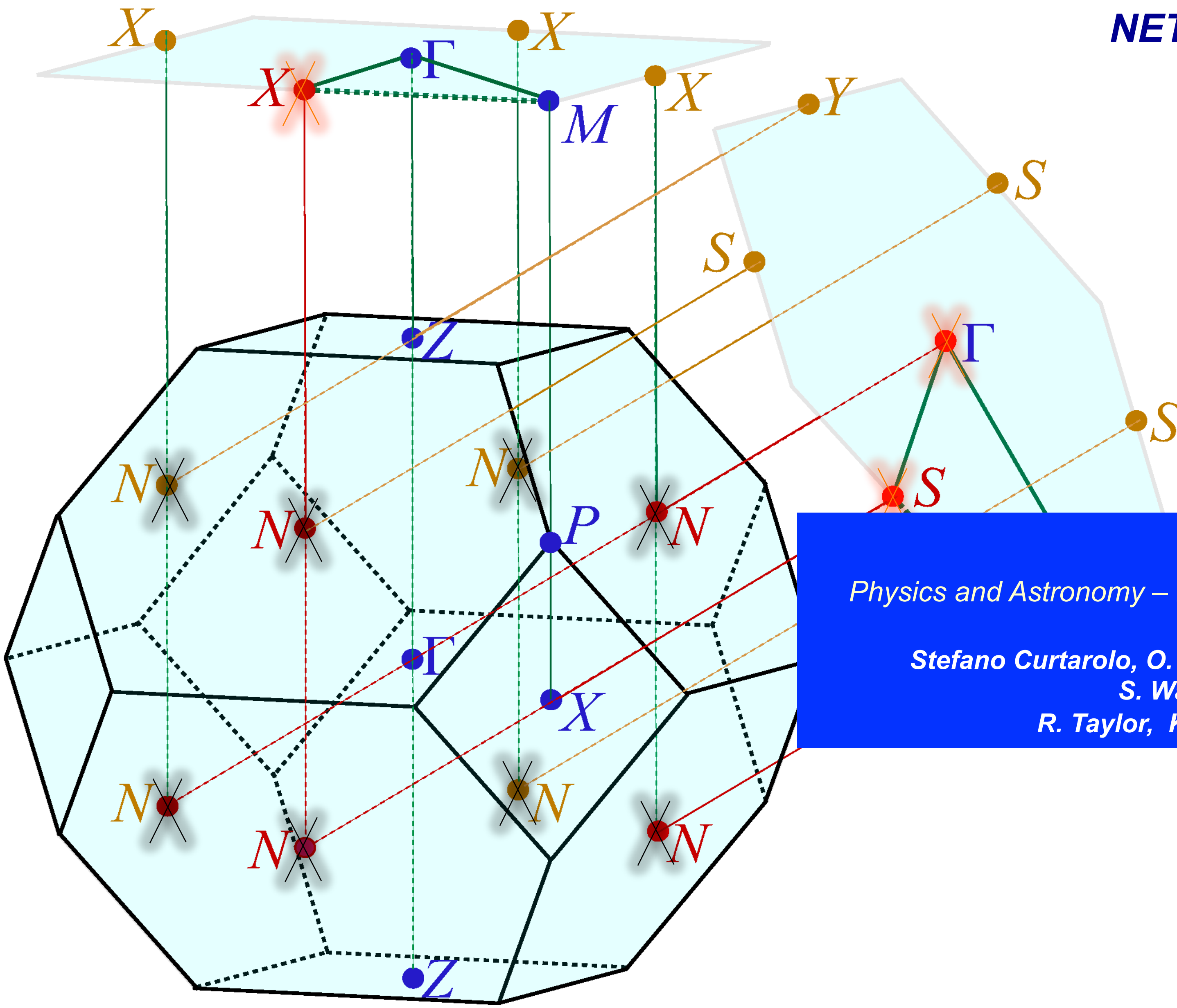
High-throughput descriptors in materials development

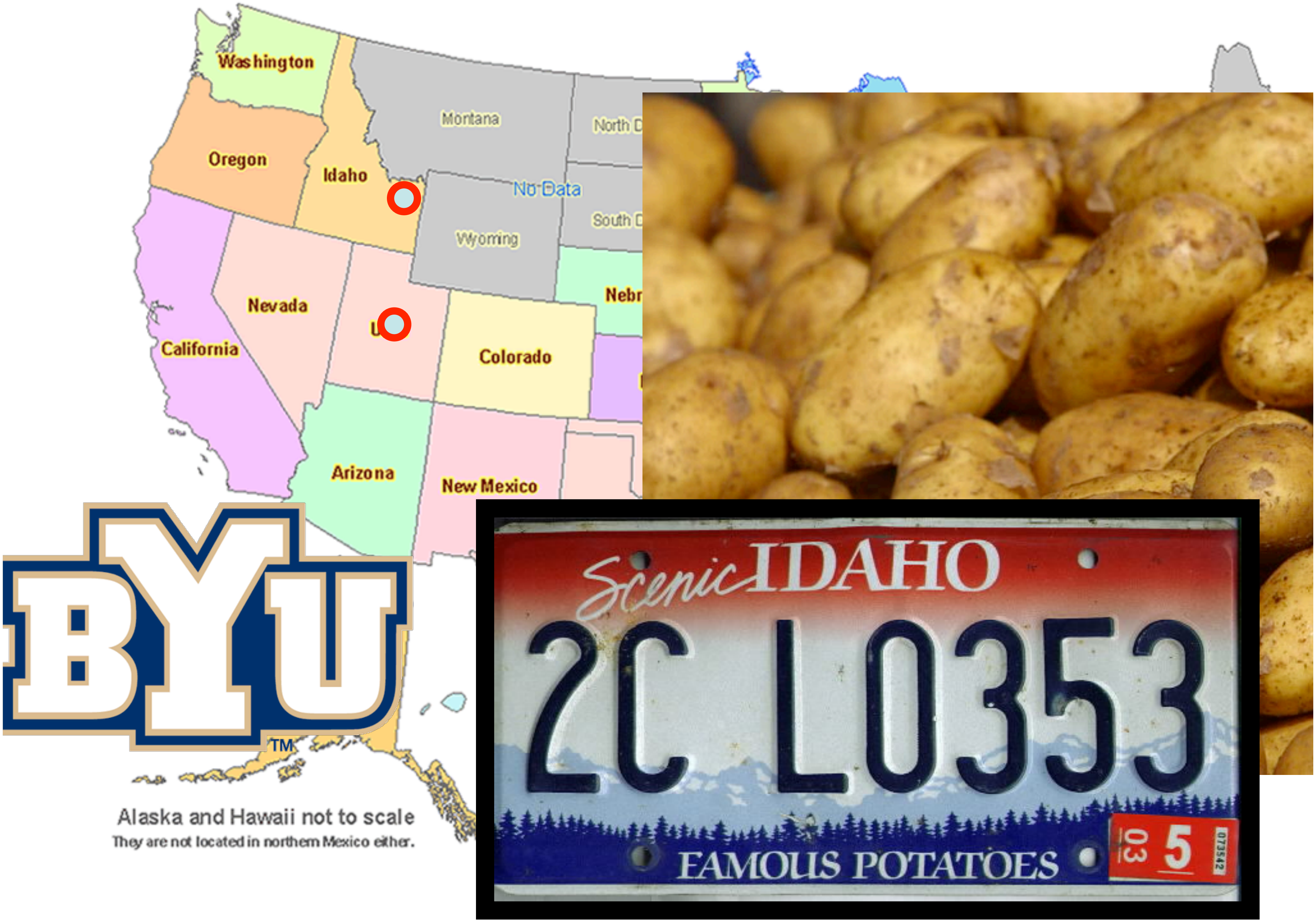
NETL, NSF, DOD-MURI



Gus L. W. Hart

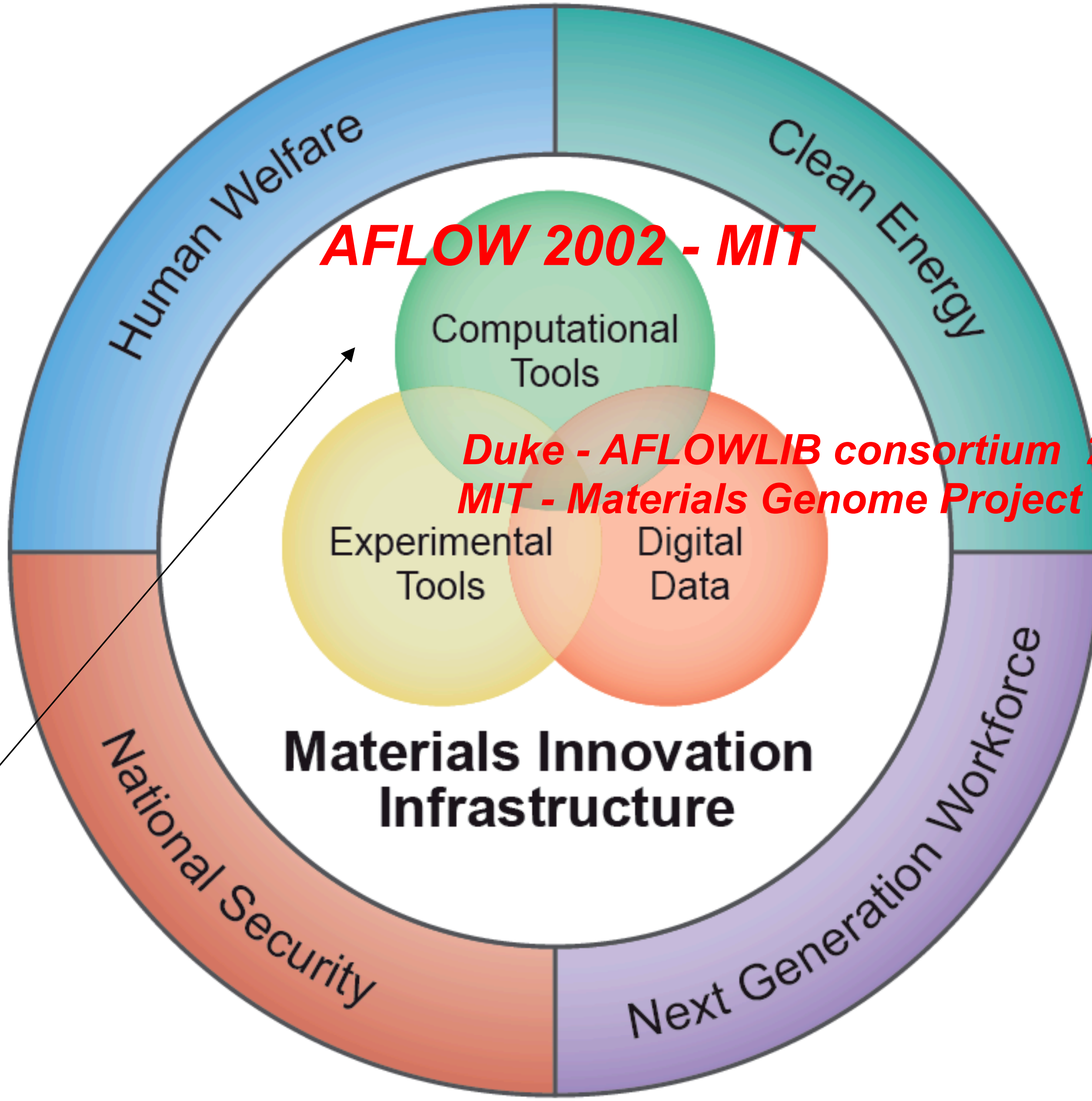
*Physics and Astronomy – **Brigham Young University***

Stefano Curtarolo, O. Levy, I. Takeuchi, J. Carrete, S. Wang, M. Buongiorno Nardelli, R. Taylor, K. Yang, N. Mingo, S. Sanvito


Washington
Oregon
Idaho
Montana
No Data
Wyoming
Nevada
California
Colorado
Arizona
New Mexico
Alaska and Hawaii not to scale
They are not located in northern Mexico either.
Scenic IDAHO
2C L0353
FAMOUS POTATOES
03 5

Materials Genome Initiative

AFLOW 2002 - MIT



Duke - AFLOWLIB consortium 2010

MIT - Materials Genome Project 2011

Curtarolo, Morgan, Persson, Rodgers, **Ceder**, *Predicting Crystal Structures with **Data Mining** of Quantum Calculations*, Phys. Rev. Lett. **91**, 135503 (2003).

AFLOW: automatic flow of calculations and analysis

COMPUTATIONAL MATERIALS GENOME

procedures of synthesis. Is there another way? Indeed, this is the burgeoning area of computational materials science called 'high-throughput' (HT) computational materials design. It is based on the marriage between computational quantum-mechanical–thermodynamic approaches[1,2] and a multitude of techniques rooted in database construction and intelligent data mining[3]. The concept is simple yet powerful: create a large database containing the calculated thermodynamic and electronic properties of existing and hypothetical materials, and then intelligently interrogate the data-

early,

exist-

ones

nature materials

REVIEW ARTICLE

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

The high-throughput highway to computational materials design

Curtarolo*, Hart, Buongiorno Nardelli, Mingo, Sanvito, Levy

DOI: 10.1038/NMAT3568 (March 2013)

COMPUTATIONAL High-Throughput

The practical implementation of computational HT is highly non-trivial. The method is employed in three strictly connected steps: (i) virtual materials growth: thermodynamic and electronic structure calculations of materials[3,23]; (ii) rational materials storage: systematic storage of the information in database repositories[24,25]; (iii) materials characterization and selection: data analysis aimed at selecting novel materials or gaining new physical insights[15,19,26].

nature materials

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MATERIALS GENOME: genes+descriptors

Table 1 | Examples of descriptors introduced in the literature. Nature Mater. **12**, 191 (2013)

Problem	Combination of materials properties (gene)	Descriptor
Structure stability: convex hull of an alloy system	Formation enthalpy (H_f) as a function of concentration (x) and the enthalpies (H) of A and B.	$H_f(x) = H(A_{1-x}B_x) - (1-x)H(A) - xH(B)$
Phase stability in off-lattice alloys PRL **91**, 135503 (2003)	Spectral decomposition of alloy vector-energies ($E_{n,p}$, n-rows = species, p-columns = configurations) with principal-component-analysis coefficients (α	$E_{n,p} \simeq \alpha_1 E_{n,1} + \cdots + \alpha_{p-1} E_{n,p-1} + \epsilon(d)$
Nano PR	Ratio of the av) (ref. 15).	
Topol Nat	Variational rat rbit derivative stra at k, a_0 lattice)[16].	
Powe l (spec cy) PRL **108**, 068701 (2012)	Ratio of the m ident solar energy densit on-hole recombinatio E)) — versus bandgap energy (E_g)[62].	
Non-proportionality in scintillators IEEE Trans. Nucl. Sci. **56**, 2989 (2009)	Maximum mismatch between effective masses of electrons (m_e) and holes (m_h)[75].	$\hat{\chi}_{np} \equiv \max\left(\frac{m_e}{m_h}, \frac{m_h}{m_e}\right)$
Morphotropic phase boundary piezoelectrics PRB **84**, 014103 (2011)	Energy proximity between tetragonal, rhombohedra and rotational distortions (ΔE_p). Angular coordinate (α_{AB}) of the energy minimum in the A–B off-centerings energy map for ABO_3 systems[79].	$\Delta E_p \lesssim 0.5$ eV $\alpha_{AB} \approx 45°$

the “problem”

qualitative picture

quantitative picture

Automation is key

NEED fast standards

Calculate electronic structure of all reported compounds

- *ICSD ~150,000 (well defined ~50%)*
- *Work out all the prototype definitions/symmetries:*
- *Define standards in reciprocal space (on-line):*

  a highly complex solution to an apparently simple problem
- *Obtain LDAU parameters when required*
- *Adiabatic U*
- *Automatic switch to LS coupling when required*
- *Calculate stability, if necessary*
- *Discover properties through correlations*
- *Make ONLINE Tools*
- *Use results as **STARTING POINTS***
- *Works for VASP and QE*

STANDARD in Real Space and Reciprocal Space

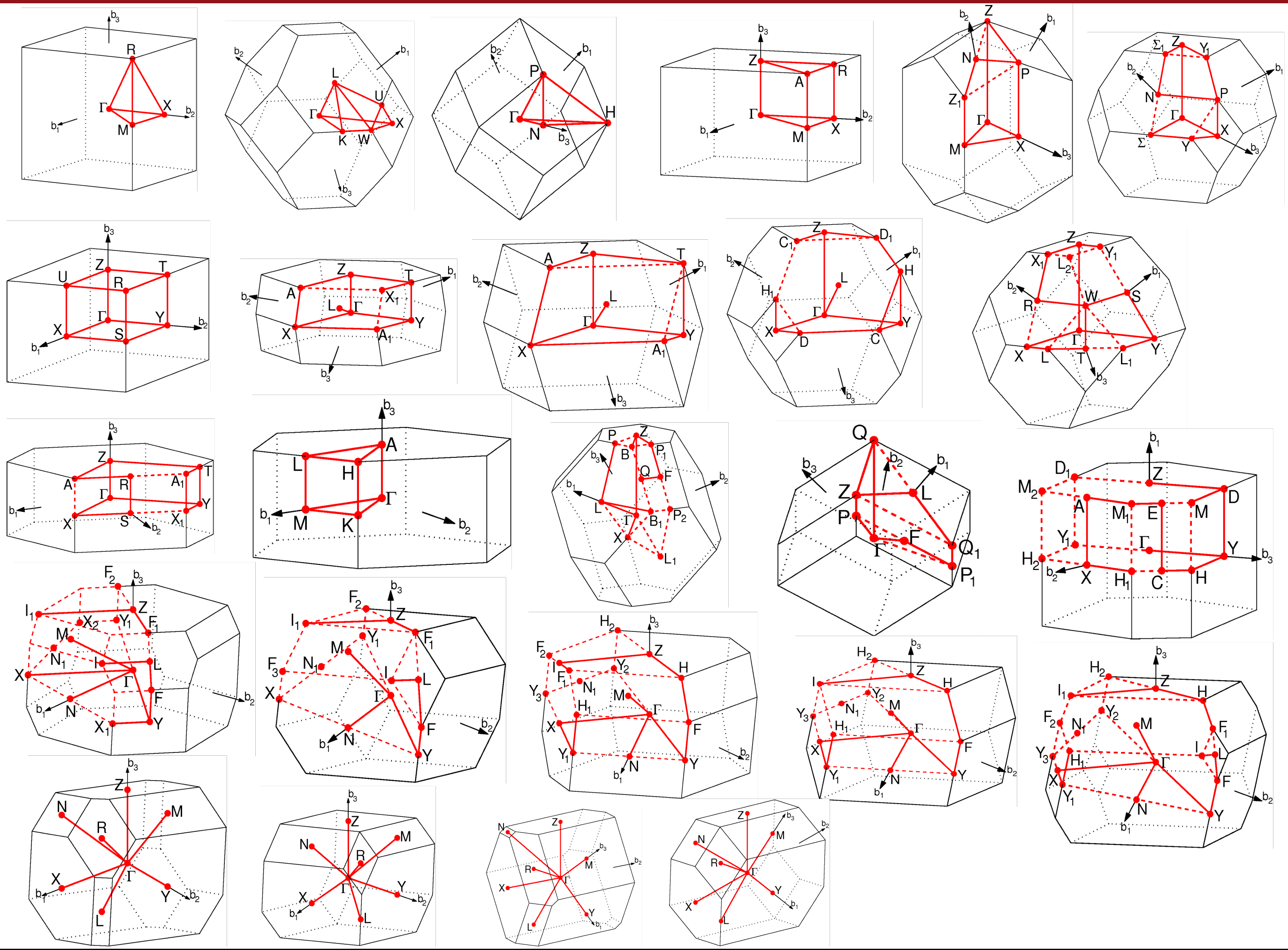
Algorithm has 25 self consistent points

$$\boxed{(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)_{BL}^{n+1} = \mathrm{Dual}\left[\mathrm{Minkowski}_{BL^*}\left[\mathrm{Dual}\left[(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)_{BL}^{n}\right]\right]\right]}$$

14 Bravais Lattices → 25 Brillouin Zones → 25 Bravais Definitions

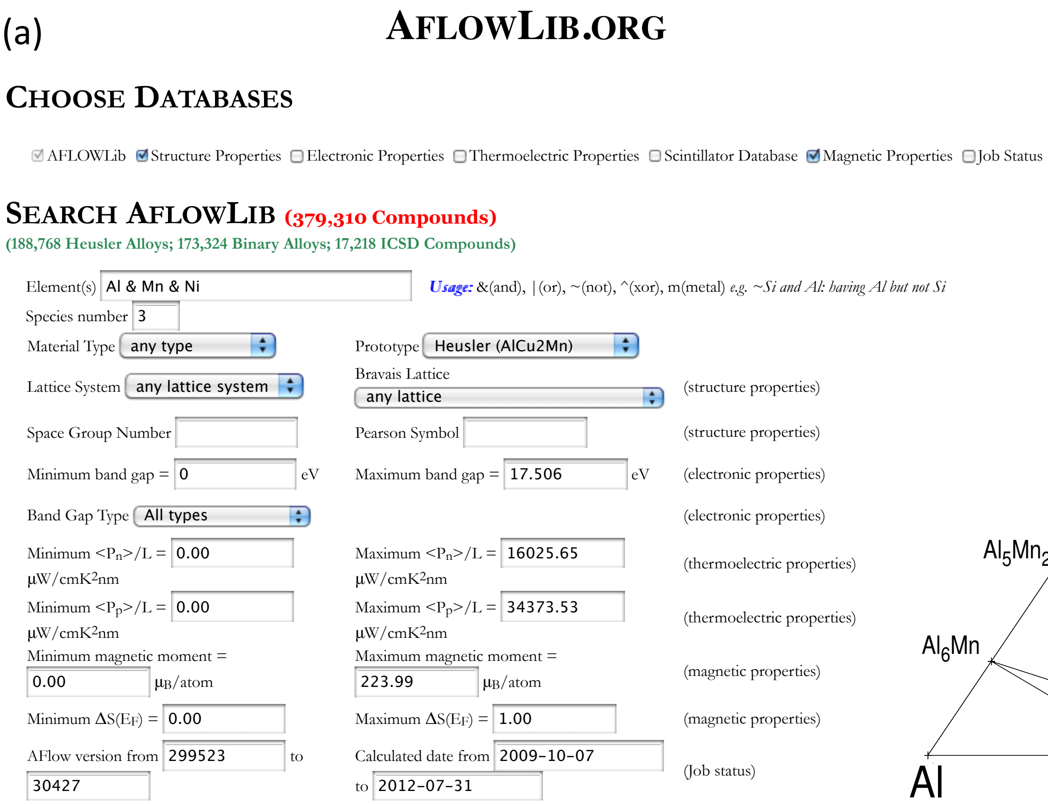
CUBIC: cub, bcc, fcc
TETRAGONAL: tet, bct_1, bct_2
ORTHORHOMBIC: orc, $orcf_1$, $orcf_2$, $orcf_2$, orci, orcc
HEXAGONAL/TRIGONAL: hex, rhl_1, rhl_2
MONOCLINIC: mcl, $mclc_1$, $mclc_2$, $mclc_3$, $mclc_4$, $mclc_5$
TRICLINIC: tri_{1a}, tri_{2a}, tri_{1b}, tri_{2b}

STANDARD in Real Space and Reciprocal Space

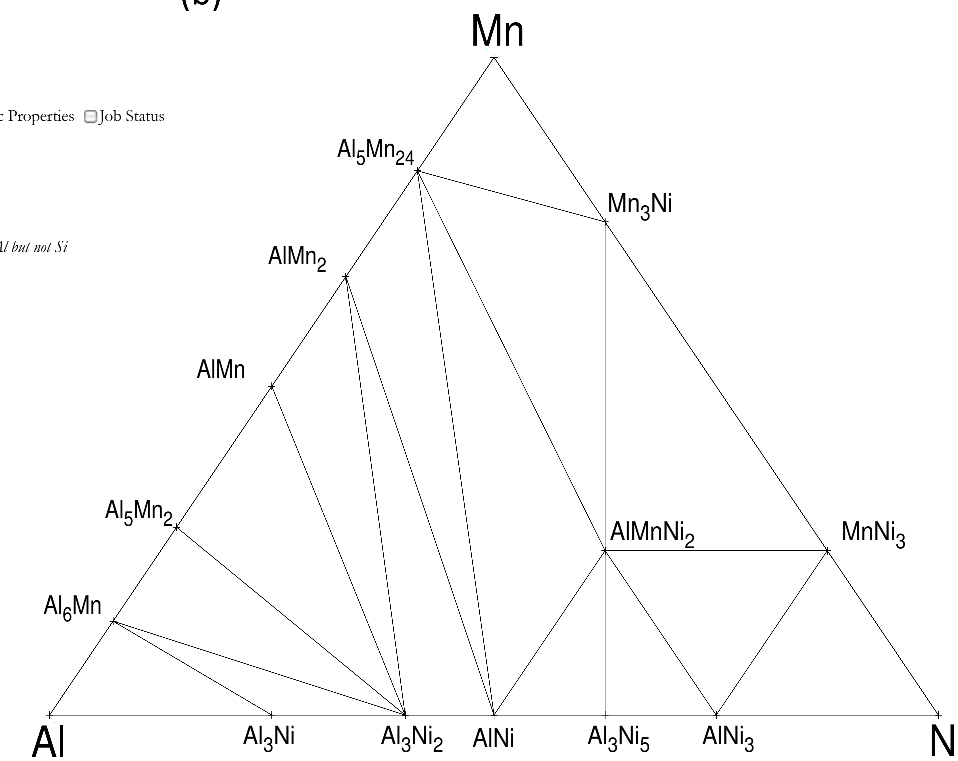


Repository of quantum mechanics calculations

(a)



(b)

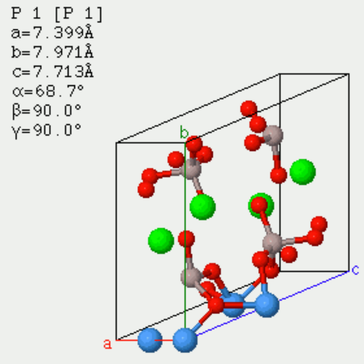


Curtarolo *et al.*, *“AFLOWLIB.ORG: a distributed materials properties repository from high-throughput ab initio calculations”*, Comp. Mat. Sci. **58**, 227-235 (2012).

$Al_1Ca_1O_5Ta_1$ (ICSD# 99001)

Real Space Lattices

Lattices:	a = 7.40Å b = 7.97Å c = 7.71Å α = 68.69° β = 90.00° γ = 90.00°
Volume:	423.76Å^3
Unit Cell Atom Number:	32
Space Group Number:	14
Pearson Symbol:	mP32
Lattice Primitive:	MCL Al1Ca1O5Ta1 #14.0 - (Al1Ca1O5Ta1_ICSD_99
Lattice Variation:	MCL
Crystal Family:	Monoclinic
Crystal System:	Monoclinic
Crystal Class:	Monoclinic-prismatic
Point Group (Hermann Mauguin):	2/m PGXTAL
Point Group (Schoenflies):	C_2h
Point Group Orbifold:	2*
Point Group Type:	centrosymmetric
Point Group Order:	4
Point Group Structure:	2 X Cyclic
Superlattice Primitive unit cell:	MCL
Superlattice Variation:	MCL
Pearson Symbol Superlattice:	mP32



☑ Turn spin off

☐ Show atom labels

ball and stick

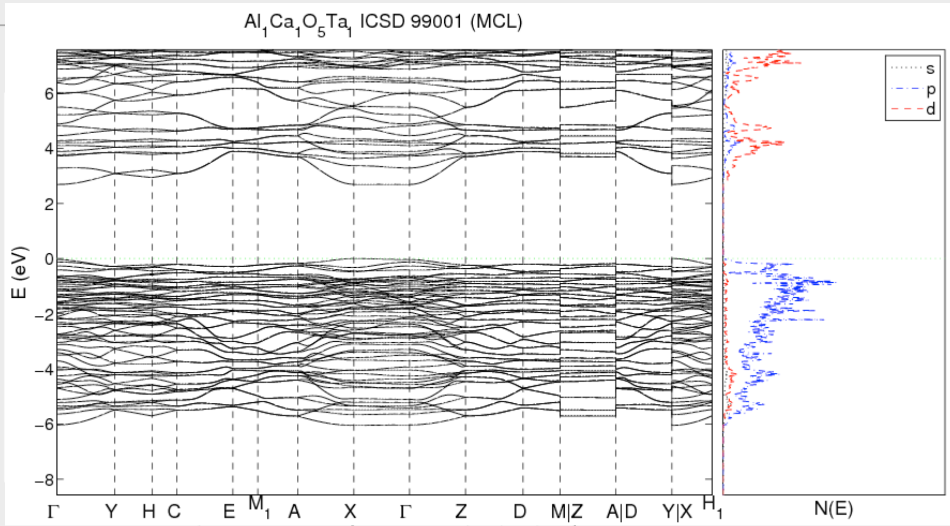
Density:	5.45 g/cm^3
Band Gap:	2.68 eV
Fit Band Gap:	4.53 eV
Band Gap Type:	Indirect
Electron Mass:	6.66 (m_0)
Hole Mass:	2.85 (m_0)

Reciprocal Space Lattices

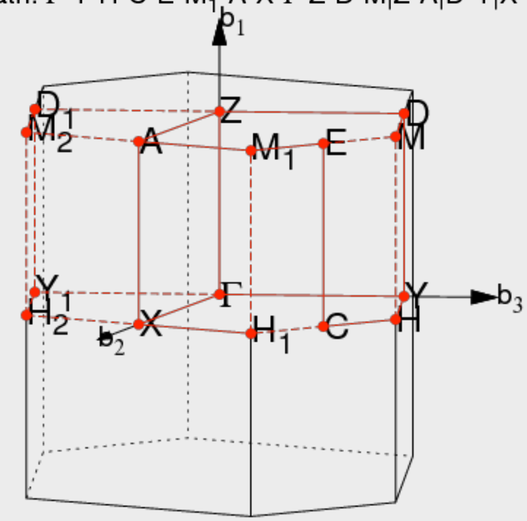
Reciprocal Lattices:	a = 0.85Å b = 0.85Å c = 0.87Å α = 111.31° β = 90.00° γ = 90.00°
Volume:	0.59 Å^{-3}
Lattice Primitive:	MCL
Lattice Variation:	MCL

Electronic Properties

Band Structure



MCL path: Γ-Y-H-C-E-M_1-A-X-Γ-Z-D-M|Z-A|D-Y|X-H_1



aflowlib

Comp. Mat. Sci. **49**, 299-312 (2010)

Repository of quantum mechanics calculations

geometrical-structural search (with formation energies)

thermoelectric data (power factors etc.)

▲Name [1]	ICSD Number [1]	Bravais Lattice	Number of Atoms	<Pn>/L (μW/cmK²nm) [4]	<Pn1>/L (μW/cmK²nm) [4]	<Pn2>/L (μW/cmK²nm) [4]	<Pn3>/L (μW/cmK²nm) [4]	<Pp>/L (μW/cmK²nm) [4]	<Pp1>/L (μW/cmK²nm) [4]	<Pp2>/L (μW/cmK²nm) [4]	<Pp3>/L (μW/cmK²nm) [4]	Sn (μV/K) [4]	Sp (μV/K) [4]
$F_3Fe_1K_1$	15424	CUB (Cubic)	5	0.15	0.15	0.15	0.15	2.17	2.17	2.17	2.17	-116.36	91.29
$F_3Fe_1Rb_1$	49586	CUB (Cubic)	5	0.24	0.24	0.24	0.24	1.50	1.48	1.51	1.51	-91.73	91.04
$Fe_1La_1O_3$	29118	CUB (Cubic)	5	0.31	0.31	0.31	0.31	2.00	2.00	2.00	2.00	-139.02	92.92

$Ag_2Fe_1S_4Sn_1$	42534	BCT (Tetragonal)	8	121 (I-42m)	tI16	4.77

magnetic properties (if you want rare-earth-free magnets/spintronics)

scintillation properties/search

▲Name [1]	ICSD Number [1]	Bravais Lattice	Number of Atoms	Magnetic Moment (μB/atom) [5]	Spin Polarization (1/atom) [5]	Spin Decomposition (μB)
$Ag_1Fe_1O_2$	2786	HEX (Hexagonal)	8	1.25	0.00	{0.039,0.039,4.303,4.303,0.258,0.258,0.258,0.258}
$Ag_1Fe_1O_2$	31919	RHL (Rhombohedral)	4	1.25	0.00	{0.039,4.303,0.258,0.258}
$Ag_2Fe_1S_4Sn_1$	42534	BCT (Tetragonal)	8	0.50	0.00	{0.016,0.016,3.631,0.024,0.024,0.024,0.024,0.016}

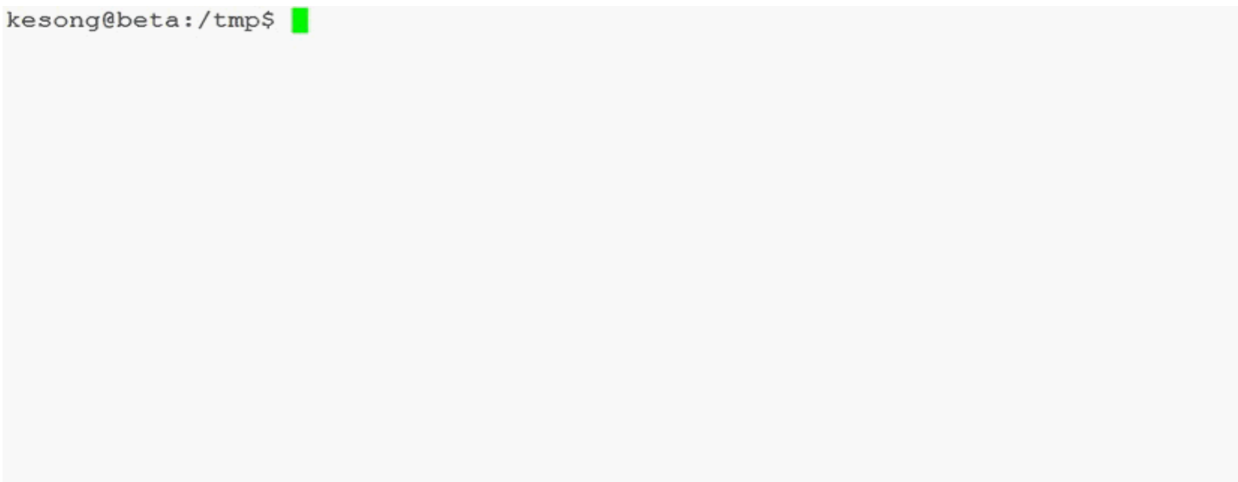
F_2Fe_1	9166	TET (Tetragonal)	6	2.63 (I)	4.46	0.49	0.48	190.80	5.47	388.39	7.15	15.23	2.86700	

aflowlib

www.aflowlib.org

Automatic Generation of Databases

Creating "aflow.in" input files:



HT Computational Tools (AFLOW)

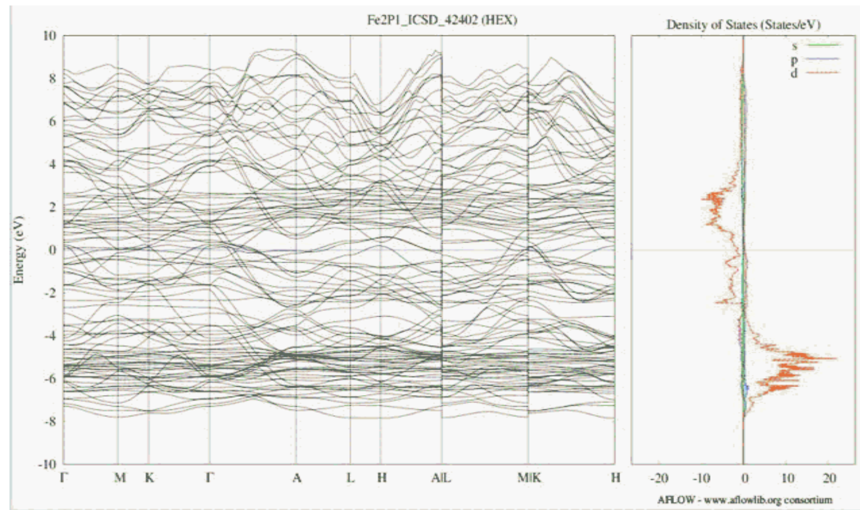
VASP

Materials Database (AFLOWLIB)

AFLOWLIB.ORG: a distributed materials properties repository from HT ab initio calculations, Comp. Mat. Sci. **58**, 227 (2012)

Automatic data/visualization analysis

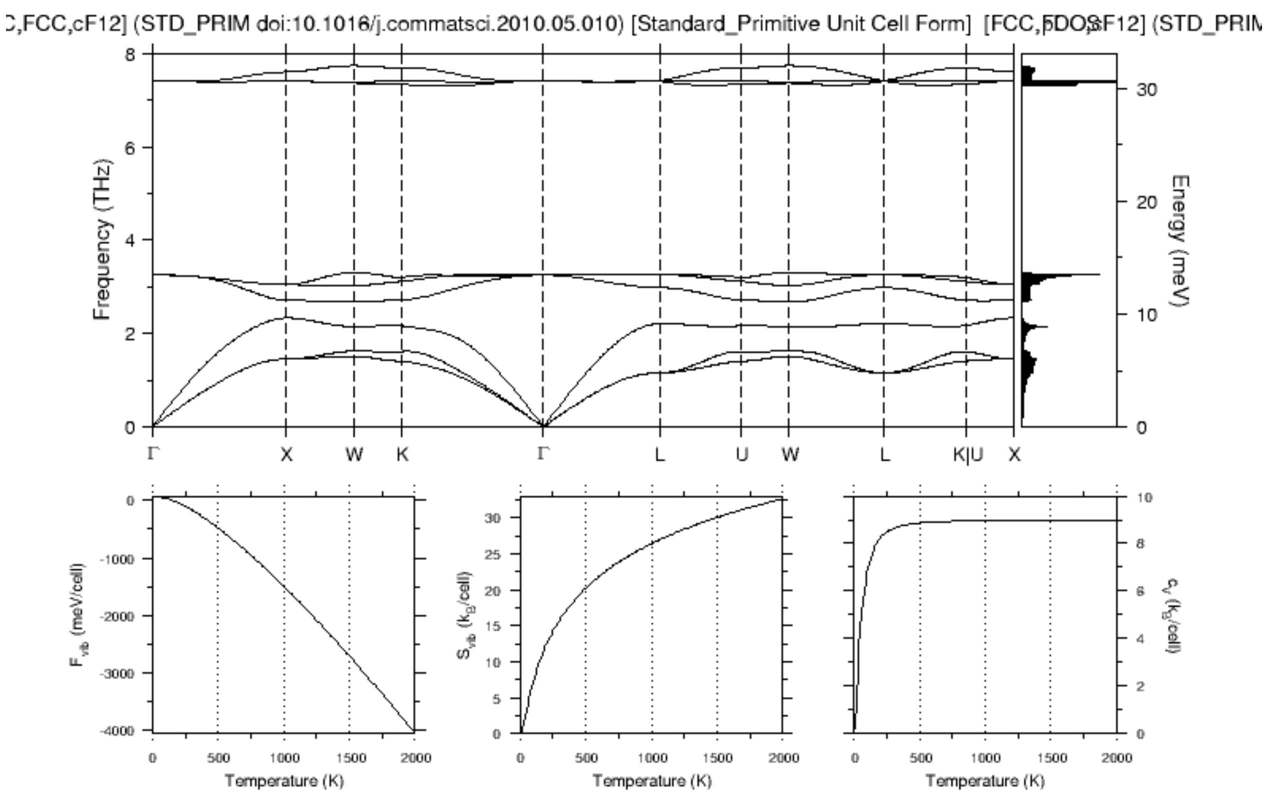
Extract general materials properties: structural, electronic, magnetic properties…



Develop new high-throughput programs based on the desired materials properties

AFLOW: an automatic framework for high-throughput materials discovery, Comp. Mat. Sci. **58**, 218-226 (2012)

Vibrational Free energy



EXAMPLE: Topological Insulators

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Nanosintered thermoelectrics PRX **1**, 021012 (2011)	Ratio of the average power factor (<P>) to the grain size (L) (ref. 15).	$\hat{\chi}_{\mathrm{thermo}} \equiv \frac{<P>}{L}$
Topological insulators (epitaxial growth) Nature Mater. **11**, 614 (2012)	Variational ratio of spin–orbit distortion versus non-spin-orbit derivative strain (E_k^{SOC}, E_k^{noSOC}, spin/no spin-orbit bandgaps at k, a_0 lattice)[16].	$\hat{\chi}_{\mathrm{TI}} \equiv -\frac{E_k^{\mathrm{SOC}}(a_0)/a_0}{\delta E_k^{\mathrm{noSOC}}(a)_0/\delta a_0 \vert_{a_0}}$
Power conversion efficiency of a solar cell (spectroscopic limited maximum efficiency) PRL **108**, 068701 (2012)	Ratio of the maximum output power density (P_m) to the incident solar energy density (P_{in}) — a function (η) of the radiative electron–hole recombination current (f_r) and the photon absorptivity ($\alpha(E)$) — versus bandgap energy (E_g)[62].	$\eta(\alpha(E), f_r) = P_m/P_{in}$; E_g
Non-proportionality in scintillators IEEE Trans. Nucl. Sci. **56**, 2989 (2009)	Maximum mismatch between effective masses of electrons (m_e) and holes (m_h)[75].	$\hat{\chi}_{np} \equiv \max\left(\frac{m_e}{m_h}, \frac{m_h}{m_e}\right)$
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top. insul.

EXAMPLE: Topological Insulators

TI: insulator inside and conductor in the surface. The conducting state is protected by the symmetry of the system (inversion and time reversal).

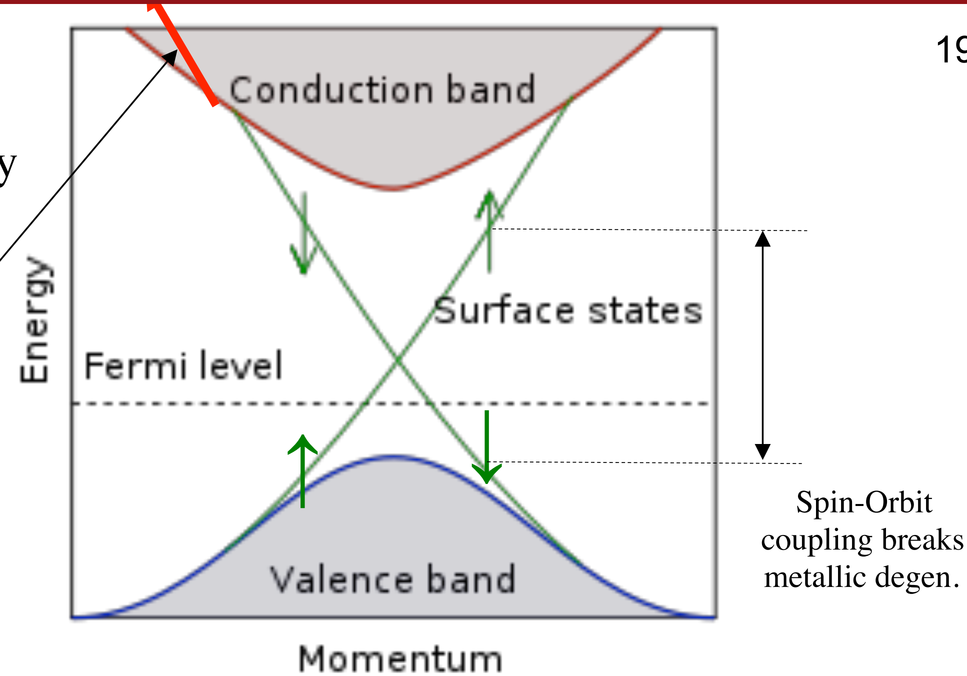
Fu, Kane, Mele, PRL **98**, 106803 (2007).
Hasan, Kane, Rev. Mod. Phys. **82**, 3045 (2010).
Haldane, PRL **61**, 2015 (1988).
Nielssen, Ninomiya, Phys. Lett. 130B, 389 (1983).

$$\hat{h}(\mathbf{k}) = \mathbf{h}(\mathbf{k})/|\mathbf{h}(\mathbf{k})|.$$

$$n = \frac{1}{4\pi}\int d^2\mathbf{k}(\partial_{k_x}\hat{h} \times \partial_{k_y}\hat{h}) \cdot \hat{h} \quad \text{(Berry Phase)}$$

number of times $\hat{h}(\mathbf{k})$ wraps around the unit sphere

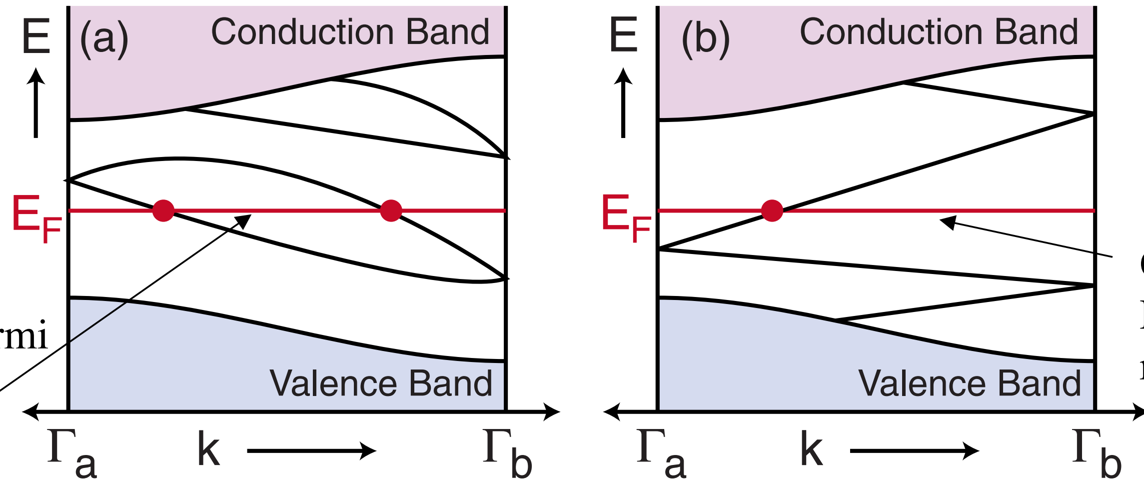
each Dirac point contributes $\pm e^2/2h$ to σ_{xy}



Cones come in doubles (even).
Insulating state = cancellation => $\sigma_{xy}=0$
Quantum Hall State = summation => $\sigma_{xy}\neq 0$

EXAMPLES: going alloys and going surfaces

Surface *2D BZ*
Surface states



EVEN crossing 2D Fermi surface: destructable by troubles

ODD crossing 2D Fermi surface: resistant

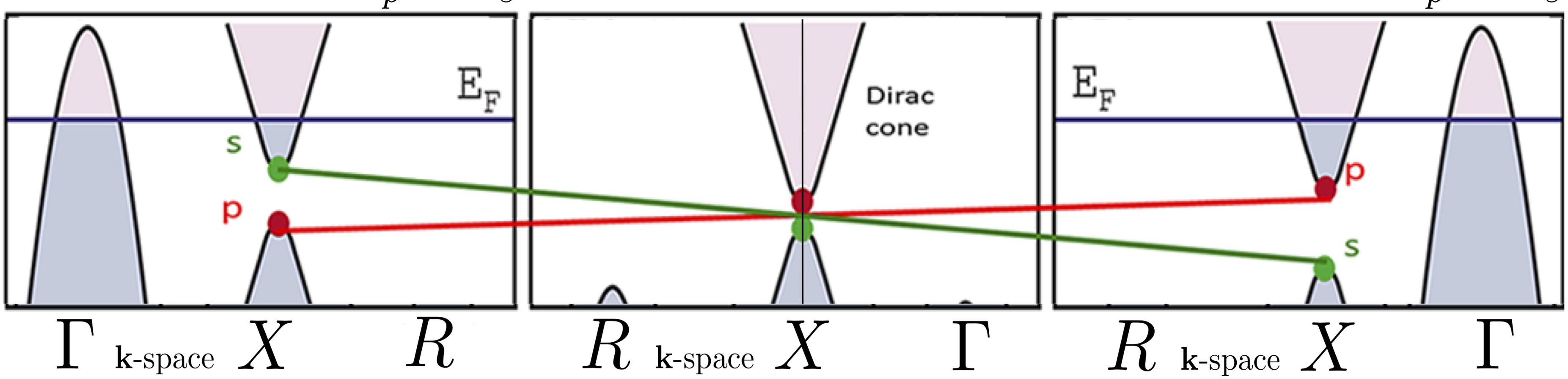
Time Reversal Invariant Momenta (TRIMs)

$$\Gamma_{i=(n_1 n_2 n_3)} = (n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3)/2, \quad \text{with} \quad n_j = 0, \quad 1.$$

(a) **Bulk:** Roto-translational invariant (Noether's theorem) $\rightarrow E^{SOC} < 0 \rightarrow E_p < E_s$

(c) **Surface**: TRIM points (eigenpoints solid-solution disorder operator)

(b) **Interface**: Roto-translational variant (Noether's theorem) $\rightarrow E^{SOC} \sim 0 \rightarrow E_p > E_s$



EXAMPLE

- *Scan the aflowlib.org library*
- *Need of a **DESCRIPTOR (need to grow… epixially).***
- *search for combination of heavy metals (potential strong spin-orbit coupling)*
- *search for ideal band structures with appropriate gaps*
- *calculate band structure with LS (thousand of compounds)*
- *calculate the bands for surfaces to see localized conducting surface stares*
- *usually they contain Bi and/or Sb,Te, Pb.*

nature materials

ARTICLES

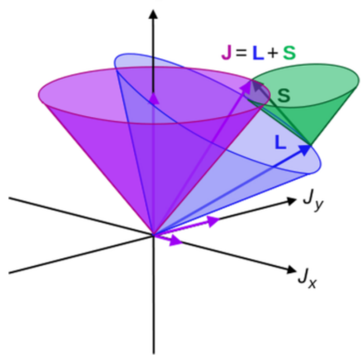
PUBLISHED ONLINE: XX MONTH XXXX | DOI: 10.1038/NMAT3332

A search model for topological insulators with high-throughput robustness descriptors

Kesong Yang[1], Wahyu Setyawan[2], Shidong Wang[1], Marco Buongiorno Nardelli[3,4] and Stefano Curtarolo[1,4,5]★

Nature Materials, ***11****(7), 614-619 (2012) DOI: 10.1038/nmat3332*

Let's precess, epitaxially !



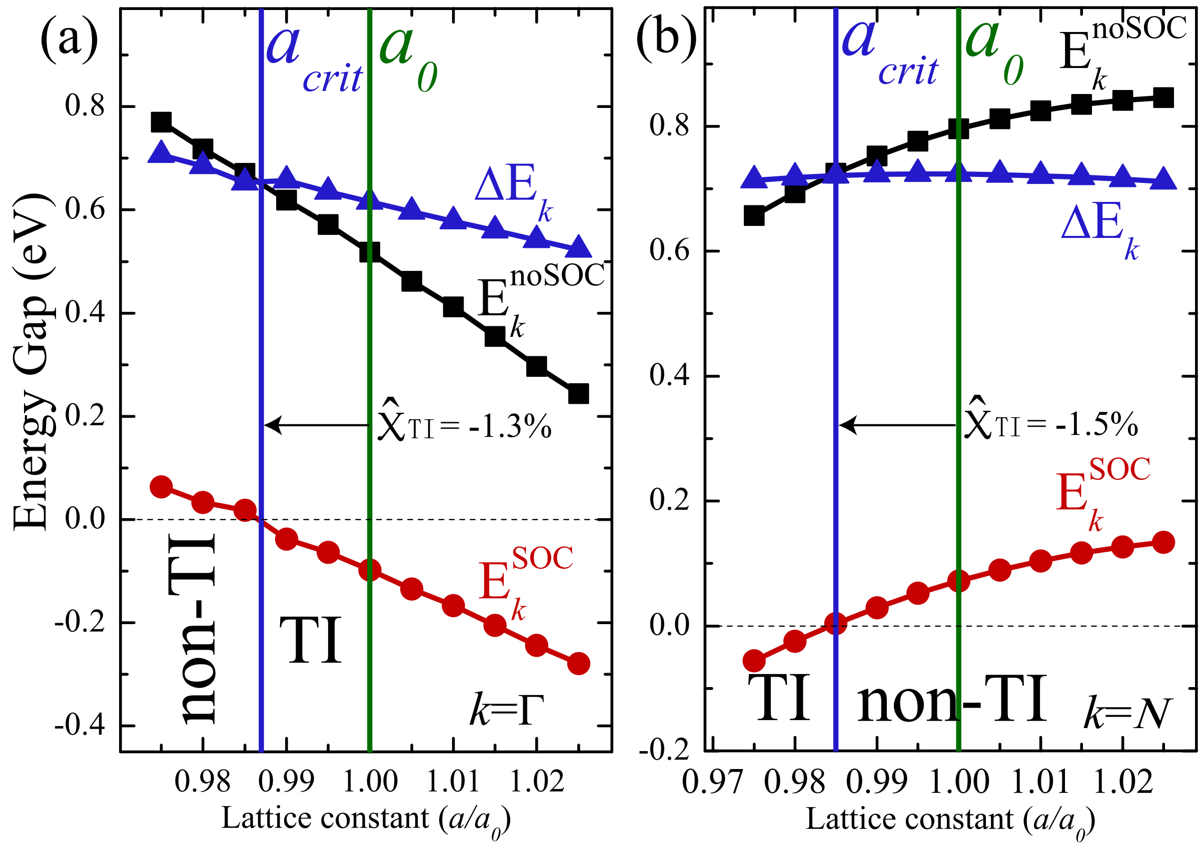
α) SPIN orbit calculations are expensive

β) LS due to electrons precessing near cores

γ) E^{soc}-E^{noSOC} ~ const

δ) simulated epitaxial strain with E^{noSOC}

robustness descriptor varitional ("quasi-meaningful" quantity)

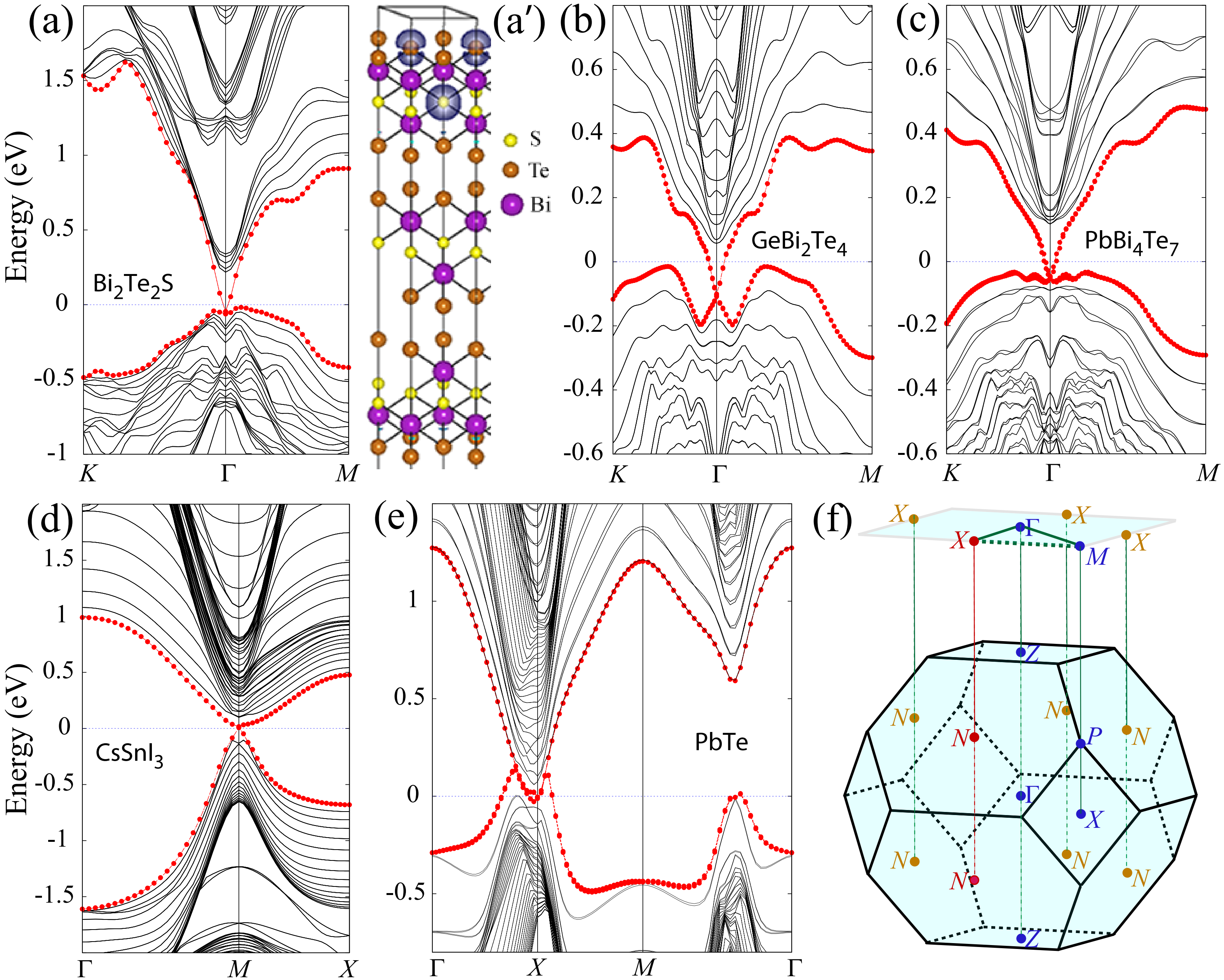


Bi_2Te_2S at $k = \Gamma$ — PbTe at $k = N$

covalent systems — *ionic compounds*

$$\hat{\chi}_{\mathrm{TI}} \equiv -\frac{E_k^{\mathrm{SOC}}(a_0)/a_0}{\delta E_k^{\mathrm{noSOC}}(a)/\delta(a)\big|_{a_0}}$$

top. insul.


(a)
(a′)
(b)
(c)
(d)
(e)
(f)
Energy (eV)
Bi2Te2S
GeBi2Te4
PbBi4Te7
CsSnI3
PbTe
S
Te
Bi
K
Γ
M
X
Z
N
P

top. insul.

New compounds: tern. halides: Cs{Sn,Pb,Ge}{Cl,Br,I}$_3$

Table 1 | Properties of bulk and simulated epitaxial structures.

	Bulk						Simulated epitaxial growth (*a* optimized, *c*/*a* free)									
Compound	Space group	ICSD # ref. 31	Pearson symbol	Latt. ref. 39	Exp. a_0, c_0	DFT a_0, c_0	Pearson symbol	Latt. cleav.	a_{crit} (Å)	E_k^{SOC} 'ref'	Ref. lattice	E_g^{SOC} 'ref'	TRIM (mult.)	ΔE_k @ (a_0, c_0)	E_k^{SOC} @ (a_0, c_0)	$\hat{\chi}_{TI}$ (%)
Sb_2Te_2S	$R\bar{3}m$	–	hR5	rhl_1	–	4.192 31.001	hR5	rhl_1 (0001)	$1.006a_0$ $0.993c_0$	−0.106	$1.019a_0$ $0.975c_0$	0.106 (D)	Γ (1)	0.21	0.043	0.6 PF
Bi_2Te_2S Fig. 2a	$R\bar{3}m$	617050	hR5	rhl_1	4.33 30.07	4.297 31.513	hR5	rhl_1 (0001)	$0.987a_0$ $1.013c_0$	−0.089	a_0 c_0	0.089 (D)	Γ (1)	0.62	−0.089	−1.3 R
$SnSb_2Te_4$	$R\bar{3}m$	30392	hR7	rhl_1	4.312 41.72	4.389 42.347	hR7	rhl_1 (0001)	$0.999a_0$ $0.998c_0$	−0.065	$1.011a_0$ $0.984c_0$	0.065 (D)	Z(1)	0.22	0.013	−0.1 PF
$PbSb_2Te_4$	$R\bar{3}m$	250250	hR7	rhl_1	4.35 41.712	4.413 42.792	hR7	rhl_1 (0001)	$0.988a_0$ $1.011c_0$	−0.017	a_0 c_0	0.017 (D)	Z(1)	0.35	−0.017	−1.2 R
$PbBi_4Se_7$	$P\bar{3}m1$	ref. 49	hP12	hex	4.25 22.68	4.216 23.839	hP12	hex (0001)	$1.018a_0$ $0.971c_0$	−0.016	$1.023a_0$ $0.966c_0$	0.016 (D)	A(1)	0.41	0.128	2.3 PF
$CsSnCl_3$	$Pm\bar{3}m$	28082	cP5	cub	5.504 5.504	5.618 5.618	tP5	tet (001)	$0.951a_0$ $1.022c_0$	−0.281	$0.936a_0$ $1.209c_0$	0.111 (I)	A(1)	0.34	0.646	−4.9 HF
$CsPbCl_3$	$Pm\bar{3}m$	29072	cP5	cub	5.605 5.605	5.733 5.733	tP5	tet (001)	$0.914a_0$ $1.037c_0$	−0.450	$0.890a_0$ $1.050c_0$	0.354 (I)	A(1)	1.11	1.073	−8.6 HF
$CsGeBr_3$	$Pm\bar{3}m$	80320	cP5	cub	5.36 5.36	5.603 5.603	tP5	tet (001)	$0.955a_0$ $1.022c_0$	−0.055	$0.952a_0$ $1.023c_0$	0.026 (I)	A(1)	0.16	0.591	−4.5 HF
$CsSnBr_3$	$Pm\bar{3}m$	4071	cP5	cub	5.795 5.795	5.884 5.884	tP5	tet (001)	$0.972a_0$ $1.010c_0$	−0.099	$0.965a_0$ $1.013c_0$	0.099 (D)	A(1)	0.34	0.288	−2.8 PF
$CsPbBr_3$	$Pm\bar{3}m$	29073	cP5	cub	5.874 5.874	5.993 5.993	tP5	tet (001)	$0.934a_0$ $1.024c_0$	−0.120	$0.926a_0$ $1.027c_0$	0.120 (D)	A(1)	1.11	0.641	−6.6 HF
$CsSnI_3$ Fig. 2d	$Pm\bar{3}m$	69997	cP5	cub	6.219 6.219	6.272 6.272	tP5	tet (001)	$0.993a_0$ $1.002c_0$	−0.335	$0.960a_0$ $1.013c_0$	0.169 (I)	A(1)	0.39	0.070	−0.7 PF
SnTe	$Fm\bar{3}m$	52489	cF8	fcc	4.471 6.323	4.528 6.404	tI4	bct_2 (001)	$1.027a_0$ $0.998c_0$	−0.058	$1.010a_0$ $0.999c_0$	0.058 (D)	N (4)	0.15	−0.107	2.7 VR

Properties of bulk structure: compound (∗ indicates experimental validation), space group, ICSD number[31], Pearson symbol, Bravais lattice[39], experimental and DFT equilibrium lattices a, c in (Å). Properties under the simulated epitaxial growth condition: Pearson symbol, Bravais lattice with conventional cleavage Miller indices, critical value for band inversion (a_{crit}), SOC band energy difference ($E_k^{SOC}(ref.)$) at the TRIM with the reference lattice, reference lattice, SOC band-gap at the reference lattice (direct/indirect) ($E_g^{SOC}(ref.)$), TRIMs having band inversion with multiplicity[39], SOC energy-gap discrepancy (ΔE_k) at the *ab initio* equilibrium lattice, SOC band energy difference ($E_k^{SOC}(a_0)$) at the TRIM with the *ab initio* equilibrium lattice, HT-descriptor ($\hat{\chi}_{TI}$). The labels below $\hat{\chi}_{TI}$ indicate: F(fragile), R(robust), VR(very robust), PF(potentially feasible), and HF(hardly feasible) (structural and electronic data is available by following the links listed in the Supplementary Information Extended Table).

novel ternary halides

if $E_k^{\mathrm{SOC}}(a_0) \leq 0$, **robustness**:
$|\hat{\chi}_{\mathrm{TI}}| \leq 1\% \Rightarrow$ fragile,
$1\% < |\hat{\chi}_{\mathrm{TI}}| \leq 2\% \Rightarrow$ robust,
$2\% < |\hat{\chi}_{\mathrm{TI}}| \Rightarrow$ very-robust.

if $E_k^{\mathrm{SOC}}(a_0) > 0$, **feasibility**:
$|\hat{\chi}_{\mathrm{TI}}| \leq 3\% \Rightarrow$ potentially-feasible,
$3\% < |\hat{\chi}_{\mathrm{TI}}| \Rightarrow$ hardly-feasible.

EXAMPLE: Thermoelectrics

without the constant relaxation time approximation

Table 1 | Examples of descriptors introduced in the literature. Nature Mater. **12**, 191 (2013)

Problem	Combination of materials properties (gene)	Descriptor
Structure stability: convex hull of an alloy system	Formation enthalpy (H_f) as a function of concentration (x) and the enthalpies (H) of A and B.	$H_f(x) = H(A_{1-x}B_x) - (1-x)H(A) - xH(B)$
Phase stability in off-lattice alloys PRL **91**, 135503 (2003)	Spectral decomposition of alloy vector-energies ($E_{n,p}$, n-rows = species, p-columns = configurations) with principal-component-analysis coefficients (α_i) and truncation error ($\epsilon(d)$) (ref. 3).	$E_{n,p} \simeq \alpha_1 E_{n,1} + \cdots + \alpha_{p-1} E_{n,p-1} + \epsilon(d)$
Nanosintered thermoelectrics PRX **1**, 021012 (2011)	Ratio of the average power factor (<P>) to the grain size (L) (ref. 15).	$\hat{\chi}_{\mathrm{thermo}} \equiv \frac{<P>}{L}$
Topological insulators (epitaxial growth) Nature Mater. **11**, 614 (2012)	Variational ratio of spin–orbit distortion versus non-spin-orbit derivative strain (E_k^{SOC}, E_k^{noSOC}, spin/no spin-orbit bandgaps at k, a_0 lattice)[16].	$\hat{\chi}_{\mathrm{TI}} \equiv - \frac{E_k^{\mathrm{SOC}}(a_0)/a_0}{\delta E_k^{\mathrm{noSOC}}(a)_0/\delta a_0 \vert_{a_0}}$
Power conversion efficiency of a solar cell (spectroscopic limited maximum efficiency) PRL **108**, 068701 (2012)	Ratio of the maximum output power density (P_m) to the incident solar energy density (P_{in}) — a function (η) of the radiative electron–hole recombination current (f_r) and the photon absorptivity ($\alpha(E)$) — versus bandgap energy (E_g)[62].	$\eta(\alpha(E), f_r) = P_m/P_{in}; E_g$
Non-proportionality in scintillators IEEE Trans. Nucl. Sci. **56**, 2989 (2009)	Maximum mismatch between effective masses of electrons (m_e) and holes (m_h)[75].	$\hat{\chi}_{np} \equiv \max\left(\frac{m_e}{m_h}, \frac{m_h}{m_e}\right)$
Morphotropic phase boundary piezoelectrics PRB **84**, 014103 (2011)	Energy proximity between tetragonal, rhombohedra and rotational distortions (ΔE_p). Angular coordinate (α_{AB}) of the energy minimum in the A–B off-centerings energy map for ABO_3 systems[79].	$\Delta E_p \le 0.5$ eV $\alpha_{AB} \approx 45°$

EXAMPLE: Thermoelectricity

Thermoelectrics: convert flow of electronic entropy in electronic current

$$ZT = \frac{\sigma S^2 T}{\kappa}$$

$$P = \sigma S^2$$

$$ZT > 1 \Rightarrow S > 156\mu\mathrm{V/K}$$

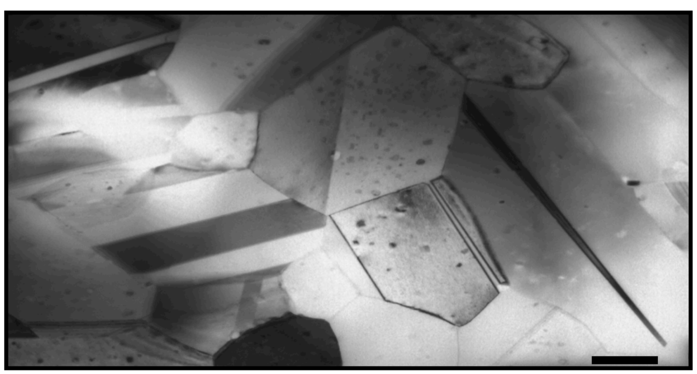
from Wiedemann-Franz law (room T)

constant or decrease less than k

must increase

$$ZT = \frac{\sigma S^2 T}{\kappa}$$

must decrease



sintering
polycrystalline

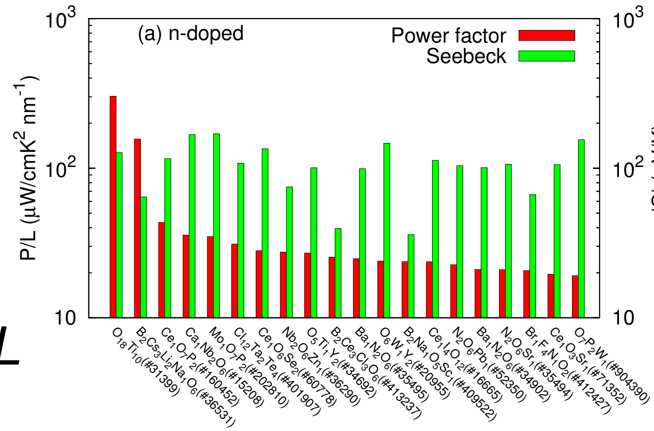
Bi_2Te_3

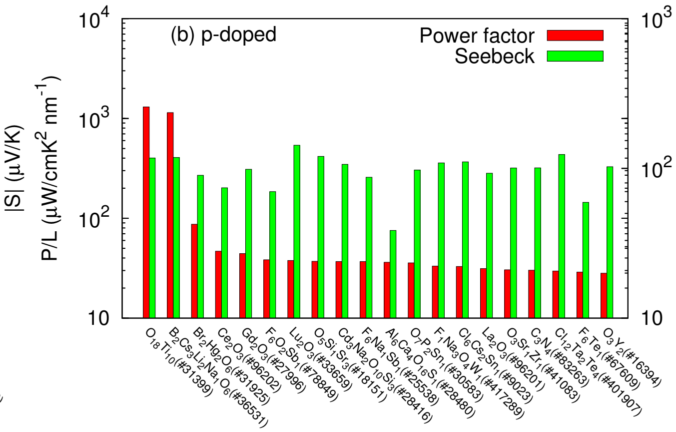
Courtesy: G. Bernard-Granger, LITEN, CEA-Grenoble.

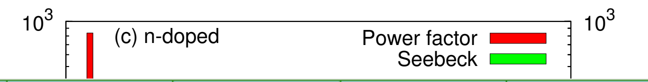
power factor

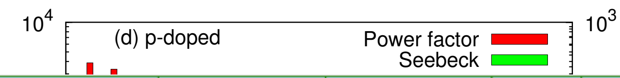
For sintered, depends on directions, project on principal axes

$X_{thermo}=\langle P\rangle/L$



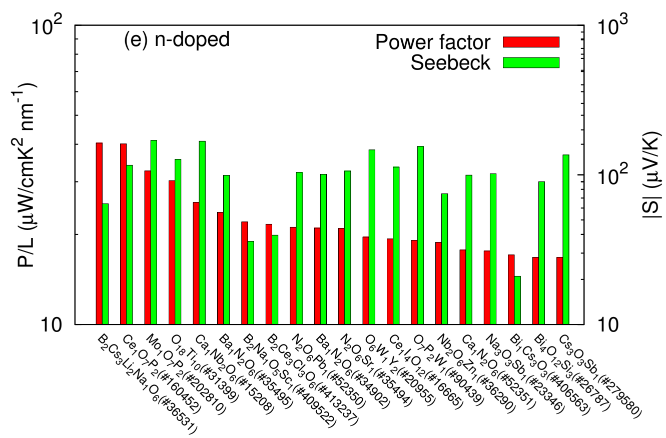


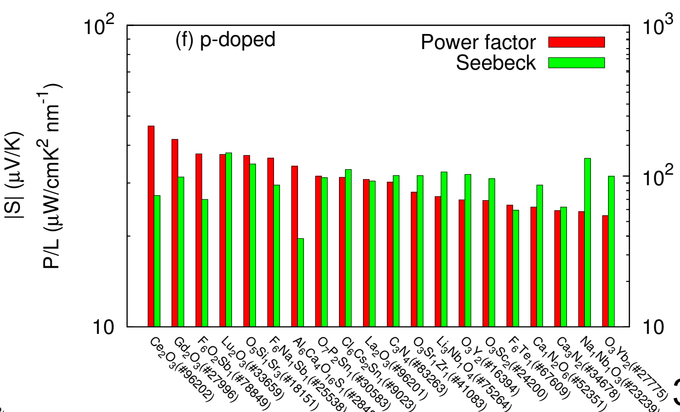




▲Name [1]	ICSD Number [1]	Bravais Lattice	Number of Atoms	$\langle P_n\rangle/L$ (μW/cmK²nm) [4]	$\langle P_{n1}\rangle/L$ (μW/cmK²nm) [4]	$\langle P_{n2}\rangle/L$ (μW/cmK²nm) [4]	$\langle P_{n3}\rangle/L$ (μW/cmK²nm) [4]	$\langle P_p\rangle/L$ (μW/cmK²nm) [4]	$\langle P_{p1}\rangle/L$ (μW/cmK²nm) [4]	$\langle P_{p2}\rangle/L$ (μW/cmK²nm) [4]	$\langle P_{p3}\rangle/L$ (μW/cmK²nm) [4]	S_n (μV/K) [4]	S_p (μV/K) [4]
$F_3Fe_1K_1$	15424	CUB (Cubic)	5	0.15	0.15	0.15	0.15	2.17	2.17	2.17	2.17	-116.36	91.29
$F_3Fe_1Rb_1$	49586	CUB (Cubic)	5	0.24	0.24	0.24	0.24	1.50	1.48	1.51	1.51	-91.73	91.04
$Fe_1La_1O_3$	29118	CUB (Cubic)	5	0.31	0.31	0.31	0.31	2.00	2.00	2.00	2.00	-139.02	92.92

max P_i/L





PRX **1**, 021012 (2011)

High-Throughput Materials Exploration

AgAl, AgAs, AgAu, AgB, AgBi, AgCd, AgCo, AgCr, AgCu, AgFe, AgGa, AgGe, AgHf, AgHg, AgIn, AgIr, AgLa, AgMg, AgMn, AgMo, AgNb, AgNi, AgOs, AgP, AgPb, AgPd, AgPt, AgRe, AgRh, AgRu, AgSb, AgSc, AgSe, AgSi, AgSn, AgTa, AgTc, AgTe, AgTi, AgV, AgW, AgY, AgZn, AgZr, AlAs, AlAu, AlB, AlBi, AlCd, AlCo, AlCr, AlCu, AlFe, AlGa, AlGe, AlCo, AlHf, AlHg, AlHf, AlPd, AlPt, AlSc, AlIn, AlIr, AlLa, AlMg, AlMn, AlMo, AlNb, AlNi, AlOs, AlP, AlPb, AlPd, AlPt, AlRe, AlRh, AlRu, AlSb, AlSc, AlSe, AlSi, AlSn, AlTa, AlTc, AlTe, AlTi, AlV, AlW, AlY, AlZn, AlZr, AsAu, AsB, AsBi, AsCd, AsCo, AsCr, AsCu, AsFe, AsGa, AsGe, AsHf, AsHg, AsIn, AsIr, AsLa, AsMg, AsMn, AsMo, AsNb, AsNi, AsOs, AsP, AsPb, AsPd, AsPt, AsRe, AsRh, AsRu, AsSb, AsSc, AsSe, AsSi, AsSn, AsTa, AsTc, AsTe, AsTi, AsV, AsW, AsY, AsZn, AsZr, AuB, AuBi, AuCd, AuCo, AuCr, AuCu, AuFe, AuGa, AuGe, AuHf, AuHg, AuIn, AuIr, AuLa, AuMg, AuMn, AuMo, AuNb, AuNi, AuOs, AuP, AuPb, AuPd, AuPt, AuRe, AuRh, AuRu, AuSb, AuSc, AuSe, AuSi, AuSn, AuTa, AuTc, AuTe, AuTi, AuV, AuW, AuY, AuZn, AuZr, BaHf, BaMg, BaPd, BaPt, BeHf, BeCd, BeCo, BeMg, BeMn, BeOs, BePd, BePt, BeRe, BeRh, BeRu, BeSc, BeTc, BeTi, BeTl, BeY, BeZn, BeZr, BBi, BCd, BCo, BCr, BCu, BFe, BGa, BGe, BHf, BHg, BIn, BIr, BLa, BMg, BMn, BMo, BNb, BNi, BOs, BP, BPb, BPd, BPt, BRe, BRh, BRu, BSb, BSc, BSe, BSi, BSn, BTa, BTc, BTe, BTi, BV, BW, BY, BZn, BZr, BiCd, BiCo, BiCr, BiCu, BiFe, BiGa, BiGe, BiHf, BiHg, BiIn, BiIr, BiLa, BiMg, BiMn, BiMo, BiNb, BiNi, BiOs, BiP, BiPb, BiPd, BiPt, BiRe, BiRh, BiRu, BiSb, BiSc, BiSe, BiSi, BiSn, BiTa, BiTc, BiTe, BiTi, BiV, BiW, BiY, BiZn, BiZr, BHf, CaHf, CaMg, CaPd, CaPt, CdCo, CdCr, CdCu, CdFe, CdGa, CdGe, CdHf, CdHg, CdIn, CdIr, CdLa, CdMg, CdMn, CdMo, CdNb, CdNi, CdOs, CdP, CdPb, CdPd, CdPt, CdRe, CdRh, CdRu, CdSb, CdSc, CdSe, CdSi, CdSn, CdTa, CdTc, CdTe, CdTi, CdTl, CdV, CdW, CdY, CdZn, CdZr, CeMg, CNi, CoCr, CoCu, CoFe, CoGa, CoGe, CoHf, CoHg, CoIn, CoIr, CoLa, CoMg, CoMn, CoMo, CoNb, CoNi, CoOs, CoP, CoPb, CoPd, CoPt, CoRe, CoRh, CoRu, CoSb, CoSc, CoSe, CoSi, CoSn, CoTa, CoTc, CoTe, CoTi, CoTl, CoV, CoW, CoY, CoZn, CoZr, CrCu, CrFe, CrGa, CrGe, CrHf, CrHg, CrIn, CrIr, CrLa, CrMg, CrMn, CrMo, CrNb, CrNi, CrOs, CrP, CrPb, CrPd, CrPt, CrRe, CrRh, CrRu, CrSb, CrSc, CrSe, CrSi, CrSn, CrTa, CrTc, CrTe, CrTi, CrV, CrW, CrY, CrZn, CrZr, CsPd, CuFe, CuGa, CuGe, CuHf, CuHg, CuIn, CuIr, CuLa, CuMg, CuMn, CuMo, CuNb, CuNi, CuOs, CuP, CuPb, CuPd, CuPt, CuRe, CuRh, CuRu, CuSb, CuSc, CuSe, CuSi, CuSn, CuTa, CuTc, CuTe, CuTi, CuV, CuW, CuY, CuZn, CuZr, FeGa, FeGe, FeHf, FeHg, FeIn, FeIr, FeLa, FeMg, FeMn, FeMo, FeNb, FeNi, FeOs, FeP, FePb, FePd, FePt, FeRe, FeRh, FeRu, FeSb, FeSc, FeSe, FeSi, FeSn, FeTa, FeTc, FeTe, FeTi, FeV, FeW, FeY, FeZn, FeZr, GaGe, GaHf, GaHg, GaIn, GaIr, GaLa, GaMg, GaMn, GaMo, GaNb, GaNi, GaOs, GaP, GaPb, GaPd, GaPt, GaRe, GaRh, GaRu, GaSb, GaSc, GaSe, GaSi, GaSn, GaTa, GaTc, GaTe, GaTi, GaV, GaW, GaY, GaZn, GaZr, GaMg, GdMg, GeHf, GeHg, GeIn, GeIr, GeLa, GeMg, GeMn, GeMo, GeNb, GeNi, GeOs, GeP, GePb, GePd, 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SrPd, SrPt, TaMg, TaTc, TaTe, TaTi, TaV, TaW, TaY, TaZn, TaZr, TcTe, TcTi, TcTl, TcV, TcW, TcY, TcZn, TcZr, TeTi, TeV, TeW, TeY, TeZn, TeZr, TiMg, TiTl, TiV, TiW, TiY, TiZn, TiZr, TlY, TlZn, TlZr, VMg, VW, VY, VZn, VZr, WMg, WY, WZn, WZr, YMg, YZn, YZr, ZnMg, ZnZr, ZrMg

High-Throughput Materials Exploration

AgAl, AgAs, AgAu, AgB, AgBi, AgCd, AgCo, AgCr, AgCu, AgFe, AgGa, AgGe, AgHf, AgHg, AgIn, AgIr, AgLa, AgMg, AgMn, AgMo, AgNb, AgNi, AgOs, AgP, AgPb, AgPd, AgPt, AgRe, AgRh, AgRu, AgSb, AgSc, AgSe, AgSi, AgSn, AgTa, AgTc, AgTe, AgTi, AgV, AgW, AgY, AgZn, AgZr, AlAs, AlAu, AlB, AlBi, AlCd, AlCo, AlCr, AlCu, AlFe, AlGa, AlGe, AlCo, AlHf, AlHg, AlHf, AlPd, AlPt, AlSc, AlIn, AlIr, AlLa, AlMg, AlMn, AlMo, AlNb, AlNi, AlOs, AlP, AlPb, AlPd, AlPt, AlRe, AlRh, AlRu, AlSb, AlSc, AlSe, AlSi, AlSn, AlTa, AlTc, AlTe, AlTi, AlV, AlW, AlY, AlZn, AlZr, AsAu, AsB, AsBi, AsCd, AsCo, AsCr, AsCu, AsFe, AsGa, AsGe, AsHf, AsHg, AsIn, AsIr, AsLa, AsMg, AsMn, AsMo, AsNb, AsNi, AsOs, AsP, AsPb, AsPd, AsPt, AsRe, AsRh, AsRu, AsSb, AsSc, AsSe, AsSi, AsSn, AsTa, AsTc, AsTe, AsTi, AsV, AsW, AsY, AsZn, AsZr, AuB, AuBi, AuCd, AuCo, AuCr, AuCu, AuFe, AuGa, AuGe, AuHf, AuHg, AuIn, AuIr, AuLa, AuMg, AuMn, AuMo, AuNb, AuNi, AuOs, AuP, AuPb, AuPd, AuPt, AuRe, AuRh, AuRu, AuSb, AuSc, AuSe, AuSi, AuSn, AuTa, AuTc, AuTe, AuTi, AuV, AuW, AuY, AuZn, AuZr, BaHf, BaMg, BaPd, BaPt, BeHf, BeCd, BeCo, BeMg, BeMn, BeOs, BePd, BePt, BeRe, BeRh, BeRu, BeSc, BeTc, BeTi, BeTl, BeY, BeZn, BeZr, BBi, BCd, BCo, BCr, BCu, BFe, BGa, BGe, BHf, BHg, BIn, BIr, BLa, BMg, BMn, BMo, BNb, BNi, BOs, BP, BPb, BPd, BPt, BRe, BRh, BRu, BSb, BSc, BSe, BSi, BSn, BTa, BTc, BTe, BTi, BV, BW, BY, BZn, BZr, BiCd, BiCo, BiCr, BiCu, BiFe, BiGa, BiGe, BiHf, BiHg, BiIn, BiIr, BiLa, BiMg, BiMn, BiMo, BiNb, BiNi, BiOs, BiP, BiPb, BiPd, BiPt, BiRe, BiRh, BiRu, BiSb, BiSc, BiSe, BiSi, BiSn, BiTa, BiTc, BiTe, BiTi, BiV, BiW, BiY, BiZn, BiZr, BHf, CaHf, CaMg, CaPd, CaPt, CdCo, CdCr, CdCu, CdFe, CdGa, CdGe, CdHf, CdHg, CdIn, CdIr, CdLa, CdMg, CdMn, CdMo, CdNb, CdNi, CdOs, CdP, CdPb, CdPd, CdPt, CdRe, CdRh, CdRu, CdSb, CdSc, CdSe, CdSi, CdSn, CdTa, CdTc, CdTe, CdTi, CdTl, CdV, CdW, CdY, CdZn, CdZr, CeMg, CNi, CoCr, CoCu, CoFe, CoGa, CoGe, CoHf, CoHg, CoIn, CoIr, CoLa, CoMg, CoMn, CoMo, CoNb, CoNi, CoOs, CoP, CoPb, CoPd, CoPt, CoRe, CoRh, CoRu, CoSb, CoSc, CoSe, CoSi, CoSn, CoTa, CoTc, CoTe, CoTi, CoTl, CoV, CoW, CoY, CoZn, CoZr, CrCu, CrFe, CrGa, CrGe, CrHf, CrHg, CrIn, CrIr, CrLa, CrMg, CrMn, CrMo, CrNb, CrNi, CrOs, CrP, CrPb, CrPd, CrPt, CrRe, CrRh, CrRu, CrSb, CrSc, CrSe, CrSi, CrSn, CrTa, CrTc, CrTe, CrTi, CrV, CrW, CrY, CrZn, CrZr, CsPd, CuFe, CuGa, CuGe, CuHf, CuHg, CuIn, CuIr, CuLa, CuMg, CuMn, CuMo, CuNb, CuNi, CuOs, CuP, CuPb, CuPd, CuPt, CuRe, CuRh, CuRu, CuSb, CuSc, CuSe, CuSi, CuSn, CuTa, CuTc, CuTe, CuTi, CuV, CuW, CuY, CuZn, CuZr, FeGa, FeGe, FeHf, FeHg, FeIn, FeIr, FeLa, FeMg, FeMn, FeMo, FeNb, FeNi, FeOs, FeP, FePb, FePd, FePt, FeRe, FeRh, FeRu, FeSb, FeSc, FeSe, FeSi, FeSn, FeTa, FeTc, FeTe, FeTi, FeV, FeW, FeY, FeZn, FeZr, GaGe, GaHf, GaHg, GaIn, GaIr, GaLa, GaMg, GaMn, GaMo, GaNb, GaNi, GaOs, GaP, GaPb, GaPd, GaPt, GaRe, GaRh, GaRu, GaSb, GaSc, GaSe, GaSi, GaSn, GaTa, GaTc, GaTe, GaTi, GaV, GaW, GaY, GaZn, GaZr, GaMg, GdMg, GeHf, GeHg, GeIn, GeIr, GeLa, GeMg, GeMn, GeMo, GeNb, GeNi, GeOs, GeP, GePb, GePd, GePt, GeRe, GeRh, GeRu, GeSb, GeSc, GeSe, GeSi, GeSn, GeTa, GeTc, GeTe, GeTi, GeV, GeW, GeY, GeZn, GeZr, GeMg, HfHg, HfIn, HfIr, HfK, HfLa, HfLi, HfMg, HfMn, HfMo, HfNa, HfNb, HfNi, HfOs, HfP, HfPb, HfPd, HfPt, HfRe, HfRh, HfRu, HfSb, HfSc, HfSe, HfSi, HfSn, HfSn, HfSr, HfTa, HfTc, HfTe, HfTi, HfTl, HfV, HfW, HfY, HfZn, HfZr, HgIn, HgIr, HgLa, HgMg, HgMn, HgMo, HgNb, HgNi, HgOs, HgP, HgPb, HgPd, HgPt, HgRe, HgRh, HgRu, HgSb, HgSc, HgSe, HgSi, HgSn, HgTa, HgTc, HgTe, HgTi, HgV, HgW, HgY, HgZn, HgZr, InIr, InLa, InMg, InMn, InMo, InNb, InNi, InOs, InP, InPb, InPd, InPt, InRe, InRh, InRu, InSb, InSc, InSe, InSi, InSn, InTa, InTc, InTe, InTi, InV, InW, InY, InZn, InZr, IrLa, IrMg, IrMn, IrMo, IrNb, IrNi, IrOs, IrP, IrPb, IrPd, IrPt, IrRe, IrRh, IrRu, IrSb, IrSc, IrSe, IrSi, IrSn, IrTa, IrTc, IrTe, IrTi, IrV, IrW, IrY, IrZn, IrZr, KMg, KPd, KPt, LaMg, LaMn, LaMo, LaNb, LaNi, LaOs, LaP, LaPb, LaPd, LaPt, LaRe, LaRh, LaRu, LaSb, LaSc, LaSe, LaSi, LaSn, LaTa, LaTc, LaTe, LaTi, LaV, LaW, LaY, LaZn, LaZr, list, LiMg, LiPd, LiPt, MgMn, MgMo, MgNb, MgNi, MgOs, MgP, MgPb, MgPd, MgPt, MgRe, MgRh, MgRu, MgSb, MgSc, MgSe, MgSi, MgSn, MgTa, MgTc, MgTe, MgTi, MgTl, MgV, MgW, MgY, MgZn, MgZr, MnMo, MnNb, MnNi, MnOs, MnP, MnPb, MnPd, MnPt, MnRe, MnRh, MnRu, MnSb, MnSc, MnSe, MnSi, MnSn, MnTa, MnTc, MnTe, MnTi, MnV, MnW, MnY, MnZn, MnZr, MoMg, MoNb, MoNi, MoOs, MoP, MoPb, MoPd, MoPt, MoRe, MoRh, MoRu, MoSb, MoSc, MoSe, MoSi, MoSn, MoTa, MoTc, MoTe, MoTi, MoV, MoW, MoY, MoZn, MoZr, NaMg, NaPd, NaPt, NbMg, NbNi, NbOs, NbP, NbPb, NbPd, NbPt, NbRe, NbRh, NbRu, NbSb, NbSc, NbSe, NbSi, NbSn, NbTa, NbTc, NbTe, NbTi, NbV, NbW, NbY, NbZn, NbZr, NiOs, NiP, NiPb, NiPd, NiPt, NiRe, NiRh, NiRu, NiSb, NiSc, NiSe, NiSi, NiSn, NiTa, NiTc, NiTe, NiTi, NiV, NiW, NiY, NiZn, NiZr, OsMg, OsP, OsPb, OsPd, OsPt, OsRe, OsRh, OsRu, OsSb, OsSc, OsSe, OsSi, OsSn, OsTa, OsTc, OsTe, OsTi, OsTl, OsV, OsW, OsY, OsZn, OsZr, PbMg, PbPd, PbPt, PbRe, PbRh, PbRu, PbSb, PbSc, PbSe, PbSi, PbSn, PbTa, PbTc, PbTe, PbTi, PbV, PbW, PbY, PbZn, PbZr, PdPt, PdRe, PdRh, PdRu, PdSb, PdSc, PdSe, PdSi, PdSn, PdTa, PdTc, PdTe, PdTi, PdV, PdW, PdY, PdZn, PdZr, PPb, PPd, PPt, PRe, PRh, PRu, PSb, PSc, PSe, PSi, PSn, PT
PtW, PtY, PtZn, PtZr, PV, PW, PY, PZn, PZr, RbMg, RbPd, RbPt, ReMg, ReRh, Re
ReZr, RhMg, RhRu, RhSb, RhSc, RhSe, RhSi, RhSn, RhTa, RhTc, RhTe, RhTi, Rh
RuTi, RuTl, RuV, RuW, RuY, RuZn, RuZr, SbSc, SbSe, SbSi, SbSn, SbTa, SbTc, Sb
ScV, ScW, ScY, ScZn, ScZr, SeSi, SeSn, SeTa, SeTc, SeTe, SeTi, SeV, SeW, SeY, Se
SnTa, SnTc, SnTe, SnTi, SnV, SnW, SnY, SnZn, SnZr, SrMg, SrPd, SrPt, TaMg, TaTc,
TeW, TeY, TeZn, TeZr, TiMg, TiTl, TiV, TiW, TiY, TiZn, TiZr, TlY, TlZn, TlZr, VMg, VW,

S. Curtarolo, O. Levy, W. Setyawan,
I. Takeuchi, A. Kolmogorov, S. Wang,
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R. Taylor, Z. Wang, K. Yang, N. Mingo, S. Sanvito

High-Throughput Materials Exploration

AgAl, AgAs, AgAu, AgB, AgBi, AgCd, AgCo, AgCr, AgCu, AgFe, AgGa, AgGe, AgHf, AgHg, AgIn, AgIr, AgLa, AgMg, AgMn, AgMo, AgNb, AgNi, AgOs, AgP, AgPb, AgPd, AgPt,
AgRe, AgRh, AgRu, AgSb, AgSc, AgSe, AgSi, … Cd, AlCo, AlCr, AlCu, AlFe, AlGa, AlGe, AlCo,
AlHf, AlHg, AlHf, AlPd, AlPt, AlSc, AlIn, All … AlSb, AlSc, AlSe, AlSi, AlSn, AlTa, AlTc, AlTe,
AlTi, AlV, AlW, AlY, AlZn, AlZr, AsAu, AsB … AsMg, AsMn, AsMo, AsNb, AsNi, AsOs, AsP,
AsPb, AsPd, AsPt, AsRe, AsRh, AsRu, AsSb … uBi, AuCd, AuCo, AuCr, AuCu, AuFe, AuGa,
AuGe, AuHf, AuHg, AuIn, AuIr, AuLa, AuM … b, AuSc, AuSe, AuSi, AuSn, AuTa, AuTc, AuTe,
AuTi, AuV, AuW, AuY, AuZn, AuZr, BaHf, … h, BeRu, BeSc, BeTc, BeTi, BeTl, BeY, BeZn,
BeZr, BBi, BCd, BCo, BCr, BCu, BFe, BGa … BRe, BRh, BRu, BSb, BSc, BSe, BSi, BSn, BTa,
BTc, BTe, BTi, BV, BW, BY, BZn, BZr, BiC … BiNb, BiNi, BiOs, BiP, BiPb, BiPd, BiPt, BiRe,
BiRh, BiRu, BiSb, BiSc, BiSe, BiSi, BiSn, Bi … o, CdCr, CdCu, CdFe, CdGa, CdGe, CdHf,
CdHg, CdIn, CdIr, CdLa, CdMg, CdMn, C … dSc, CdSe, CdSi, CdSn, CdTa, CdTc, CdTe,
CdTi, CdTl, CdV, CdW, CdY, CdZn, CdZr, CeMg, CNi, CoCr, CoCu, CoFe, CoGa, CoGe, CoHf, CoHg, CoIn, CoIr, CoLa, CoMg, CoMn, CoMo, CoNb, CoNi, CoOs,
CoP, CoPb, CoPd, CoPt, CoRe, CoRh, CoRu, CoSb, CoSc, CoSe, CoSi, CoSn, CoTa, CoTc, CoTe, CoTi, CoTl, CoV, CoW, CoY, CoZn, CoZr, CrCu, CrFe, CrGa,
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GeSc, GeSe, GeSi, GeSn, GeTa, GeTc, GeTe, GeTi, GeV, GeW, GeY, GeZn, GeZr, GeMg, HfHg, HfIn, HfIr, HfK, HfLa, HfLi, HfMg, HfMn, HfMo, HfNa, HfNb, HfNi, HfOs,
HfP, HfPb, HfPd, HfPt, HfRe, HfRh, HfRu, HfSb, HfSc, HfSe, HfSi, HfSn, HfSn, HfSr, HfTa, HfTc, HfTe, HfTi, HfTl, HfV, HfW, HfY, HfZn, HfZr, HgIn, HgIr, HgLa, HgMg,
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InIr, InLa, InMg, InMn, InMo, InNb, InNi, InOs, InP, InPb, InPd, InPt, InRe, InRh, InRu, InSb, InSc, InSe, InSi, InSn, InTa, InTc, InTe, InTi, InV, InW, InY, InZn, InZr, IrLa, IrMg,
IrMn, IrMo, IrNb, IrNi, IrOs, IrP, IrPb, IrPd, IrPt, IrRe, IrRh, IrRu, IrSb, IrSc, IrSe, IrSi, IrSn, IrTa, IrTc, IrTe, IrTi, IrV, IrW, IrY, IrZn, IrZr, KMg, KPd, KPt, LaMg, LaMn, LaMo,
LaNb, LaNi, LaOs, LaP, LaPb, LaPd, LaPt, LaRe, LaRh, LaRu, LaSb, LaSc, LaSe, LaSi, LaSn, LaTa, LaTc, LaTe, LaTi, LaV, LaW, LaY, LaZn, LaZr, list, LiMg, LiPd, LiPt, MgMn,
MgMo, MgNb, MgNi, MgOs, MgP, MgPb, MgPd, MgPt, MgRe, MgRh, MgRu, MgSb, MgSc, MgSe, MgSi, MgSn, MgTa, MgTc, MgTe, MgTi, MgTl, MgV, MgW, MgY, MgZn, MgZr,
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NbY, NbZn, NbZr, NiOs, NiP, NiPb, NiPd, NiPt, NiRe, NiRh, NiRu, NiSb, NiSc, NiSe, NiSi, NiSn, NiTa, NiTc, NiTe, NiTi, NiV, NiW, NiY, NiZn, NiZr, OsMg, OsP, OsPb,
OsPd, OsPt, OsRe, OsRh, OsRu, OsSb, OsSc, OsSe, OsSi, OsSn, OsTa, OsTc, OsTe, OsTi, OsTl, OsV, OsW, OsY, OsZn, OsZr, PbMg, PbPd, PbPt, PbRe, PbRh, PbRu,
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PdW, PdY, PdZn, PdZr, PPb, PPd, PPt, PRe, PRh, PRu, PSb, PSc, PSe, PSi, PSn, PT
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TeW, TeY, TeZn, TeZr, TiMg, TiTl, TiV, TiW, TiY, TiZn, TiZr, TlY, TlZn, TlZr, VMg, VW,

~1300 systems and counting
~170,000 calculations
~100 million cpu hours

S. Curtarolo, O. Levy, W. Setyawan,
I. Takeuchi, A. Kolmogorov, S. Wang,
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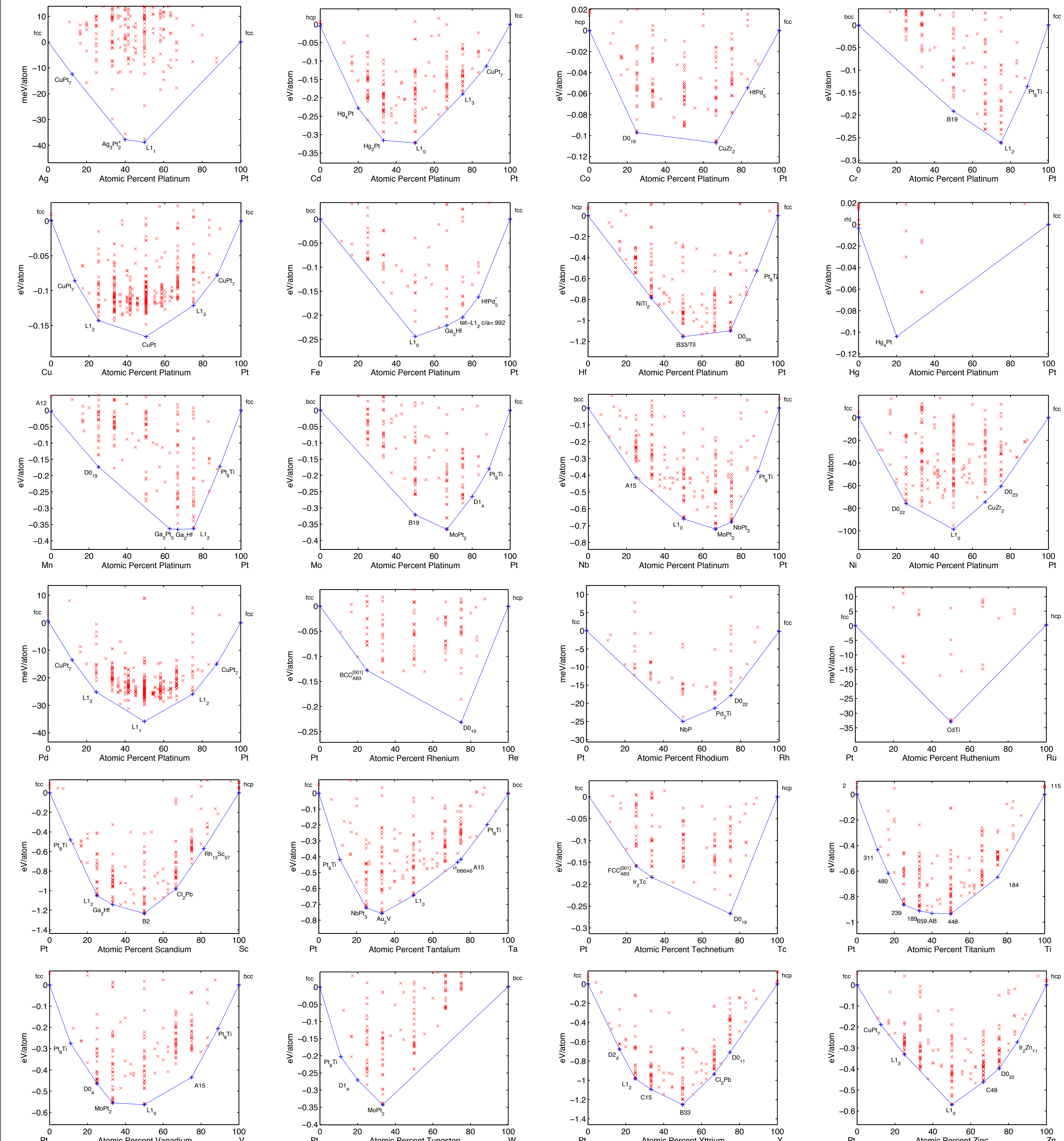

	Os	Ru	Ir	Rh	Pt	Pd
Y			B2	B2	B27 B33	? B33
Sc		B2	B2	B2	B2	B2
Zr	B2	B2	NiTi	NiTi B33	TlI B33	? B33
Hf	B2	B2	? B27	B2 B27	B33	? B33
Ti	B2	B2	? $L1_0$	? $L1_0$	B19 NiTi	B19 —
Nb		? —	$L1_0$	$L1_0$	B19 $L1_0$	
Ta		? —	$L1_0$	IrTa —	— $L1_0$	B11
V		B11 —	$L1_0$	$L1_0$	B19 $L1_0$	? —
Mo			B19	B19	B19	
W			B19		? —	
Cr			— B19		$L1_0$ B19	
Tc	$\overline{\text{B19}}$	$\overline{\text{B19}}$	$\overline{\text{B19}}$	$\overline{\text{B19}}$		$\overline{\text{RhRu*}}$
Re	$\overline{\text{B19}}$	$\overline{\text{B19}}$	$\overline{\text{B19}}$	$\overline{\text{B19}}$		
Mn	$\overline{\text{B19}}$		$L1_0$ B19	B2	$L1_0$ —	$L1_0$ —
Fe			— NbP	B2 —	$L1_0$	
Os		$\overline{\text{B19}}$		$\overline{\text{RhRu*}}$		
Ru	$\overline{\text{B19}}$		$\overline{\text{B19}}$	$\overline{\text{RhRu*}}$	$\overline{\text{CdTi}}$	
Co					$L1_0$ —	
Ir		$\overline{\text{B19}}$		$\overline{\text{W2}}$		
Rh	$\overline{\text{RhRu*}}$	$\overline{\text{RhRu*}}$	$\overline{\text{W2}}$		— NbP	
Ni			— NbP		$L1_0$	
Pt		$\overline{\text{CdTi}}$		— NbP		$\overline{L1_1}$
Pd					$\overline{L1_1}$	
Au						? NbP
Ag					? $L1_1$	$\overline{L1_1}$
Cu					$L1_1$	? B2
Hg						$L1_0$
Cd					$L1_0$	CuTi $L1_0$
Zn			$\overline{\text{IrZn}^{\dagger}}$	$\overline{\text{B2}}$	$L1_0$	CuTi $L1_0$

High-Throughput Materials Exploration

AgAl, AgAs, AgAu, AgB, AgBi, AgCd, AgCo, AgCr, AgCu, AgFe, AgGa, AgGe, AgHf, AgHg, AgIn, AgIr, AgLa, AgMg, AgMn, AgMo, AgNb, AgNi, AgOs, AgP, AgPb, AgPd, AgPt, AgRe, AgRh, AgRu, AgSb, AgSc, AgSe, AgSi, AgSn, AgTa, AgTc, AgTe, AgTi, AgV, AgW, AgY, AgZn, AgZr, AlAs, AlAu, AlB, AlBi, AlCd, AlCo, AlCr, AlCu, AlFe, AlGa, AlGe, AlCo, AlHf, AlHg, AlHf, AlPd, AlPt, AlSc, AlIn, AlIr, AlLa, AlMg, AlMn, AlMo, AlNb, AlNi, AlOs, AlP, AlPb, AlPd, AlPt, AlRe, AlRh, AlRu, AlSb, AlSc, AlSe, AlSi, AlSn, AlTa, AlTc, AlTe, AlTi, AlV, AlW, AlY, AlZn, AlZr, AsAu, AsB, AsBi, AsCd, AsCo, AsCr, AsCu, AsFe, AsGa, AsGe, AsHf, AsHg, AsIn, AsIr, AsLa, AsMg, AsMn, AsMo, AsNb, AsNi, AsOs, AsP, AsPb, AsPd, AsPt, AsRe, AsRh, AsRu, AsSb, AsSc, AsSe, AsSi, AsSn, AsTa, AsTc, AsTe, AsTi, AsV, AsW, AsY, AsZn, AsZr, AuB, AuBi, AuCd, AuCo, AuCr, AuCu, AuFe, AuGa, AuGe, AuHf, AuHg, AuIn, AuIr, AuLa, AuMg, AuMn, AuMo, AuNb, AuNi, AuOs, AuP, AuPb, AuPd, AuPt, AuRe, AuRh, AuRu, AuSb, AuSc, AuSe, AuSi, AuSn, AuTa, AuTc, AuTe, AuTi, AuV, AuW, AuY, AuZn, AuZr, BaHf, BaMg, BaPd, BaPt, BeHf, BeCd, BeCo, BeMg, BeMn, BeOs, BePd, BePt, BeRe, BeRh, BeRu, BeSc, BeTc, BeTi, BeTl, BeY, BeZn, BeZr, BBi, BCd, BCo, BCr, BCu, BFe, BGa, BGe, BHf, BHg, BIn, BIr, BLa, BMg, BMn, BMo, BNb, BNi, BOs, BP, BPb, BPd, BPt, BRe, BRh, BRu, BSb, BSc, BSe, BSi, BSn, BTa, BTc, BTe, BTi, BV, BW, BY, BZn, BZr, BiCd, BiCo, BiCr, BiCu, BiFe, BiGa, BiGe, BiHf, BiHg, BiIn, BiIr, BiLa, BiMg, BiMn, BiMo, BiNb, BiNi, BiOs, BiP, BiPb, BiPd, BiPt, BiRe, BiRh, BiRu, BiSb, BiSc, BiSe, BiSi, BiSn, BiTa, BiTc, BiTe, BiTi, BiV, BiW, BiY, BiZn, BiZr, BHf, CaHf, CaMg, CaPd, CaPt, CdCo, CdCr, CdCu, CdFe, CdGa, CdGe, CdHf, CdHg, CdIn, CdIr, CdLa, CdMg, CdMn, CdMo, CdNb, CdNi, CdOs, CdP, CdPb, CdPd, CdPt, CdRe, CdRh, CdRu, CdSb, CdSc, CdSe, CdSi, CdSn, CdTa, CdTc, CdTe, CdTi, CdTl, CdV, CdW, CdY, CdZn, CdZr, CeMg, CNi, CoCr, CoCu, CoFe, CoGa, CoGe, CoHf, CoHg, CoIn, CoIr, CoLa, CoMg, CoMn, CoMo, CoNb, CoNi, CoOs, CoP, CoPb, CoPd, CoPt, CoRe, CoRh, CoRu, CoSb, CoSc, CoSe, CoSi, CoSn, CoTa, CoTc, CoTe, CoTi, CoTl, CoV, CoW, CoY, CoZn, CoZr, CrCu, CrFe, CrGa, CrGe, CrHf, CrHg, CrIn, CrIr, CrLa, CrMg, CrMn, CrMo, CrNb, CrNi, CrOs, CrP, CrPb, CrPd, CrPt, CrRe, CrRh, CrRu, CrSb, CrSc, CrSe, CrSi, CrSn, CrTa, CrTc, CrTe, CrTi, CrV, CrW, CrY, CrZn, CrZr, CsPd, CuFe, CuGa, CuGe, CuHf, CuHg, CuIn, CuIr, CuLa, CuMg, CuMn, CuMo, CuNb, CuNi, CuOs, CuP, CuPb, CuPd, CuPt, CuRe, CuRh, CuRu, CuSb, CuSc, CuSe, CuSi, CuSn, CuTa, CuTc, CuTe, CuTi, CuV, CuW, CuY, CuZn, CuZr, FeGa, FeGe, FeHf, FeHg, FeIn, FeIr, FeLa, FeMg, FeMn, FeMo, FeNb, FeNi, FeOs, FeP, FePb, FePd, FePt, FeRe, FeRh, FeRu, FeSb, FeSc, FeSe, FeSi, FeSn, FeTa, FeTc, FeTe, FeTi, FeV, FeW, FeY, FeZn, FeZr, GaGe, GaHf, GaHg, GaIn, GaIr, GaLa, GaMg, GaMn, GaMo, GaNb, GaNi, GaOs, GaP, GaPb, GaPd, GaPt, GaRe, GaRh, GaRu, GaSb, GaSc, GaSe, GaSi, GaSn, GaTa, GaTc, GaTe, GaTi, GaV, GaW, GaY, GaZn, GaZr, GaMg, GdMg, GeHf, GeHg, GeIn, GeIr, GeLa, GeMg, GeMn, GeMo, GeNb, GeNi, GeOs, GeP, GePb, GePd, 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LaZn, LaZr, list, LiMg, LiPd, LiPt, MgMn, MgMo, MgNb, MgNi, MgOs, MgP, MgPb, MgPd, MgPt, MgRe, MgRh, MgRu, MgSb, MgSc, MgSe, MgSi, MgSn, MgTa, MgTc, MgTe, MgTi, MgTl, MgV, MgW, MgY, MgZn, MgZr, MnMo, MnNb, MnNi, MnOs, MnP, MnPb, MnPd, MnPt, MnRe, MnRh, MnRu, MnSb, MnSc, MnSe, MnSi, MnSn, MnTa, MnTc, MnTe, MnTi, MnV, MnW, MnY, MnZn, MnZr, MoMg, MoNb, MoNi, MoOs, MoP, MoPb, MoPd, MoPt, MoRe, MoRh, MoRu, MoSb, MoSc, MoSe, MoSi, MoSn, MoTa, MoTc, MoTe, MoTi, MoV, MoW, MoY, MoZn, MoZr, NaMg, NaPd, NaPt, NbMg, NbNi, NbOs, NbP, NbPb, NbPd, NbPt, NbRe, NbRh, NbRu, NbSb, NbSc, NbSe, NbSi, NbSn, NbTa, NbTc, NbTe, NbTi, NbV, NbW, NbY, NbZn, NbZr, NiOs, NiP, NiPb, NiPd, NiPt, NiRe, NiRh, NiRu, NiSb, NiSc, NiSe, NiSi, NiSn, NiTa, NiTc, NiTe, NiTi, NiV, NiW, NiY, NiZn, NiZr, OsMg, OsP, OsPb, OsPd, OsPt, OsRe, OsRh, OsRu, OsSb, OsSc, OsSe, OsSi, OsSn, OsTa, OsTc, OsTe, OsTi, OsTl, OsV, OsW, OsY, OsZn, OsZr, PbMg, PbPd, PbPt, PbRe, PbRh, PbRu, PbSb, PbSc, PbSe, PbSi, PbSn, PbTa, PbTc, PbTe, PbTi, PbV, PbW, PbY, PbZn, PbZr, PdPt, PdRe, PdRh, PdRu, PdSb, PdSc, PdSe, PdSi, PdSn, PdTa, PdTc, PdTe, PdTi, PdV, PdW, PdY, PdZn, PdZr, PPb, PPd, PPt, PRe, PRh, PRu, PSb, PSc, PSe, PSi, PSn, PTa, PTc, PTe, PTi, PtRe, PtRh, PtRu, PtSb, PtSc, PtSe, PtSi, PtSn, PtTa, PtTc, PtTe, PtTi, PtV, PtW, PtY, PtZn, PtZr, PV, PW, PY, PZn, PZr, RbMg, RbPd, RbPt, ReMg, ReRh, ReRu, ReSb, ReSc, ReSe, ReSi, ReSn, ReTa, ReTc, ReTe, ReTi, ReTl, ReV, ReW, ReY, ReZn, ReZr, RhMg, RhRu, RhSb, RhSc, RhSe, RhSi, RhSn, RhTa, RhTc, RhTe, RhTi, RhTl, RhV, RhW, RhY, RhZn, RhZr, RuMg, RuSb, RuSc, RuSe, RuSi, RuSn, RuTa, RuTc, RuTe, RuTi, RuTl, RuV, RuW, RuY, RuZn, RuZr, SbSc, SbSe, SbSi, SbSn, SbTa, SbTc, SbTe, SbTi, SbV, SbW, SbY, SbZn, SbZr, ScMg, ScSe, ScSi, ScSn, ScTa, ScTc, ScTe, ScTi, ScTl, ScV, ScW, ScY, ScZn, ScZr, SeSi, SeSn, SeTa, SeTc, SeTe, SeTi, SeV, SeW, SeY, SeZn, SeZr, SiPd, SiPt, SiSn, SiTa, SiTc, SiTe, SiTi, SiV, SiW, SiY, SiZn, SiZr, SnMg, SnPd, SnPt, SnTa, SnTc, SnTe, SnTi, SnV, SnW, SnY, SnZn, SnZr, SrMg, SrPd, SrPt, TaMg, TaTc, TaTe, TaTi, TaV, TaW, TaY, TaZn, TaZr, TcTe, TcTi, TcTl, TcV, TcW, TcY, TcZn, TcZr, TeTi, TeV, TeW, TeY, TeZn, TeZr, TiMg, TiTl, TiV, TiW, TiY, TiZn, TiZr, TlY, TlZn, TlZr, VMg, VW, VY, VZn, VZr, WMg, WY, WZn, WZr, YMg, YZn, YZr, ZnMg, ZnZr, ZrMg

High-Throughput Materials Exploration

AgAl, AgAs, AgAu, AgB, AgBi, AgCd, AgCo, AgCr, AgCu, AgFe, AgGa, AgGe, AgHf, AgHg, AgIn, AgIr, AgLa, AgMg, AgMn, AgMo, AgNb, AgNi, AgOs, AgP, AgPb, AgPd, AgPt, AgRe, AgRh, AgRu, AgSb, AgSc, AgSe, AgSi, AgSn, AgTa, AgTc, AgTe, AgTi, AgV, AgW, AgY, AgZn, AgZr, AlAs, AlAu, AlB, AlBi, AlCd, AlCo, AlCr, AlCu, AlFe, AlGa, AlGe, AlCo, AlHf, AlHg, AlHf, AlPd, AlPt, AlSc, AlIn, AlIr, AlLa, AlMg, AlMn, AlMo, AlNb, AlNi, AlOs, AlP, AlPb, AlPd, AlPt, AlRe, AlRh, AlRu, AlSb, AlSc, AlSe, AlSi, AlSn, AlTa, AlTc, AlTe, AlTi, AlV, AlW, AlY, AlZn, AlZr, AsAu, AsB, AsBi, AsCd, AsCo, AsCr, AsCu, AsFe, AsGa, AsGe, AsHf, AsHg, AsIn, AsIr, AsLa, AsMg, AsMn, AsMo, AsNb, AsNi, AsOs, AsP, AsPb, AsPd, AsPt, AsRe, AsRh, AsRu, AsSb, AsSc, AsSe, AsSi, AsSn, AsTa, AsTc, AsTe, AsTi, AsV, AsW, AsY, AsZn, AsZr, AuB, AuBi, AuCd, AuCo, AuCr, AuCu, AuFe, AuGa, AuGe, AuHf, AuHg, AuIn, AuIr, AuLa, AuMg, AuMn, AuMo, AuNb, AuNi, AuOs, AuP, AuPb, AuPd, AuPt, AuRe, AuRh, AuRu, AuSb, AuSc, AuSe, AuSi, AuSn, AuTa, AuTc, AuTe, AuTi, AuV, AuW, AuY, AuZn, AuZr, BaHf, BaMg, BaPd, BaPt, BeHf, BeCd, BeCo, BeMg, BeMn, BeOs, BePd, BePt, BeRe, BeRh, BeRu, BeSc, BeTc, BeTi, BeTl, BeY, BeZn, BeZr, BBi, BCd, BCo, BCr, BCu, BFe, BGa, BGe, BHf, BHg, BIn, BIr, BLa, BMg, BMn, BMo, BNb, BNi, BOs, BP, BPb, BPd, BPt, BRe, BRh, BRu, BSb, BSc, BSe, BSi, BSn, BTa, BTc, BTe, BTi, BV, BW, BY, BZn, BZr, BiCd, BiCo, BiCr, BiCu, BiFe, BiGa, BiGe, BiHf, BiHg, BiIn, BiIr, BiLa, BiMg, BiMn, BiMo, BiNb, BiNi, BiOs, BiP, BiPb, BiPd, BiPt, BiRe, BiRh, BiRu, BiSb, BiSc, BiSe, BiSi, BiSn, BiTa, BiTc, BiTe, BiTi, BiV, BiW, BiY, BiZn, BiZr, BHf, CaHf, CaMg, CaPd, CaPt, CdCo, CdCr, CdCu, CdFe, CdGa, CdGe, CdHf, CdHg, CdIn, CdIr, CdLa, CdMg, CdMn, CdMo, CdNb, CdNi, CdOs, CdP, CdPb, CdPd, CdPt, CdRe, CdRh, CdRu, CdSb, CdSc, CdSe, CdSi, CdSn, CdTa, CdTc, CdTe, CdTi, CdTl, CdV, CdW, CdY, CdZn, CdZr, CeMg, CNi, CoCr, CoCu, CoFe, CoGa, CoGe, CoHf, CoHg, CoIn, CoIr, CoLa, CoMg, CoMn, CoMo, CoNb, CoNi, CoOs, CoP, CoPb, CoPd, CoPt, CoRe, CoRh, CoRu, CoSb, CoSc, CoSe, CoSi, CoSn, CoTa, CoTc, CoTe, CoTi, CoTl, CoV, CoW, CoY, CoZn, CoZr, CrCu, CrFe, CrGa, CrGe, CrHf, CrHg, CrIn, CrIr, CrLa, CrMg, CrMn, CrMo, CrNb, CrNi, CrOs, CrP, CrPb, CrPd, CrPt, CrRe, CrRh, CrRu, CrSb, CrSc, CrSe, CrSi, CrSn, CrTa, CrTc, CrTe, CrTi, CrV, CrW, CrY, CrZn, CrZr, CsPd, CuFe, CuGa, CuGe, CuHf, CuHg, CuIn, CuIr, CuLa, CuMg, CuMn, CuMo, CuNb, CuNi, CuOs, CuP, CuPb, CuPd, CuPt, CuRe, CuRh, CuRu, CuSb, CuSc, CuSe, CuSi, CuSn, CuTa, CuTc, CuTe, CuTi, CuV, CuW, CuY, CuZn, CuZr, FeGa, FeGe, FeHf, FeHg, FeIn, FeIr, FeLa, FeMg, FeMn, FeMo, FeNb, FeNi, FeOs, FeP, FePb, FePd, FePt, FeRe, FeRh, FeRu, FeSb, FeSc, FeSe, FeSi, FeSn, FeTa, FeTc, FeTe, FeTi, FeV, FeW, FeY, FeZn, FeZr, GaGe, GaHf, GaHg, GaIn, GaIr, GaLa, GaMg, GaMn, GaMo, GaNb, GaNi, GaOs, GaP, GaPb, GaPd, GaPt, GaRe, GaRh, GaRu, GaSb, GaSc, GaSe, GaSi, GaSn, GaTa, GaTc, GaTe, GaTi, GaV, GaW, GaY, GaZn, GaZr, GaMg, GdMg, GeHf, GeHg, GeIn, GeIr, GeLa, GeMg, GeMn, GeMo, GeNb, GeNi, GeOs, GeP, GePb, GePd, GePt, GeRe, GeRh, GeRu, GeSb, GeSc, GeSe, GeSi, GeSn, GeTa, GeTc, GeTe, GeTi, GeV, GeW, GeY, GeZn, GeZr, GeMg, HfHg, HfIn, HfIr, HfK, HfLa, HfLi, HfMg, HfMn, HfMo, HfNa, HfNb, HfNi, HfOs, HfP, HfPb, HfPd, HfPt, HfRe, HfRh, HfRu, HfSb, HfSc, HfSe, HfSi, HfSn, HfSn, HfSr, HfTa, HfTc, HfTe, HfTi, HfTl, HfV, HfW, HfY, HfZn, HfZr, HgIn, HgIr, HgLa, HgMg, HgMn, HgMo, HgNb, HgNi, HgOs, HgP, HgPb, HgPd, HgPt, HgRe, HgRh, HgRu, HgSb, HgSc, HgSe, HgSi, HgSn, HgTa, HgTc, HgTe, HgTi, HgV, HgW, HgY, HgZn, HgZr, InIr, InLa, InMg, InMn, InMo, InNb, InNi, InOs, InP, InPb, InPd, InPt, InRe, InRh, InRu, InSb, InSc, InSe, InSi, InSn, InTa, InTc, InTe, InTi, InV, InW, InY, InZn, InZr, IrLa, IrMg,
IrMn, IrMo, IrNb, … aMg, LaMn, LaMo,
LaNb, LaNi, LaOs … LiPd, LiPt, MgMn,
MgMo, MgNb, Mg… MgY, MgZn, MgZr,
MnMo, MnNb, Mn… MnY, MnZn, MnZr,
MoMg, MoNb, Mo… oW, MoY, MoZn,
MoZr, NaMg, NaP… NbTi, NbV, NbW,
NbY, NbZn, NbZ… OsMg, OsP, OsPb,
OsPd, OsPt, OsR… bRe, PbRh, PbRu,
PbSb, PbSc, PbSe, PbSi, PbSn, PbTa, PbTc, PbTe, PbTi, PbV, PbW, PbY, PbZn, PbZr, PdPt, PdRe, PdRh, PdRu, PdSb, PdSc, PdSe, PdSi, PdSn, PdTa, PdTc, PdTe, PdTi, PdV,
PdW, PdY, PdZn, PdZr, PPb, PPd, PPt, PRe, PRh, PRu, PSb, PSc, PSe, PSi, PSn, PT…
PtW, PtY, PtZn, PtZr, PV, PW, PY, PZn, PZr, RbMg, RbPd, RbPt, ReMg, ReRh, Re…
ReZr, RhMg, RhRu, RhSb, RhSc, RhSe, RhSi, RhSn, RhTa, RhTc, RhTe, RhTi, Rh…
RuTi, RuTl, RuV, RuW, RuY, RuZn, RuZr, SbSc, SbSe, SbSi, SbSn, SbTa, SbTc, Sb…
ScV, ScW, ScY, ScZn, ScZr, SeSi, SeSn, SeTa, SeTc, SeTe, SeTi, SeV, SeW, SeY, Se…
SnTa, SnTc, SnTe, SnTi, SnV, SnW, SnY, SnZn, SnZr, SrMg, SrPd, SrPt, TaMg, TaTc,
TeW, TeY, TeZn, TeZr, TiMg, TiTl, TiV, TiW, TiY, TiZn, TiZr, TlY, TlZn, TlZr, VMg, VW,

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S. Curtarolo, O. Levy, W. Setyawan,
I. Takeuchi, A. Kolmogorov, S. Wang,
M. Jahnatek, M. Buongiorno Nardelli, M. Fornari,
R. Taylor, Z. Wang, K. Yang, N. Mingo, S. Sanvito

High-Throughput Materials Exploration

AgAl, AgAs, AgAu, AgB, AgBi, AgCd, AgCo, AgCr, AgCu, AgFe, AgGa, AgGe, AgHf, AgHg, AgIn, AgIr, AgLa, AgMg, AgMn, AgMo, AgNb, AgNi, AgOs, AgP, AgPb, AgPd, AgPt,
AgRe, AgRh, AgRu, AgSb, AgSc, AgSe, AgSi, AgSn, AgTa, AgTc, AgTe, AgTi, AgV, AgW, AgY, AgZn, AgZr, AlAs, AlAu, AlB, AlBi, AlCd, AlCo, AlCr, AlCu, AlFe, AlGa, AlGe, AlCo,
AlHf, AlHg, AlHf, AlPd, AlPt, AlSc, AlIn, AlIr, AlLa, AlMg, AlMn, AlMo, AlNb, AlNi, AlOs, AlP, AlPb, AlPd, AlPt, AlRe, AlRh, AlRu, AlSb, AlSc, AlSe, AlSi, AlSn, AlTa, AlTc, AlTe,
AlTi, AlV, AlW, AlY, AlZn, AlZr, AsAu, AsB, AsBi, AsCd, AsCo, AsCr, AsCu, AsFe, AsGa, AsGe, AsHf, AsHg, AsIn, AsIr, AsLa, AsMg, AsMn, AsMo, AsNb, AsNi, AsOs, AsP,
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AuGe, AuHf, AuHg, AuIn, AuIr, AuLa, AuMg, AuMn, AuMo, AuNb, AuNi, AuOs, AuP, AuPb, AuPd, AuPt, AuRe, AuRh, AuRu, AuSb, AuSc, AuSe, AuSi, AuSn, AuTa, AuTc, AuTe,
AuTi, AuV, AuW, AuY, AuZn, AuZr, BaHf, BaMg, BaPd, BaPt, BeHf, BeCd, BeCo, BeMg, BeMn, BeOs, BePd, BePt, BeRe, BeRh, BeRu, BeSc, BeTc, BeTi, BeTl, BeY, BeZn,
BeZr, BBi, BCd, BCo, BCr, BCu, BFe, BGa, BGe, BHf, BHg, BIn, BIr, BLa, BMg, BMn, BMo, BNb, BNi, BOs, BP, BPb, BPd, BPt, BRe, BRh, BRu, BSb, BSc, BSe, BSi, BSn, BTa,
BTc, BTe, BTi, BV, BW, BY, BZn, BZr, BiCd, BiCo, BiCr, BiCu, BiFe, BiGa, BiGe, BiHf, BiHg, BiIn, BiIr, BiLa, BiMg, BiMn, BiMo, BiNb, BiNi, BiOs, BiP, BiPb, BiPd, BiPt, BiRe,
BiRh, BiRu, BiSb, BiSc, BiSe, BiSi, BiSn, BiTa, BiTc, BiTe, BiTi, BiV, BiW, BiY, BiZn, BiZr, BHf, CaHf, CaMg, CaPd, CaPt, CdCo, CdCr, CdCu, CdFe, CdGa, CdGe, CdHf,
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CoP, CoPb, CoPd, CoPt, CoRe, CoRh, CoRu, CoSb, CoSc, CoSe, CoSi, CoSn, CoTa, CoTc, CoTe, CoTi, CoTl, CoV, CoW, CoY, CoZn, CoZr, CrCu, CrFe, CrGa,
CrGe, CrHf, CrHg, CrIn, CrIr, CrLa, CrMg, C u, CrSb, CrSc, CrSe, CrSi, CrSn, CrTa, CrTc,
CrTe, CrTi, CrV, CrW, CrY, CrZn, CrZr, CsPc , CuNb, CuNi, CuOs, CuP, CuPb, CuPd, CuPt,
CuRe, CuRh, CuRu, CuSb, CuSc, CuSe, CuSi, Ge, FeHf, FeHg, FeIn, FeIr, FeLa, FeMg, FeMn,
FeMo, FeNb, FeNi, FeOs, FeP, FePb, FePd, FeP eV, FeW, FeY, FeZn, FeZr, GaGe, GaHf, GaHg,
GaIn, GaIr, GaLa, GaMg, GaMn, GaMo, GaNb, Se, GaSi, GaSn, GaTa, GaTc, GaTe, GaTi, GaV,
GaW, GaY, GaZn, GaZr, GaMg, GdMg, GeHf, GePb, GePd, GePt, GeRe, GeRh, GeRu, GeSb,
GeSc, GeSe, GeSi, GeSn, GeTa, GeTc, GeTe, G , HfMg, HfMn, HfMo, HfNa, HfNb, HfNi, HfOs,
HfP, HfPb, HfPd, HfPt, HfRe, HfRh, HfRu, HfS fW, HfY, HfZn, HfZr, HgIn, HgIr, HgLa, HgMg,
HgMn, HgMo, HgNb, HgNi, HgOs, HgP, HgPb, Tc, HgTe, HgTi, HgV, HgW, HgY, HgZn, HgZr,
InIr, InLa, InMg, InMn, InMo, InNb, InNi, InOs, InP, InPb, InPd, InPt, InRe, InRh, InRu, InSb, InSc, InSe, InSi, InSn, InTa, InTc, InTe, InTi, InV, InW, InY, InZn, InZr, IrLa, IrMg,
IrMn, IrMo, IrNb, aMg, LaMn, LaMo,
LaNb, LaNi, LaOs LiPd, LiPt, MgMn,
MgMo, MgNb, Mg MgY, MgZn, MgZr,
MnMo, MnNb, Mr MnY, MnZn, MnZr,
MoMg, MoNb, Mo oW, MoY, MoZn,
MoZr, NaMg, NaP NbTi, NbV, NbW,
NbY, NbZn, NbZ OsMg, OsP, OsPb,
OsPd, OsPt, OsR PbRe, PbRh, PbRu,
PbSb, PbSc, PbSe, PbSi, PbSn, PbTa, PbTc, PbTe, PbTi, PbV, PbW, PbY, PbZn, PbZr, PdPt, PdRe, PdRh, PdRu, PdSb, PdSc, PdSe, PdSi, PdSn, PdTa, PdTc, PdTe, PdTi, PdV,
PdW, PdY, PdZn, PdZr, PPb, PPd, PPt, PRe, PRh, PRu, PSb, PSc, PSe, PSi, PSn, PT
PtW, PtY, PtZn, PtZr, PV, PW, PY, PZn, PZr, RbMg, RbPd, RbPt, ReMg, ReRh, Re
ReZr, RhMg, RhRu, RhSb, RhSc, RhSe, RhSi, RhSn, RhTa, RhTc, RhTe, RhTi, Rh
RuTi, RuTl, RuV, RuW, RuY, RuZn, RuZr, SbSc, SbSe, SbSi, SbSn, SbTa, SbTc, Sb
ScV, ScW, ScY, ScZn, ScZr, SeSi, SeSn, SeTa, SeTc, SeTe, SeTi, SeV, SeW, SeY, Se
SnTa, SnTc, SnTe, SnTi, SnV, SnW, SnY, SnZn, SnZr, SrMg, SrPd, SrPt, TaMg, TaTc,
TeW, TeY, TeZn, TeZr, TiMg, TiTl, TiV, TiW, TiY, TiZn, TiZr, TlY, TlZn, TlZr, VMg, VW,

Beyond the direct results, are there other things we can learn from the data?

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R. Taylor, Z. Wang, K. Yang, N. Mingo, S. Sanvito

High Throughput is the future...

High Throughput is the future...

Need: 3 post-docs and 4 PhD students

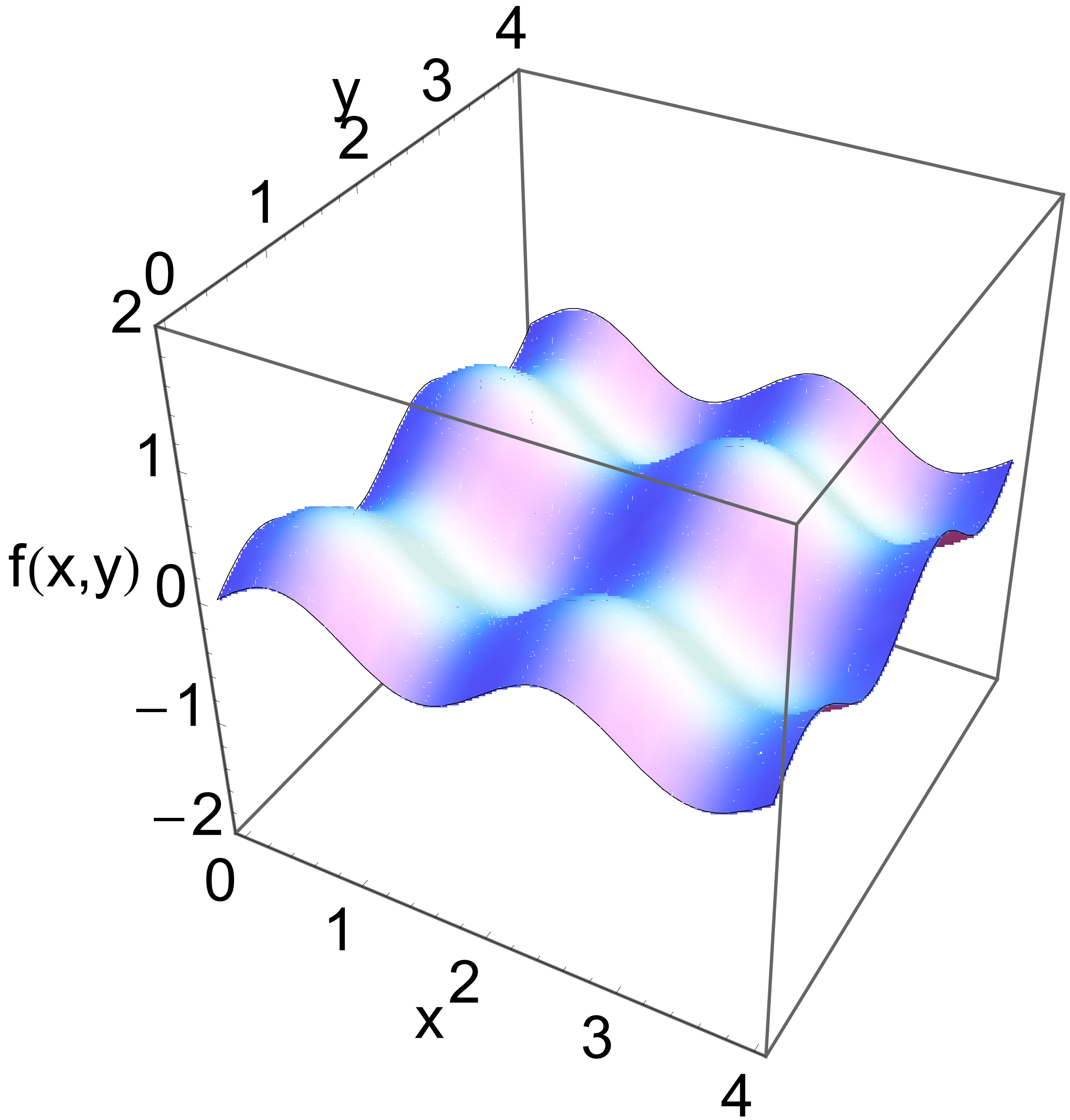
Compressed sensing model building in a nutshell: **Better models, faster**

Basic idea:

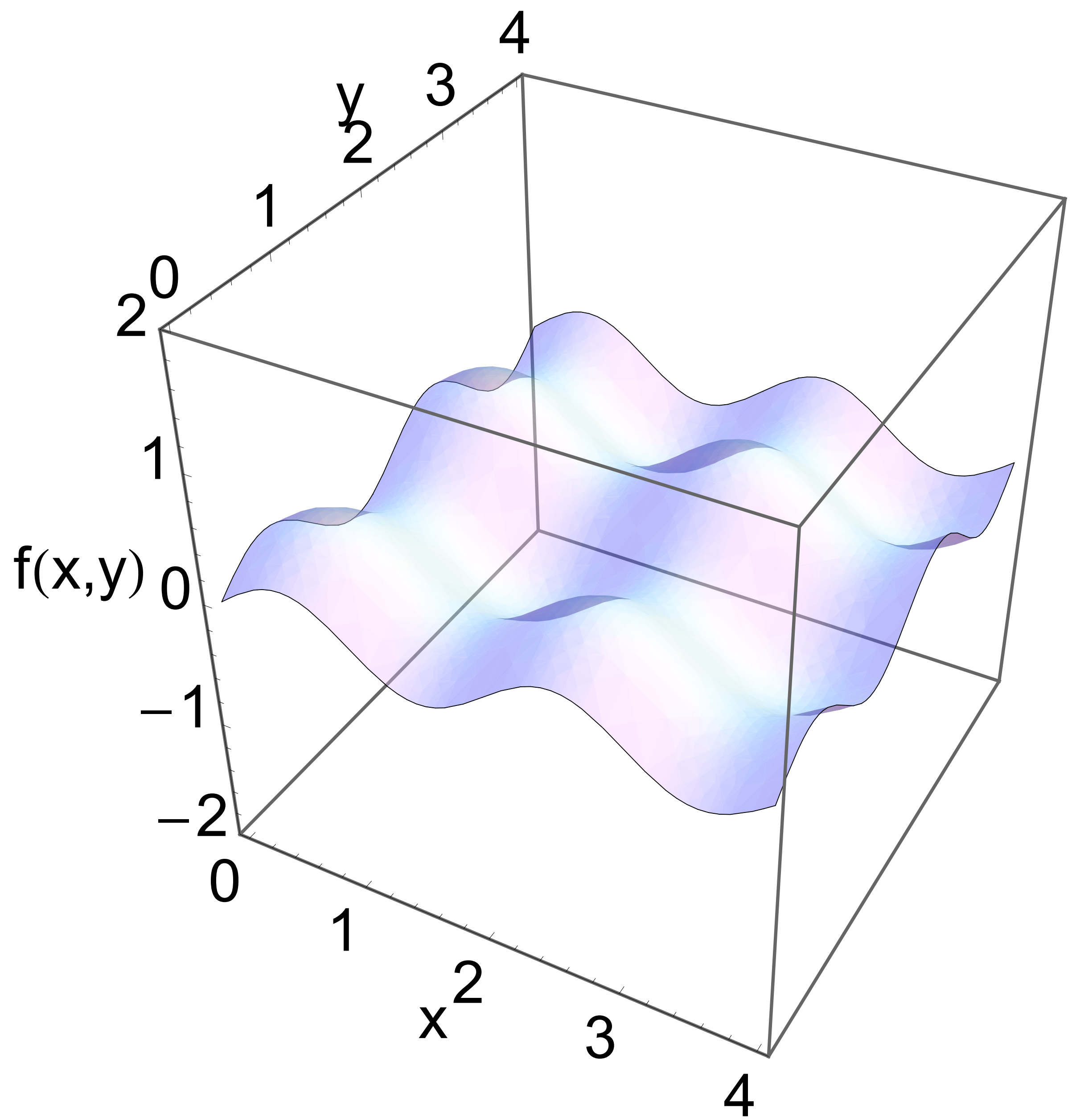
Instead of adding complexity (terms) to a model until it fits the data and predicts well...(normal approach)...

...start with an infinite set of models (containing all possible terms). Discard all models except the simplest one (Compressive Sensing approach). Surprisingly perhaps, this is really efficient.

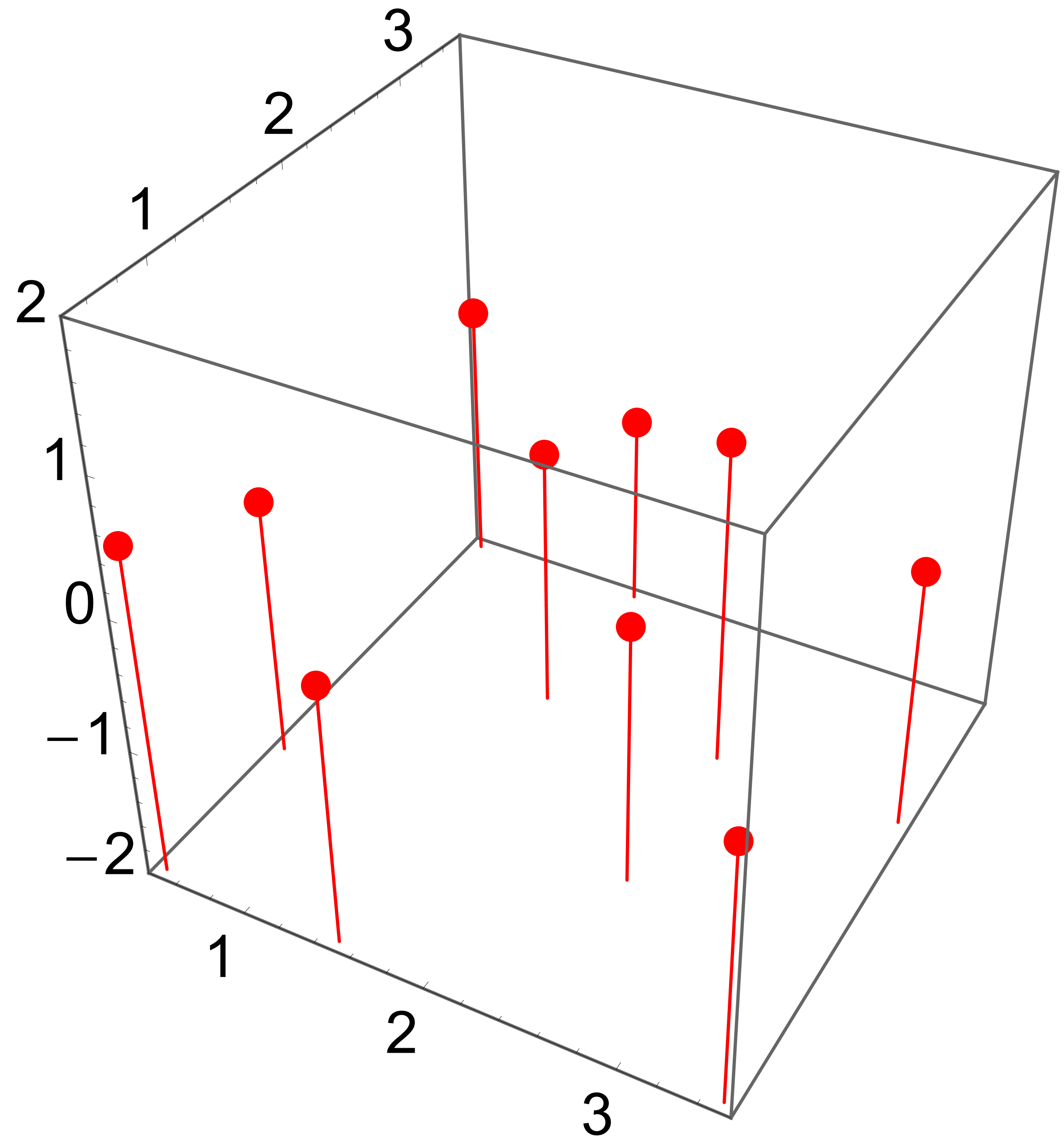
Physical quantities vs. experimental parameters



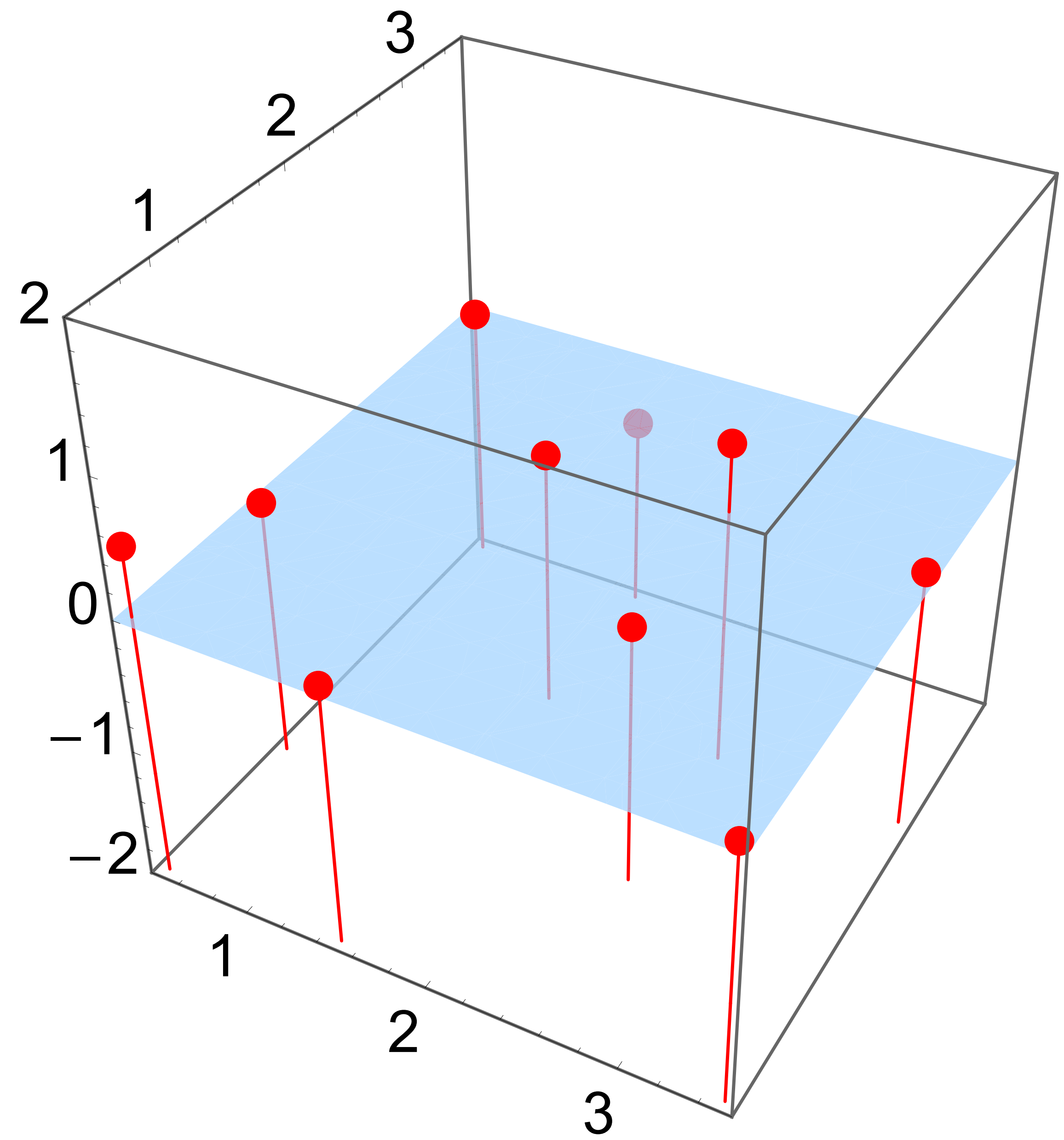
Finding functions for observables (signal recovery)



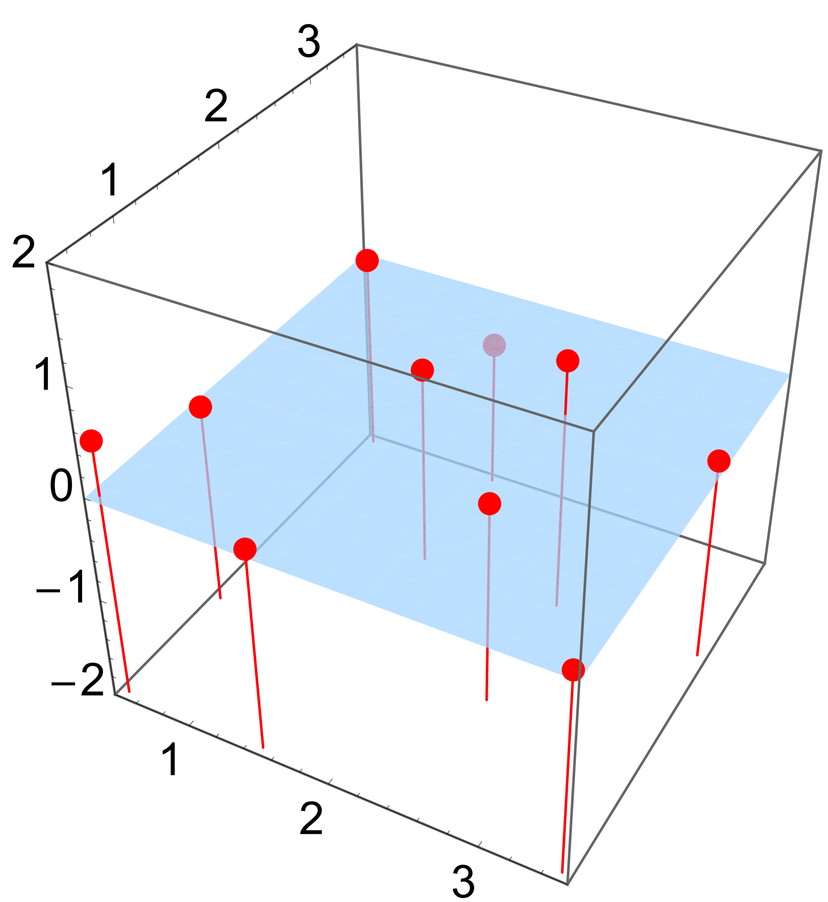
Making measurements (signal sampling)



Assume a model, least squares fitting



Assume a model, least squares fitting



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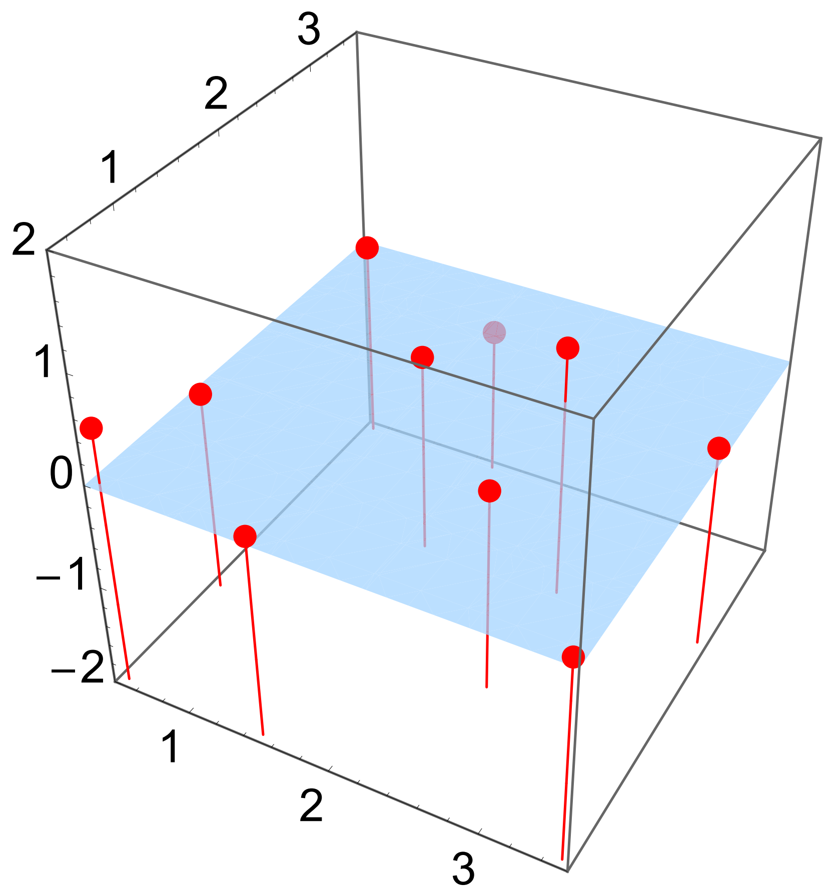
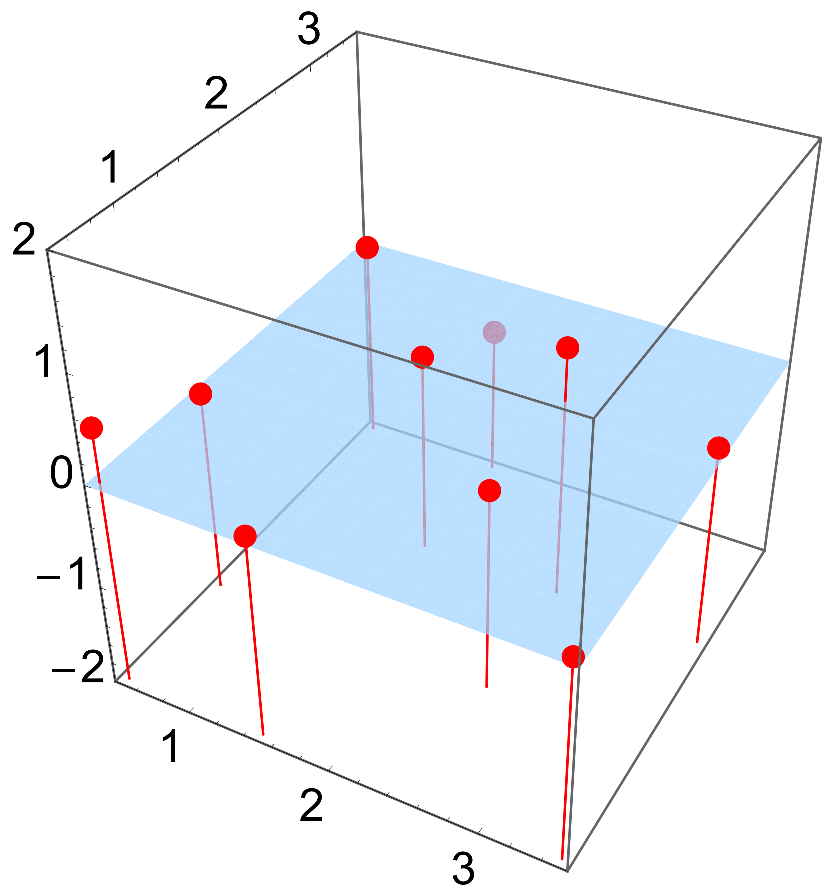


1. Model may have the wrong functional form (physics is incorrect)

Assume a model, least squares fitting



1. Model may have the wrong functional form (physics is incorrect)
2. Least-squares error may not reflect the actual errors in the measurements

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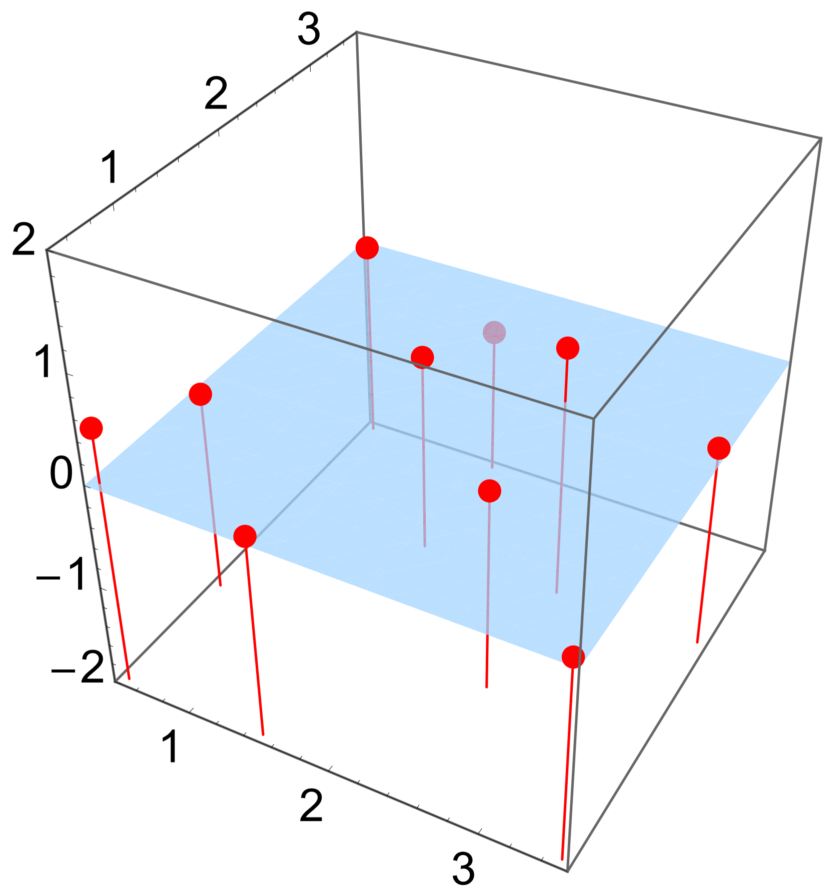

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$$\mathrm{RMSE} = \left(\sum_i |y_i - f_i|^2 \right)^{\frac{1}{2}}$$

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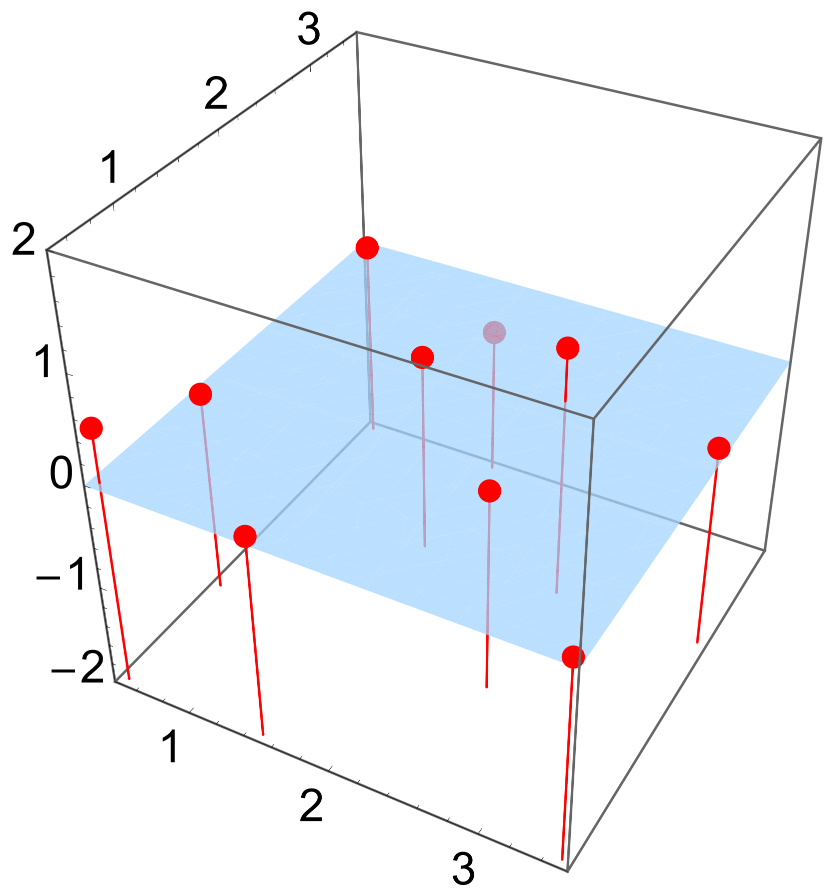

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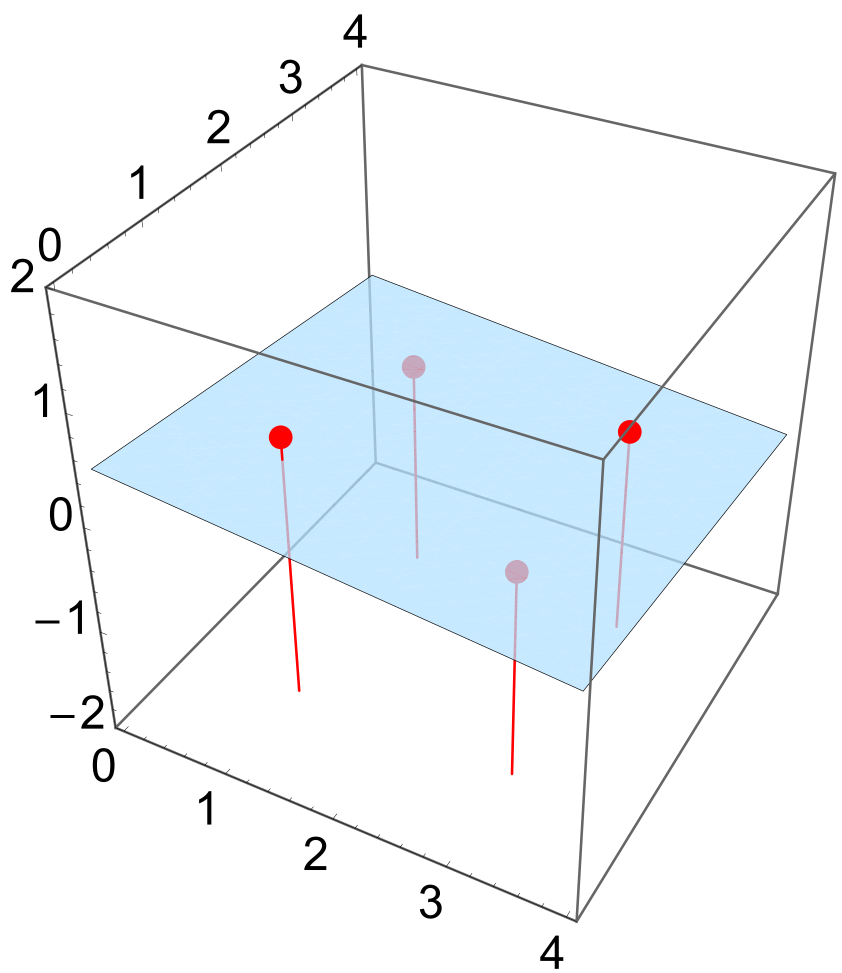
$$\mathrm{RMSE} = \left(\sum_i |y_i - f_i|^{2} \right)^{\frac{1}{2}} \equiv \ell_2 \text{ norm}$$

Going beyond a linear model fit (adding terms)

$$f(x,y) = \boxed{a_0 + a_1 x + a_2 y} + a_3 xy + a_4 x^2 + a_5 y^2 + \cdots$$



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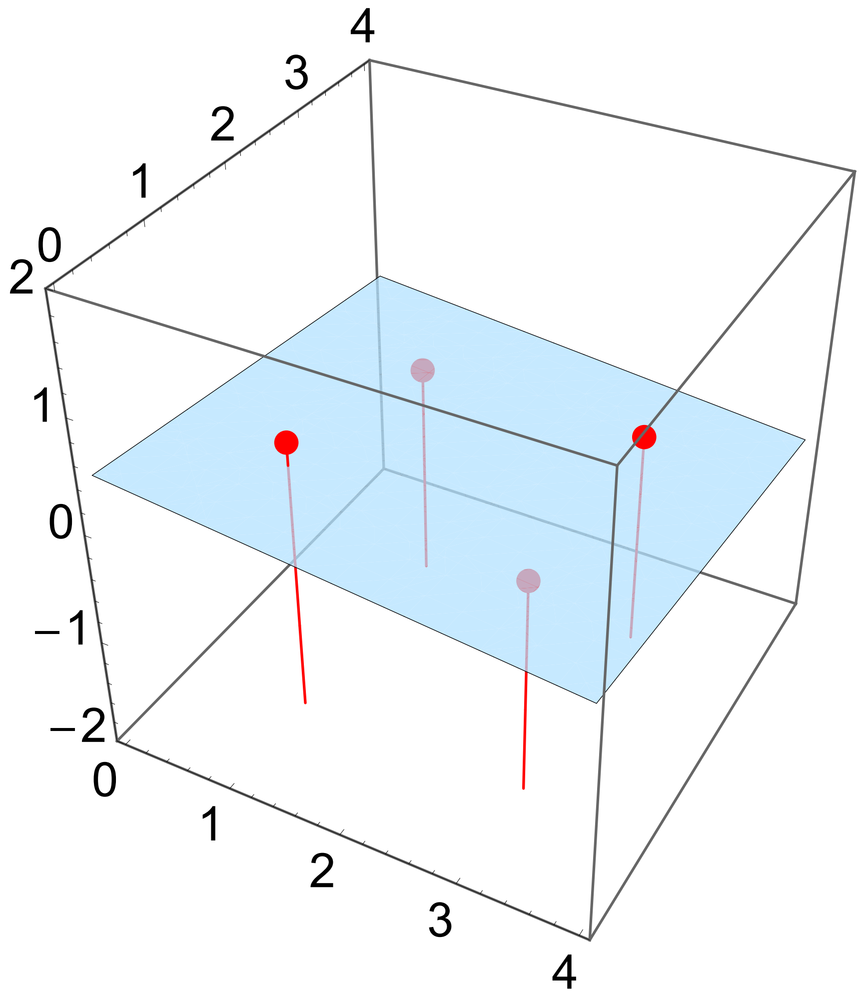

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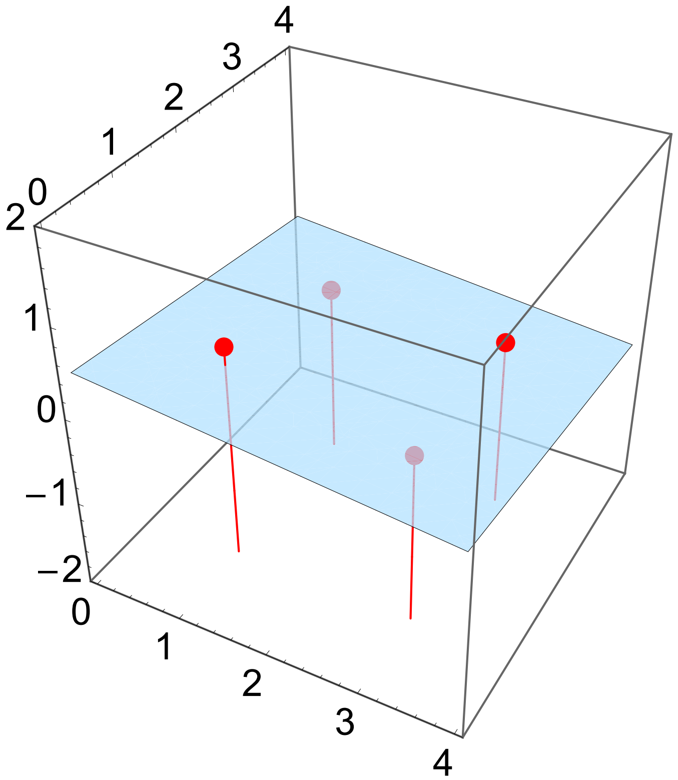

$$\begin{pmatrix} 1 & x_1 & y_1 & x_1 y_1 \\ 1 & x_2 & y_2 & x_2 y_2 \\ 1 & x_3 & y_3 & x_3 y_3 \\ 1 & x_4 & y_4 & x_4 y_4 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}$$

Sensing matrix

Going beyond a linear model fit (adding terms)

$$f(x,y) = \boxed{a_0 + a_1 x + a_2 y + a_3 xy} + a_4 x^2 + a_5 y^2 + \cdots$$

$$\begin{pmatrix} 1 & x_1 & y_1 & x_1 y_1 \\ 1 & x_2 & y_2 & x_2 y_2 \\ 1 & x_3 & y_3 & x_3 y_3 \\ 1 & x_4 & y_4 & x_4 y_4 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}$$

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$$\mathbb{M}\vec{a} = \vec{f}$$

“Solving” an under-determined problem

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$$\min_{\vec{a}} \left\{ \|\vec{a}\|_1 : \mathbb{M}\vec{a} = \vec{f} \right\}$$

"Solving" an under-determined problem

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$$\ell_1 \equiv \|\vec{u}\| = \sum_i |u_i|$$

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$$\min_{\vec{a}} \left\{ \|\vec{a}\|_1 : \mathbb{M}\vec{a} = \vec{f} \right\}$$

$$\ell_1 \equiv \|\vec{u}\| = \sum_i |u_i|$$

$$\ell_2 \equiv \left(\sum_i |u_i|^2 \right)^{\frac{1}{2}} \qquad \ell_1 \equiv \left(\sum_i |u_i|^1 \right)^{\frac{1}{1}}$$

Explain the magic

Basic ideas of Compressive Sensing

- Solution must be “sparse” in some basis
- Numerical application of ell-1 norm is fast
- Choose a big basis so that you’ve captured all the relevant components
- Like a Fourier Transform...except that you can sample way below the Nyquist frequency
- Sample points must be “uncorrelated”—selected at random from the domain.

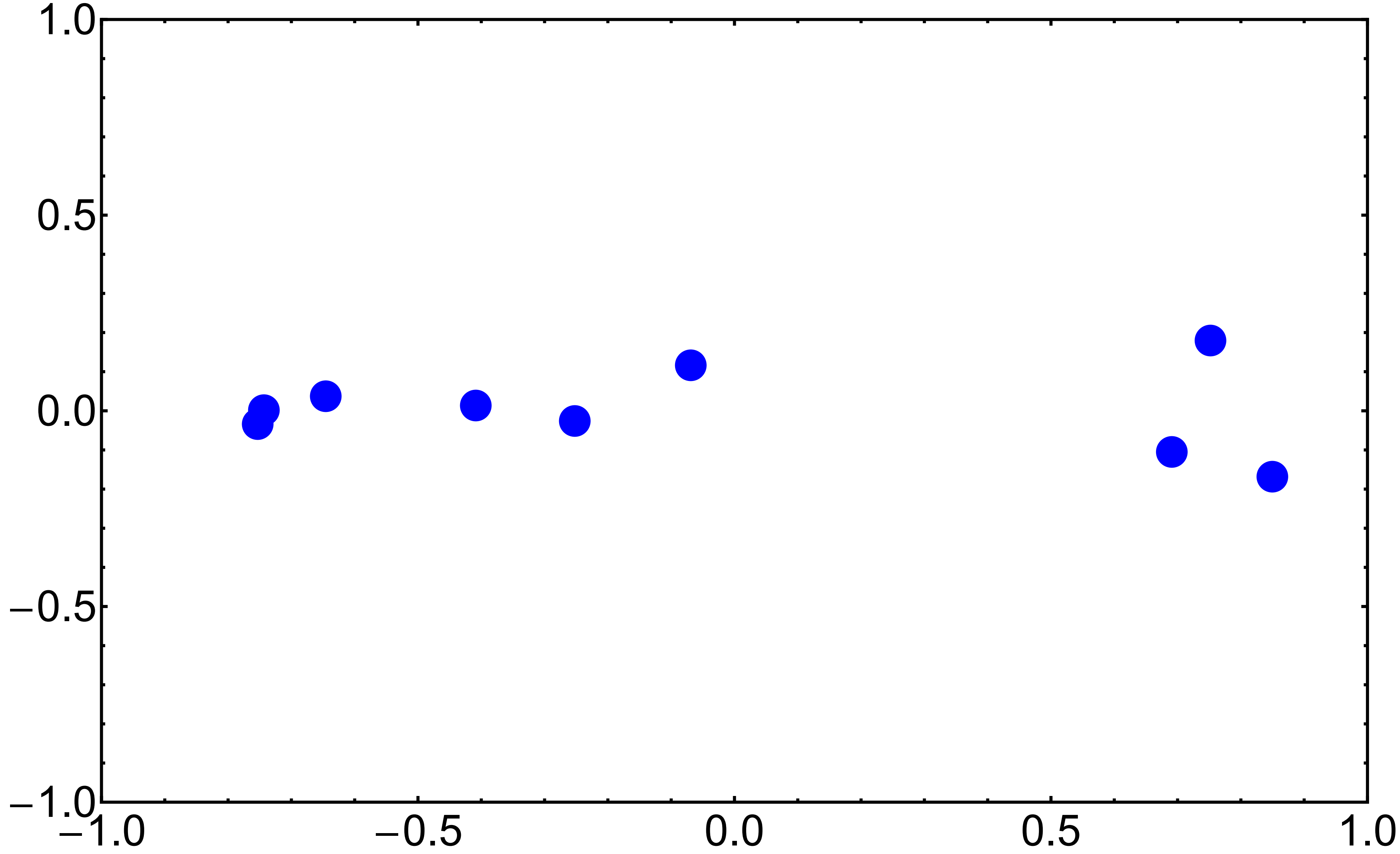
An Introduction To Compressive Sampling

[A sensing/sampling paradigm that goes against the common knowledge in data acquisition]

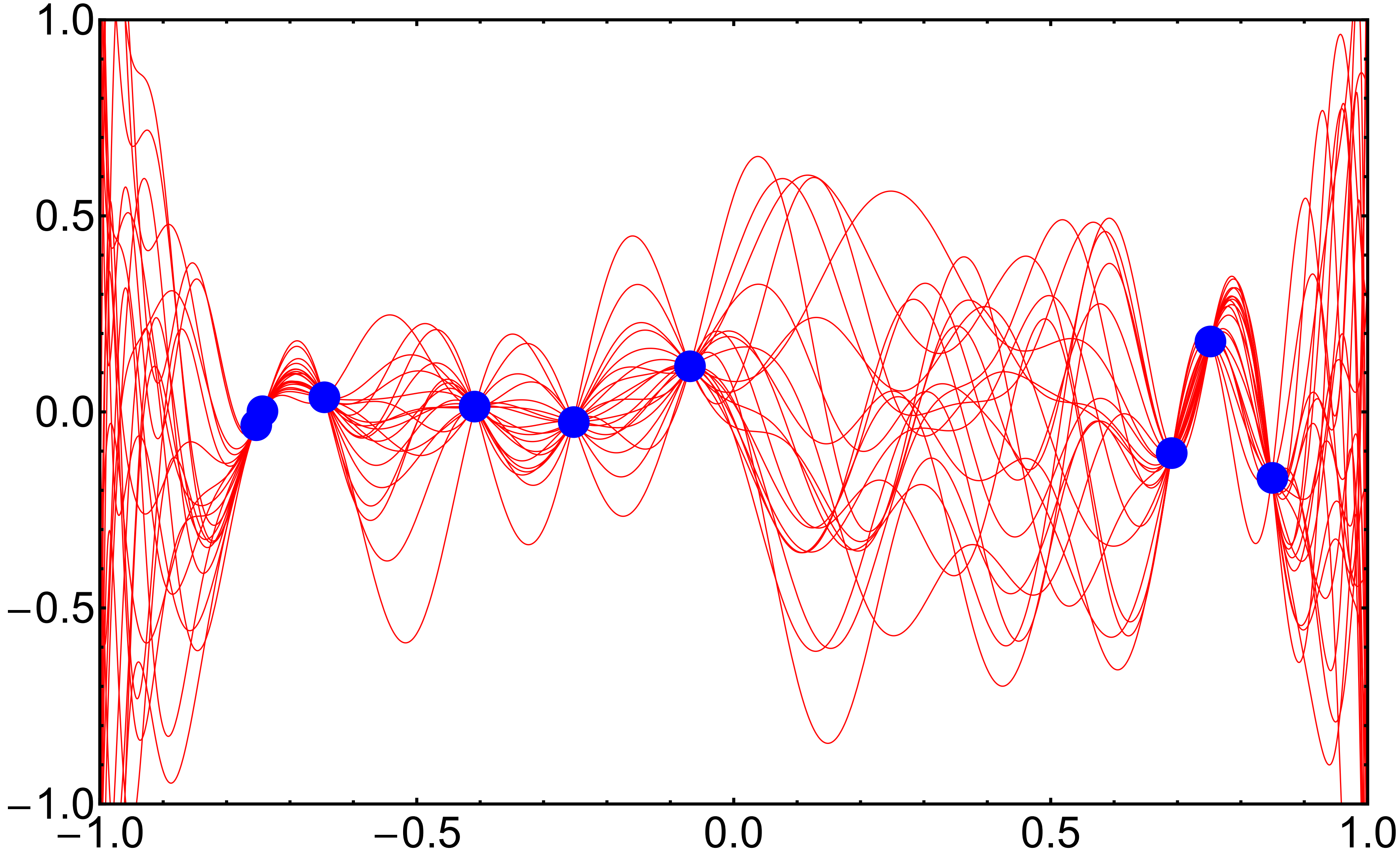
[Emmanuel J. Candès
and Michael B. Wakin]

Conventional approaches to sampling signals or images follow Shannon's celebrated theorem: the sampling rate must be at least twice the maximum frequency present in the signal (the so-called Nyquist rate). In fact, this principle underlies nearly all signal acquisition protocols used in consumer

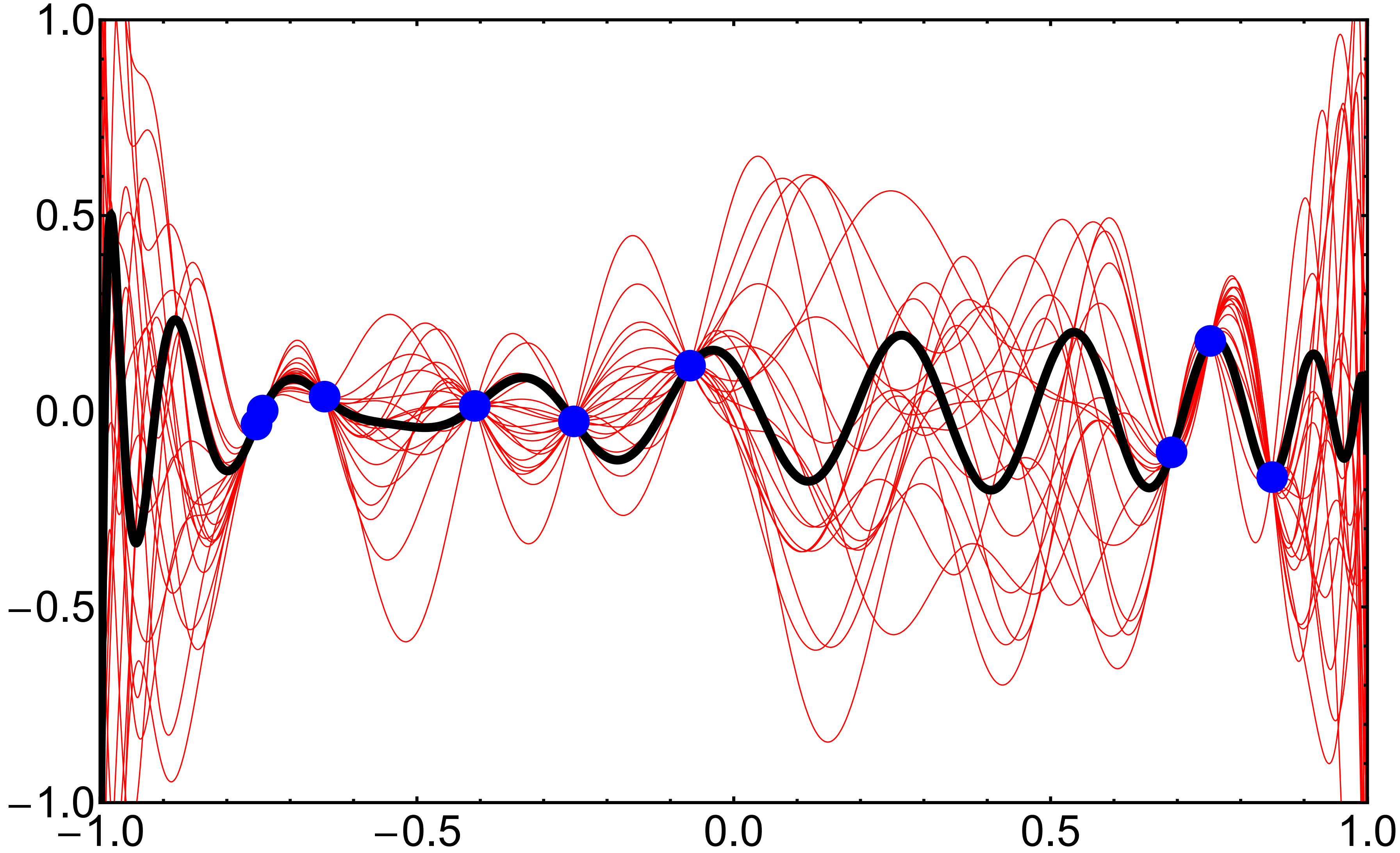
Under-determined problem: Example



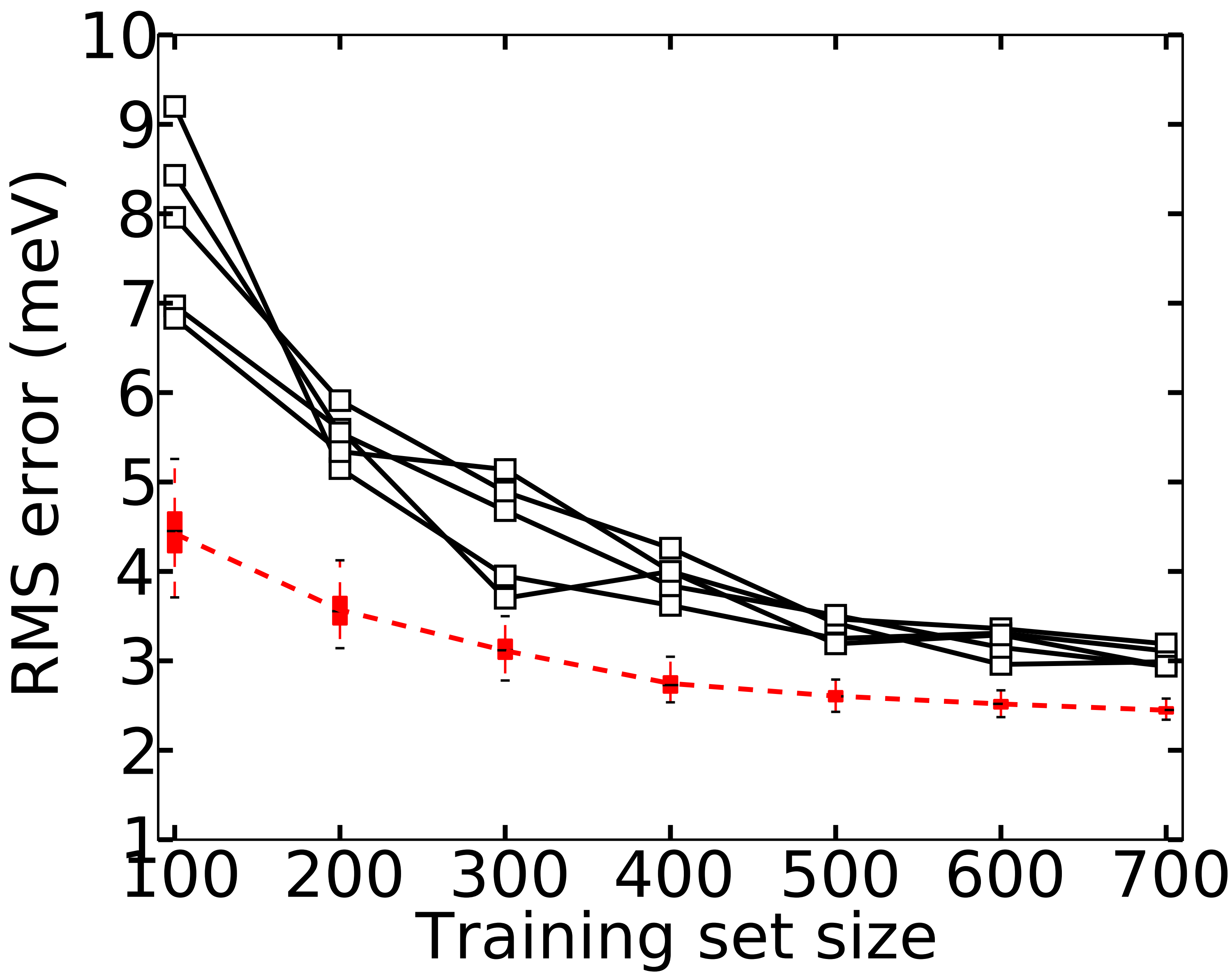
Under-determined problem: Example



Under-determined problem: Example



Bayesian Compressive Sensing vs. GA



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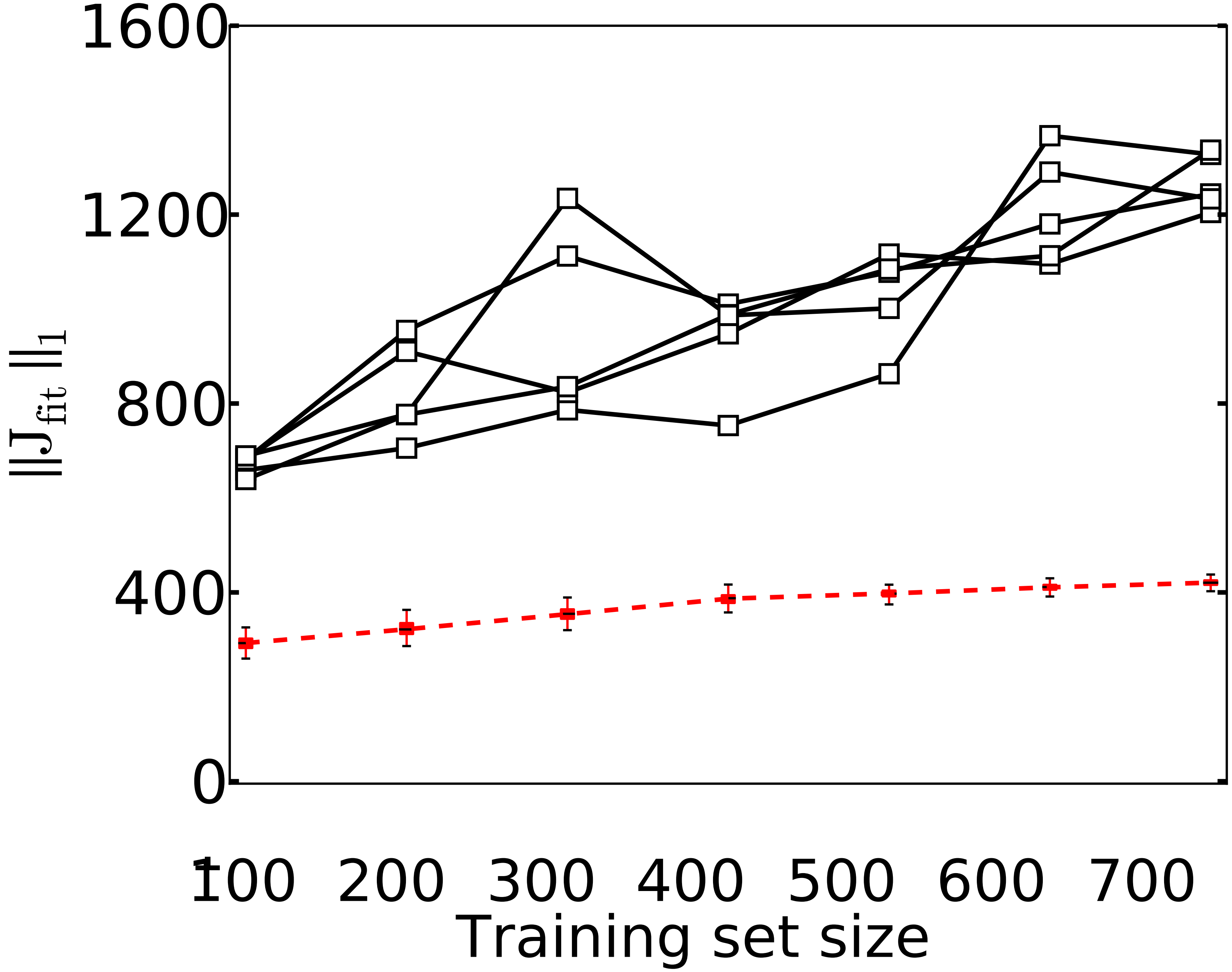

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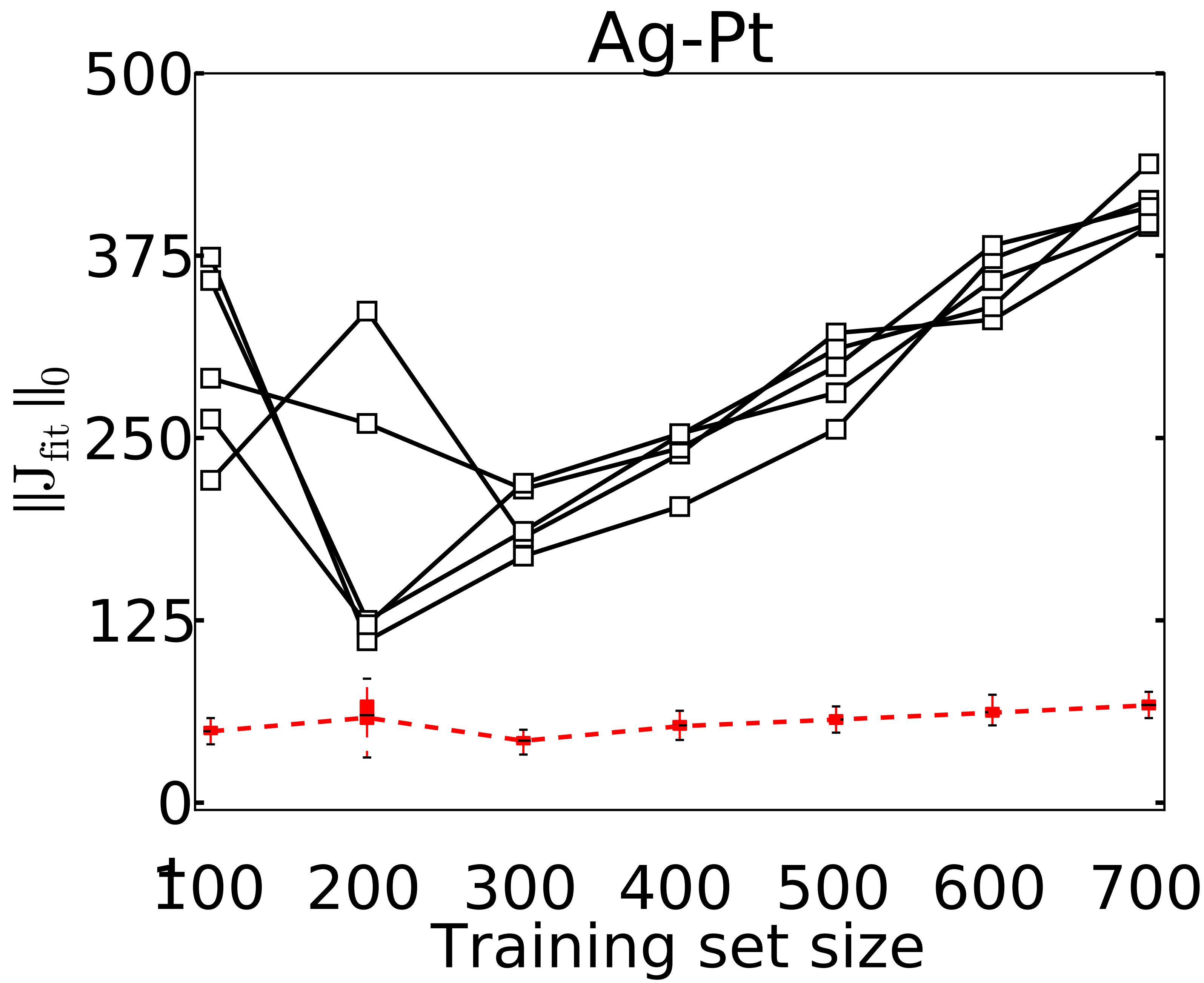

Further reading

Lance J. Nelson, Gus L. W. Hart, Fei Zhou, and Vidvuds Ozolins, "*Cluster expansion made easy with Bayesian compressive sensing,*" arXiv: 1307.2938 [cond-mat.mtrl-sci]

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