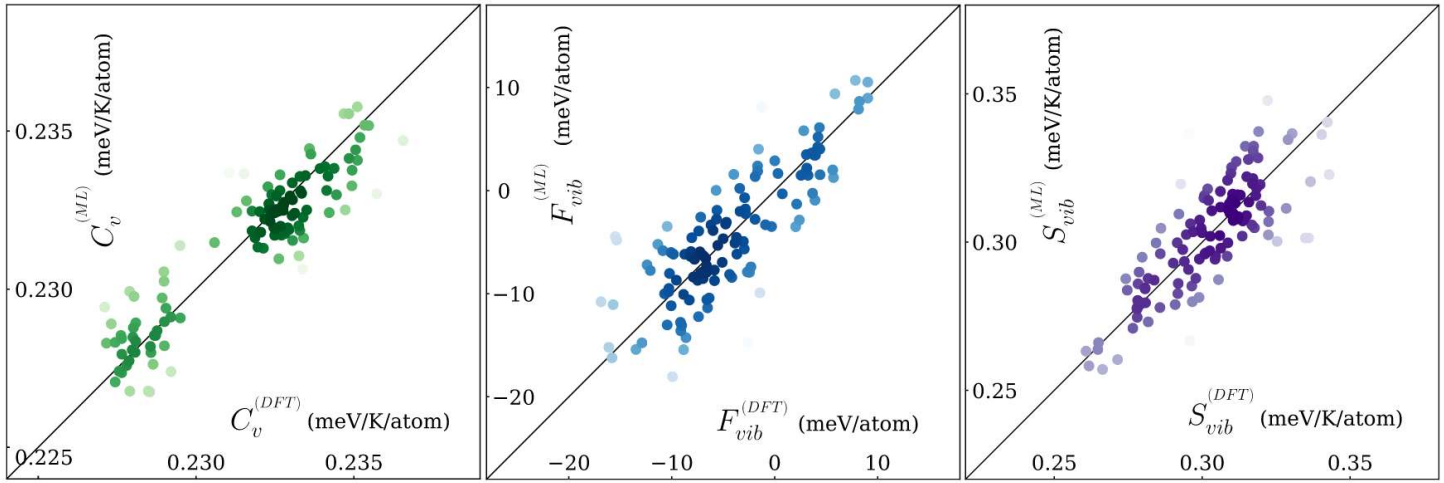
STRUCTURAL DESCRIPTORS

$$\mathbf{D}_{i,j}^{(2)\alpha} = \sum_m e^{-\left|\frac{\mathbf{r}_{ij}+\mathbf{R}_m}{a_\alpha}\right|^2} (\mathbf{r}_{ij} + \mathbf{R}_m) \otimes (\mathbf{r}_{ji} - \mathbf{R}_m)$$

$$\mathbf{D}_{s,s';i,j}^{(2)\alpha} \equiv (\delta_{s_i,s}\delta_{s_j,s'} + \delta_{s_i,s'}\delta_{s_j,s})\mathbf{D}_{i,j}^{(2)\alpha}$$

$$a_\alpha = \{1, 2, 3, ..., 30\} \text{ Å}$$





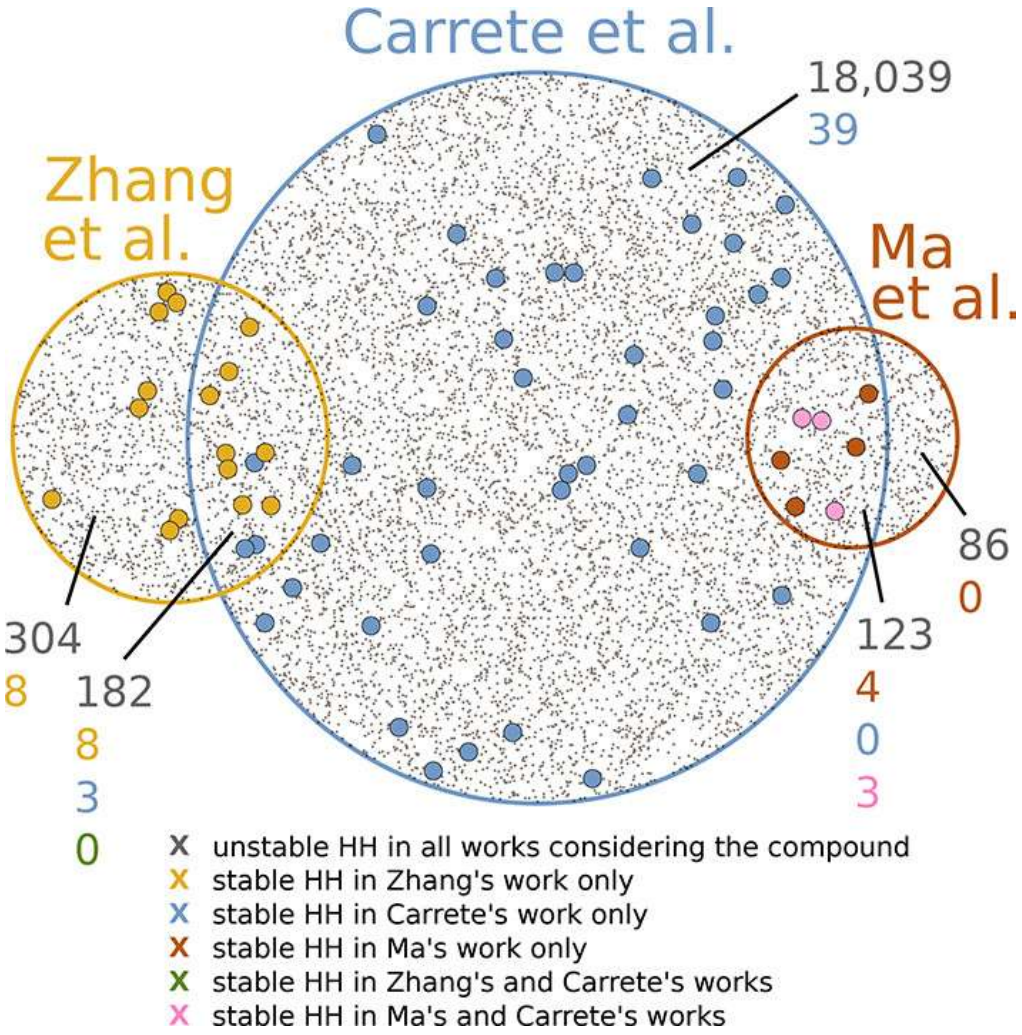
Legrain et al., arXiv:1803.09827, Journal of Chemical Information and Modeling in press

FINDING NEW COMPOUNDS

XYZ	probability	space group
ErNiBi	0.954	216[b]
TmPtBi	0.947	216[b]
ErPdBi	0.931	216[c]
MnRuSb	0.931	
TbPtBi	0.913	216[b]
TbPdBi	0.906	216[b]
TmPdBi	0.899	216[b]
EuPdBi	0.890	
MnFeSb	0.885	227[d]
LuPtBi	0.882	216[b]
YPtBi	0.864	216[b]
EuPtBi	0.861	
TiRhSb	0.861	216[e]
ScPdBi	0.854	216[b]
MnTeRh	0.846	
HfCoBi	0.844	
LuPdBi	0.831	216[b]

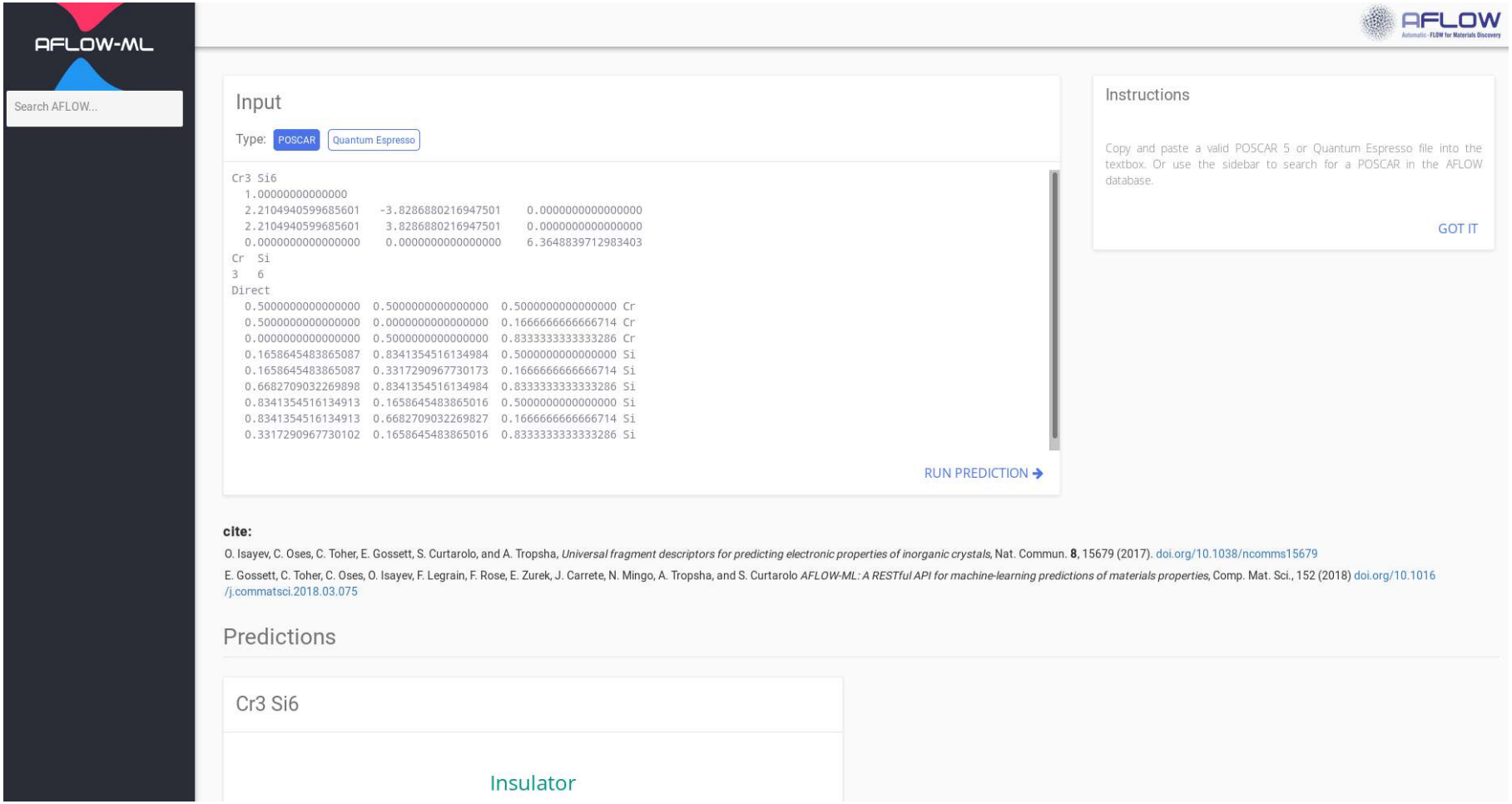
Legrain et al., The Journal of Physical Chemistry B 122, 625 (2018)

REPRODUCIBILITY



Legrain et al., The Journal of Physical Chemistry B 122, 625 (2018)

OPEN CODES AND DATABASES



EXPERIMENTAL DEMONSTRATION

J|A|C|S JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Article
pubs.acs.org/JACS

Theoretical Prediction and Experimental Realization of New Stable Inorganic Materials Using the Inverse Design Approach

Andriy Zakutayev,[†] Xiuwen Zhang,[†,‡] Arpun Nagaraja,[∥] Liping Yu,[§] Stephan Lany,[†] Thomas O. Mason,[∥] David S. Ginley,[†] and Alex Zunger*[,§]

ARTICLES
PUBLISHED ONLINE: 24 MARCH 2015 | DOI: 10.1038/NCHEM.2207
nature chemistry

Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds

Romain Gautier[1†], Xiuwen Zhang[2†], Linhua Hu[1], Liping Yu[2], Yuyuan Lin[1], Tor O. L. Sunde[1], Danbee Chon[1], Kenneth R. Poeppelmeier[1]* and Alex Zunger[2]*

ARTICLE
Received 12 Nov 2014 | Accepted 27 Apr 2015 | Published 24 Jun 2015
DOI: 10.1038/ncomms8308

Design and discovery of a novel half-Heusler transparent hole conductor made of all-metallic heavy elements

Feng Yan[1,*], Xiuwen Zhang[2,*], Yonggang G. Yu[2], Liping Yu[3], Arpun Nagaraja[1], Thomas O. Mason[1] & Alex Zunger[2]

Keynote

NOVEL HIGH-ENTROPY CARBIDES DISCOVERED BY SYNTHESIZABILITY DESCRIPTORS

Pranab Sarker[1] , Tyler Harrington[2] , Cormac Toher[1] , Kenneth Vecchio[2] , Jon-Paul Maria[3] , Donald Brenner[3] , **Stefano Curtarolo**[1] ,

CONCLUSION

- Machine learning techniques and high-throughput screening is a very good combination
- The field is still young and needs structure and solid results
- Very simple machine learning techniques can already provide a lot of interesting information

Thank you!

In collaboration with:

Natalio MINGO
Jesús CARRETE
Fleur LEGRAIN
Stefano CURTAROLO

For more: listen to
Anton BOCHKAREV’s talk.

Commissariat à l’énergie atomique et aux énergies alternatives
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