NOMAD
NOVEL MATERIALS DISCOVERY

FAIRmat

MAX-PLANCK-GESELLSCHAFT

Learning Descriptors for Materials Properties with Symbolic Regression and Compressed Sensing

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MAX-PLANCK-GESELLSCHAFT

Big Data Summer
A summer school of the BiGmax Network
Platja d'Aro, Spain, September 9 - 13, 2019

Charts/maps of materials

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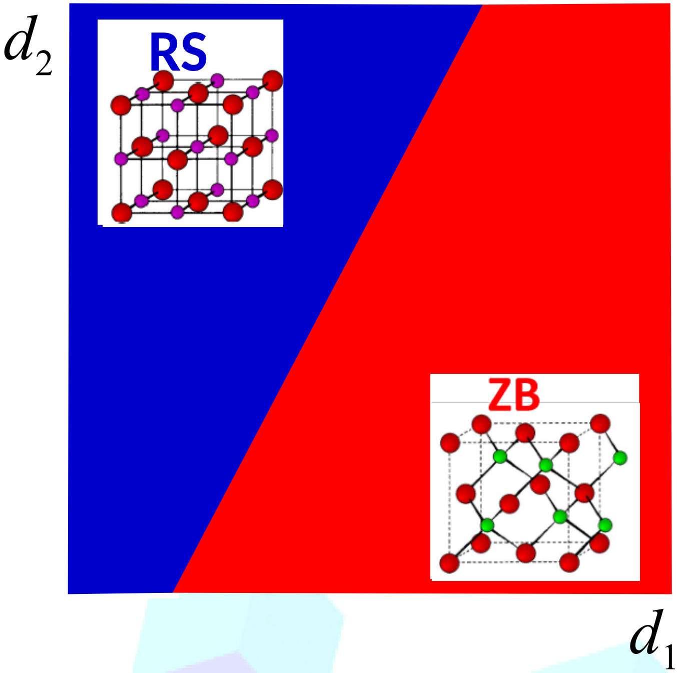

Octet binaries

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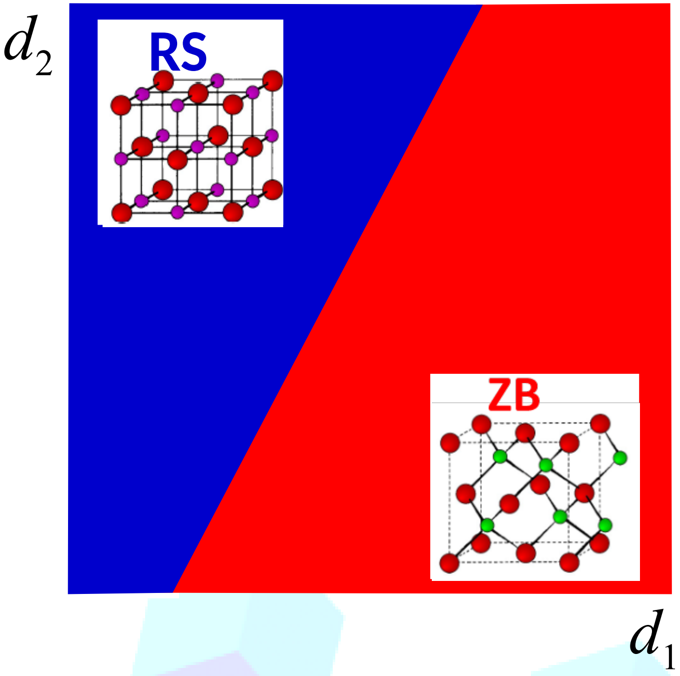

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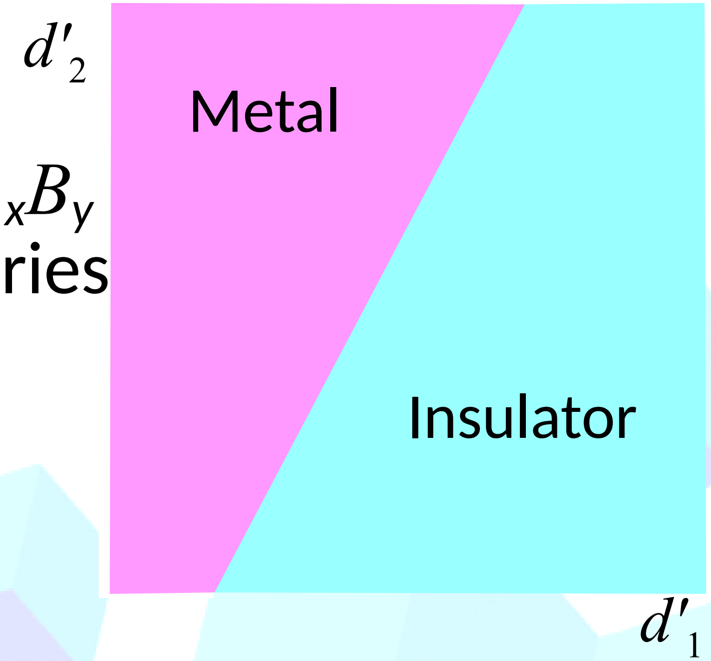
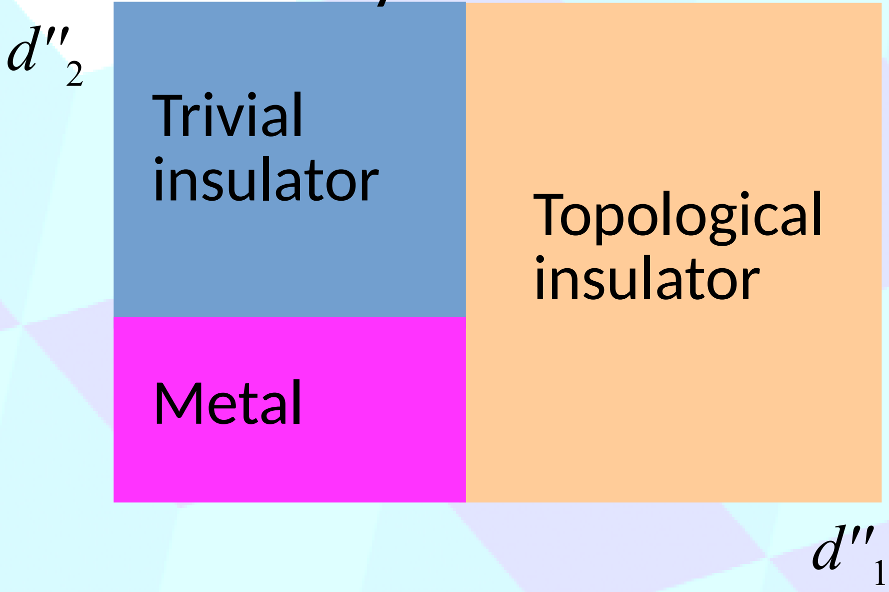


2D honeycomb materials



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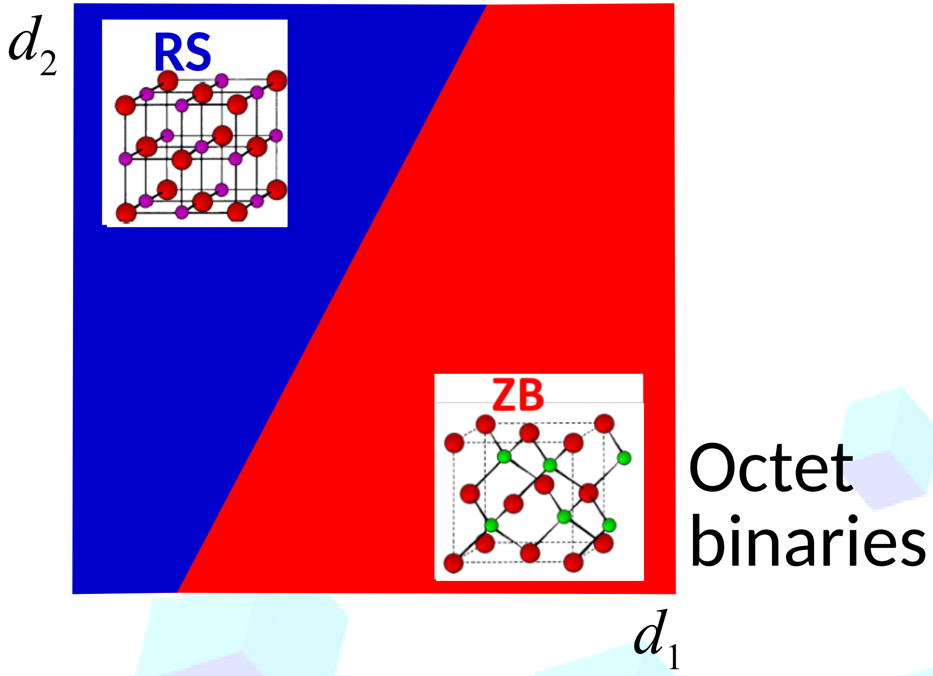
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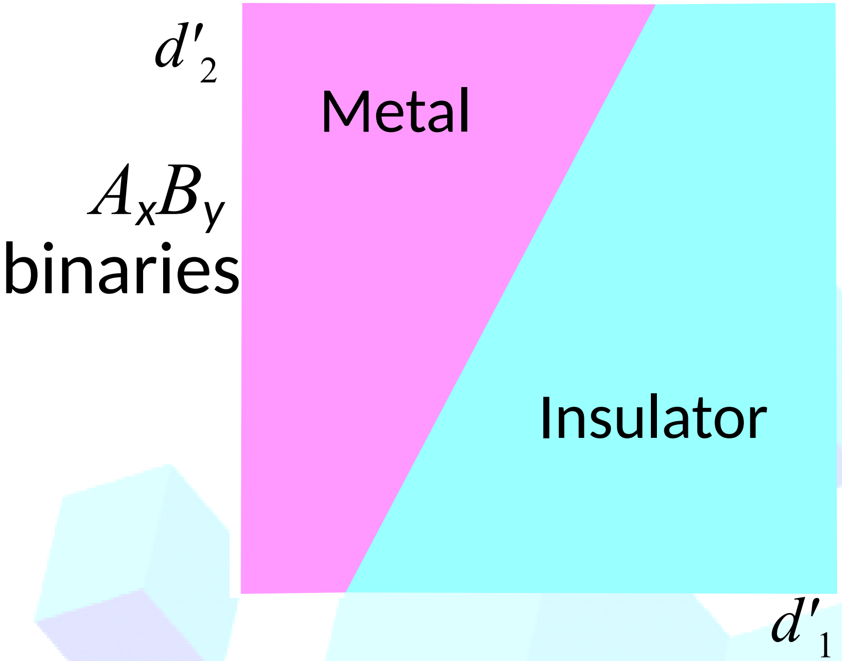
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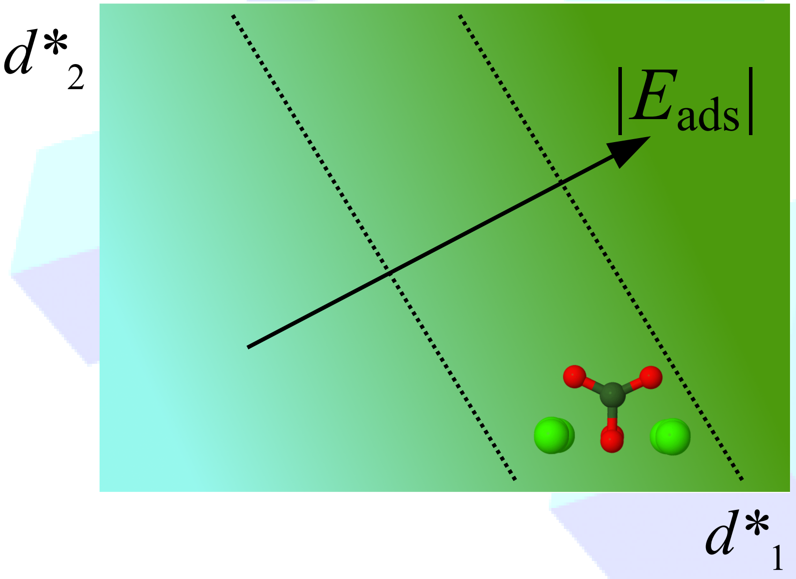
$E_{ads}(CO_2)$ on oxides



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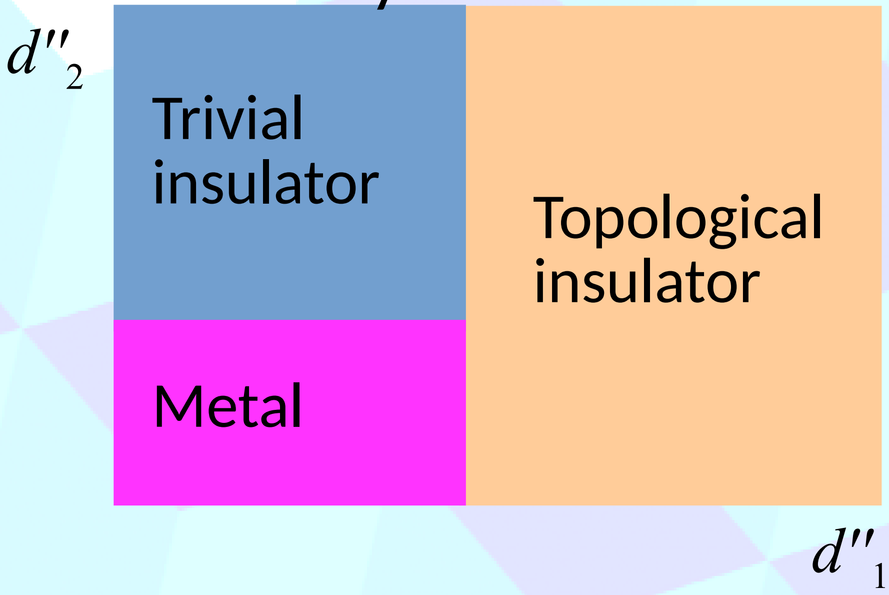

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A quantum many-body problem

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For instance, given a class of chemical compositions (e.g., via prototype formula, such as ABX_3):

- what is the most stable crystal structure of each material in the class?
- which materials are metals / topological insulators / superconductors ?
- which material has the highest melting point?
- which materials has a surface optimal for catalysing some chemical reaction?

The Big Picture

- Design of new materials:
  preparation, synthesis, and characterization is complex and costly

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- Data analytics tools will help to identify trends and anomalies in data and guide discovery of new materials

We have a dream

From the **periodic table of the elements**
to **charts of materials**

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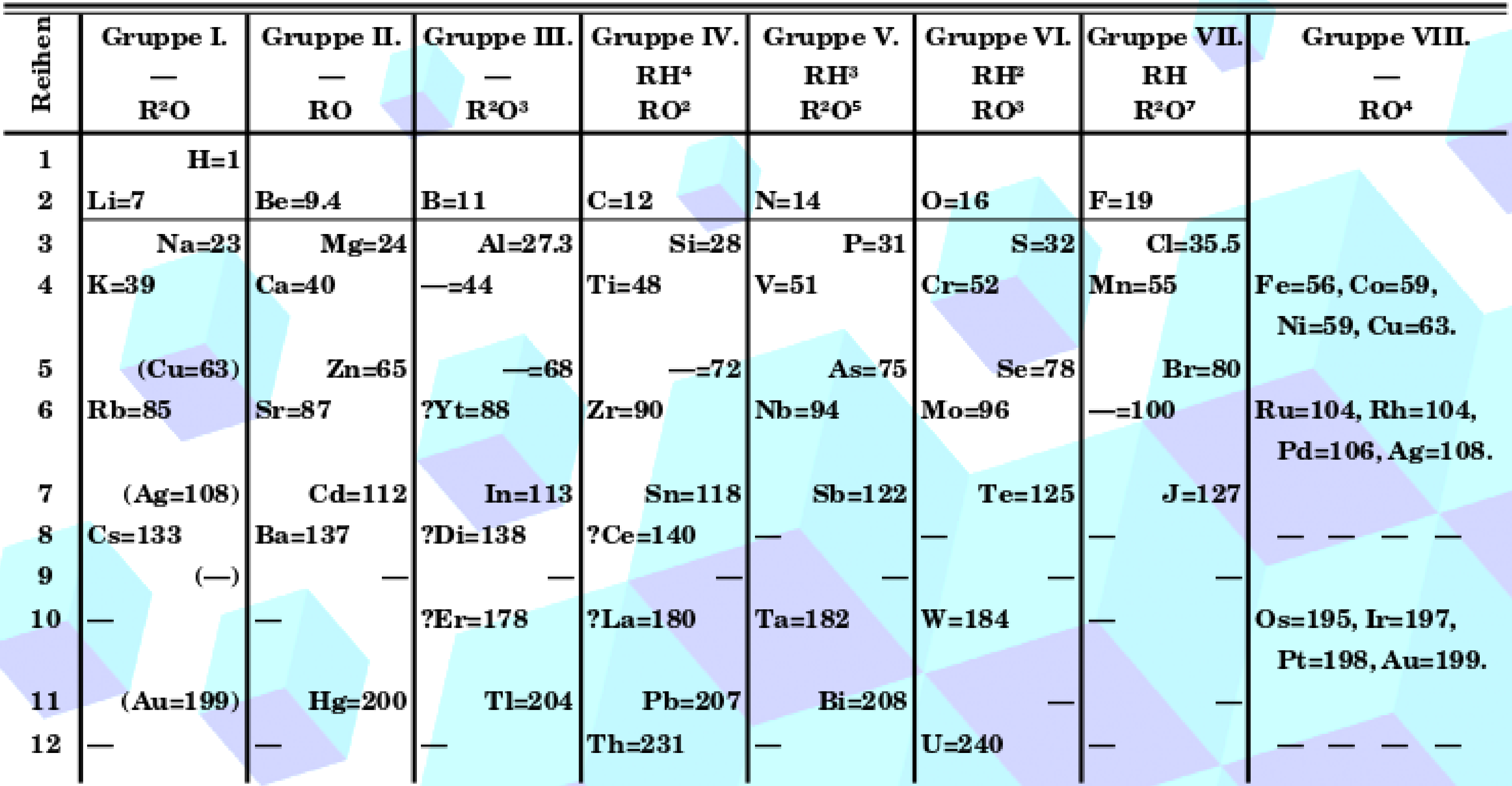
From the **periodic table of the elements** to **charts of materials**



Reihen	Gruppe I.	Gruppe II.	Gruppe III.	Gruppe IV.	Gruppe V.	Gruppe VI.	Gruppe VII.	Gruppe VIII.
	—	—	—	RH^4	RH^3	RH^2	RH	—
	R^2O	RO	R^2O^3	RO^2	R^2O^5	RO^3	R^2O^7	RO^4
1	H=1							
2	Li=7	Be=9.4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27.3	Si=28	P=31	S=32	Cl=35.5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
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11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

Mendeleev's **1871** periodic table

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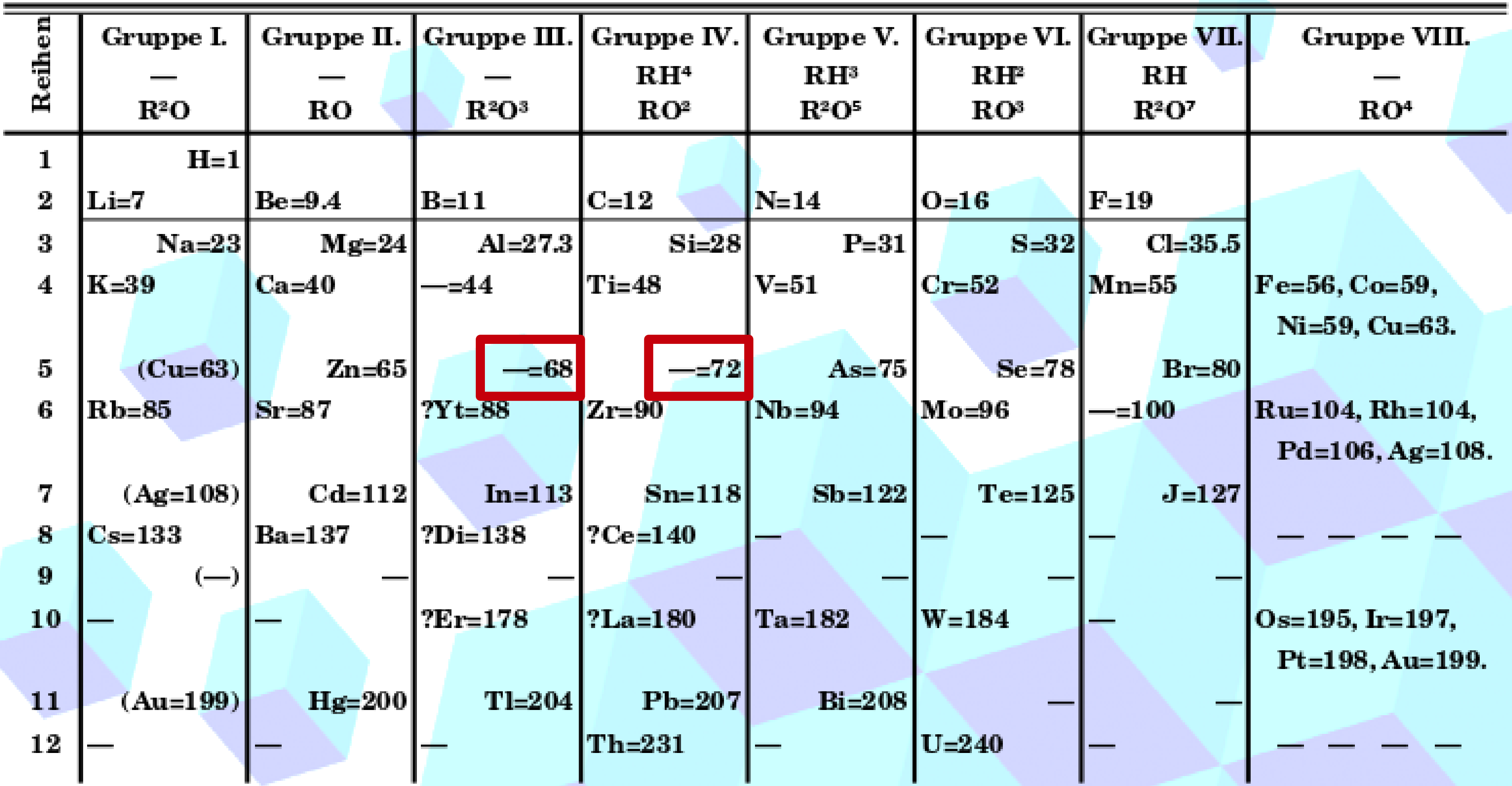

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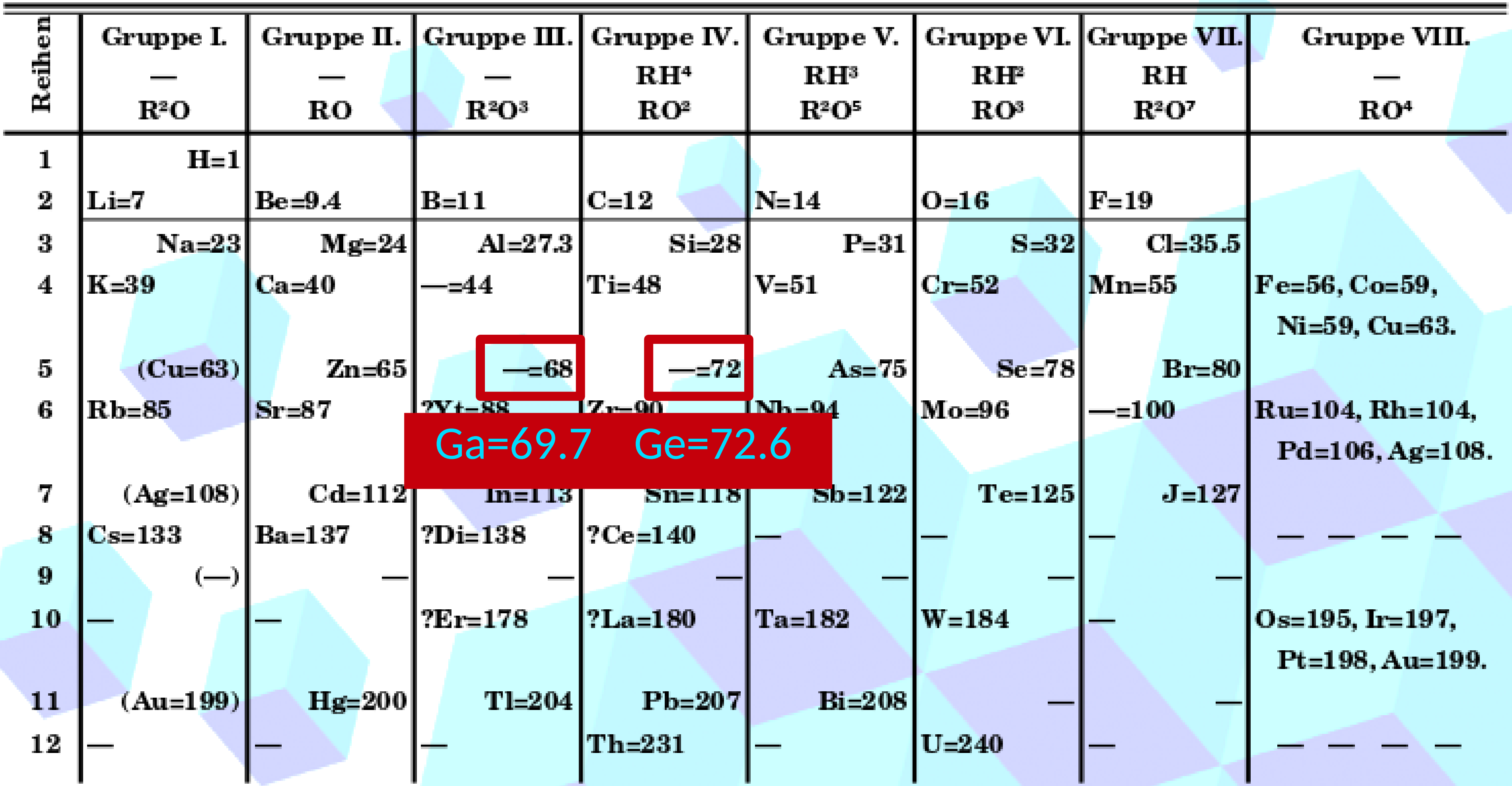

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Ga=69.7 Ge=72.6

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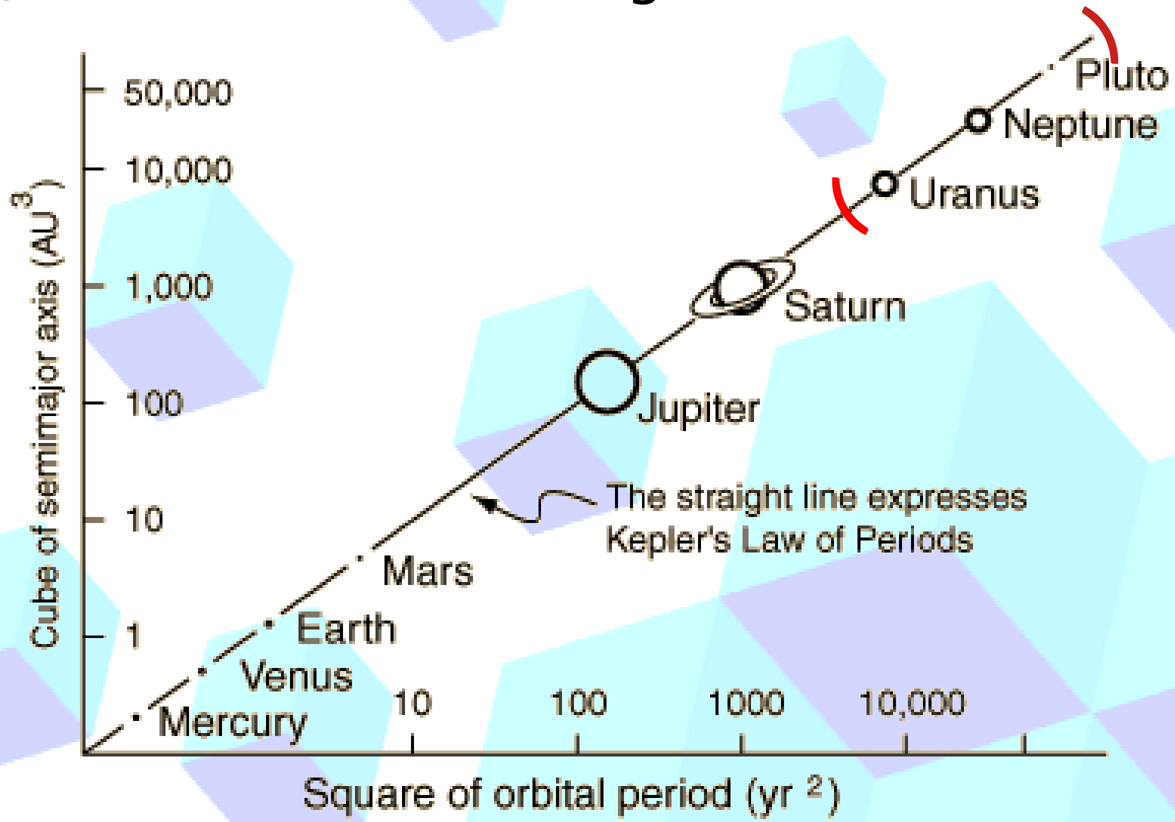

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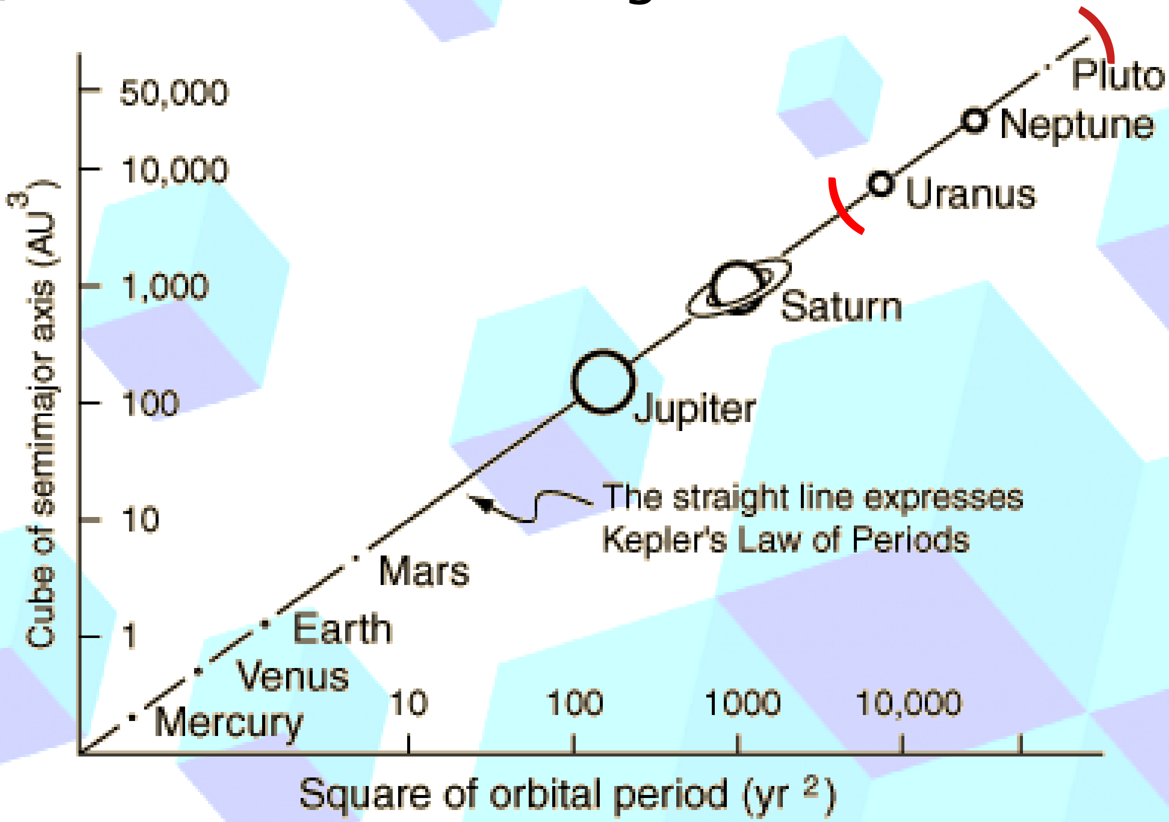

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Data
(collected by
Tycho Brahe)

↓

Statistical learning
(performed by
Johannes Kepler)

↓

Physical law
(assessed by
Isaac Newton)

Supervised (big-)data analysis: a flow chart

Training set

Calculate properties and functions

P_i, for many *materials*, i

E.g., Density-Functional Theory

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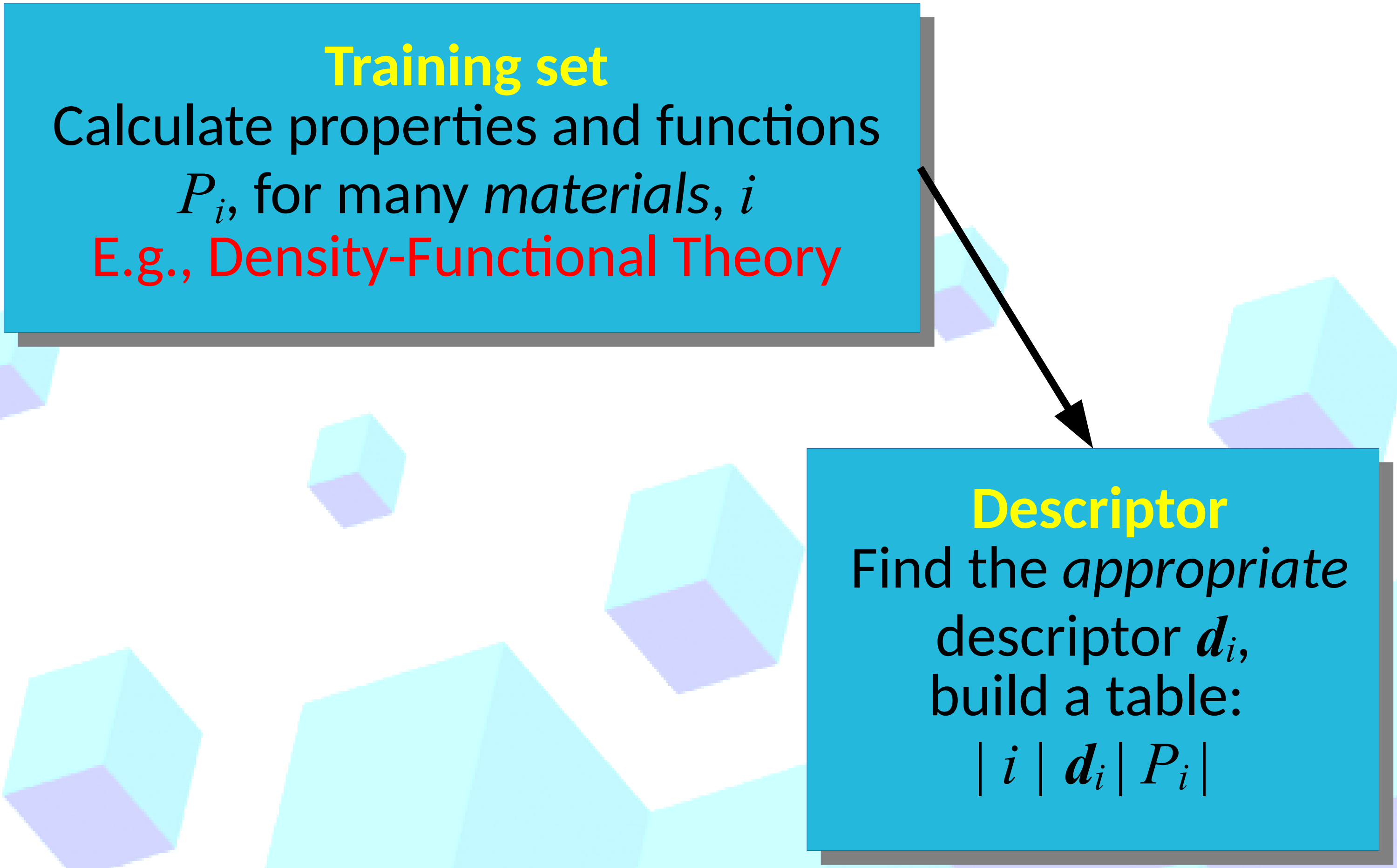

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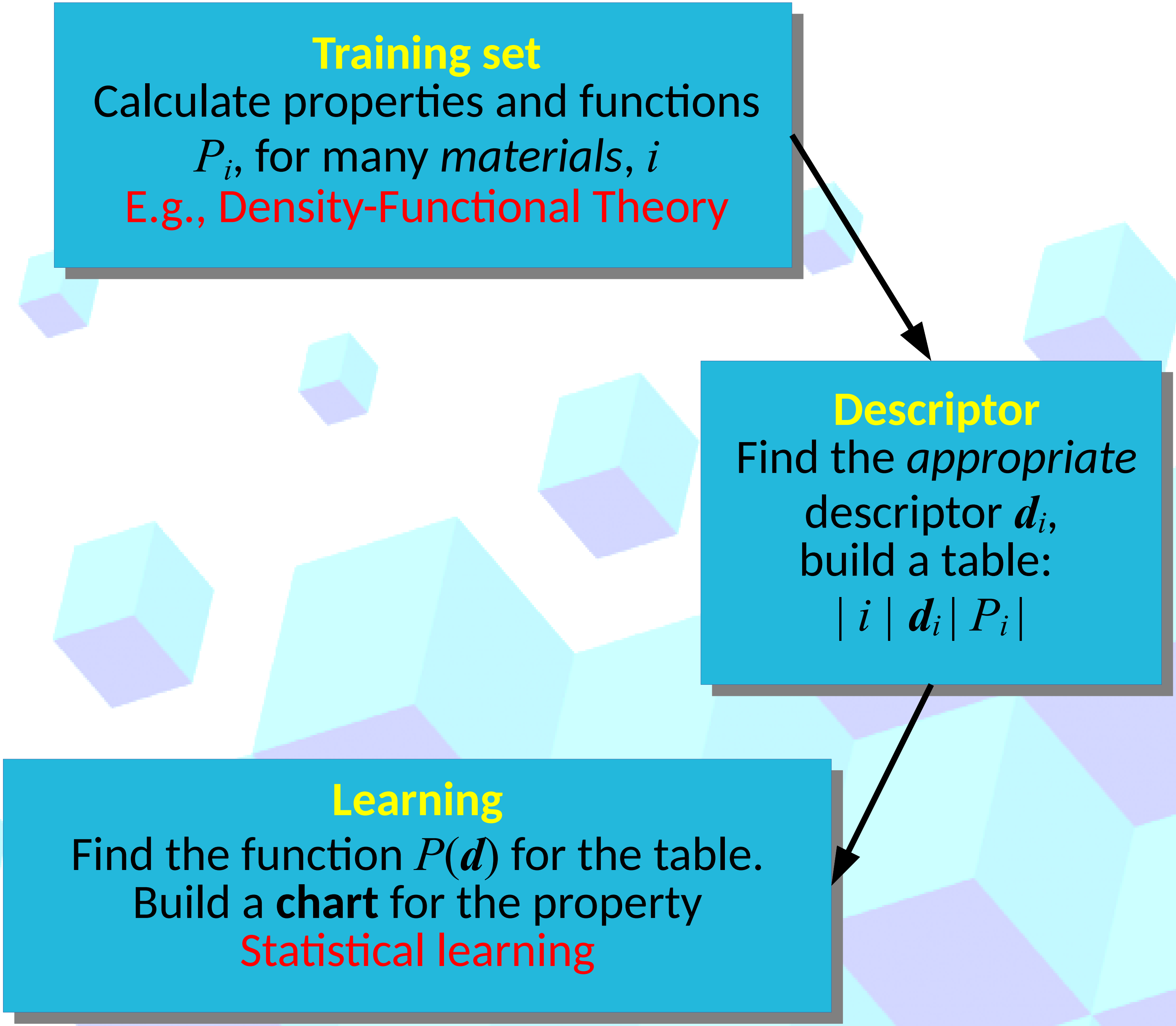

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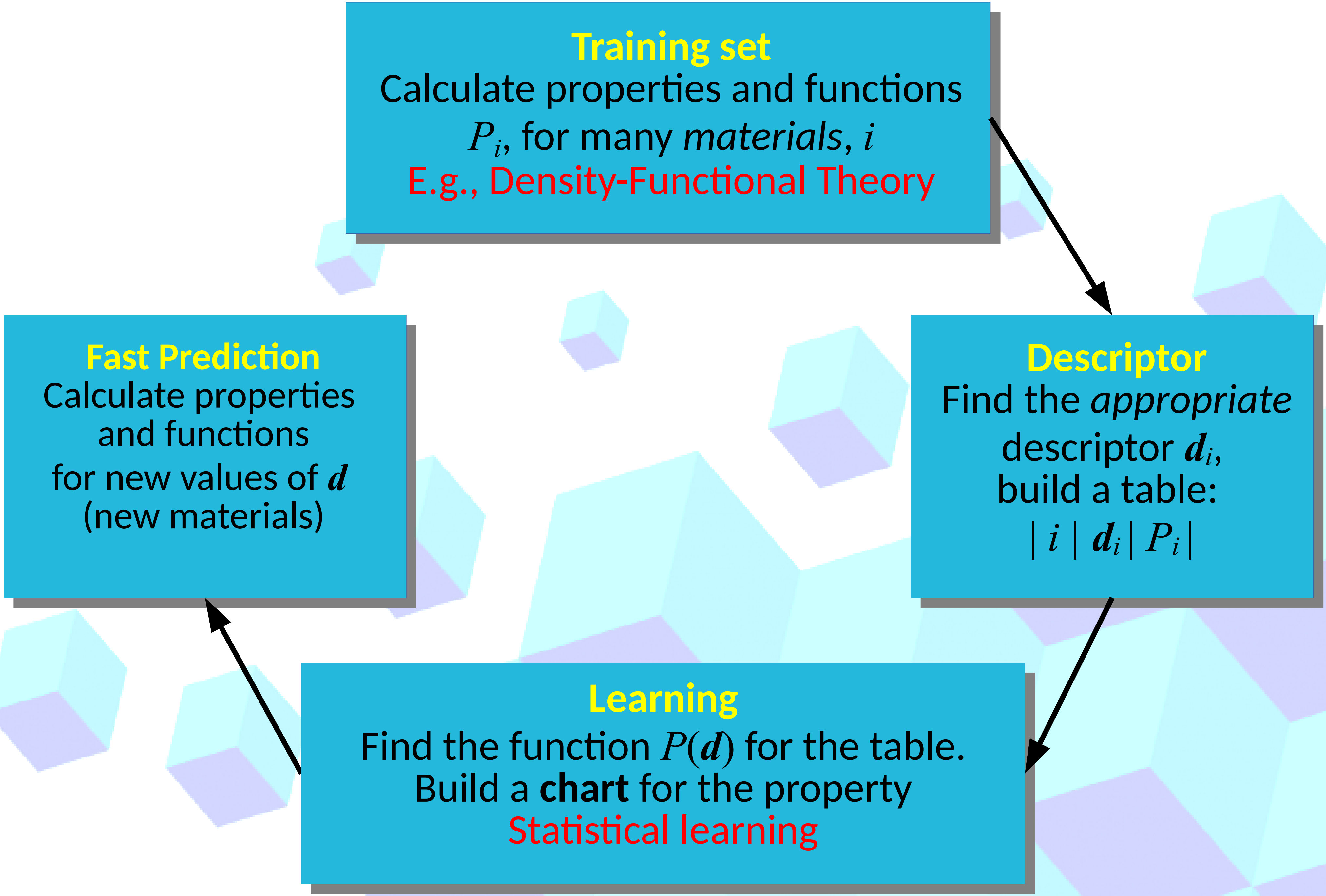

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Calculate properties
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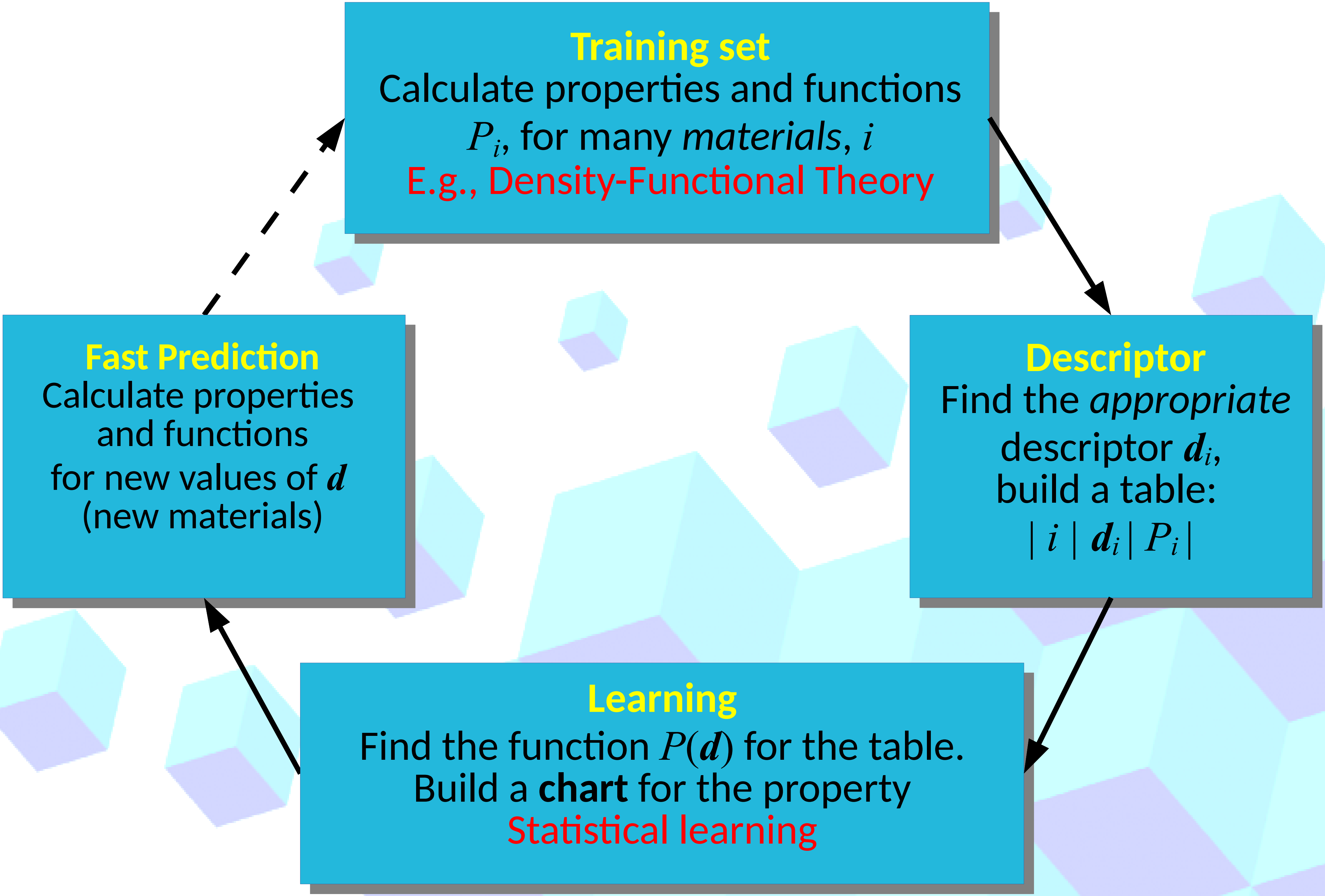

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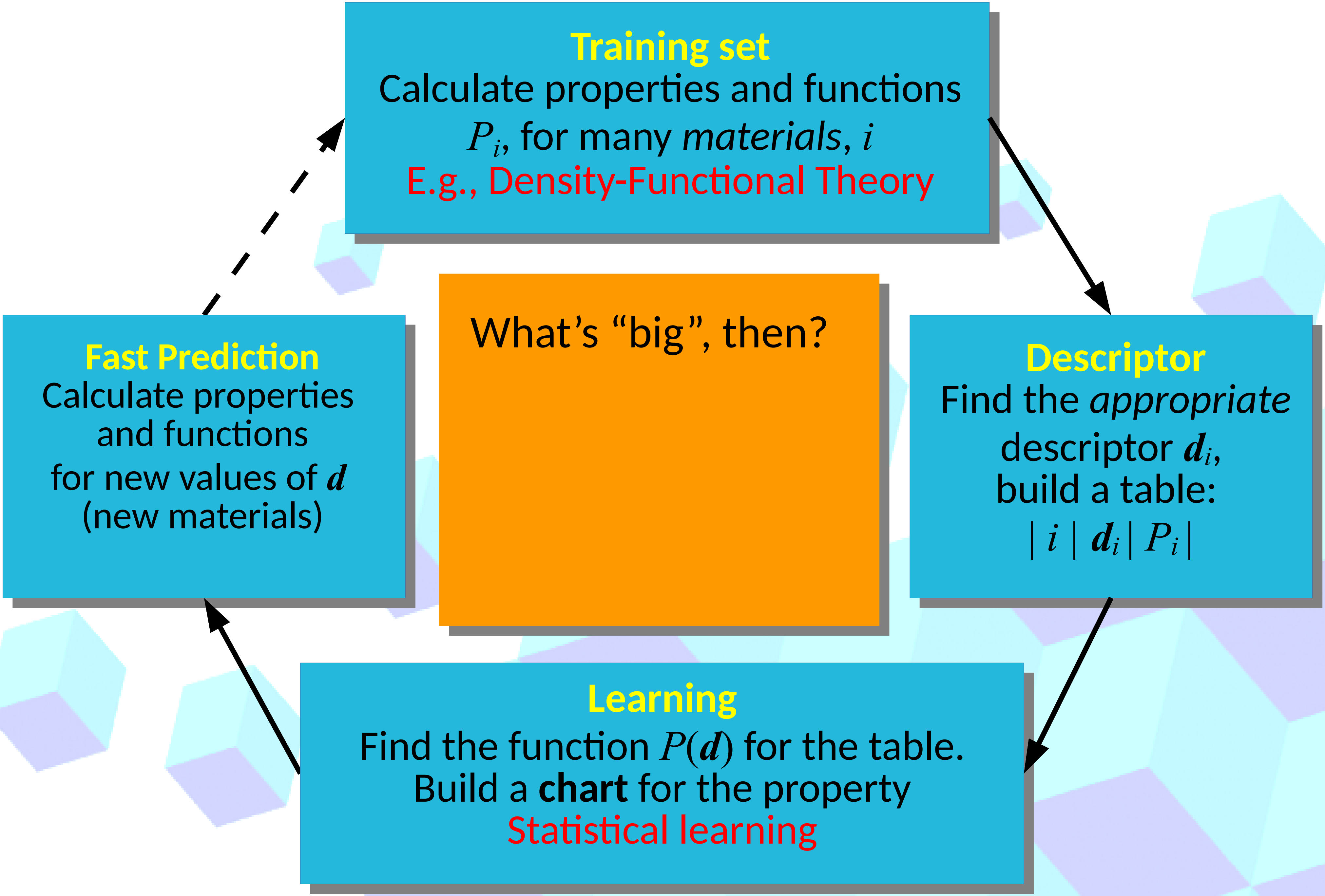

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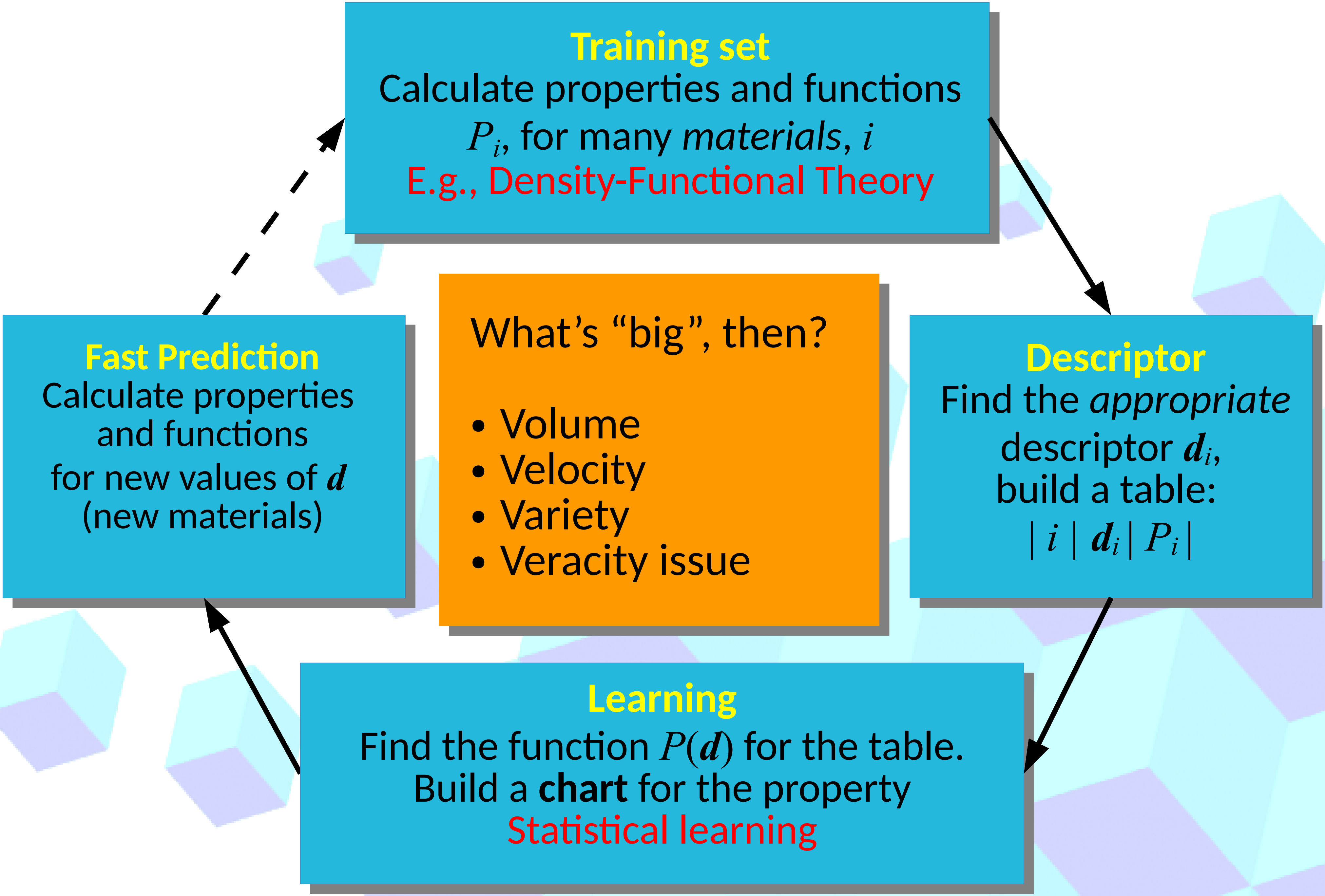

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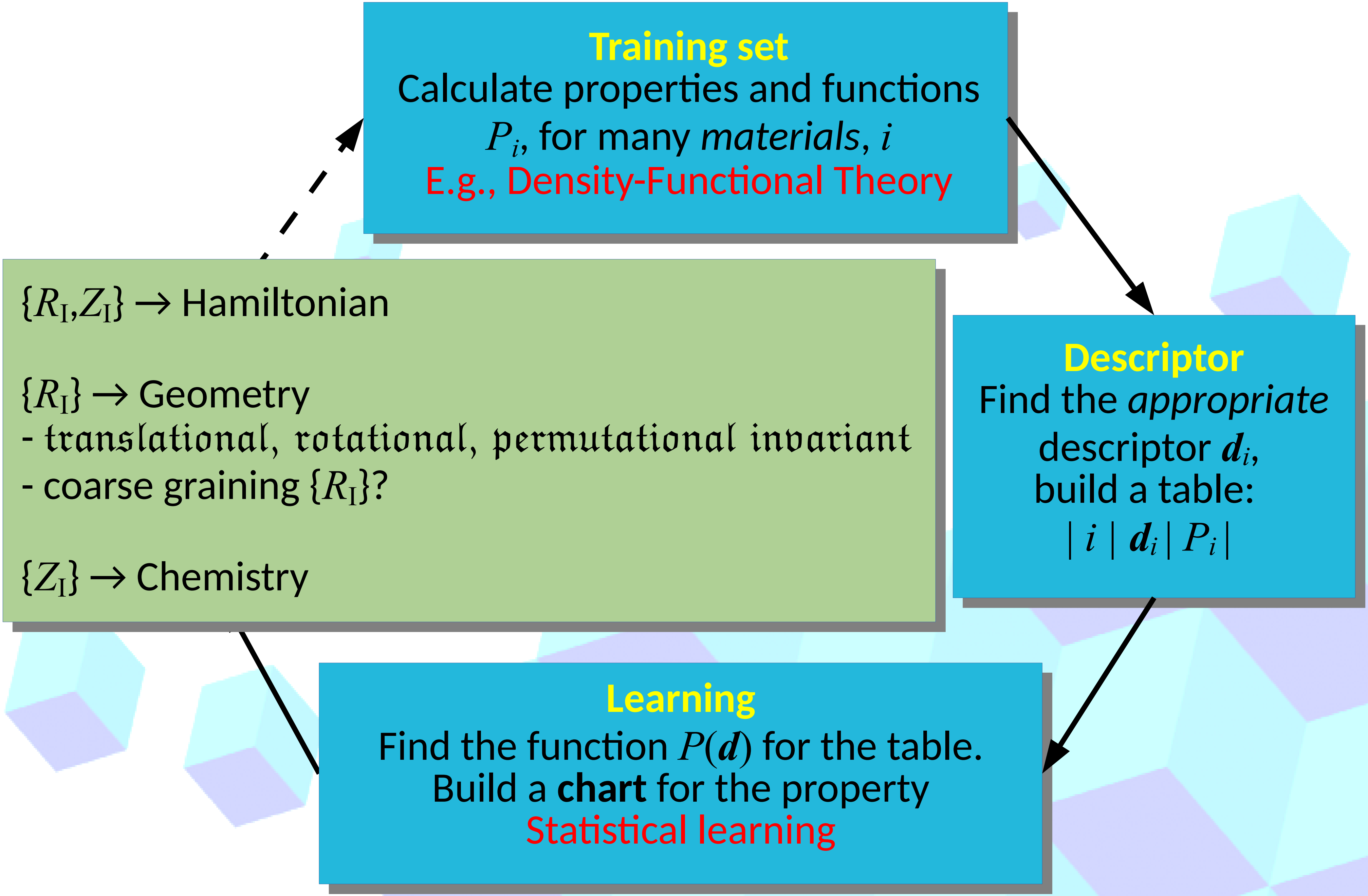
What's "big", then?

- Volume
- Velocity
- Variety
- Veracity issue

Descriptor? Don’t we know it from the start?



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$\{R_\mathrm{I}, Z_\mathrm{I}\}$ → Hamiltonian

$\{R_\mathrm{I}\}$ → Geometry
- translational, rotational, permutational invariant
- coarse graining $\{R_\mathrm{I}\}$?

$\{Z_\mathrm{I}\}$ → Chemistry

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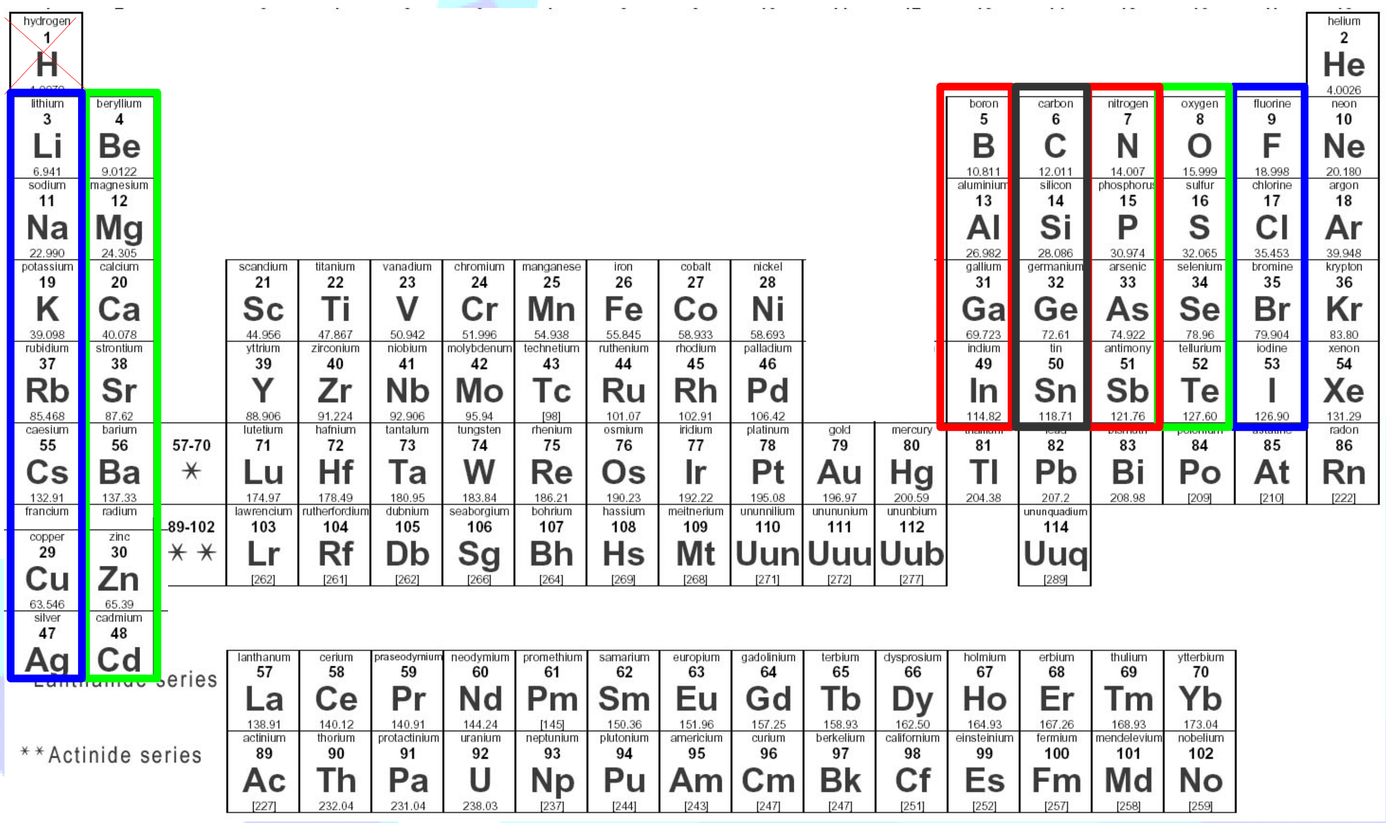
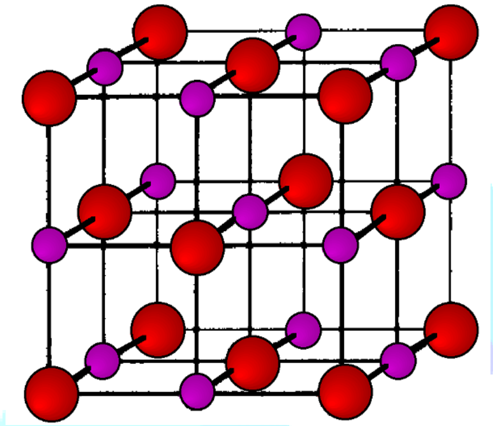
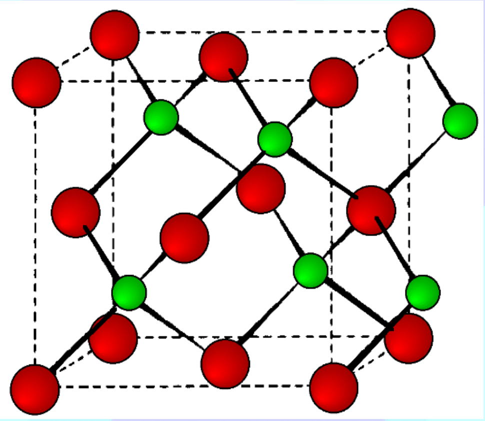
An example: predicting crystal structures from the composition

82 octet AB binary compounds


H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd In Sn Sb Te I Xe
Cs Ba 57-70 * Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra 89-102 ** Lr Rf Db Sg Bh Hs Mt Uun Uuu Uub Uuq
Cu Zn
Ag Cd
*Lanthanide series La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
**Actinide series Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No



Rock salt



Zinc blende

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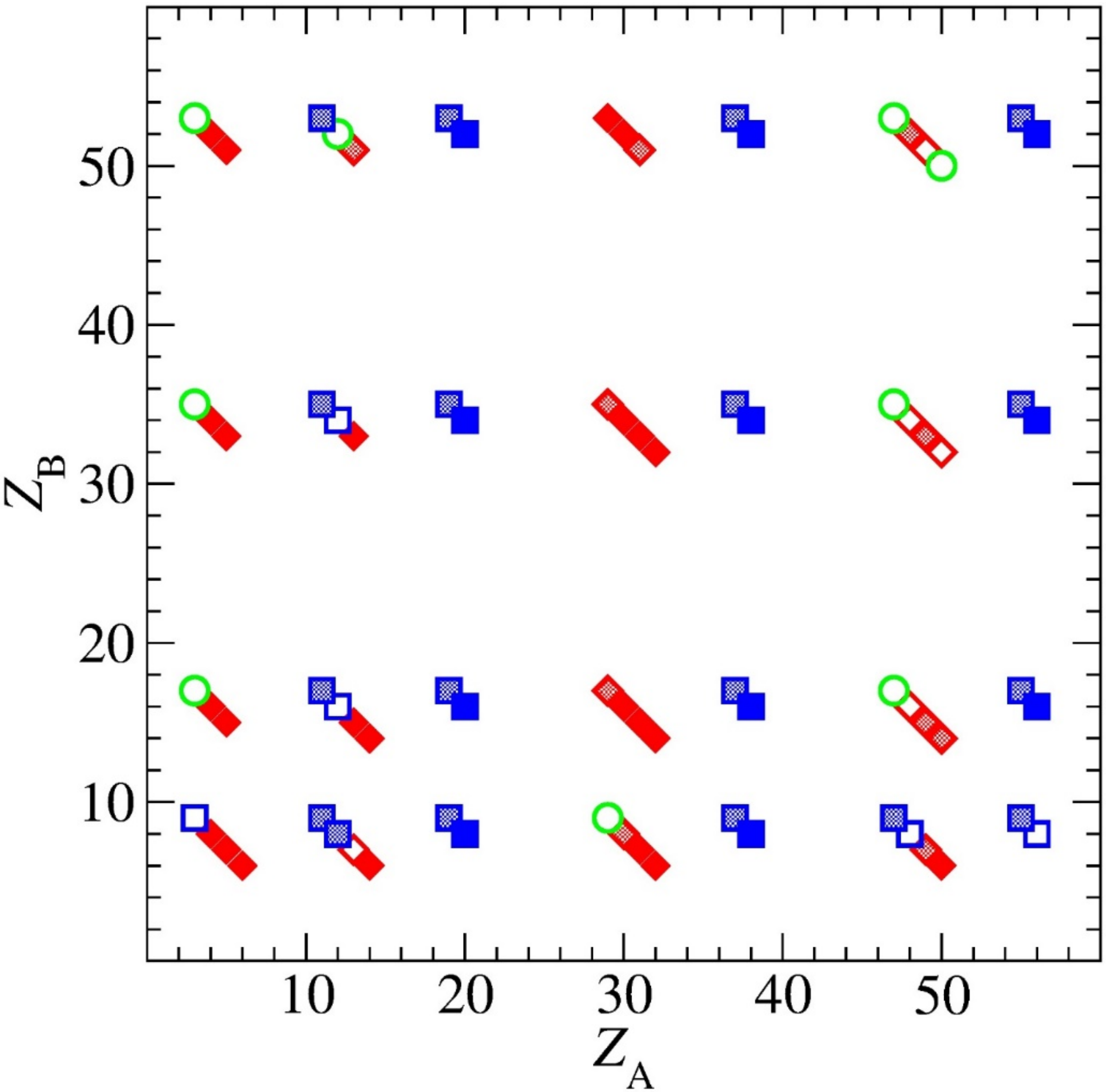

■ Rock salt

○ Rock salt/Zinc blende

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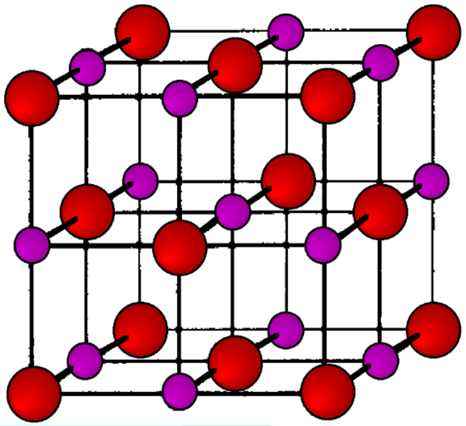

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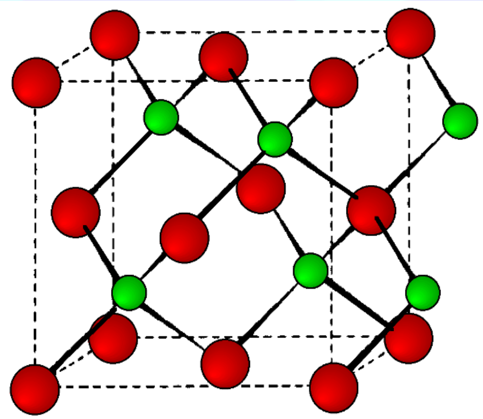

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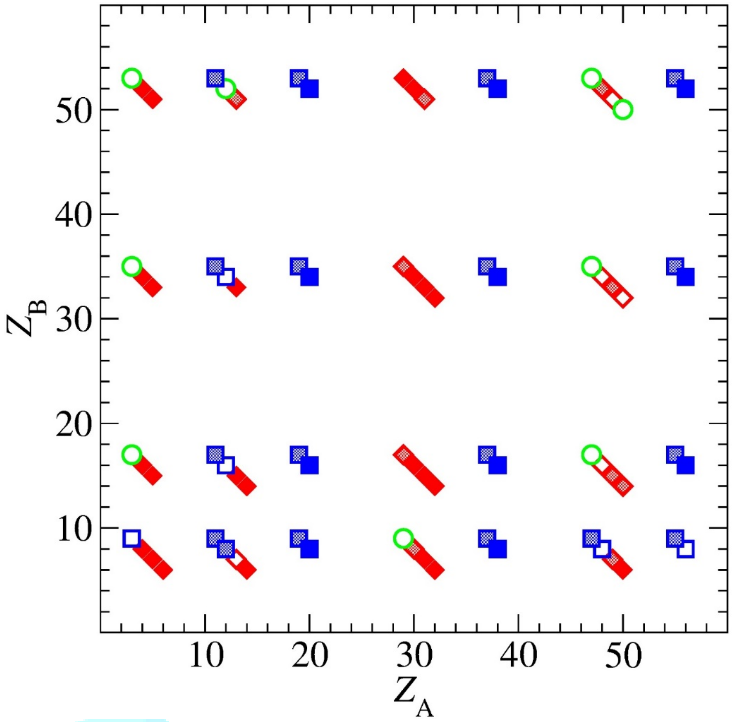

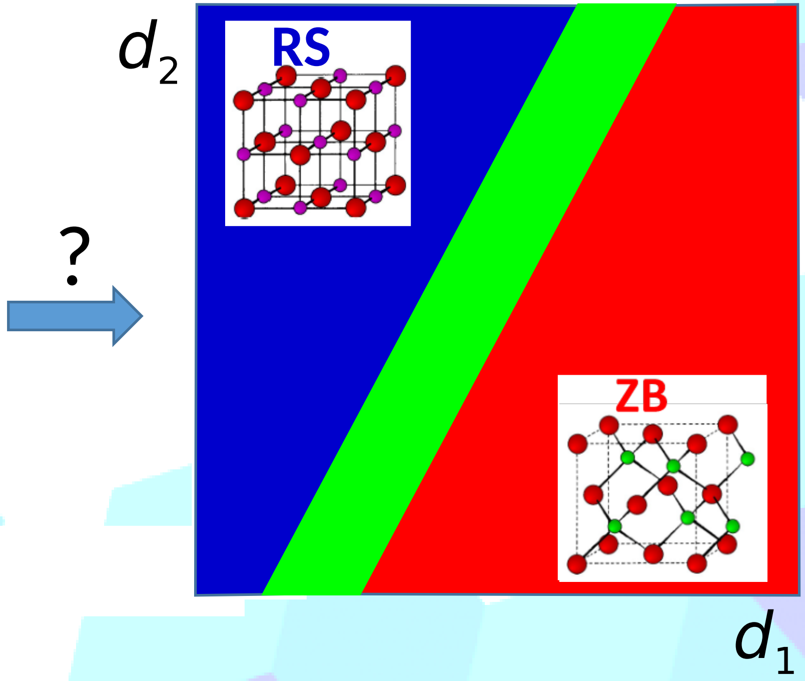

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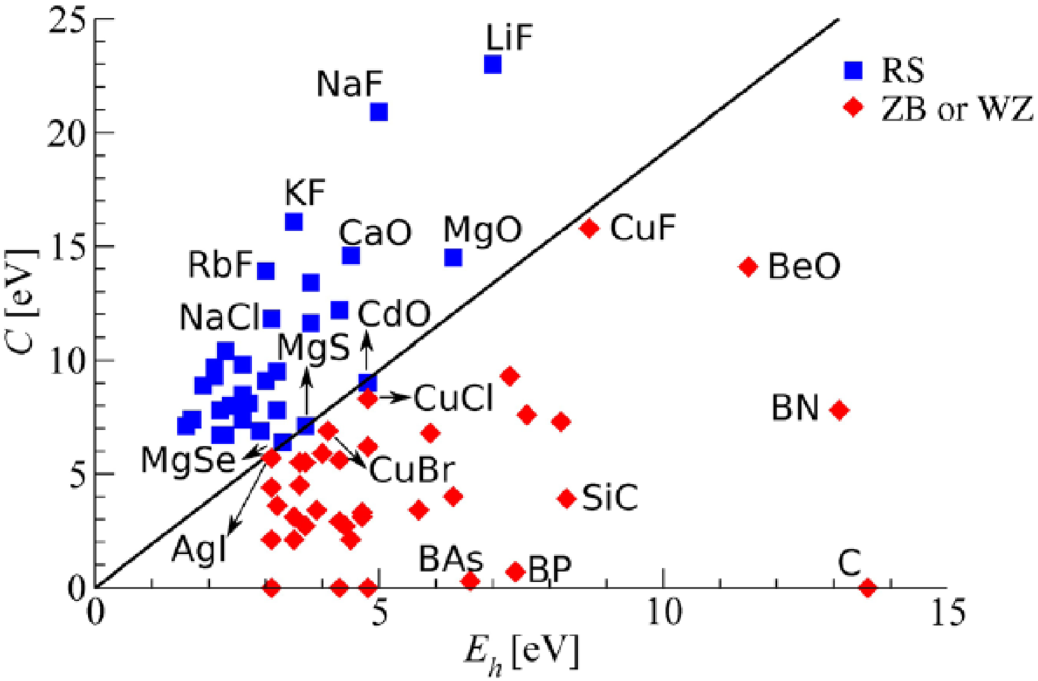

The descriptor proposed by Phillips and van Vechten in 1969-70 depends on:
- lattice parameter
- electrical conductivity

d_1

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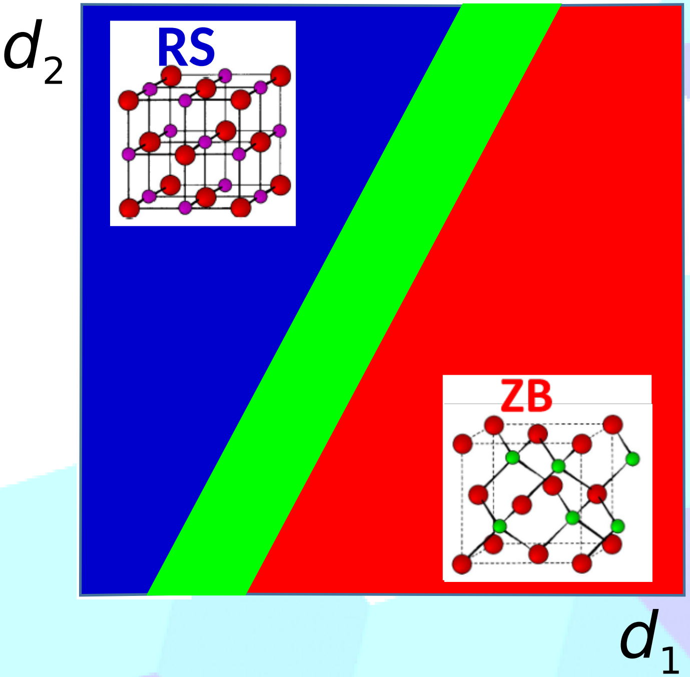
Ansatz: atomic features

- HOMO
- LUMO
- Ionization Potential
- Electron Affinity
- Radius of valence *s* orbital
- Radius of valence *p* orbital
- Radius of valence *d* orbital
- … ?

E(Rock salt) – *E*(Zinc blende)



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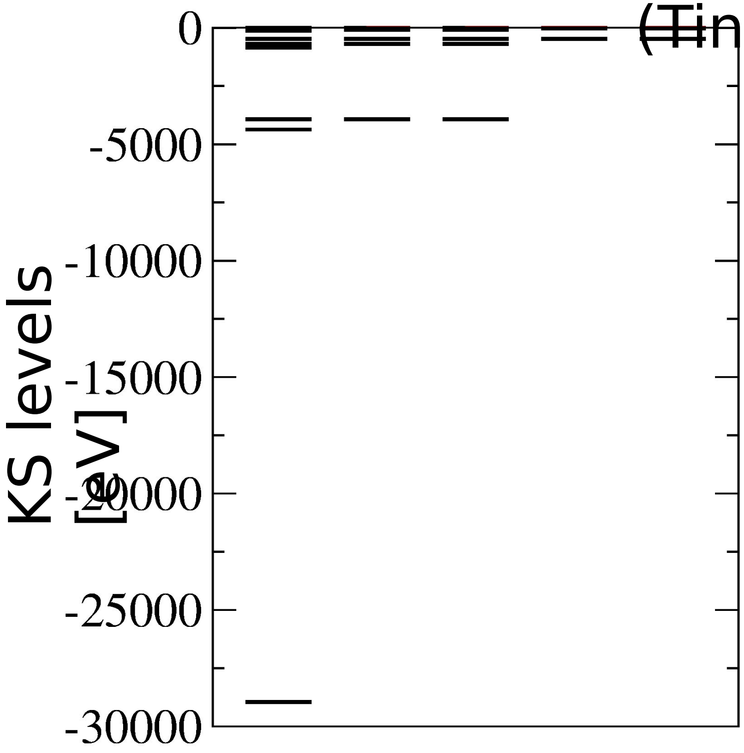
Y. Saad, D. Gao, T. Ngo, S. Bobbitt, J. R. Chelikowsky, and W. Andreoni, Phys. Rev. B 85, 104104 (2012).

Primary (atomic) features

example: Sn (Tin)



Primary (atomic) features

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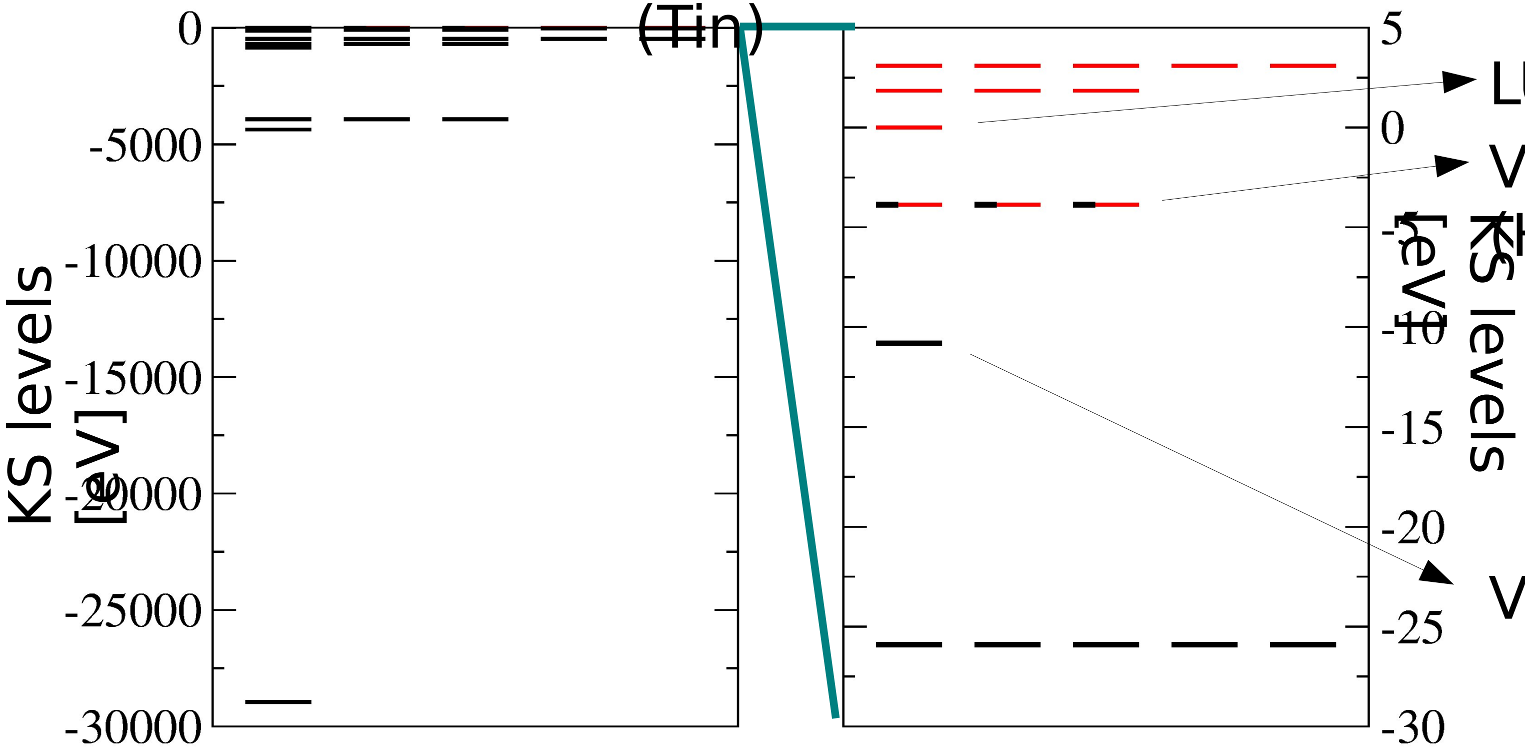


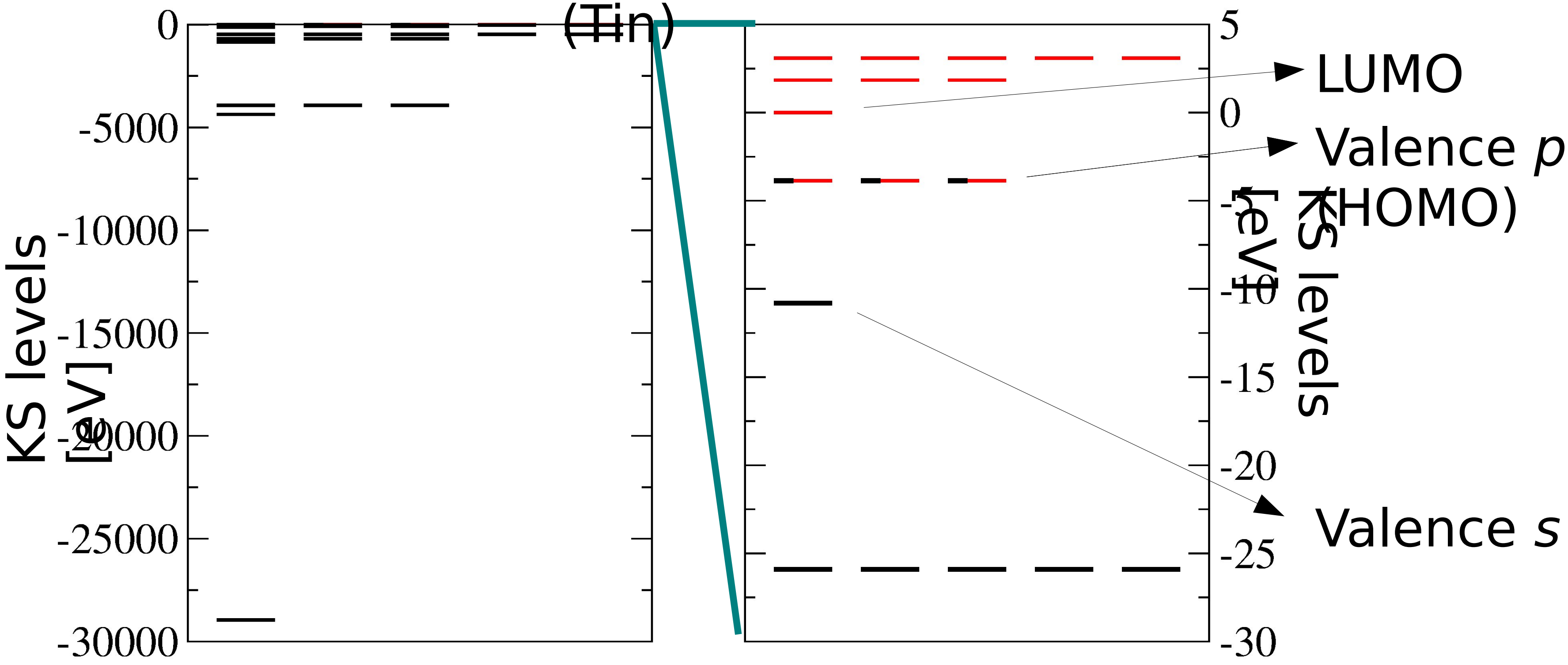
LUMO

Valence *p* (HOMO)

Valence *s*

Primary (atomic) features

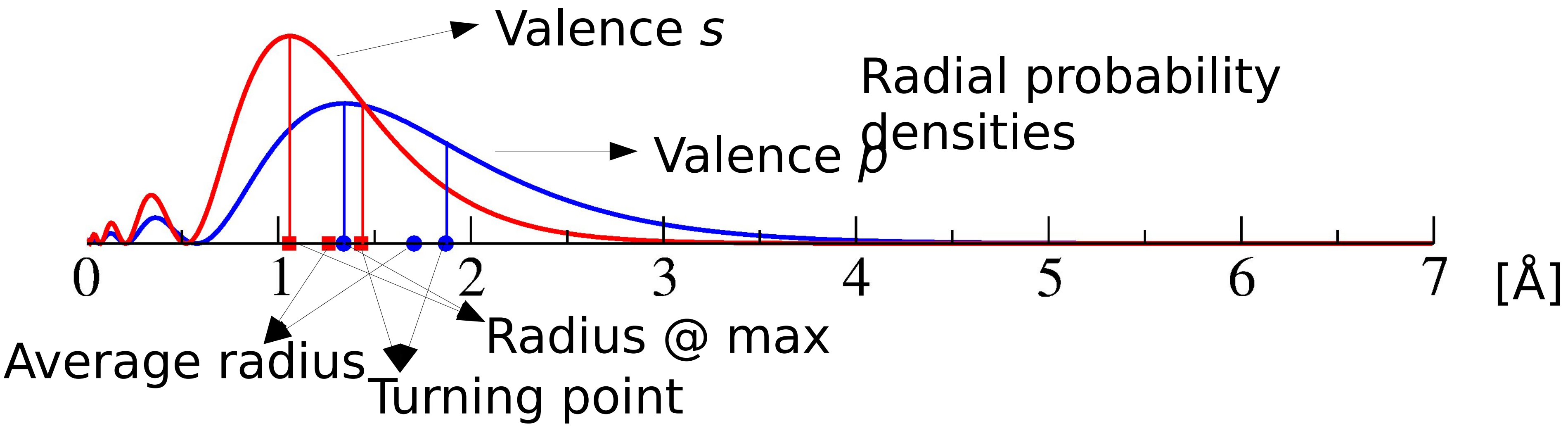
example: Sn (Tin)



LUMO

Valence *p* (HOMO)

Valence *s*



Valence *s*

Valence *p*

Radial probability densities

Average radius

Turning point

Radius @ max

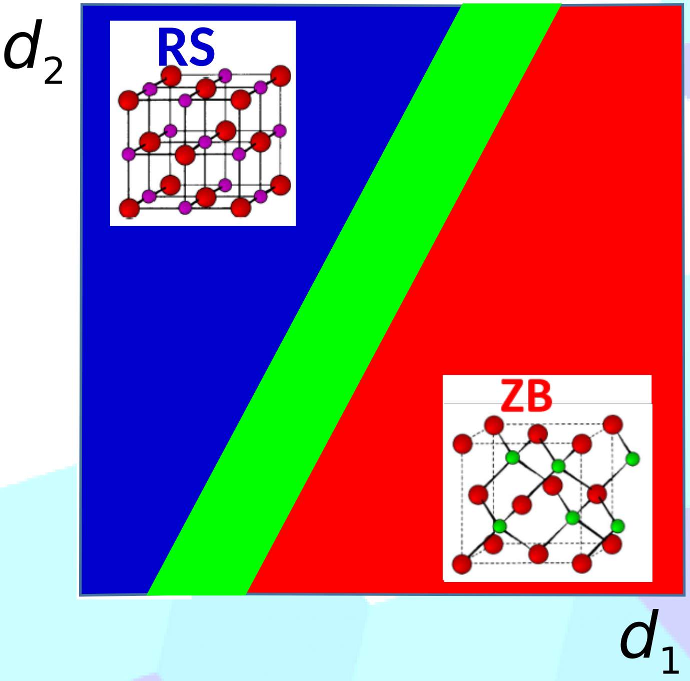
An example: predicting crystal structures from the composition

82 octet AB binary compounds

Ansatz: atomic features

- HOMO
- LUMO
- Ionization Potential
- Electron Affinity
- Radius of valence *s* orbital
- Radius of valence *p* orbital
- Radius of valence *d* orbital
- … ?

E(Rock salt) – *E*(Zinc blende)



🟦 Rock salt

○ Rock salt/Zinc blende

◆ Zinc blende

J. A. van Vechten, Phys. Rev. 182, 891 (1969).

J. C. Phillips, Rev. Mod. Phys. 42, 317 (1970).

J. John and A.N. Bloch, Phys. Rev. Lett. 33, 1095 (1974)

J. R. Chelikowsky and J. C. Phillips, Phys. Rev. B 33, 2453 (1978)

A. Zunger, Phys. Rev. B 22, 5839 (1980).

D. G. Pettifor, Solid State Commun. 51, 31 (1984).

Y. Saad, D. Gao, T. Ngo, S. Bobbitt, J. R. Chelikowsky, and W. Andreoni, Phys. Rev. B 85, 104104 (2012).

Compressed sensing

Aim: finding descriptors and learning predictive models

Ansatz:

$\boldsymbol{P} = c_1\boldsymbol{d}_1 + c_2\boldsymbol{d}_2 + \ldots\, c_n\boldsymbol{d}_n$

Where

P is the property of interest

$\boldsymbol{d}_1, \ldots\, \boldsymbol{d}_n$ are candidate features, i.e., nonlinear functions of primary features (EA, IP, …)

$c_1, \ldots\, c_{\mathrm{n}}$ are unknown coefficients, with the extra constraint that these (nonzero) coefficients should be as few as possible.

Compressed sensing

With a foreword on
dimensionality reduction

Aim: finding descriptors and learning pre models

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Linear dimensionality reduction: Principal components

Pearson, K. "On Lines and Planes of Closest
Fit to Systems of Points in Space".
Philosophical Magazine 2, 559 (1901)

Linear dimensionality reduction: Principal components

Pearson, K. "On Lines and Planes of Closest Fit to Systems of Points in Space". Philosophical Magazine 2, 559 (1901)

Orthonormal transformation of coordinates, converting a set of (possibly) linearly correlated coordinates into a new set of linearly uncorrelated (called principal or normal) components, such that the first component has the largest variance and each subsequent has the largest variance constrained to being orthogonal to all the preceding components

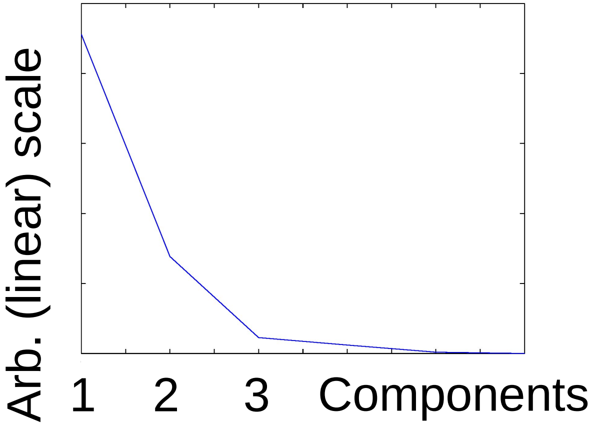
Linear dimensionality reduction: Principal components

Ansatz: atomic features

- Valence number Z_v
- Energy of valence *s* orbital E_s
- Energy of valence *p* orbital E_p
- Radius of valence *s* orbital r_s
- Radius of valence *p* orbital r_p

r_s, r_p, $E_s/\sqrt{Z_v}$, $E_p/\sqrt{z_v}$,
for A and B atoms

linearly uncorrelated (called principal or normal) components, such that the first component has the largest variance and each subsequent has the largest variance constrained to being orthogonal to all the preceding components



Saad, …, Chelikowsky, and Andreoni, PRB 85, 104104 (2012)

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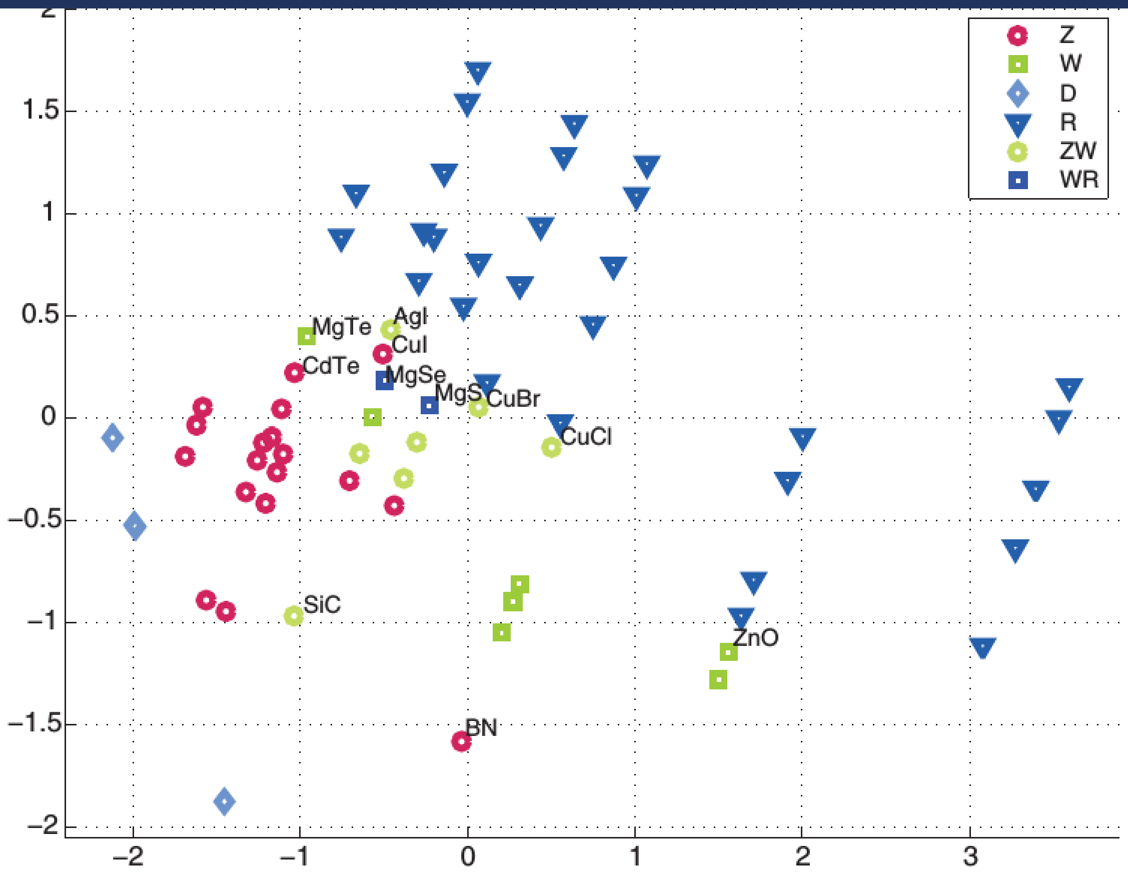

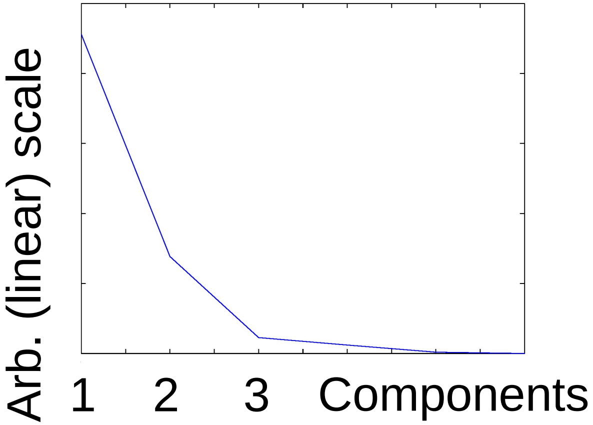

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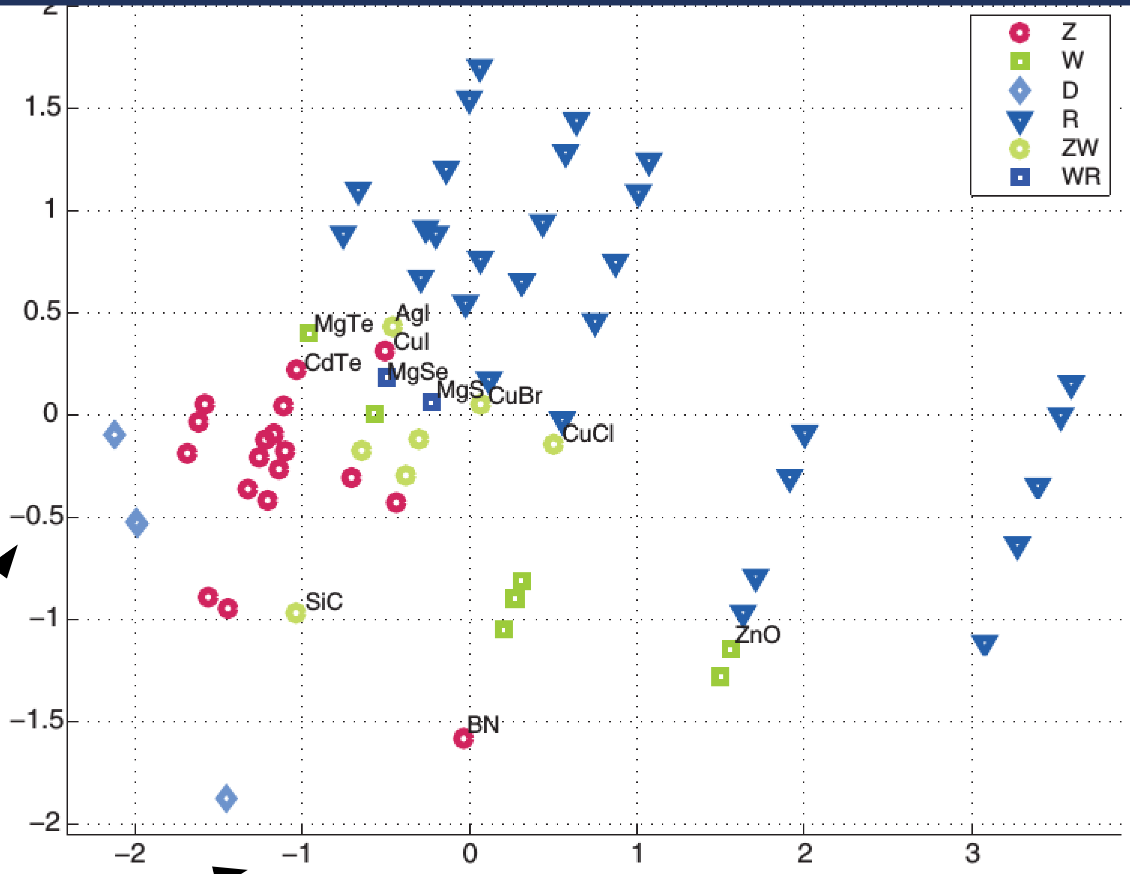
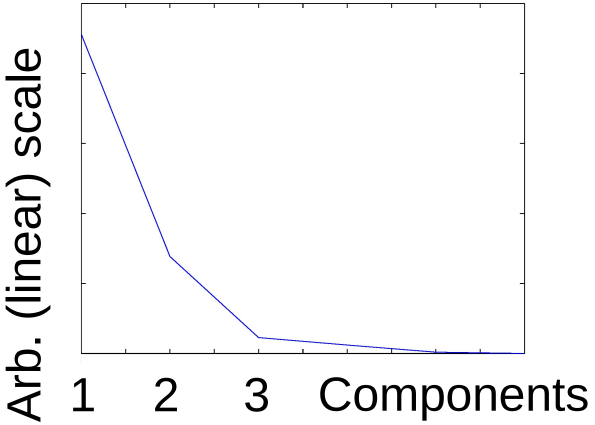


What's on the axes?

Linear combination of (possibly all) the initial dimensions



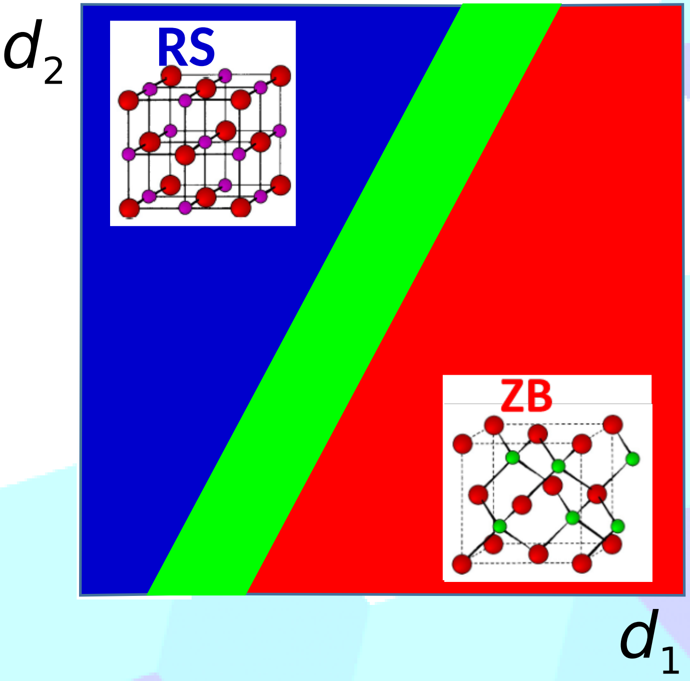
Saad, …, Chelikowsky, and Andreoni, PRB 85, 104104 (2012)

Compressed sensing: the quest for descriptors and predictive models

82 octet AB binary compounds

Ansatz: atomic features

- HOMO
- LUMO
- Ionization Potential
- Electron Affinity
- Radius of valence *s* orbital
- Radius of valence *p* orbital
- Radius of valence *d* orbital
- Thousands to billions of non-linear functions of the above



■ Rock salt
○ RS / ZB
◆ Zinc blende

$$\boldsymbol{P} = c_1\boldsymbol{d}_1 + c_2\boldsymbol{d}_2 + \dots c_n\boldsymbol{d}_n$$

E(Rock salt) – *E*(Zinc blende)

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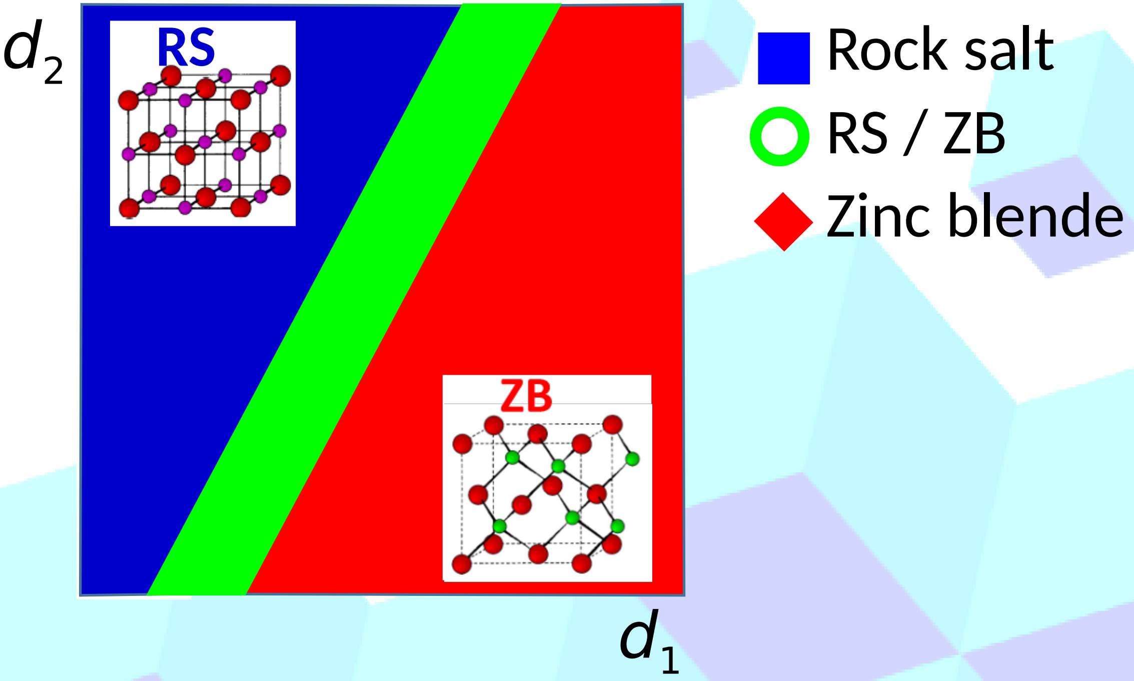
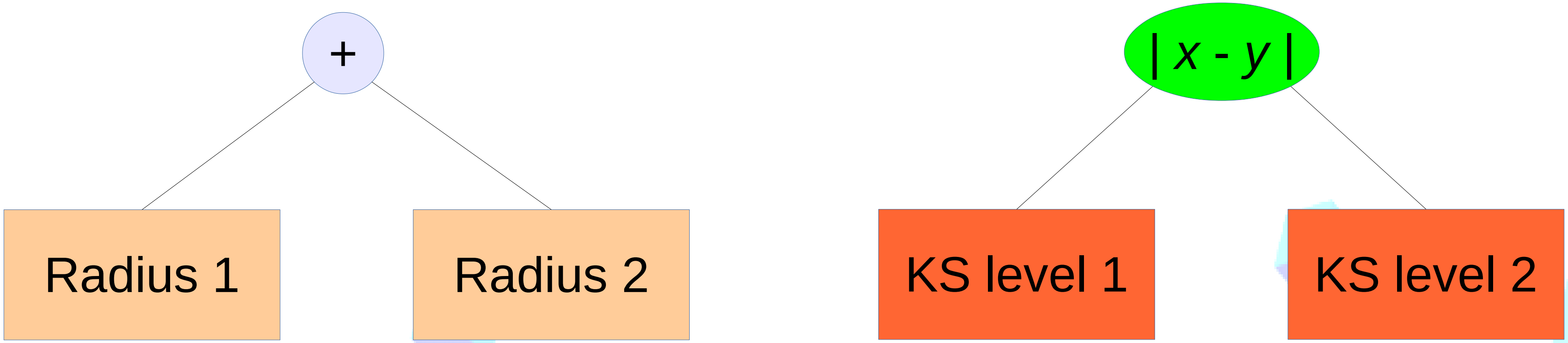


Symbolic Regression

$$\boldsymbol{P} = c_1\boldsymbol{d}_1 + c_2\boldsymbol{d}_2 + \dots c_n\boldsymbol{d}_n$$

E(Rock salt) – *E*(Zinc blende)

Systematic construction of the feature space



+

Radius 1

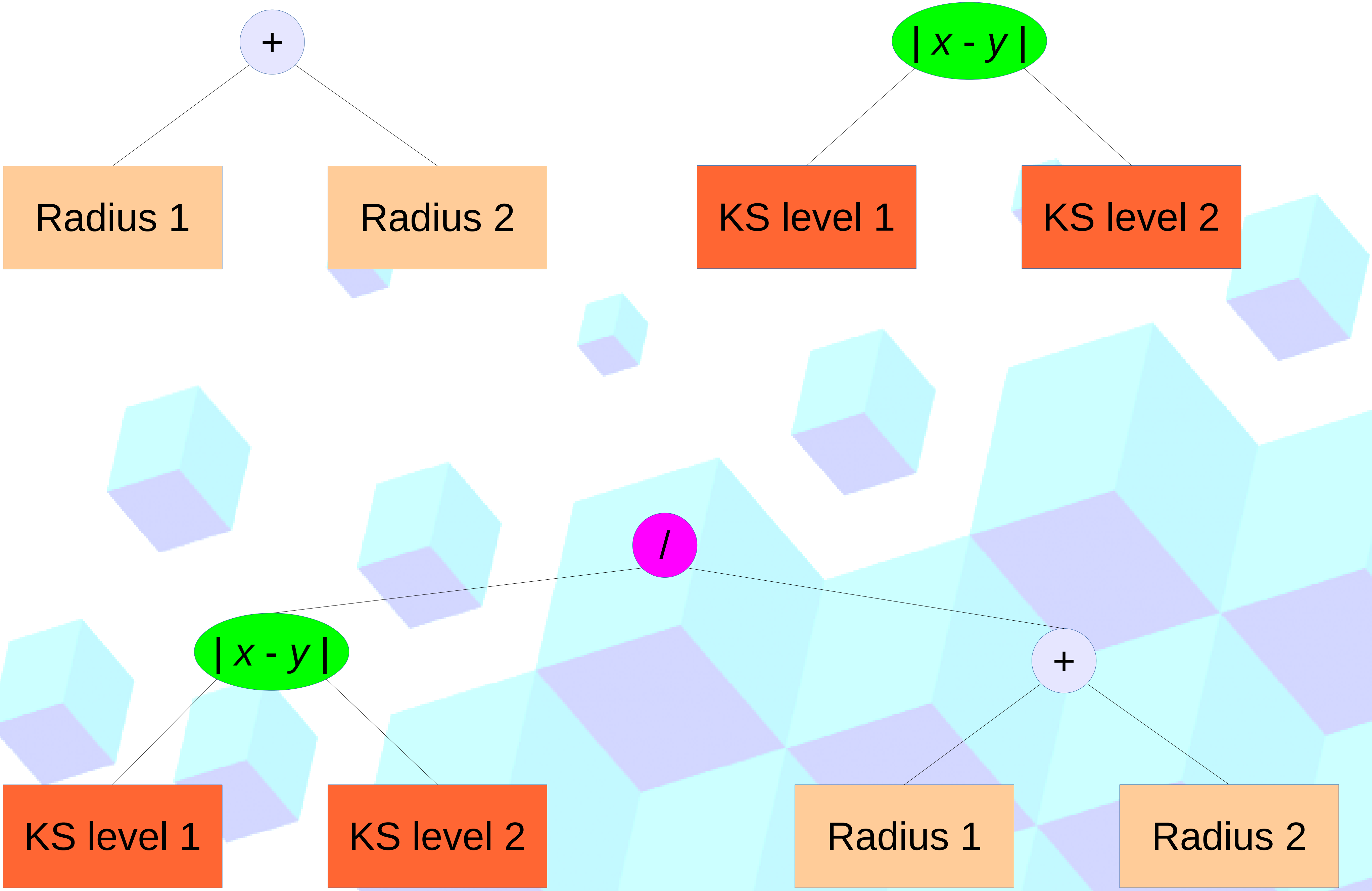
Radius 2

| *x* - *y* |

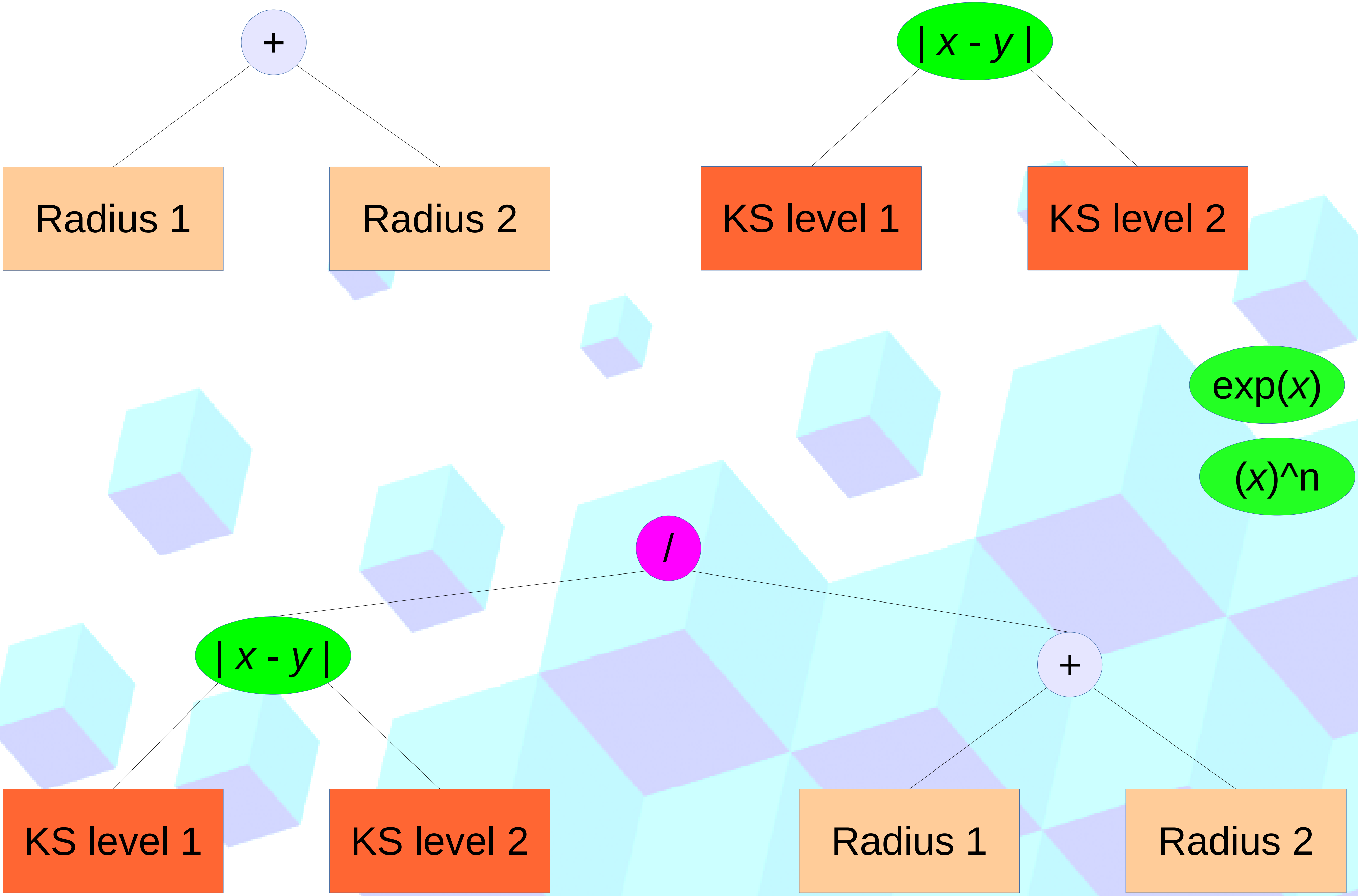
KS level 1

KS level 2

Systematic construction of the feature space



Systematic construction of the feature space



+

Radius 1

Radius 2

| x - y |

KS level 1

KS level 2

exp(x)

(x)^n

/

| x - y |

KS level 1

KS level 2

+

Radius 1

Radius 2

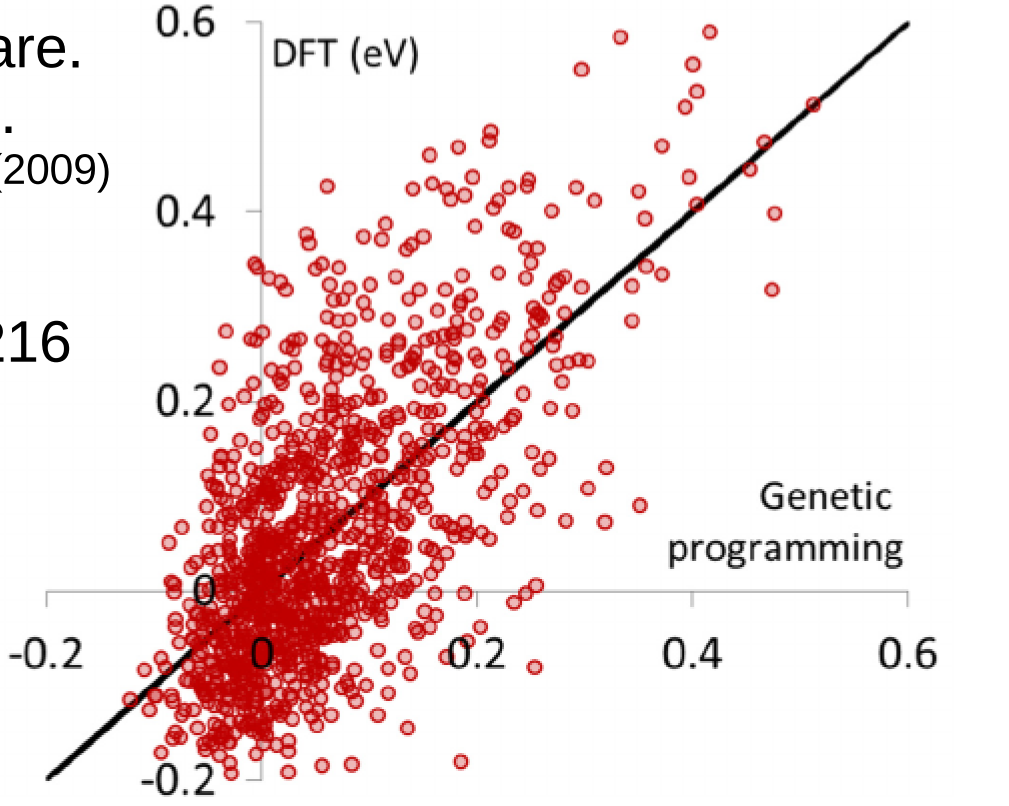
Systematic construction of the feature space: EUREQA

EUREQA: genetic programming software.
Global optimization (genetic algorithm).
Schmidt M., Lipson H., Science, Vol. 324, No. 5923, (2009)

T. Müller et al. PRB **89** 115202 (2014):
Data: ~1000 amorphous structures of 216 Si atoms (saturated)

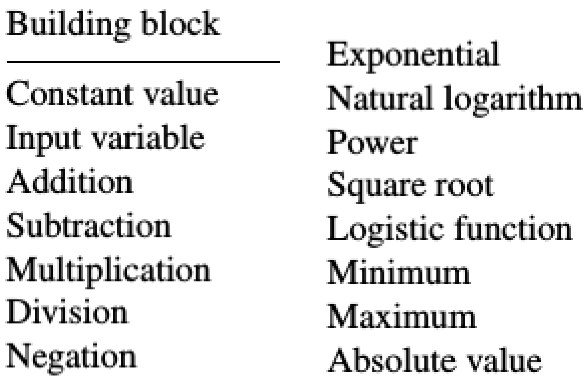
Property: hole trap depth

$$\frac{\min(1.66355,a)\max(5.37551,c) - f - bd}{g} - h\max(3.42929,e),$$



Descriptor (candidates: 242)

a The largest distance between a H atom and its nearest Si neighbor
b The shortest distance between a Si atom and its sixth-nearest Si neighbor
c The maximum bond valence sum on a Si atom
d The smallest value for the fifth-smallest relative bond length around a Si atom
e The fourth-shortest distance between a Si atom and its eighth-nearest neighbor
f The second-shortest distance between a Si atom and its fifth-nearest neighbor
g The third-shortest distance between a Si atom and its sixth-nearest neighbor
h The H-Si nearest-neighbor distance for the hydrogen atom with the fourth-smallest difference between the distances to the two Si atoms nearest to a H atom



Building block
Constant value
Input variable
Addition
Subtraction
Multiplication
Division
Negation
Exponential
Natural logarithm
Power
Square root
Logistic function
Minimum
Maximum
Absolute value

Compressed sensing: the quest for descriptors and predictive models

82 octet AB binary compounds

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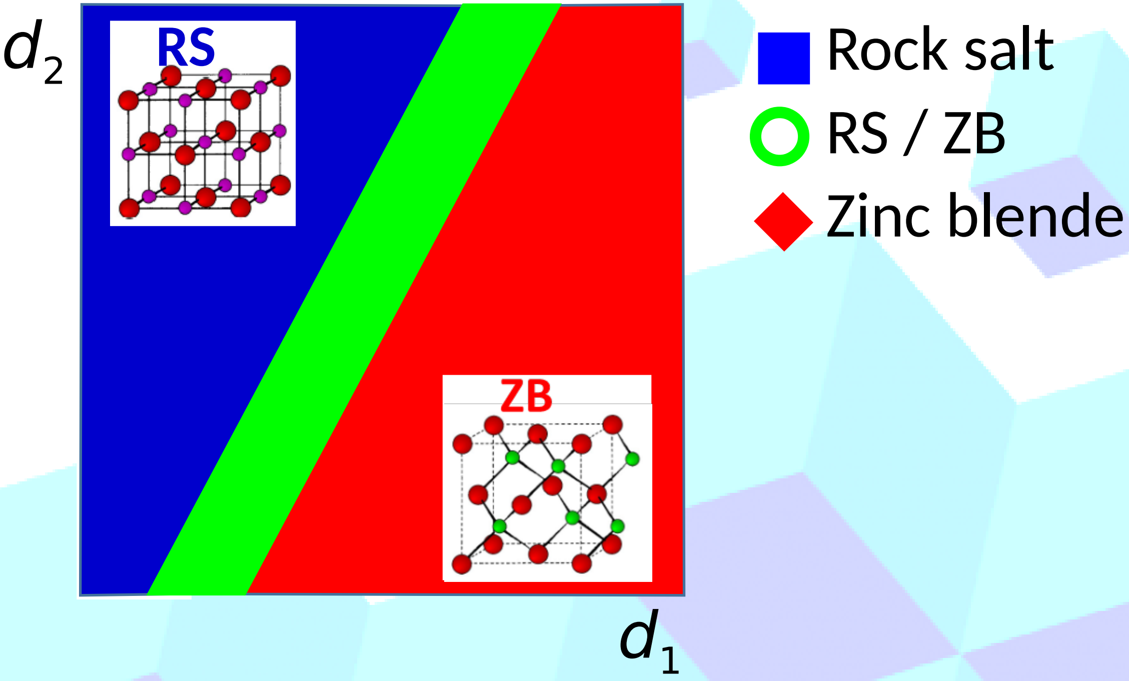

$$\boldsymbol{P} = c_1\boldsymbol{d}_1 + c_2\boldsymbol{d}_2 + \ldots\, c_n\boldsymbol{d}_n \Rightarrow \underset{\boldsymbol{c}\in\mathbb{R}^M}{\mathrm{argmin}} \|\boldsymbol{P} - \boldsymbol{D}\boldsymbol{c}\|_2^2 + \lambda\|\boldsymbol{c}\|_0$$

E(Rock salt) – *E*(Zinc blende)

Compressed sensing: the quest for descriptors and predictive models

Ideal method: regression with ℓ_0 regularization

$$\underset{\boldsymbol{c}\in\mathbb{R}^M}{\operatorname{argmin}}\left(\|\boldsymbol{P}-\boldsymbol{D}\boldsymbol{c}\|_2^2+\lambda\|\boldsymbol{c}\|_0\right)$$

Optimal solution
Non-polinomial complexity
Small # columns in ***D***

Compressed sensing: the quest for descriptors and predictive models

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Optimal solution
Non-polinomial complexity
Small # columns in ***D***

$\|\boldsymbol{c}\|_0$ # of nonzero elements of ***c***

$\|\boldsymbol{c}\|_2$ Euclidean. Square root of sum of squares of the elements of ***c***)

Compressed sensing: the quest for descriptors and predictive models

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Non-polinomial complexity
Small # columns in ***D***

$\|\boldsymbol{c}\|_0$	# of nonzero elements of ***c***
$\|\boldsymbol{c}\|_2$	Euclidean. Square root of sum of squares of the elements of ***c***)

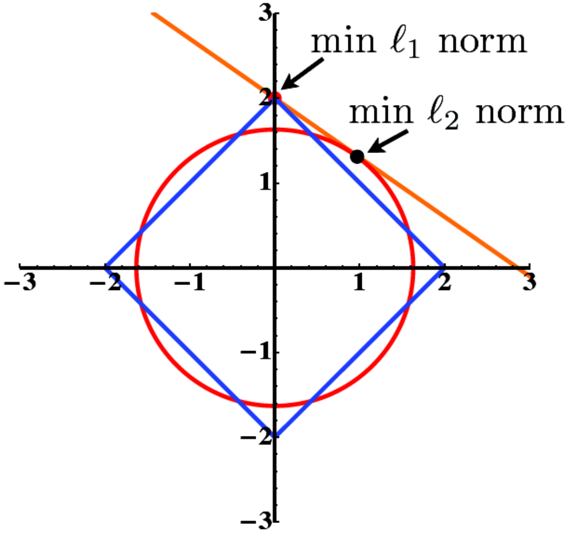
For matrices D with uncorrelated columns: LASSO

$$\underset{\boldsymbol{c}\in\mathbb{R}^M}{\operatorname{argmin}}\|\boldsymbol{P}-\boldsymbol{D}\boldsymbol{c}\|_2^2+\lambda\|\boldsymbol{c}\|_1$$

(Possibly) optimal solution
Convex optimization
Moderate # columns in ***D***

$\|\boldsymbol{c}\|_1$	“Manhattan”. Sum of absolute values of the elements of ***c***

Compressed sensing: the quest for descriptors and predictive models



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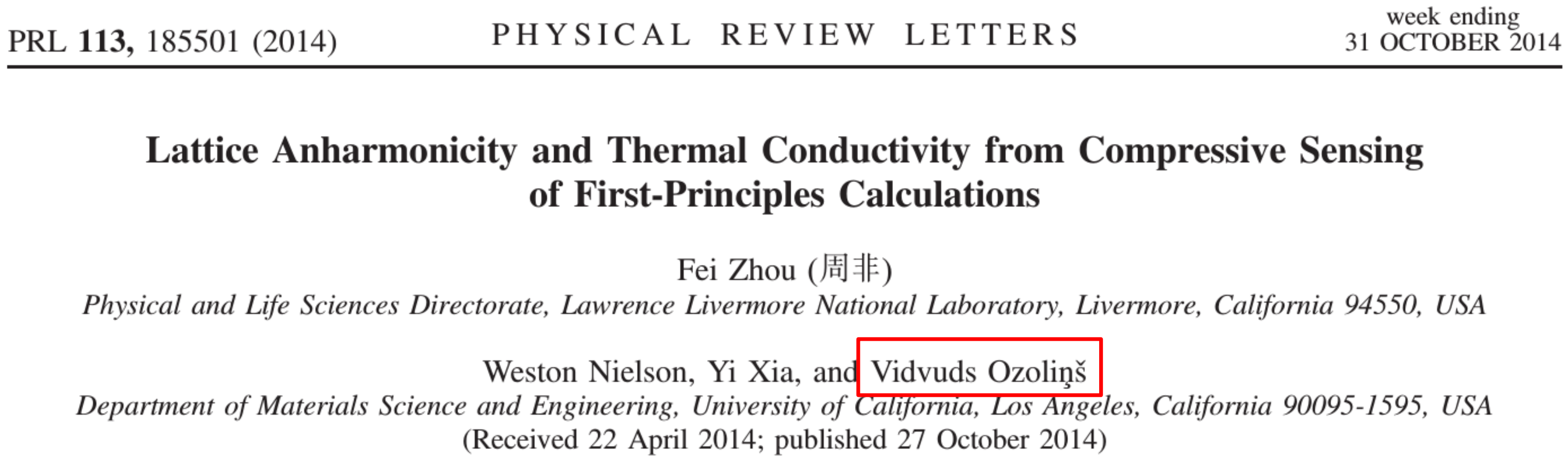
(Possibly) optimal solution
Convex optimization
Moderate # columns in ***D***

$\|\boldsymbol{c}\|_1$ “Manhattan”. Sum of absolute values of the elements of ***c***

Compressed sensing in materials science



PRL **113,** 185501 (2014) PHYSICAL REVIEW LETTERS week ending 31 OCTOBER 2014

Lattice Anharmonicity and Thermal Conductivity from Compressive Sensing of First-Principles Calculations

Fei Zhou (周非)
Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, California 94550, USA

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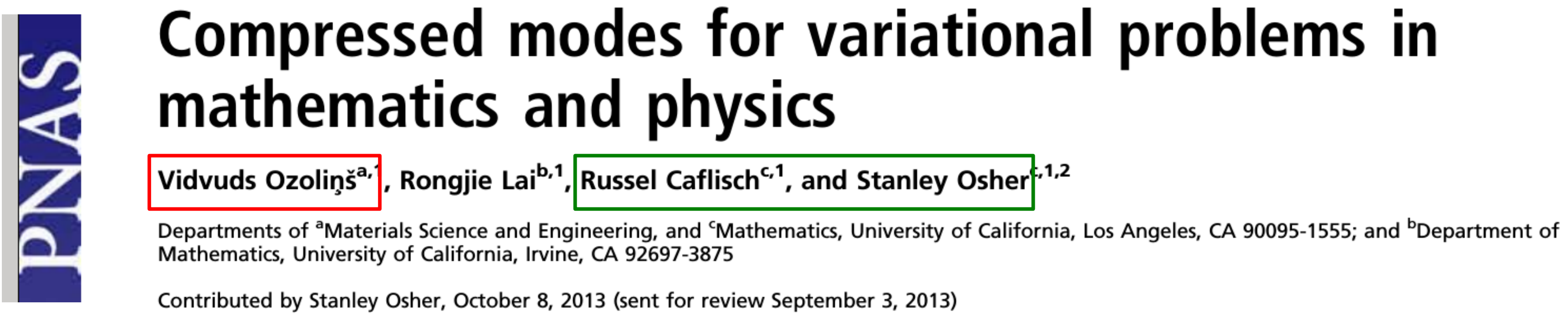
Department of Materials Science and Engineering, University of California, Los Angeles, California 90095-1595, USA

(Received 22 April 2014; published 27 October 2014)



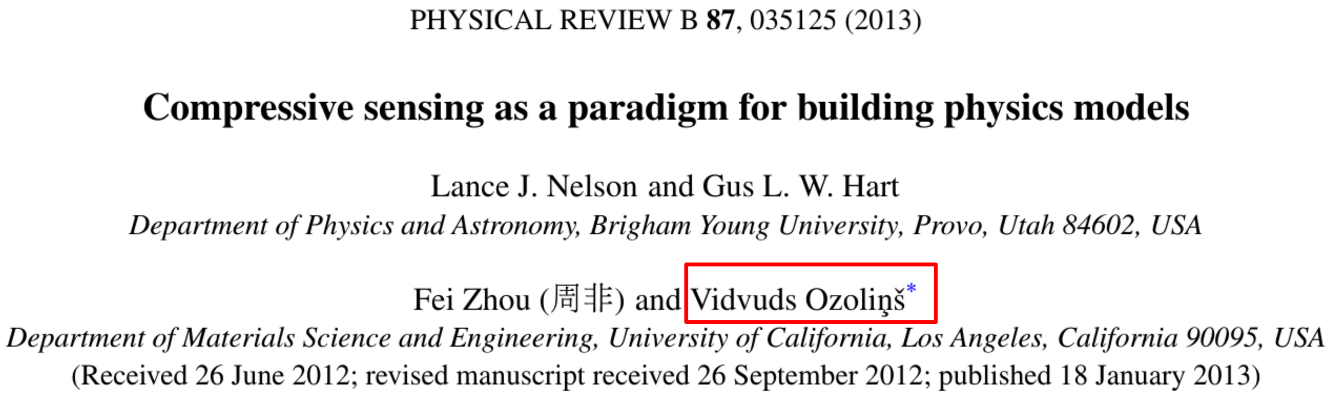
PNAS

Compressed modes for variational problems in mathematics and physics

Vidvuds Ozoliņš[a,1], Rongjie Lai[b,1], Russel Caflisch[c,1], and Stanley Osher[c,1,2]

Departments of [a]Materials Science and Engineering, and [c]Mathematics, University of California, Los Angeles, CA 90095-1555; and [b]Department of Mathematics, University of California, Irvine, CA 92697-3875

Contributed by Stanley Osher, October 8, 2013 (sent for review September 3, 2013)



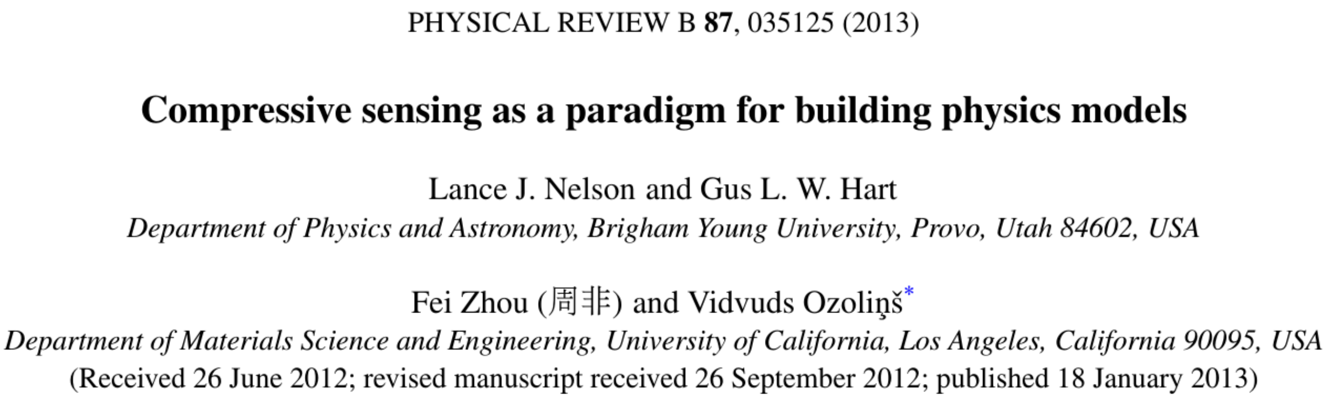
PHYSICAL REVIEW B **87**, 035125 (2013)

Compressive sensing as a paradigm for building physics models

Lance J. Nelson and Gus L. W. Hart
Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA

Fei Zhou (周非) and Vidvuds Ozoliņš*
Department of Materials Science and Engineering, University of California, Los Angeles, California 90095, USA

(Received 26 June 2012; revised manuscript received 26 September 2012; published 18 January 2013)



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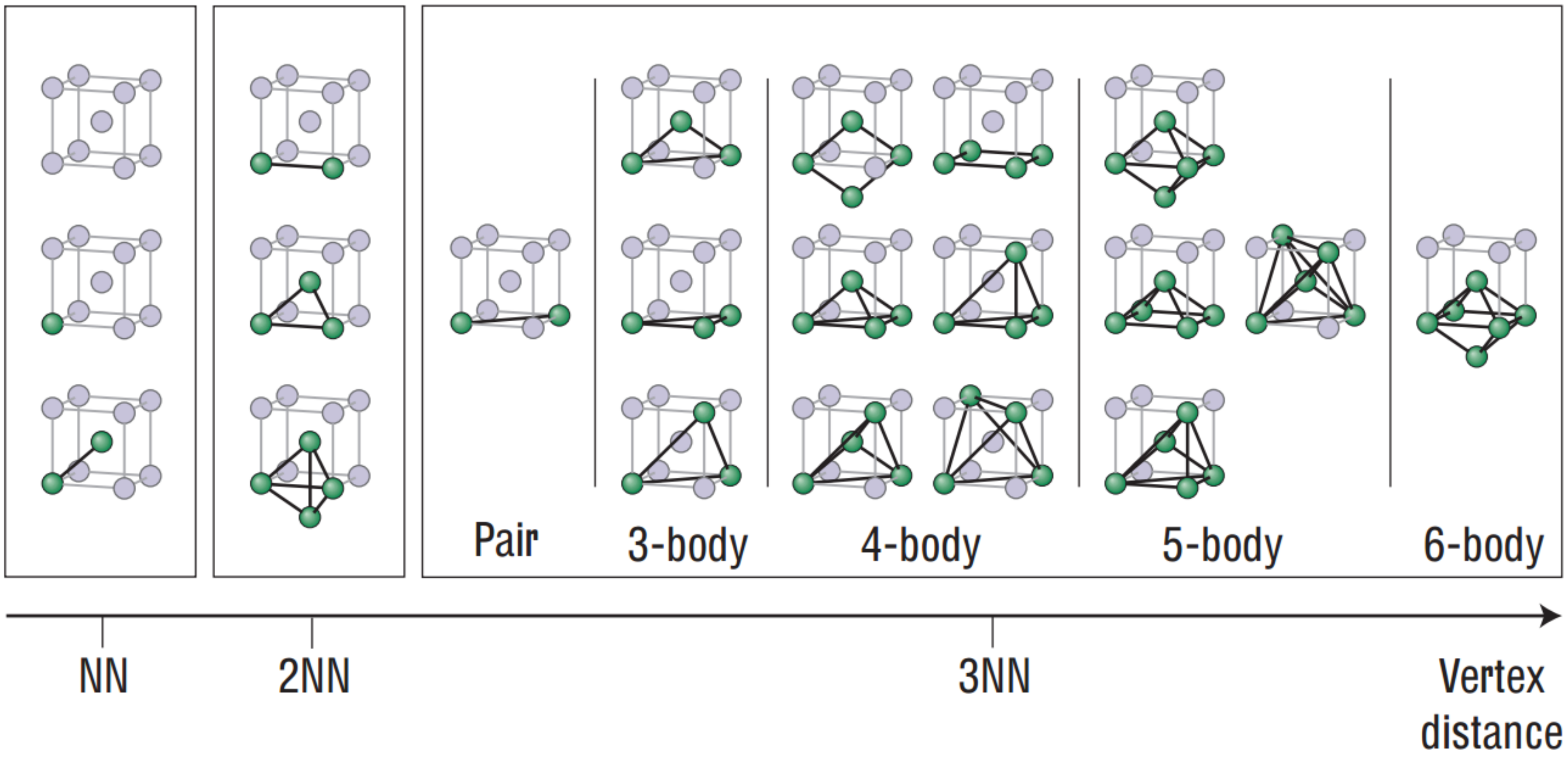
$$E(\sigma) = E_0 + \sum_f \bar{\Pi}_f(\sigma) J_f$$



Compressed sensing: the quest for descriptors and predictive models

82 octet AB binary compounds

Ansatz: atomic features

- HOMO
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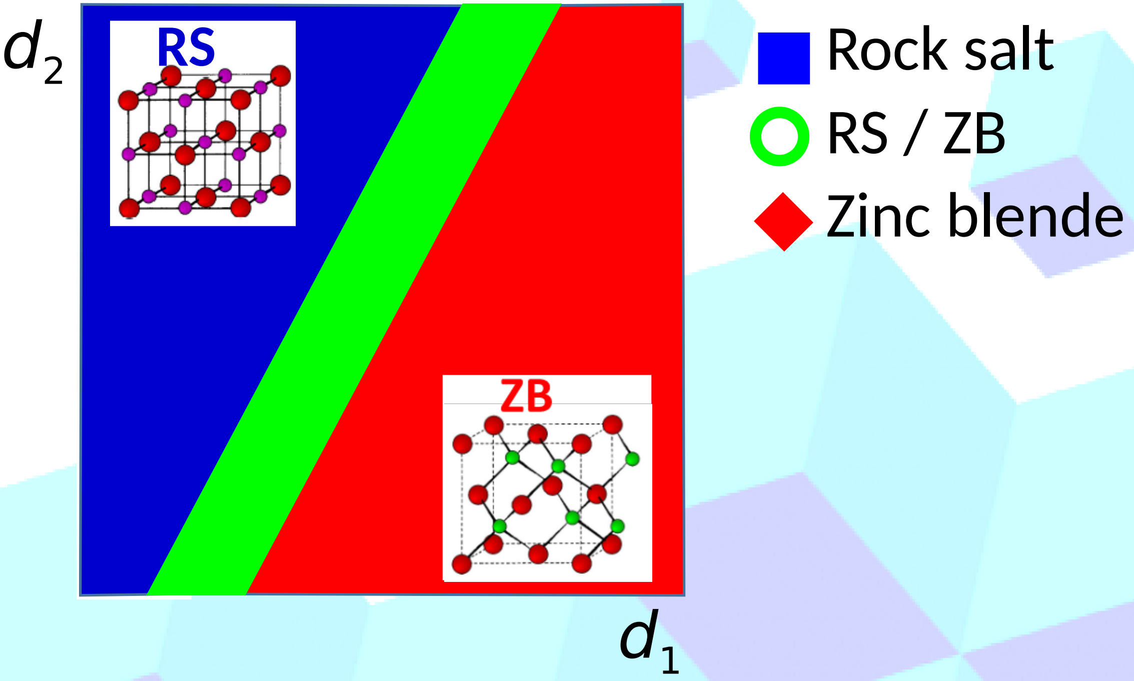

$$\boldsymbol{P} = c_1\boldsymbol{d}_1 + c_2\boldsymbol{d}_2 + \ldots\, c_n\boldsymbol{d}_n$$

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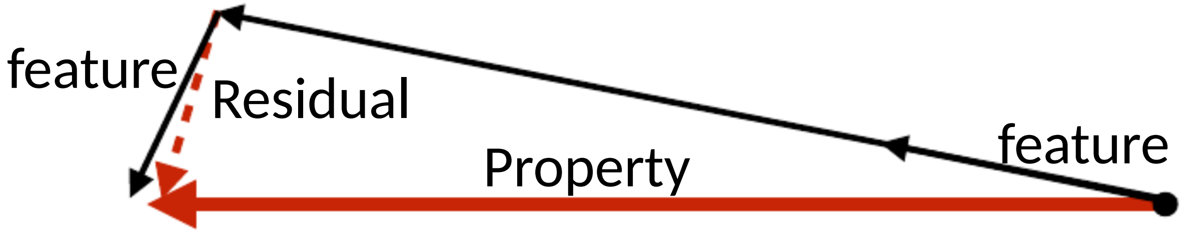
E(Rock salt) – *E*(Zinc blende)

Compressed sensing: the quest for descriptors and predictive models

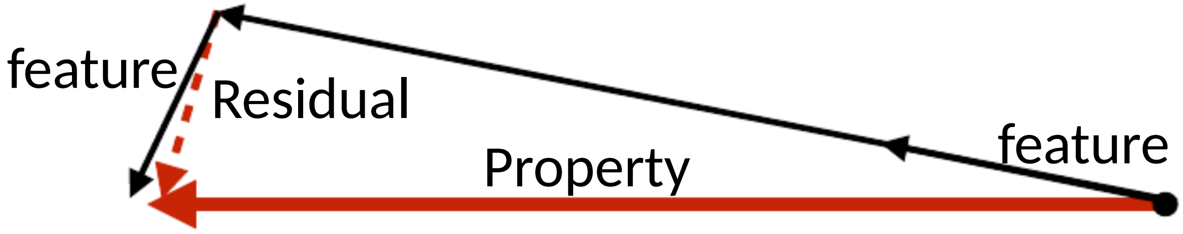
From orthogonal matching pursuit ….



Local-optimum solution
Huge # columns in D

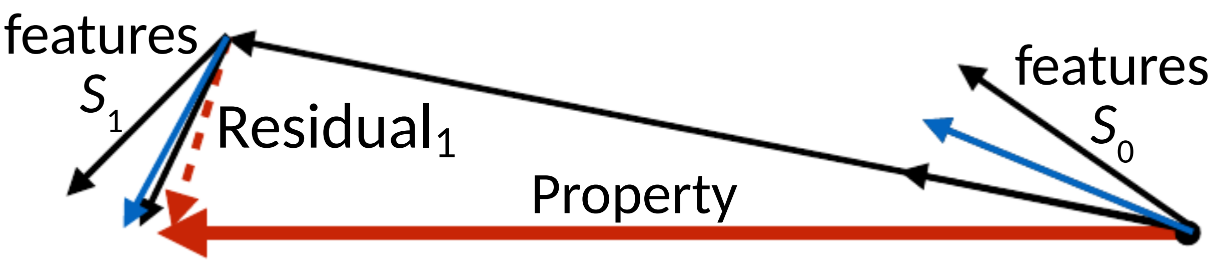
Compressed sensing: the quest for descriptors and predictive models

From orthogonal matching pursuit ….



Local-optimum solution
Huge # columns in D

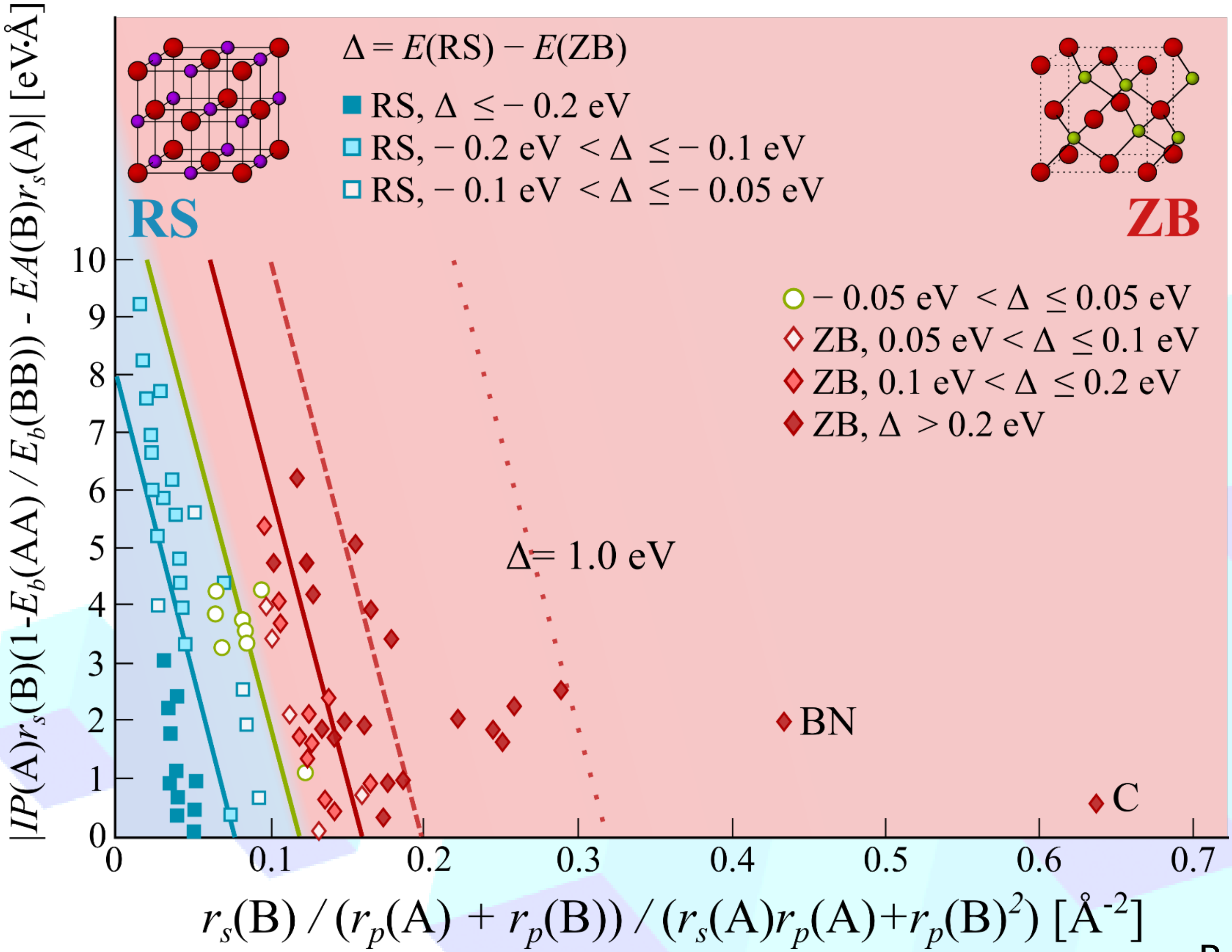
… to Sure Independence Screening + Sparsifying Operator (SISSO)



Proxy of
global-optimum solution
Huge # columns in D

R. Ouyang *et al.* PRM **2**, 083802 (2018), published 7 August 2018)

Compressed sensing: the quest for descriptors and predictive models



Structure map with SISSO, starting from 7 atomic + 6 dimer features
Feature space: 10^{11} features

R. Ouyang *et al.* PRM (2018)

Compressed sensing: the quest for descriptors and predictive models

$$\arg\min_{\boldsymbol{c}} \left(\|\boldsymbol{P} - \boldsymbol{D}\boldsymbol{c}\|_2^2 + \lambda \|\boldsymbol{c}\|_0 \right)$$

Compressed-sensing-based model identification:
Shares concepts with

Regularized regression. But: Massive sparsification.

Dimensionality reduction. But supervised, and yielding sparse, “inspectable” descriptors

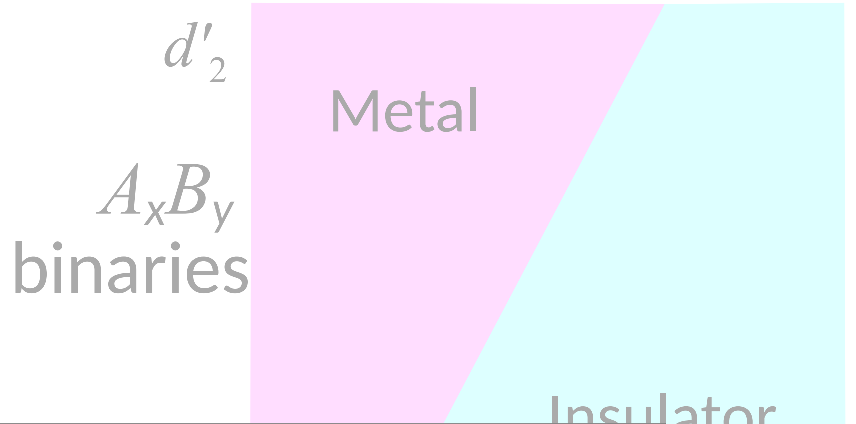
Feature/Basis-set selection/extraction. But: non-greedy solver.

Symbolic regression. But: deterministic solver.

Charts/maps of materials

$$\underset{\boldsymbol{c}\in\mathbb{R}^M}{\operatorname{argmin}}\left(\underbrace{\|\boldsymbol{P}-\boldsymbol{D}\boldsymbol{c}\|_2^2}+\lambda\|\boldsymbol{c}\|_0\right)$$

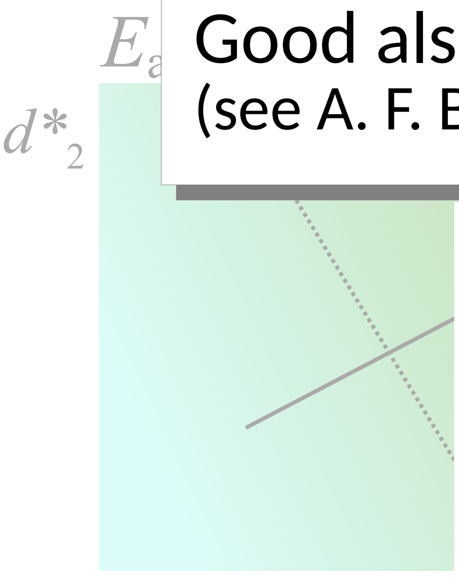
New cost function to be minimized: overlap of *convex* domains



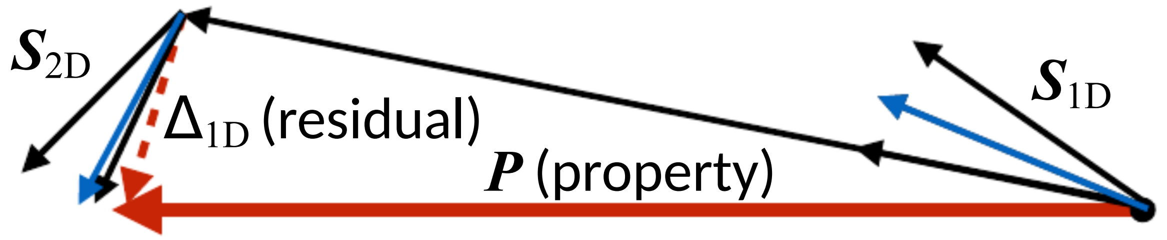
1. # points in the *convex* overlap domain
2. Area of the domain overlap
3. Distance between domains

Good also for multi-categorical problems

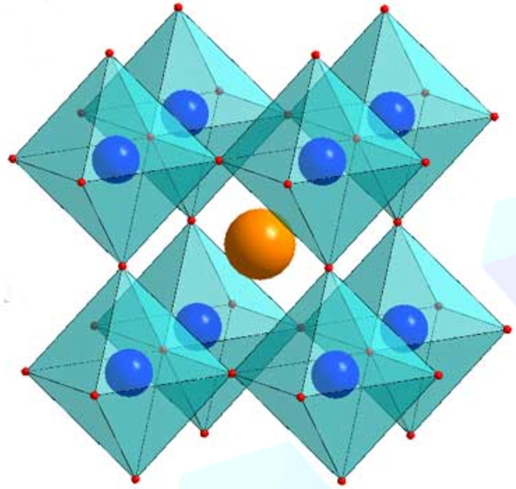
(see A. F. Bialon *et al*., Chem. Mater. **28**, 2550 (2016))



Iterative generation of feature subspaces



Perovskites' stability: an improved Goldschmidt Tolerance Factor

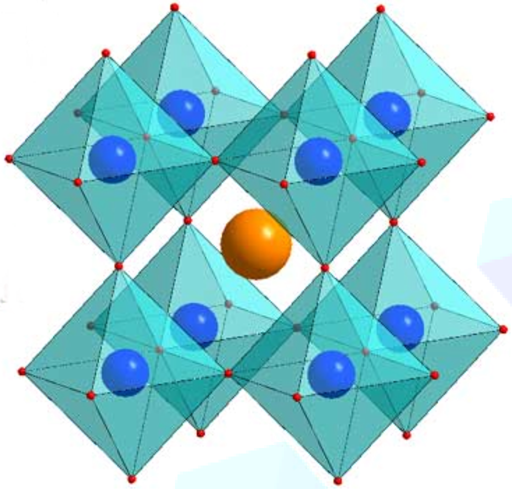


ABX$_3$

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$ → Ionic radius

Goldschmidt* stable perovskites: 0.825 < ***t*** < 1.059, accuracy 79%

Perovskites' stability: an improved Goldschmidt Tolerance Factor



ABX$_3$

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$

$$\tau = \boxed{\frac{r_X}{r_B}} - n_A \left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)} \right)$$

→ Ionic radius

→ Oxidation state

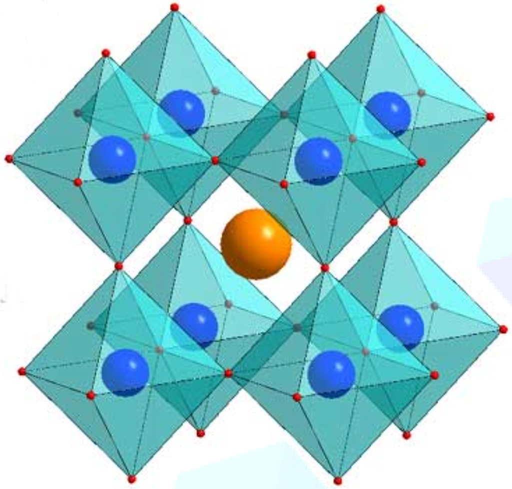
→ 1 / μ = Octahedral factor

Goldschmidt* stable perovskites: 0.825 < *t* < 1.059, accuracy 79%

Our stable perovskites: *τ* < 4.18, accuracy 92%

Bartel, Sutton, Goldsmith, Ouyang, Musgrave, LMG &Scheffler, Sci. Adv. 5, *eaav0693 (2019)*

Perovskites' stability: an improved Goldschmidt Tolerance Factor



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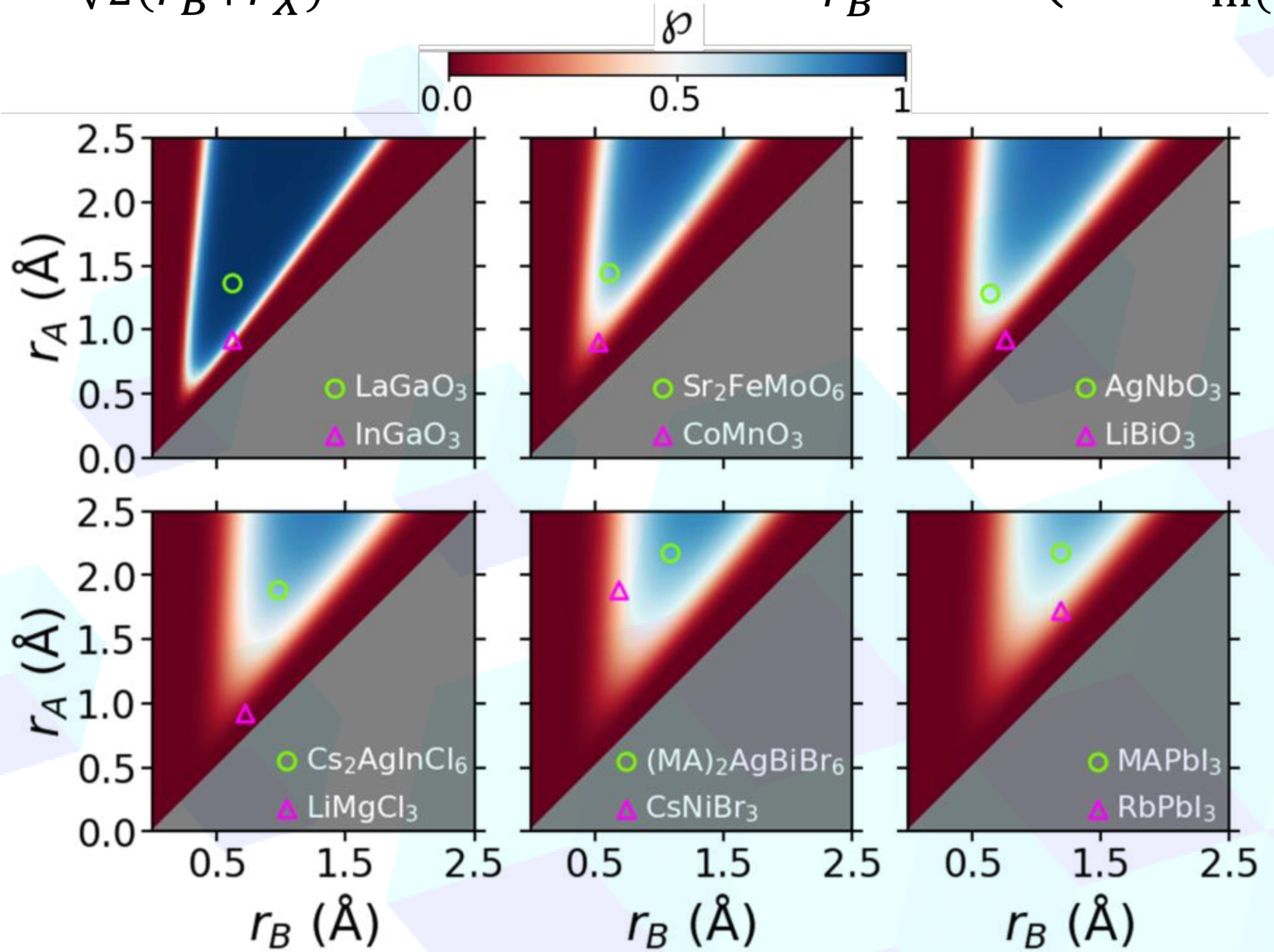
τ < 3.31 or τ > 5.92, 99% accuracy (1/3 of the training data)

τ < 3.31 or τ > 12.08, 100% accuracy (1/4 of the training data)

Bartel, Sutton, Goldsmith, Ouyang, Musgrave, LMG &Scheffler, Sci. Adv. *5, eaav0693 (2019)*

Improved Goldschmidt Tolerance Factor: Materials design

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \longrightarrow \tau = \frac{r_X}{r_B} - n_A\left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)}\right)$$



n_A →

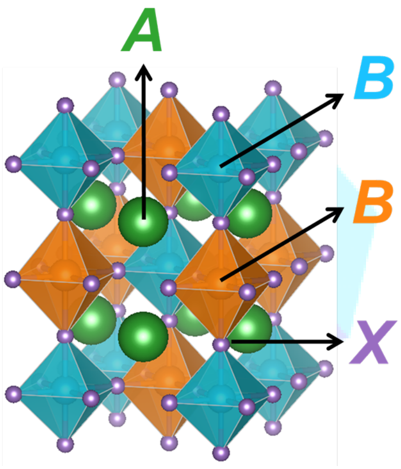
$X = O^{2-}$

$n_A = 1^+$

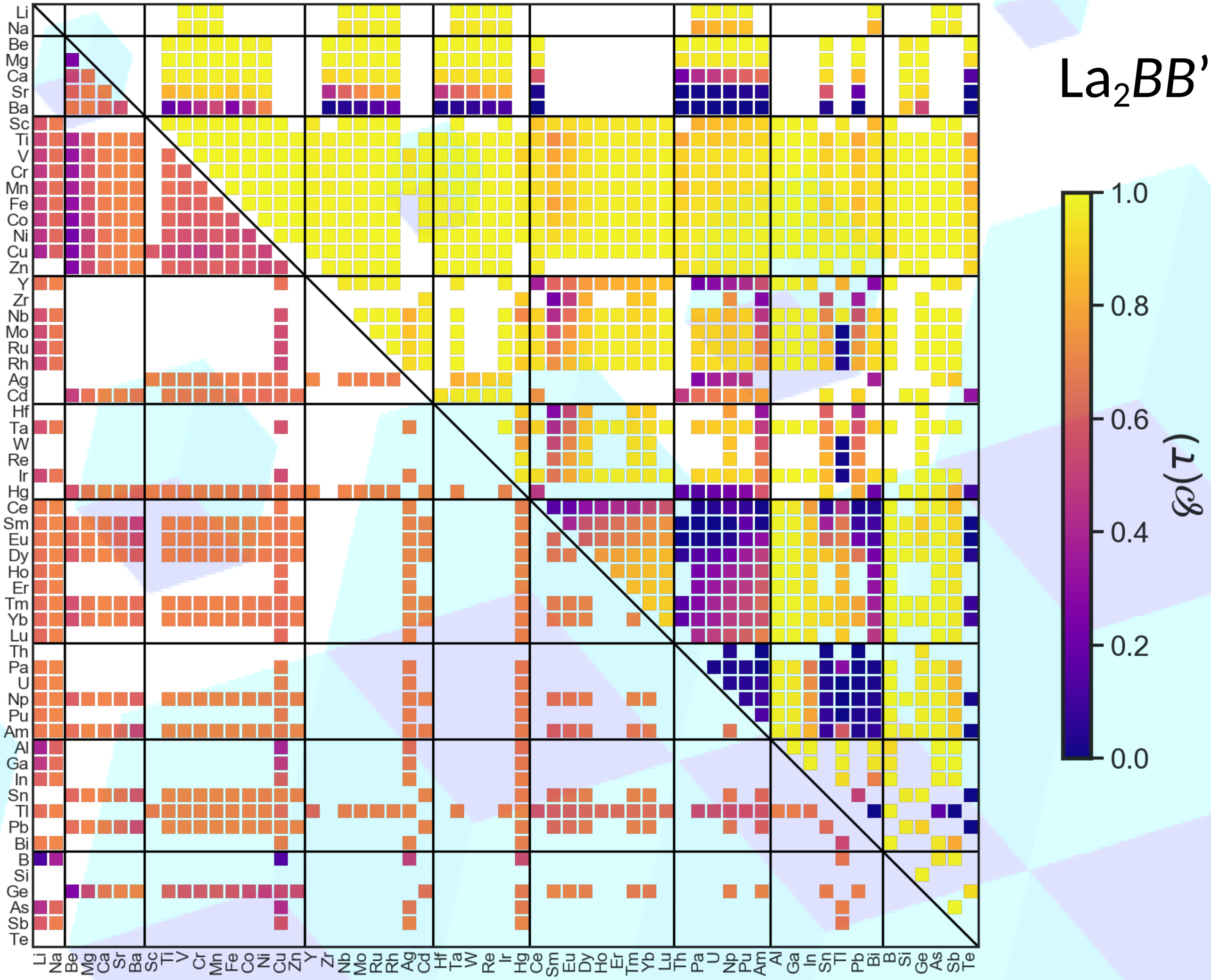
X →

Improved Goldschmidt Tolerance Factor: Extension of the materials space

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \longrightarrow \tau = \frac{r_X}{r_B} - n_A\left(n_A - \frac{r_A/r_B}{\ln(r_A/r_B)}\right)$$



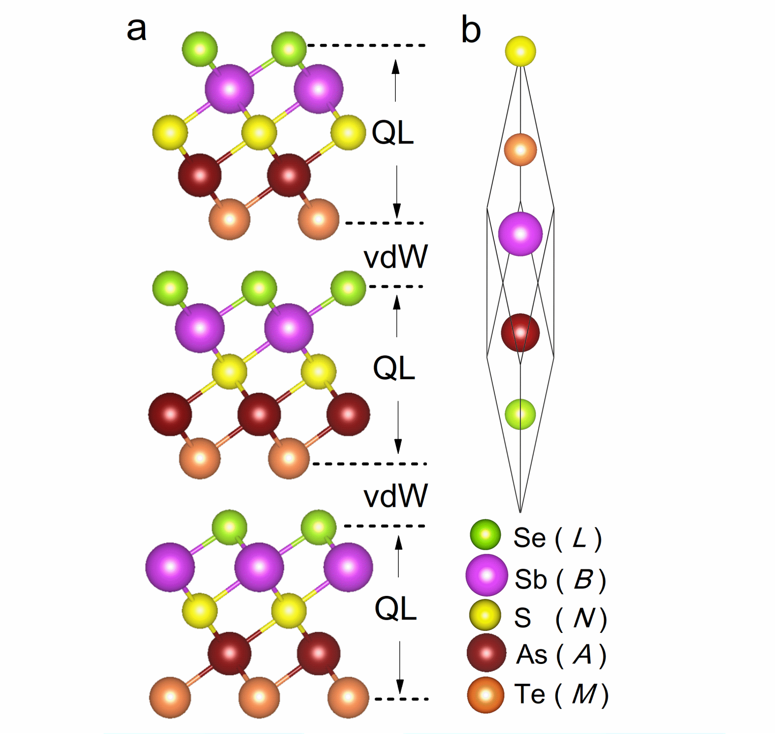
$La_2BB'O_6$



$Cs_2BB'Cl_6$

SISSO: predicting new tetradymite topological insulators

Prototype formula:
AB-LNM
AB = {As,Sb,Bi}
LNM = {S, Se,Te}



Cao, Liu, Ouyang, LMG, Zhou, Scheffler, Zhang, Carbogno, submitted (2019)

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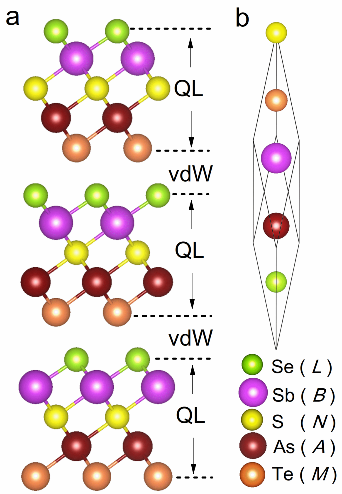
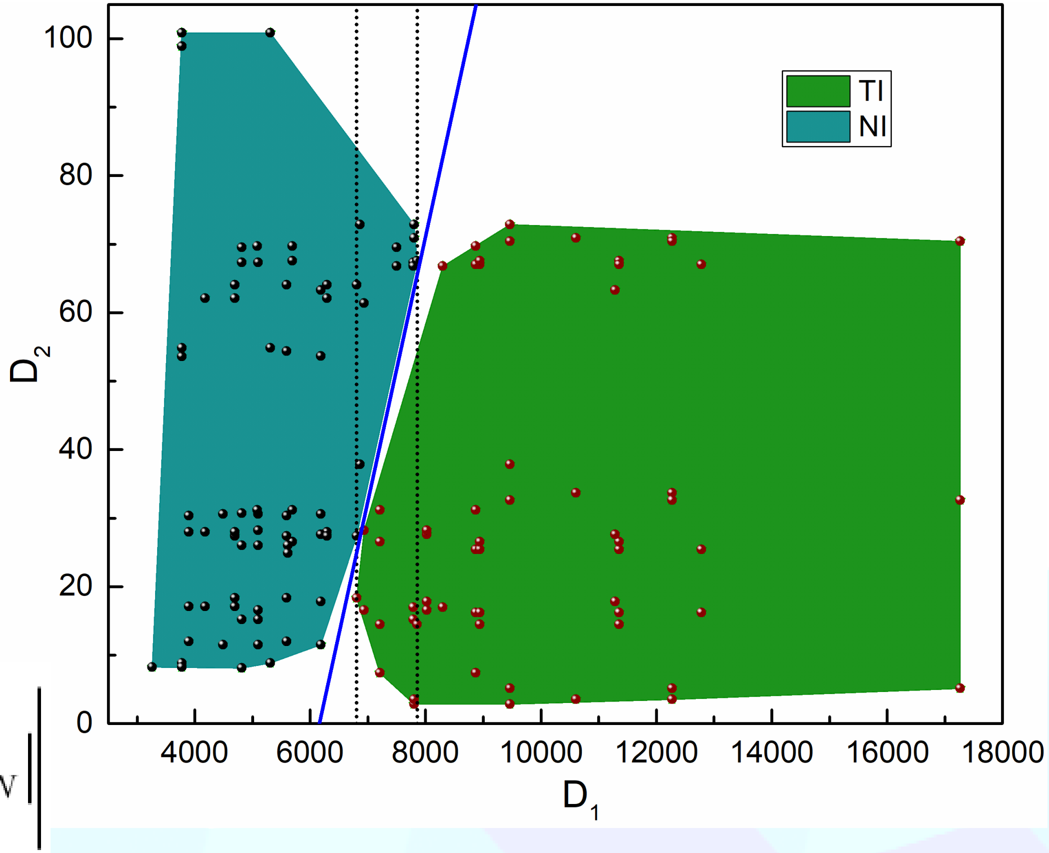


$$D_1 = (Z_A + Z_B)\cdot(Z_L + Z_M) - |Z_A Z_M - Z_B Z_L|$$

$$D_2 = \left|\frac{(\chi_M + \chi_N)\cdot Z_E}{\chi_A} - (Z_M + Z_N) - |Z_M - Z_N|\right|$$



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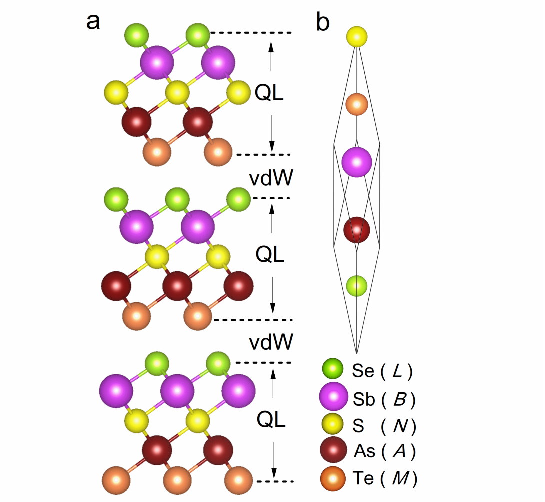

$$As_xSb_yBi_{2\text{-}x\text{-}y}S_aSe_bTe_{3\text{-}\,a\text{-}\,b}$$

$$D_1 = (Z_A + Z_B)\cdot(Z_L + Z_M) - |Z_A Z_M - Z_B Z_L|$$

$$D_2 = \left|\frac{(\chi_M + \chi_N)\cdot Z_E}{\chi_A} - (Z_M + Z_N) - |Z_M - Z_N|\right|$$

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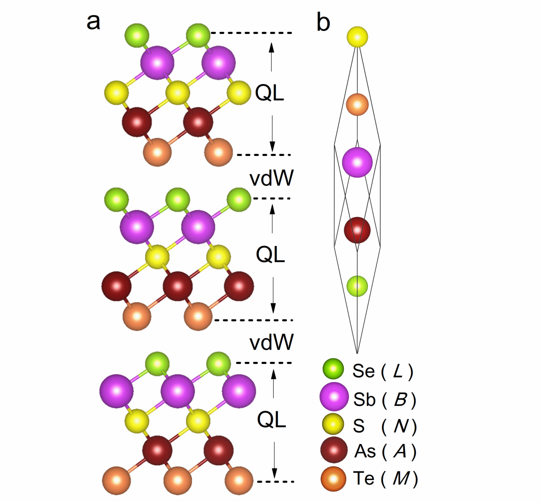
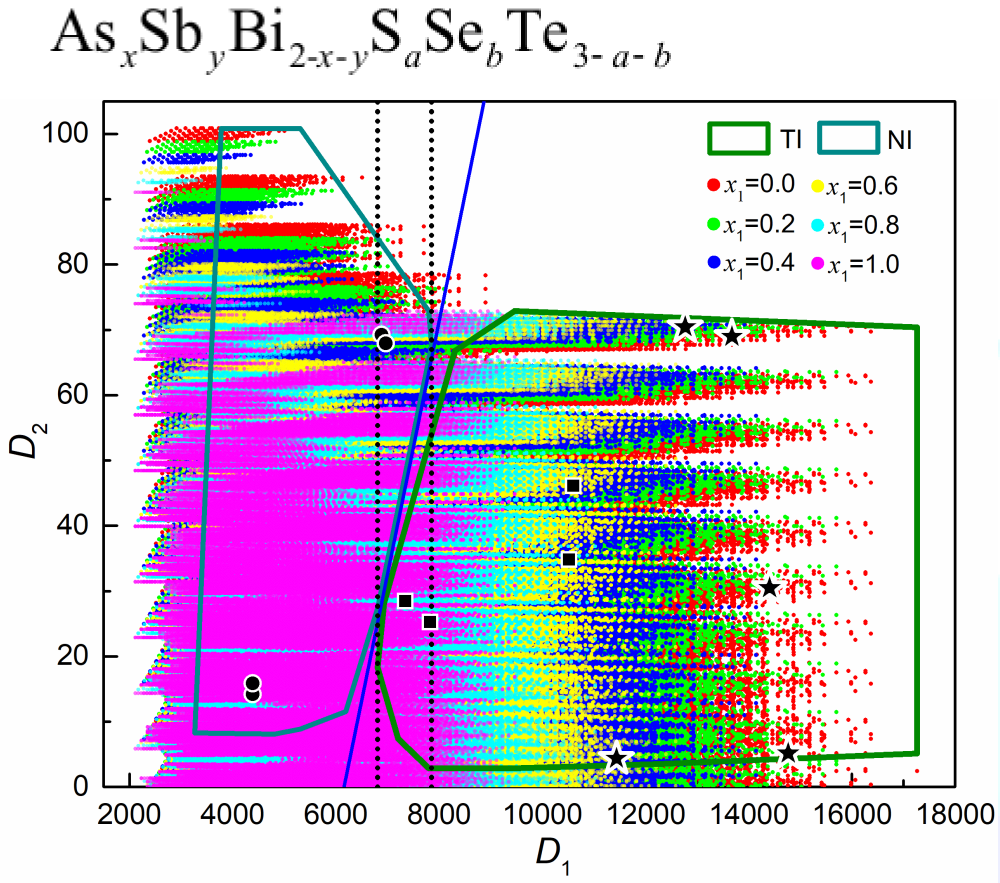


$$D_1 = (Z_A + Z_B) \cdot (Z_L + Z_M) - |Z_A Z_M - Z_B Z_L|$$

$$D_2 = \left| \frac{(\chi_M + \chi_N) \cdot Z_E}{\chi_A} - (Z_M + Z_N) - |Z_M - Z_N \right.$$



Cao, Liu, Ouyang, LMG, Zhou, Scheffler, Zhang, Carbogno, submitted (2019)

Acknowledgements

Compressed sensing and SISSO
Jan Vybiral, Runhai Ouyang, Emre Ahmetcik, Stefano Curtarolo, Christian Carbogno, Sergey Levchenko, Claudia Draxl

Application of SISSO to perovskites
Christopher J. Bartel, Christopher Sutton, Bryan R. Goldsmith, Runhai Ouyang, Charles B. Musgrave

Application of SISSO to topological insulators
Guohua Cao, Runhai Ouyang, Huijun Liu, Zizhen Zhou, Zhenyu Zhang, Christian Carbogno

And
Matthias Scheffler

NOMAD
NOVEL MATERIALS DISCOVERY

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