



第18回情報論的学習理論ワークショップ (IBIS2015)

The 18th Information-Based Induction Sciences Workshop

2015.11.25~28 つくば国際会議場

マテリアルズインフォマティクスの現状と将来展望

¹京都大学 工学研究科 材料工学専攻

²京都大学 構造材料元素戦略拠点(ESISM)

³ファインセラミックスセンター(JFCC) ナノ構造研究所

⁴NIMS 情報統合型物質・材料研究拠点(MI²I)

田中 功

米国のチャレンジ

the WHITE HOUSE PRESIDENT BARACK OBAMA

★★★★ THE WHITE HOUSE WASHINGTON ★★★★★

BLOG PHOTOS & VIDEO BRIEFING ROOM ISSUES the ADMINISTRATION

Home • The Administration • Office of Science and Technology Policy

Office of Science and Technology Policy

About OSTP | OSTP Blog | Pressroom | Divisions | R&D Budgets | Resource Library | NSTC | PC

Materials Genome Initiative: A Renaissance of American Manufacturing [Subscribe](#)

Posted by Tom Kalil and Cyrus Wadia on June 24, 2011 at 09:03 AM EST



2011 June

材料ゲノム：アメリカ製造業のルネサンスへ

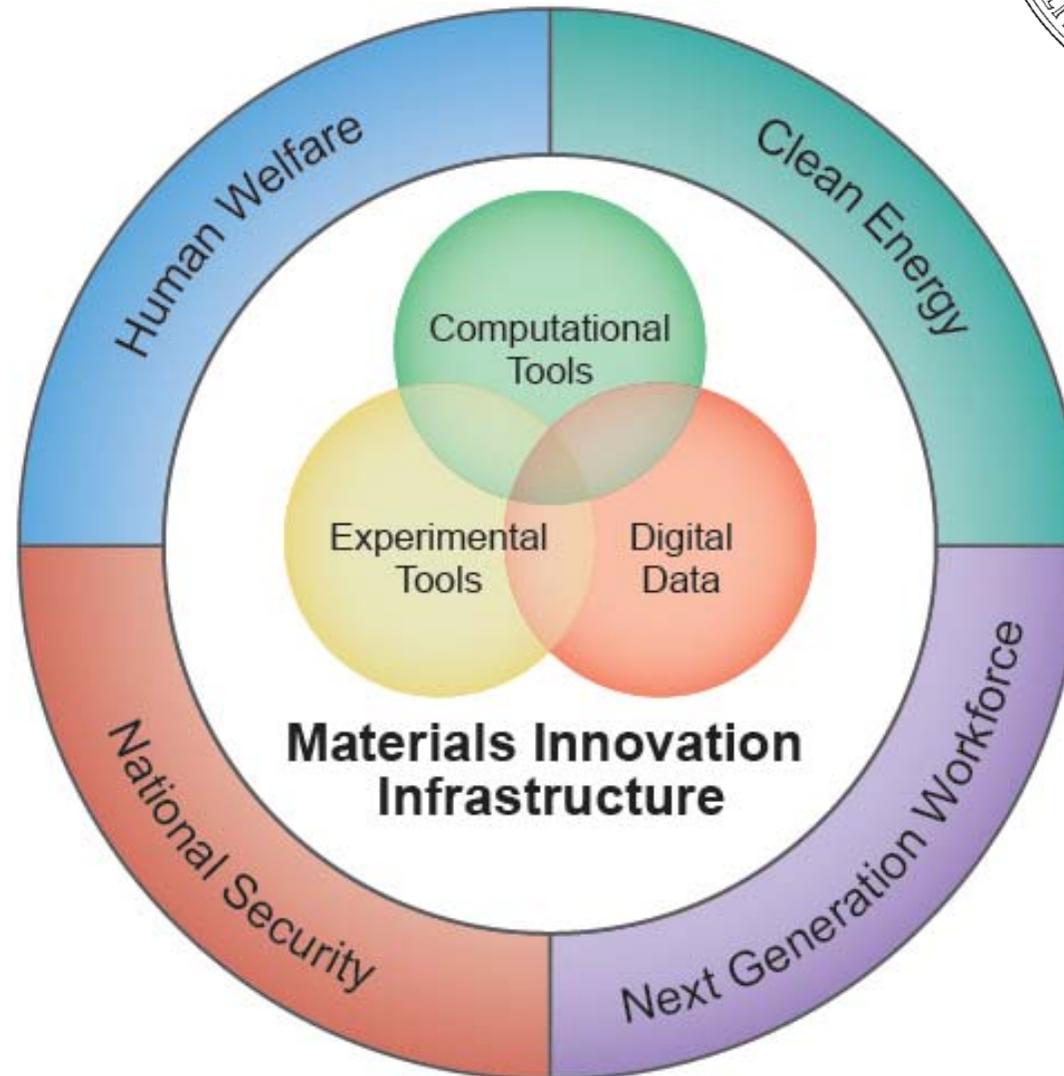
To double the speed with which we discover, develop, and manufacture new materials. **新材料の発見・開発・製品化のスピードを2倍に。**

FY12 budget includes \$100 million to launch the Materials Genome Initiative.

年間予算 1億USドル = 120億日本円

Materials Genome Initiative for Global Competitiveness

June 2011



EUのチャレンジ1



EUROPEAN CENTER OF EXCELLENCE (CoE) FOR
NOVEL MATERIALS DISCOVERY (NOMAD)

Funded by the EU Commission under the Horizon2020 programs

<http://nomad-lab.eu/>

The NOMAD CoE develops a *Materials Encyclopedia* and *Big-Data Analytics* tools for materials science and engineering. Eight complementary research groups of highest scientific standing in computational materials science along with four high-performance computer centers form the synergetic core of this CoE.



EUのチャレンジ2



Materials' Revolution: Computational Design and Discovery of Novel Materials

Swiss National Science Foundation

Vertical Projects

VP1 - Novel Materials Physics

VP2 - Novel Materials Applications



Nicola Marzari

Director
EPFL, Lausanne

Horizontal Projects

HP3 - Advanced Quantum Simulations

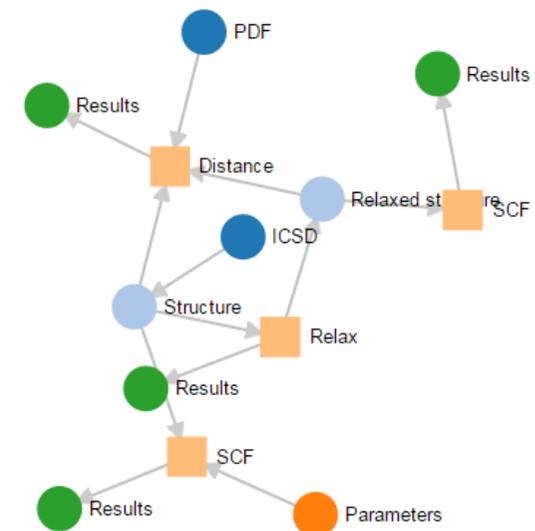
HP4 - Advanced Sampling Methods

HP5 - Materials Informatics

Platform Projects

PP6 - Informatics

PP7 - Experiments



日本のチャレンジ

2012 科学研究費・新学術領域

『ナノ構造情報』

『マテリアルズ・インフォマティクス』

2013

採択

JSTでの調査



2014

実施中



2015

NIMSイノベーションハブ 開始

JSTさきがけ開始

2016

情報統合型物質・材料研究拠点

MI²I
(情報統合型物質・材料開発イニシアティブ)

- 人材糾合
- データ科学との新たな融合
- 新しい物質・材料科学手法の開発・蓄積・普及と人材育成
- データプラットフォーム構築：情報統合型物質・材料開発手法のパッケージ化・システム化
- 産業界への有効ソリューションの短期での開発・提供

NIMS 拠点運営室

拠点長	副拠点長
寺倉 清之	小出 康夫

さきがけ

理論・実験・計算科学とデータ科学が連携・融合した先進的マテリアルズインフォマティクスのための基盤技術の構築

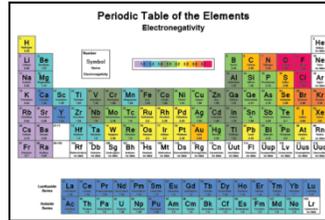
研究総括

常任 真司(東京大学 大学院理学系研究科 教授)

2017

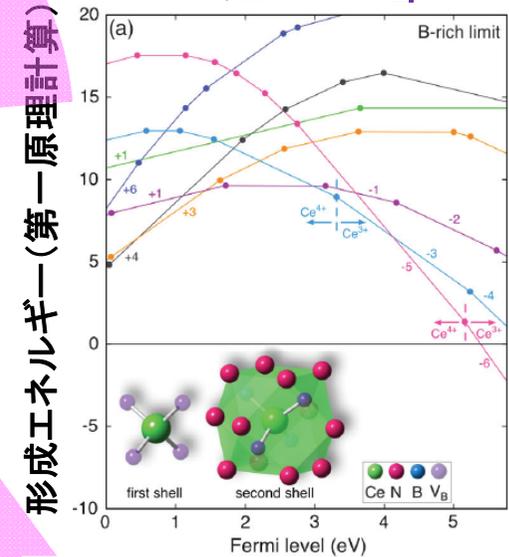
マツカワ形成メカニズムの常法

材料設計



最適化

シミュレーション



情報論的 学習理論

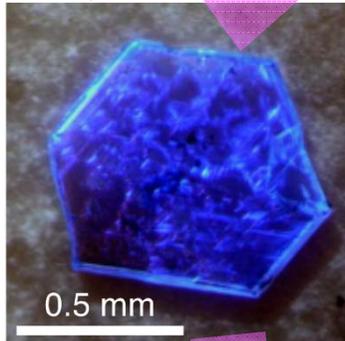
理論計算

物理法則：

古典力学，電磁気学，
熱・統計力学，量子力学
等に立脚

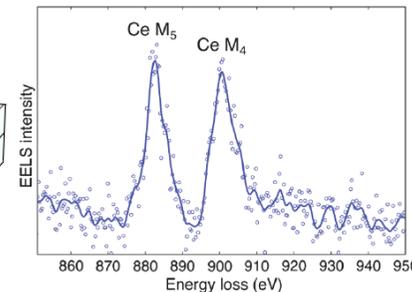
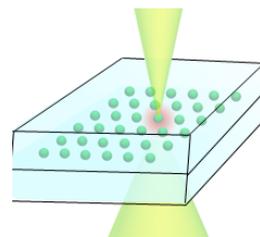
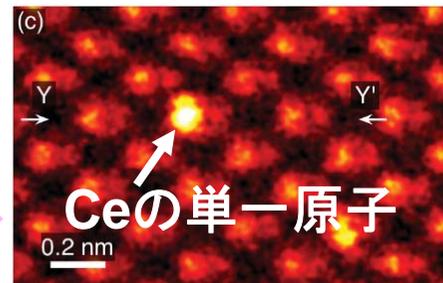
解析

合成実験



特性

解析実験



ニーズ

シーズ

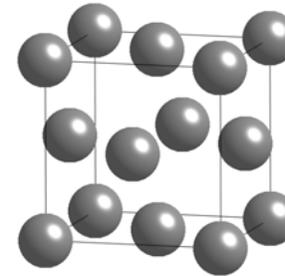


(無機)材料科学のキャストの例： 結晶性物質

A periodic table of elements. The elements from Boron (B) to Argon (Ar) in the second and third periods are highlighted in green. Aluminum (Al) is highlighted in blue. Other elements are in various colors: red, pink, light blue, dark blue, yellow, and purple.

Periodic Table

Al

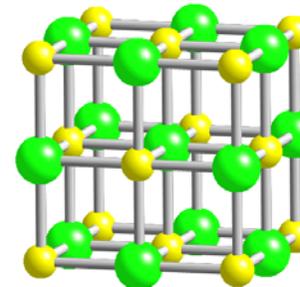


face centered cubic structure



light metal tube

NaCl

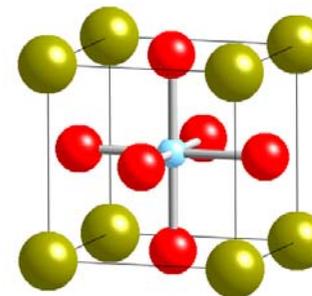


rock salt structure

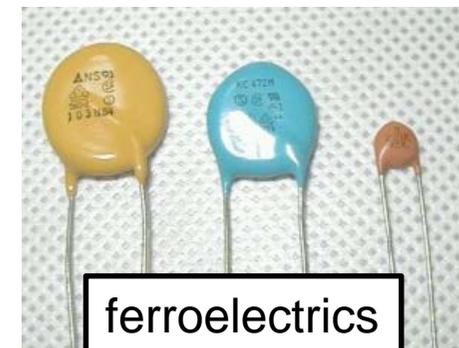


table salt

BaTiO₃



perovskite structure



ferroelectrics

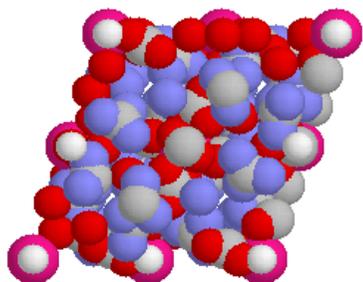
Enormous number of chemical combinations

1 2 13 14 15 16 17 18
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 Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Lr Rf Db Sg Bh Hs Mt Ds Rg Uub Uut Uuq Uup Uuh Uus Uuo
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No

Periodic Table

Number of chemical elements	Number of chemical combinations (only for simple composition ratio)
1	~100
2	~100,000
3	~10,000,000
4	~1,000,000,000

Inorganic Crystal Structure Database (ICSD)



FIZ/NIST
Inorganic
Crystal
Structure
Database

Version 1.9.6

Database 2015-1

Fachinformationszentrum,
Karlsruhe
National Institute of Standards
and Technology, Gaithersburg

Days left on license 110

Getting Structure Types

c2015 by Fachinformationszentrum Karlsruhe, and the U.S.
Secretary of Commerce on behalf of the United States. All
rights reserved.

World largest database
for **known inorganic crystals**.

177,000 crystal structures
→ 55,000 structures
excluding duplicates.

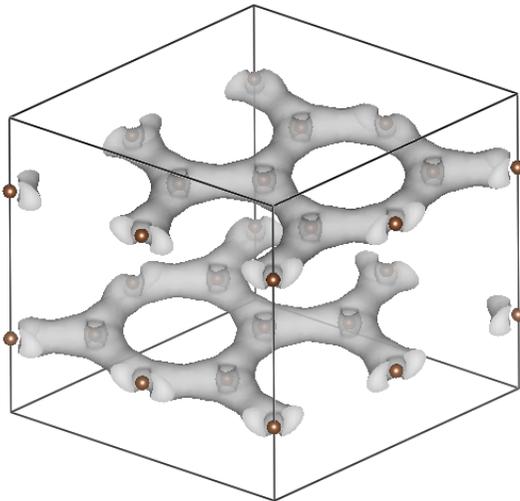
9,100 structure prototypes
(e.g. rock-salt, perovskite, ...)

Number of chemical elements	Number of structure prototypes in ICSD
1	120
2	1,700
3	4,700
4	4,300

First Principles Calculations

Useful to fill the gap between enormous number of chemical combinations and experimental database.

Electronic structure calculations entirely based on quantum theory without using empirical parameters.



Total energy

Force/Stress

Electronic/Magnetic structures

Physical properties

.....

First Principles Calculations

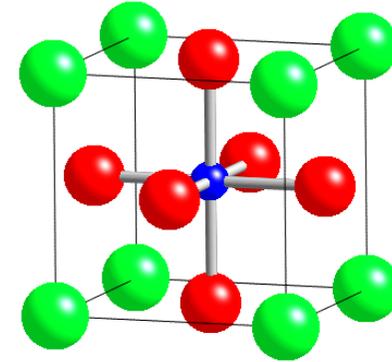
INPUT
Space Group
Unit Cell Parameters
Atoms / Atomic Number and Coordinates

Density Functional Theory Calculations

$$\left(-\frac{1}{2}\nabla^2 + V_{ion}(\vec{r}) + \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' + v_{XC}(\vec{r}) \right) \psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r})$$

OUTPUT

Total Energy
Stress / Force
Electronic Structures



SrTiO₃
(cubic perovskite)
Space Group $Pm\bar{3}m$
1 x Sr + 1 x Ti + 3 x O
= 5 atoms/unit cell

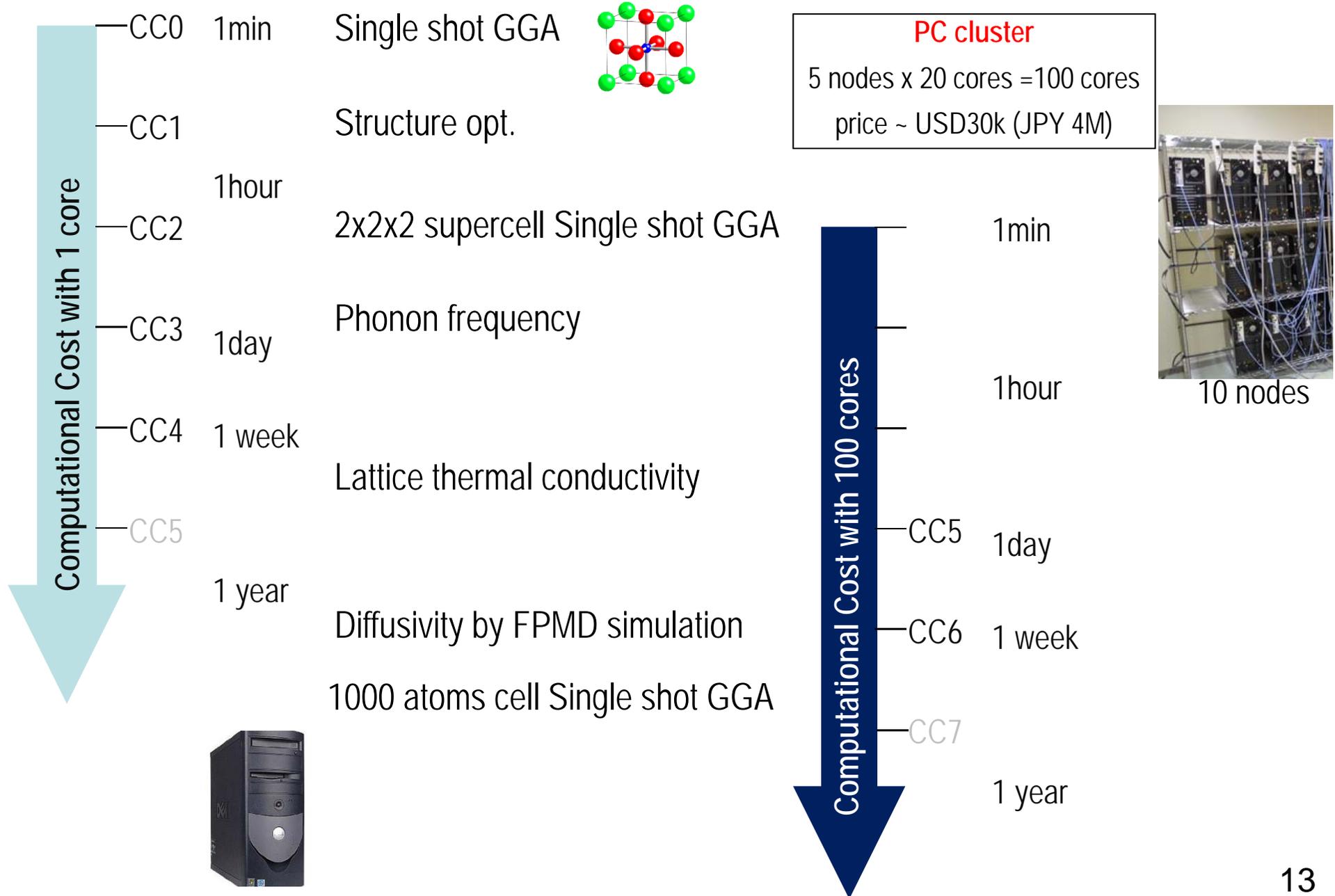
structure optimization

Computational Cost

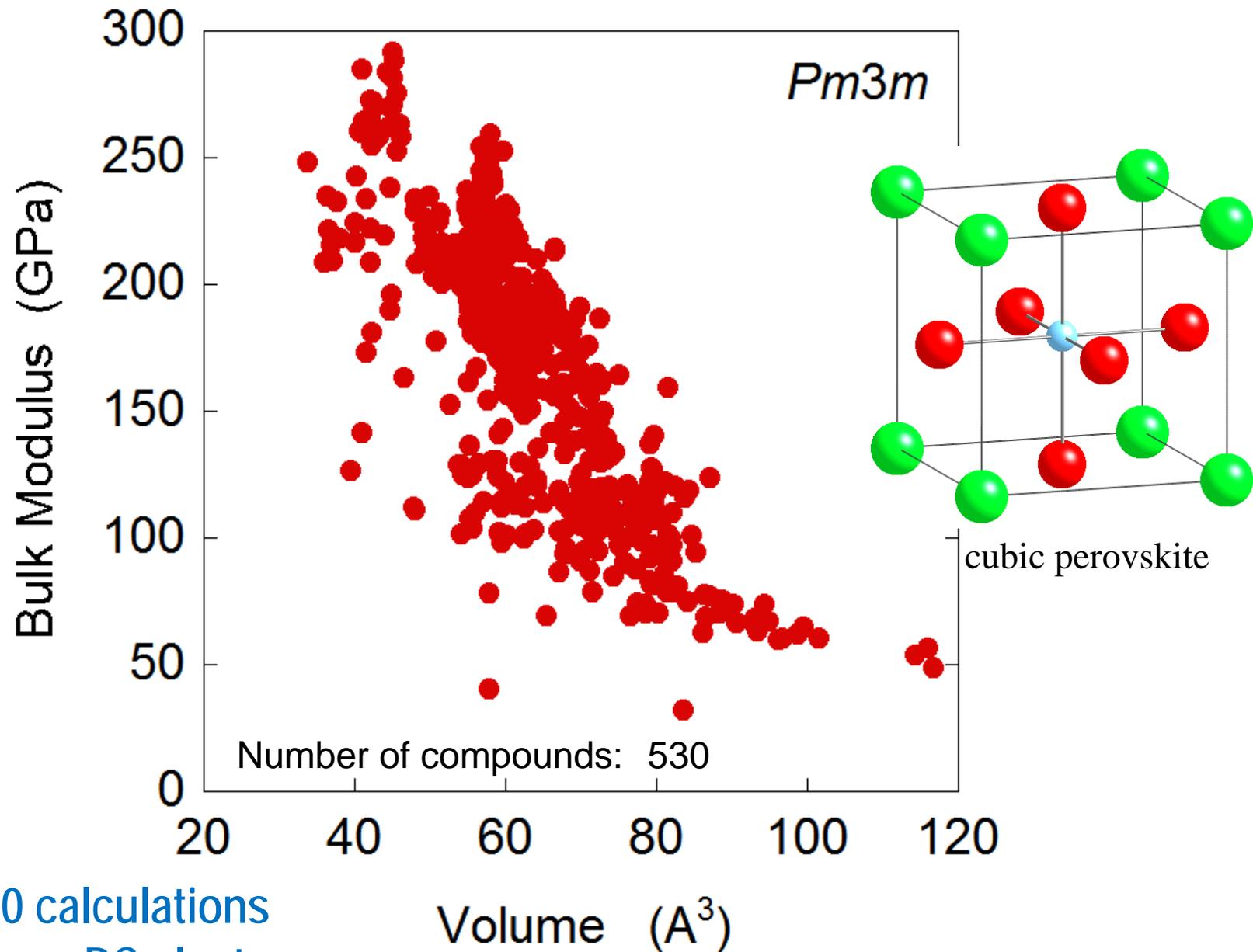
CC0 x 10 = CC1

Computational Cost 0 (CC0)

Cost for First Principles Calculations



A set of DFT calculations during a lunch break



CC1 x 530 calculations
by a 100 core PC cluster

Materials Project @MIT

<https://materialsproject.org/>

ICSD収録の構造データについて、生成エネルギーやバンドギャップなどの第一原理計算結果

The Materials Project

Harnessing the power of supercomputing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Learn more](#) [Tutorials](#) [Sign In or Register](#) to start using

Electronic Structure

Click and drag to zoom

Indirect X-F bandgap = 7.7511 eV

Density of States

sign indicates spin ↑ ↓

MATERIAL
TbF₃

Material Details

- Final Magnetic Moment: 0.0000 μ_B
- Formation Energy/Atom: -4.1520 eV
- Energy Above Hull: 0.0000 eV
- Density: 7.16 g/cm³
- Space Group: Hermann Mauguin Pbnm, Hall -P 2c 2ab

EXPLORE MATERIALS
Search for materials information by chemistry, composition, or property

EXPLORE BATTERIES
Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

VISUALIZE STABILITY
Generate phase and pourbaix diagrams to find stable phases and study reaction pathways

INVENT STRUCTURES
Design new compounds with our structure editor and substitution algorithms

CALCULATE
Calculate the enthalpy of 10,000+ reactions and compare with experimental values

Database Statistics

58251	41831	1766
COMPOUNDS	BANDSTRUCTURES	ELASTIC TENSORS

Materials Project @MIT

<https://materialsproject.org/>

ICSD収録の構造データについて、生成エネルギーやバンドギャップなどの第一原理計算結果

The screenshot displays the Materials Project search interface. On the left is a sidebar with search filters: 'Imareite' in the search bar, 'Submit' button, 'Band Gap (eV)' slider (1 to 10), 'Energy Above Hull' slider (0), 'Formation Energy' slider (-27 to -0.1), '# unit cell sites' slider (2), 'Density' slider (0 to 12.8), 'Volume' slider (7 to 2233), 'Crystal Systems' dropdown (Any), and 'Has bandstructure' checkbox. Below these are navigation links: BATTERY PROPERTIES, PHASE DIAGRAM, POURBAIX DIAGRAM, CALCULATE RXN, STRUCTURE EDITOR, PREDICT STRUCTURE, THERMO, and COMPARE ELEMENTS.

The main area features a periodic table with elements highlighted in green (Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La-Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Ac-Lr, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr). Below the table are filter buttons: Band Gap, E Above Hull, Formation Energy Per Atom, Nsites, Density, and Volume. A '50 records per page' dropdown and a 'Batch Structures' button are also present. On the right are 'Show / hide columns', 'Copy', 'Print', and 'Export' buttons.

Materials Id	Formula	Spacegroup	Formation Energy (eV)	E Above Hull (eV)	Band Gap (eV)	Nsites	Density (gm/cc)	Volume	
mp-1216	YbO	Fm $\bar{3}$ m	-3.649	0	3.46	2	11.723	26.777	<input type="checkbox"/>
mp-2624	AlSb	F $\bar{4}$ 3m	-0.164	0	1.227	2	4.078	60.561	<input type="checkbox"/>
mp-22905	LiCl	Fm $\bar{3}$ m	-2.107	0	6.25	2	2.058	34.202	<input type="checkbox"/>
mp-23259	LiBr	Fm $\bar{3}$ m	-1.548	0	4.923	2	3.442	41.899	<input type="checkbox"/>
mp-1087	SrS	Fm $\bar{3}$ m	-2.151	0	2.497	2	3.566	55.732	<input type="checkbox"/>
mp-1479	BP	F $\bar{4}$ 3m	-0.412	0	1.243	2	2.953	23.5	<input type="checkbox"/>
mp-1265	MgO	Fm $\bar{3}$ m	-3.071	0	4.445	2	3.471	19.279	<input type="checkbox"/>
mp-1000	BaTe	Fm $\bar{3}$ m	-1.789	0	1.593	2	4.938	89.091	<input type="checkbox"/>
mp-13031	MgSe	F $\bar{4}$ 3m	-1.255	0	2.548	2	3.175	54.014	<input type="checkbox"/>
mp-2667	CsAu	Pm $\bar{3}$ m	-0.327	0	1.024	2	6.514	84.089	<input type="checkbox"/>
mp-22702	LiF	Fm $\bar{3}$ m	-0.482	0	0.084	2	0.044	16.208	<input type="checkbox"/>

Discovery of new low thermal conductivity materials

First-Principles Anharmonic Lattice-Dynamics Calculations and Bayesian Optimization



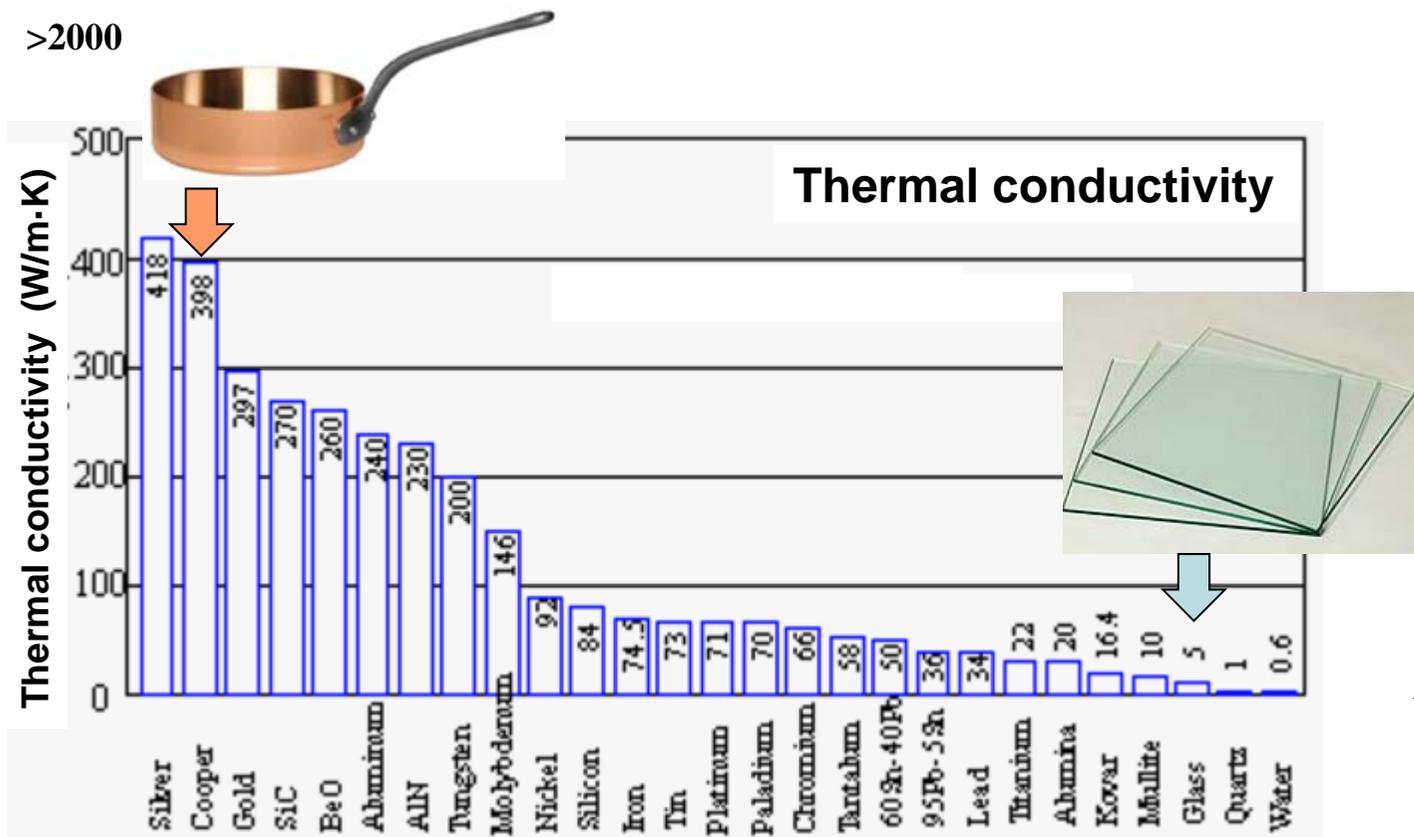
Atsuto Seko, Atsushi Togo, Hiroyuki Hayashi,

Koji Tsuda, Laurent Chaput, and IT

Discovery of ultra-low thermal conductivity materials of 0.1 W/m·K level in ICSD database (55,000 crystals)



diamond
>2000



Background

Thermal Conductivity (TC)

$$\kappa = \kappa_{\text{electronic}} + \kappa_{\text{lattice}}$$

Lattice Thermal Conductivity (LTC)

- ✓ Reliable experimental dataset is limited (< 100 crystals).
- ✓ Reliable first principles calculations are **very expensive**.
(**CC5 class** : 1 day/100 cores for 1 simple crystal.)
- ✓ Little knowledge to predict LTC deductively.
(Chemistry-structure-LTC relationships are not clear.)

Materials search has been made through “modification” of known compounds showing high/low LTC.

Thermoelectric materials

Essential for utilizing otherwise waste heat.

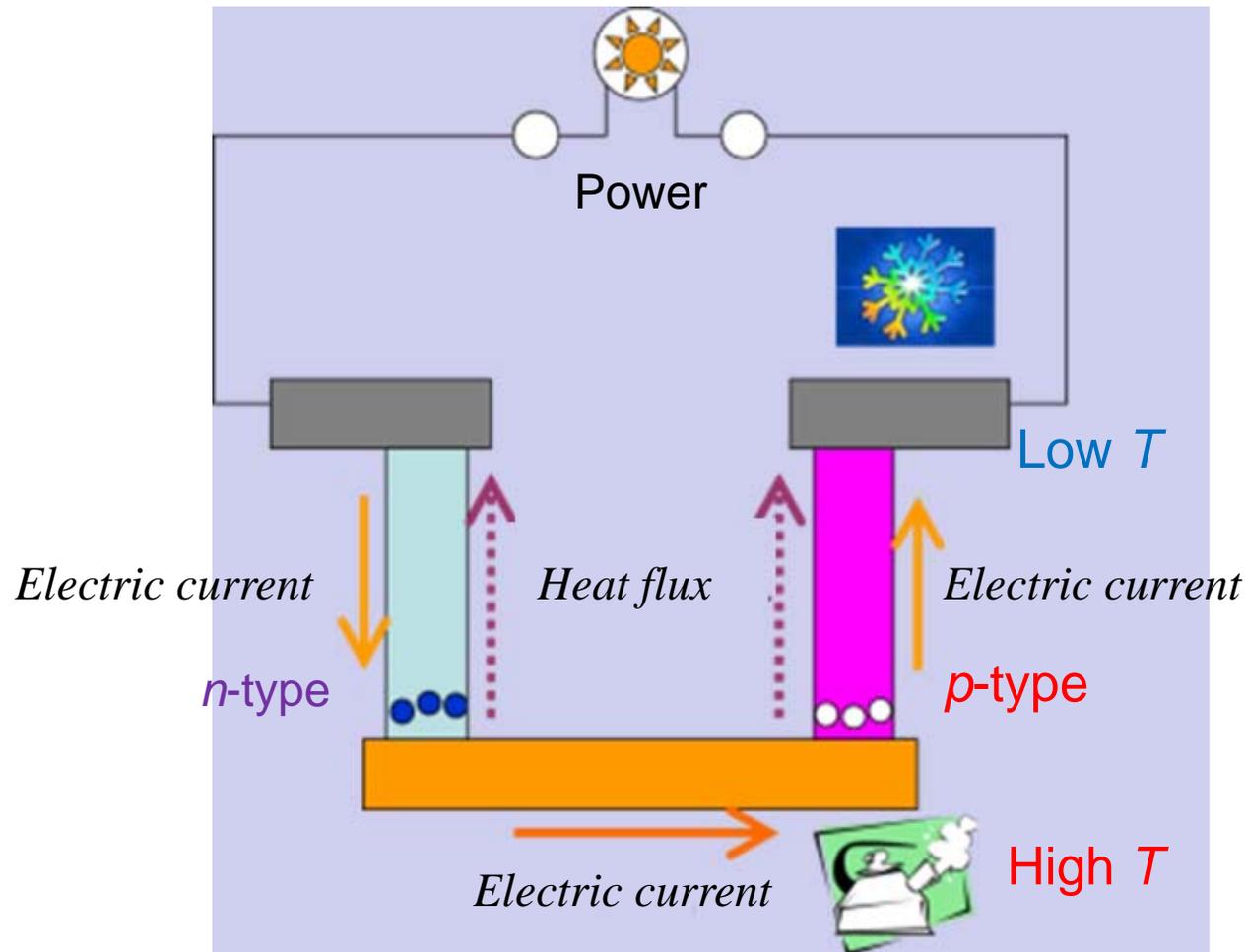


Figure of Merit

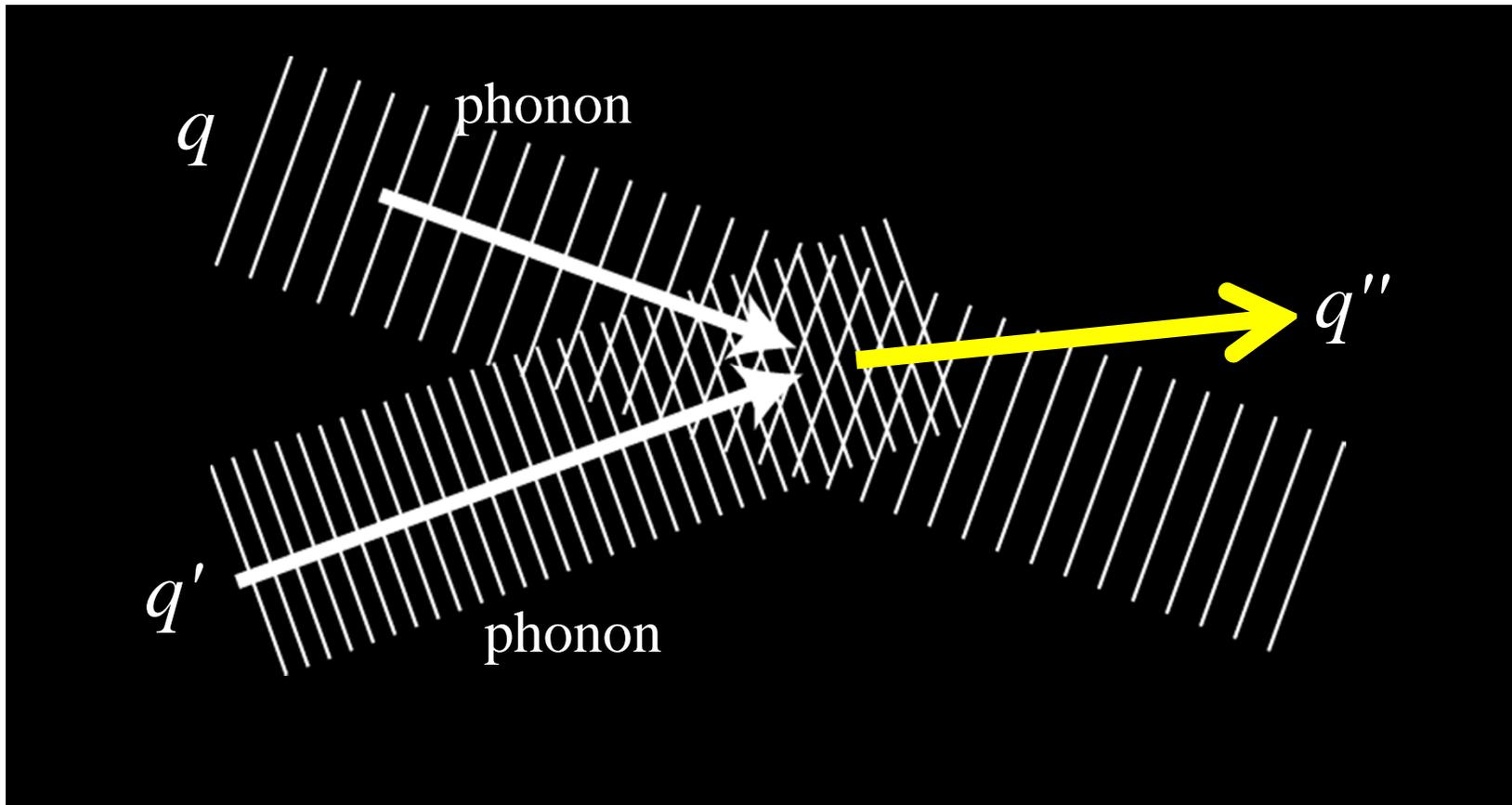
$$ZT = \frac{S^2 \sigma}{\kappa} T$$

S : Seebeck coefficient
 σ : electrical conductivity
 κ : **thermal conductivity**

Physical origin of thermal resistivity

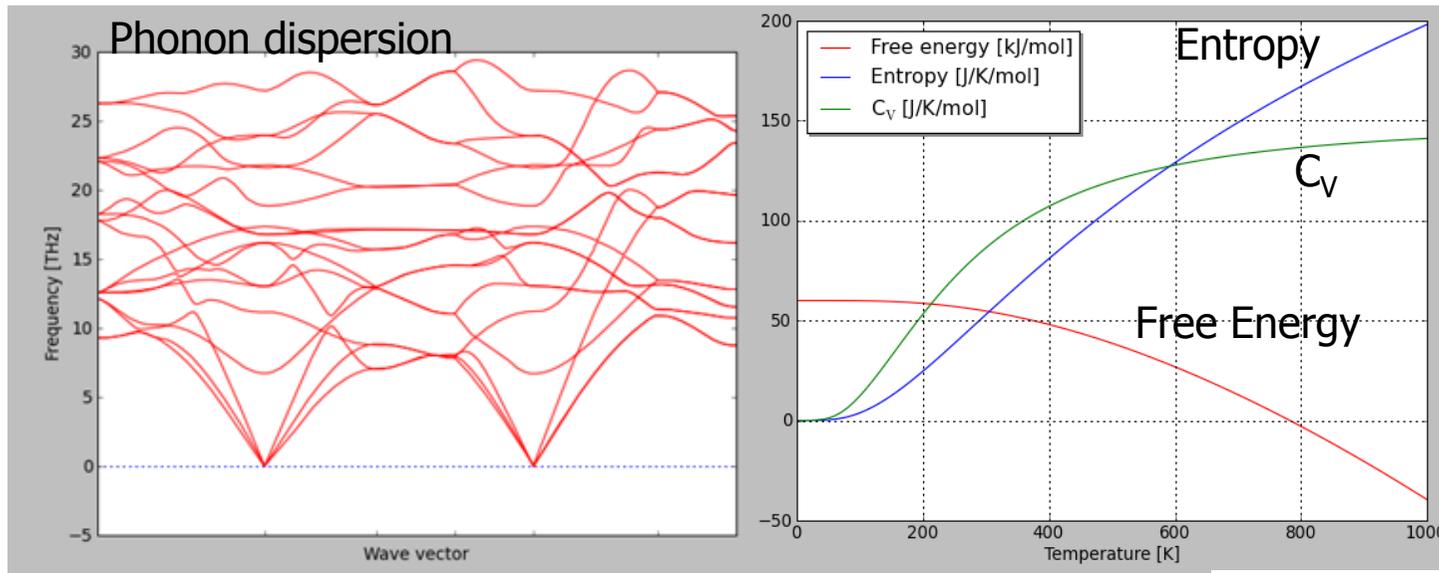
Phonon-phonon scattering (phonon anharmonicity)

Harmonic phonons do not interact.

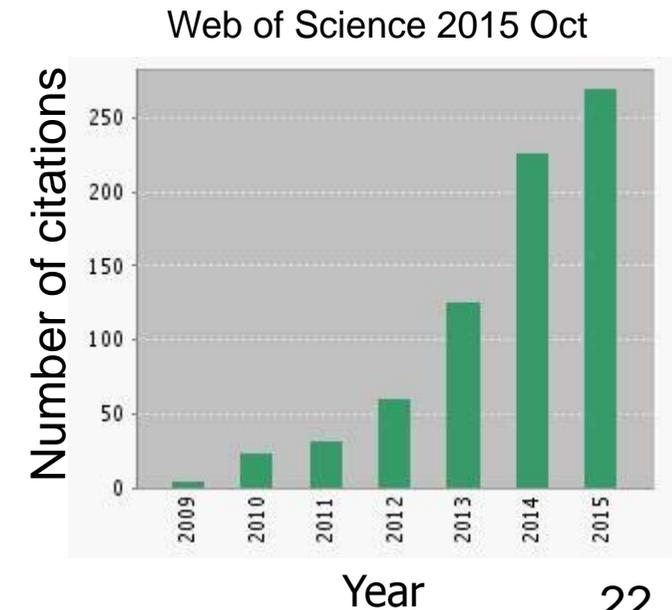
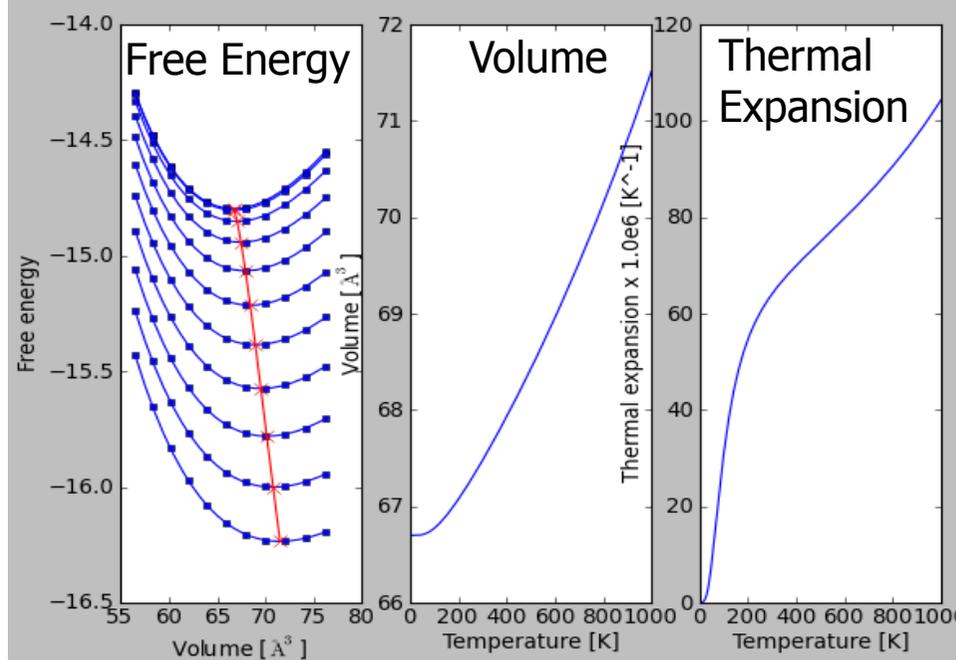


phonopy: open source for ab-initio phonon calcs

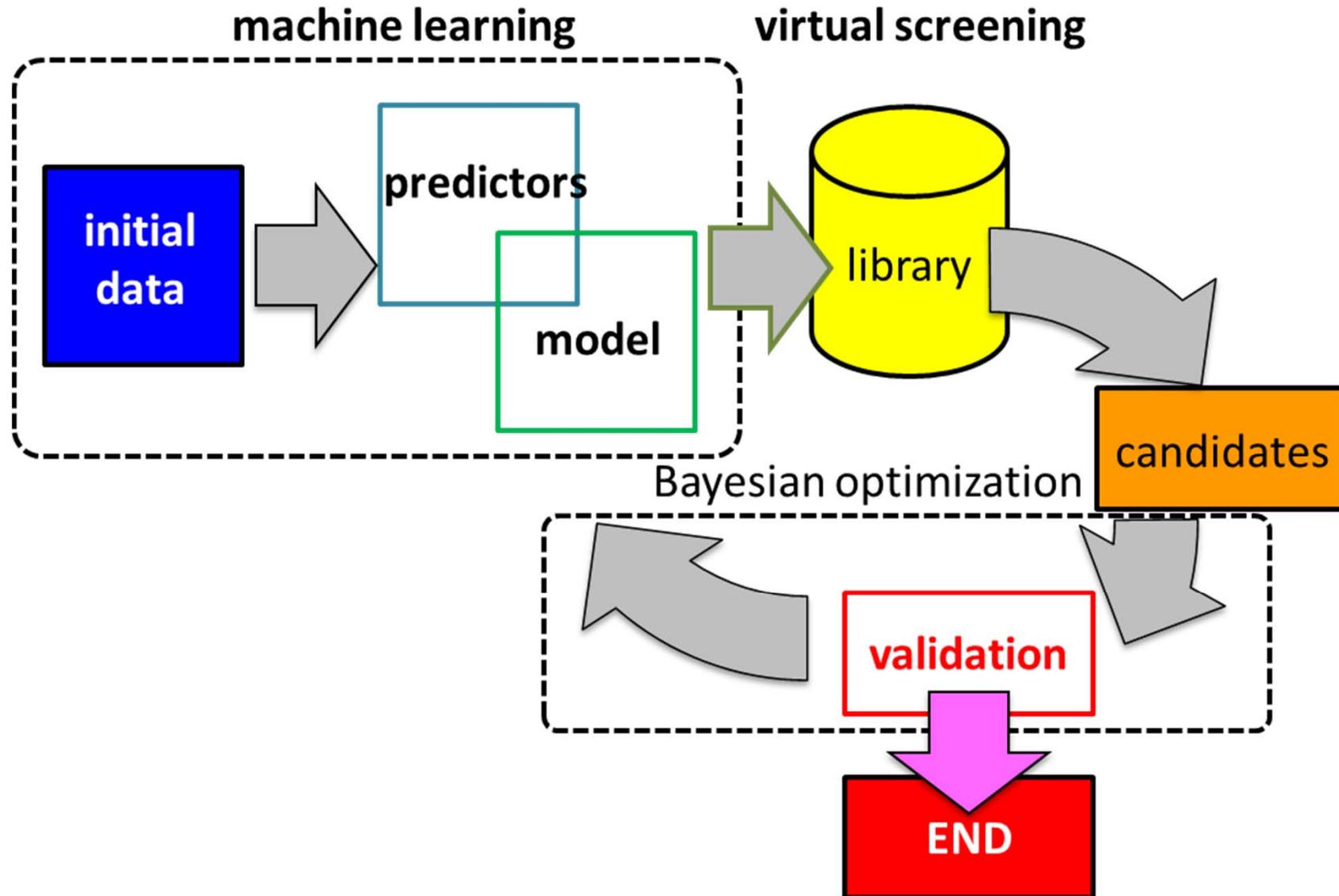
<http://phonopy.sf.net/>



Atsushi TOGO
Kyoto Univ.

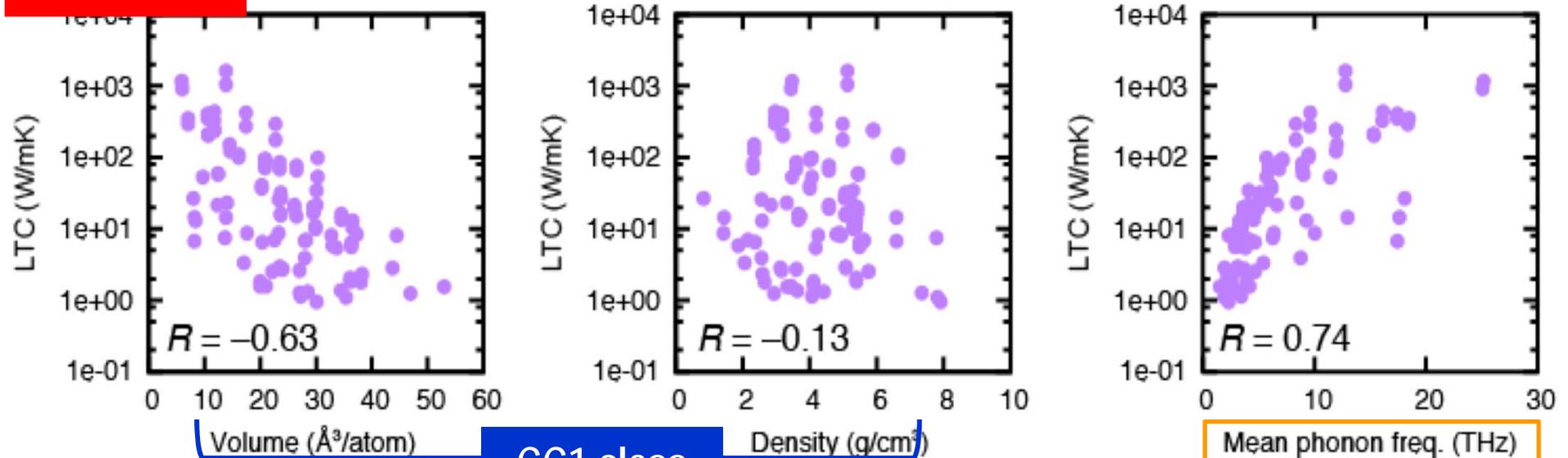


Virtual Screening

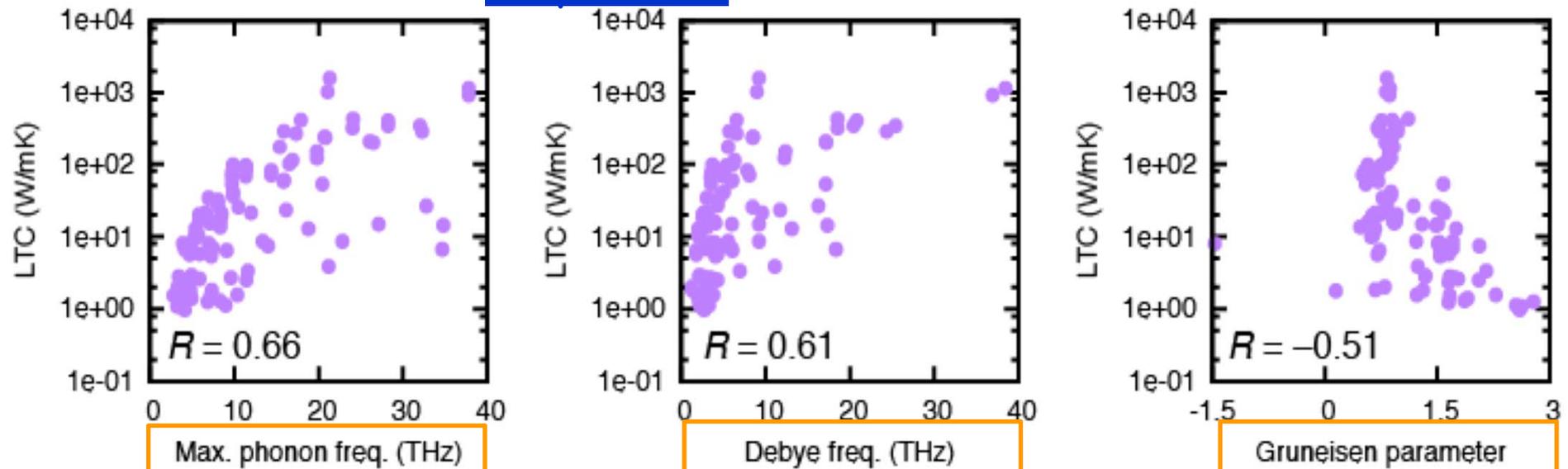


Correlations between LTC and predictors

CC5 class



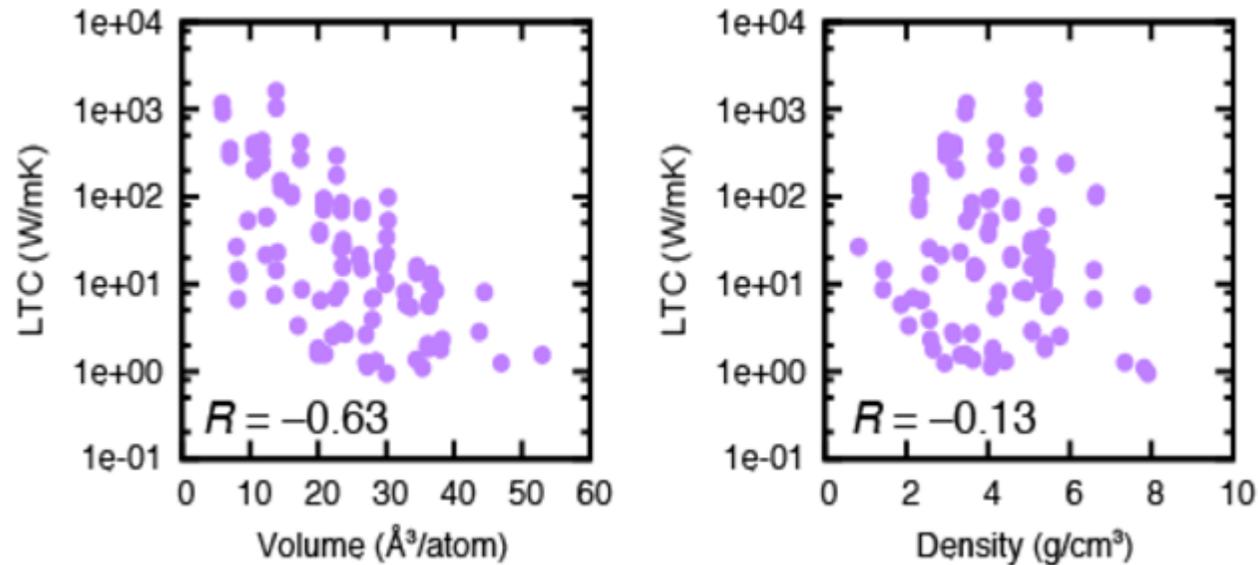
CC1 class



CC3 class

Candidates of descriptors for LTC

Model 1: Volume V and Density ρ



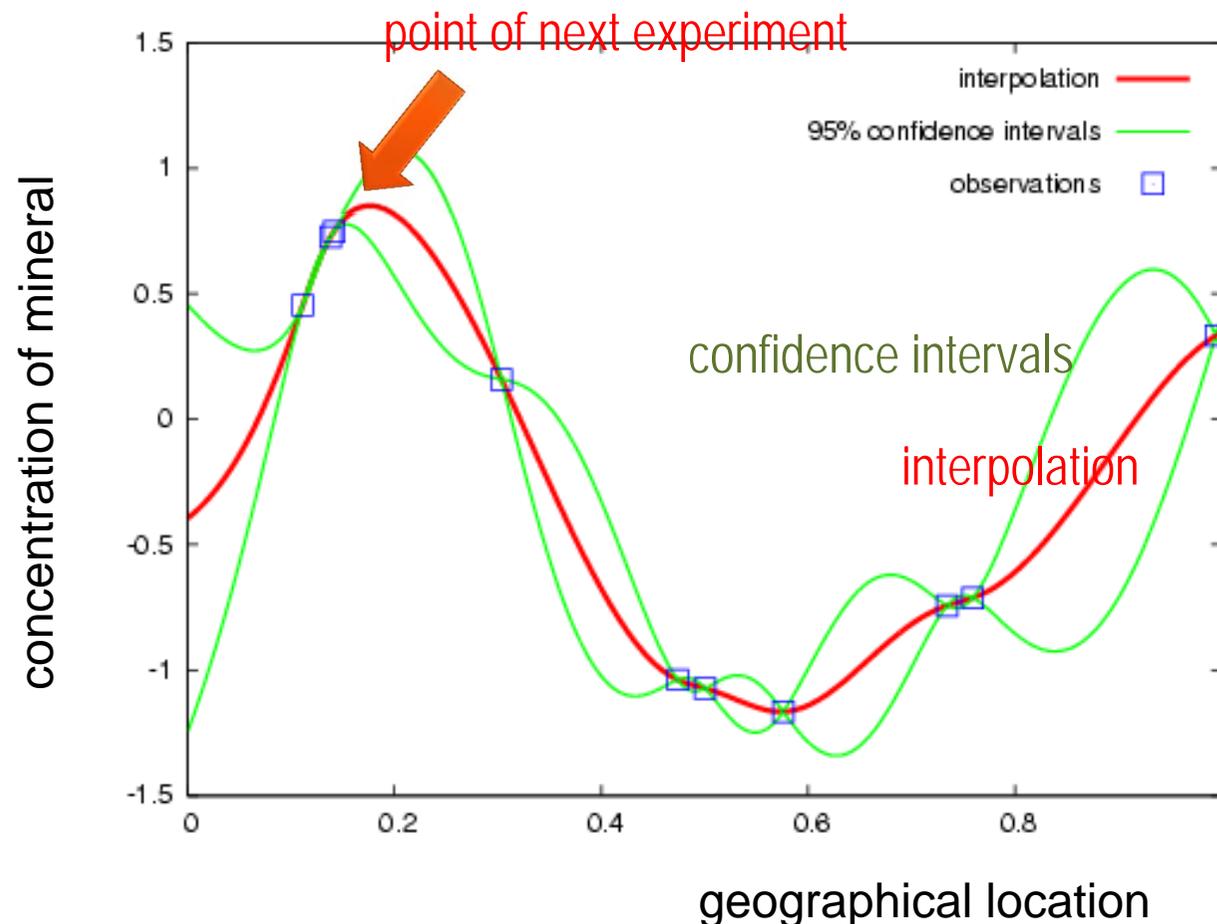
Model 2: Model 1 + primitive elemental descriptors

	H	Li	Be	B	C	N	O	F	...
LiH	1	1	0	0	0	0	0	0	
LiF	0	1	0	0	0	0	0	1	
BeO	0	0	1	0	0	0	1	0	
BN	0	0	0	1	0	1	0	0	
...									

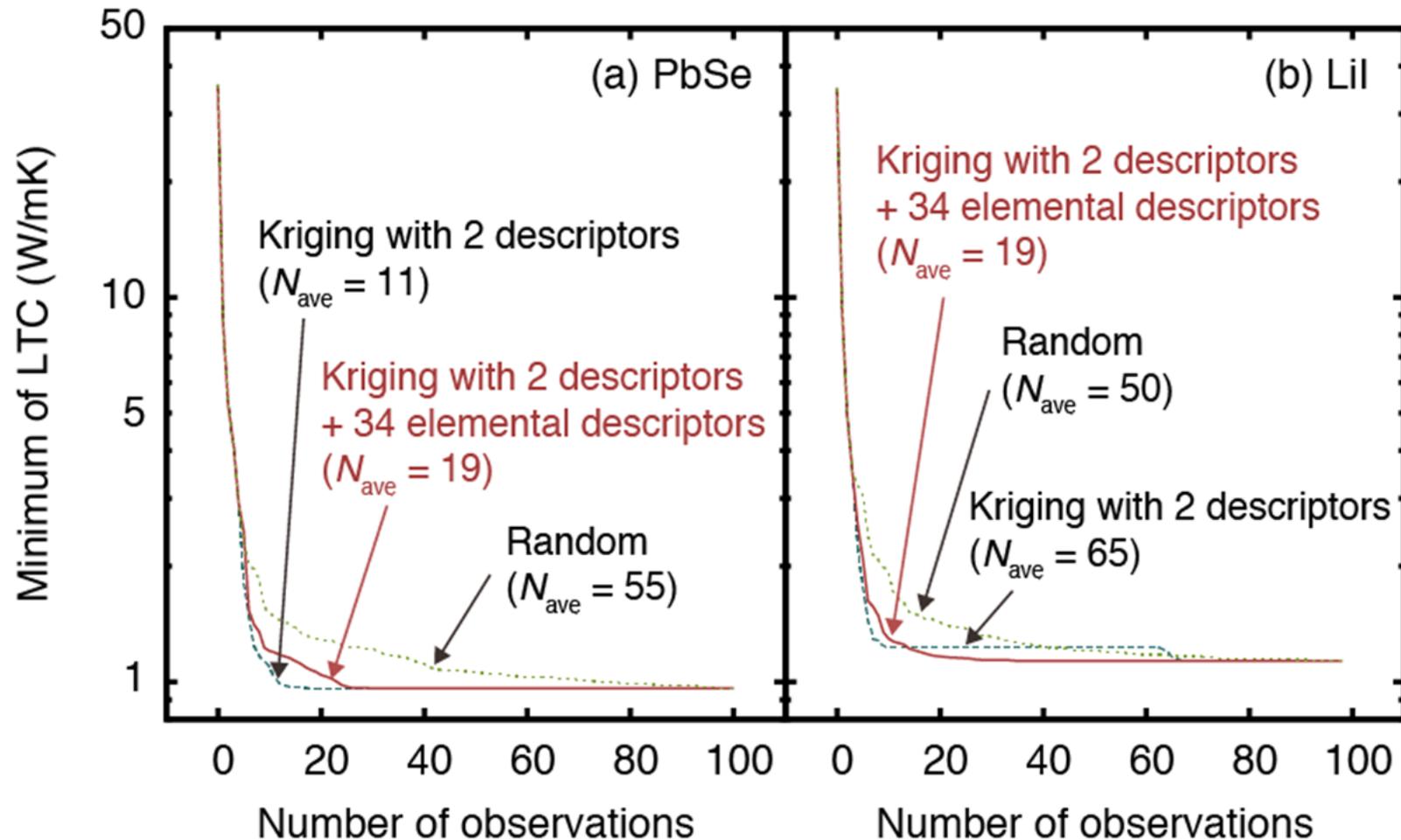
Toward discovery of new low LTC materials

Kriging

Interpolation method for which the interpolated values are modeled by a Gaussian process governed by prior covariances, originally from geo-statistics.



Kriging using 101 ab-initio LTC data



First prediction was made using $N_0 (=5)$ LTC data and GPR.

Use of 34 elemental descriptors on top of V and ρ is found to be effective to overcome an outlier problem.

Ranking of LTC for 54,779 compounds in ICSD library

Z-score

“Virtual screening”

$$Z(x^*) = [f(x^*) - f_{\text{best}}] / \sqrt{v(x^*)}$$

$$f = -\log \kappa_L$$

The higher Z-score, the lower predicted LTC !

	Materials Id	Formula	Z-score
1	mp-23517	RbPbI3	1.90
2	mp-571465	PbI2	1.76
3	mp-28564	Rb4PbBr6	1.56
4	mp-23053	PbI2	1.56
5	mp-22997	PbBrCl	1.56
6	mp-23043	RbPb2Br5	1.45
7	mp-22883	PbI2	1.44
8	mp-567503	PbI2	1.43
9	mp-540839	CsPbI3	1.40
10	mp-569595	PbI2	1.34
11	mp-567246	PbI2	1.34
12	mp-23436	Cs4PbBr6	1.34
13	mp-505148	ThPbI6	1.34
14	mp-22893	PbI2	1.34
15	mp-567199	PbI2	1.32
16	mp-580202	PbI2	1.32
17	mp-600089	CsPbBr3	1.31
18	mp-640058	PbI2	1.31
19	mp-574189	PbI2	1.30
20	mp-567542	PbI2	1.30
21	mp-540789	PbI2	1.30
22	mp-567178	PbI2	1.29
23	mp-567629	CsPbBr3	1.29
24	mp-672671	PbI2	1.28
25	mp-561320	PbS	1.27
26	mp-680205	PbI2	1.25
27	mp-29883	Rb3PbCl5	1.25
28	mp-567681	CsPbBr3	1.24
29	mp-608081	Rb3Pb4Au	1.18
30	mp-27552	TlPbI3	1.17
31	mp-674972	Rb6Pb5Cl16	1.15
32	mp-31508	KPb2Br5	1.15
33	mp-771814	CaPbI6	1.14

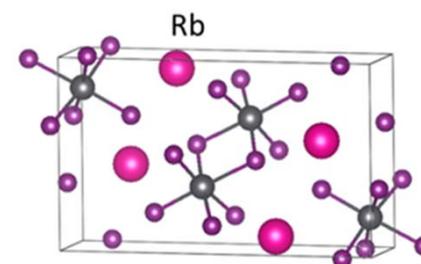
	Materials Id	Formula	Z-score
34	mp-23037	CsPbCl3	1.14
35	mp-675524	CsPbCl3	1.14
36	mp-675022	CsPbCl3	1.14
37	mp-23475	Rb2PbCl6	1.13
38	mp-29212	Tl4PbI6	1.12
39	mp-581775	Cs5(KPb6)3	1.09
40	mp-23380	Tl3PbI5	1.08
41	mp-630851	Cs3NaPb4	1.07
42	mp-574070	Cs4Pb9	1.05
43	mp-674339	Tl6PbI10	1.04
44	mp-23425	Cs2PbCl6	1.03
45	mp-771691	CaPbI6	1.01
46	mp-756313	CaPbI4	0.99
47	mp-673703	Rb3Bi7Pb3(IO)10	0.99
48	mp-680463	Rb4Pb9	0.97
49	mp-755943	CaPbI4	0.96
50	mp-622294	Hg2Pb(SBr)2	0.96
51	mp-21525	RbPb	0.96
52	mp-571638	Rb2Cu(BrCl)2	0.90
53	mp-756136	CaPbI4	0.90
54	mp-31317	La3PbI3	0.88
55	mp-756451	CaPbI4	0.88
56	mp-753670	CaPbI4	0.87
57	mp-569879	Cs2Ta6PbCl18	0.86
58	mp-570753	Tl3PbBr5	0.86
59	mp-27451	Tl3PbBr5	0.85
60	mp-569238	Cs3LiI4	0.85
61	mp-755977	CaPbI4	0.84
62	mp-680159	CsTa6PbCl18	0.84
63	mp-557719	PbS	0.82
64	mp-755056	CaPbI4	0.82
65	mp-771827	Ca3Pb3I14	0.81
66	mp-754540	CaPbI4	0.81

	Materials Id	Formula	Z-score
67	mp-622106	Ba5Pb3	0.81
68	mp-771877	Ca3Pb3I14	0.80
69	mp-621612	AgPb2Br5	0.80
70	mp-21246	Ba2Pb	0.78
71	mp-37163	Ag2HgI4	0.78
72	mp-569465	Cs2Nb6PbCl18	0.77
73	mp-554116	BaPb2BrF5	0.76
74	mp-674993	KPb2Cl5	0.73
75	mp-607267	KPb2Cl5	0.72
76	mp-3	Cs	0.71
77	mp-27662	CsI2Br	0.71
78	mp-20136	BaPb	0.70
79	mp-573579	Cs	0.70
80	mp-672241	Cs	0.70
81	mp-11832	Cs	0.70
82	mp-1	Cs	0.69
83	mp-639727	Cs	0.69
84	mp-569225	Mo6PbI14	0.67
85	mp-541112	ZrI4	0.66
86	mp-28077	PbBr2	0.66
87	mp-569866	Cs6K7	0.64
88	mp-31288	La5Pb3I	0.64
89	mp-554245	BaPb2IF5	0.64
90	mp-613652	PbClF	0.63
91	mp-5811	CsPbF3	0.61
92	mp-570355	PbCl4	0.61
93	mp-20282	CsPbF3	0.60
94	mp-579536	CsCu2ICl2	0.60
95	mp-22969	PbIF	0.59
96	mp-559470	AgPbBrO	0.58
97	mp-674359	Tl3PbCl5	0.58
98	mp-30519	Tl3PbCl5	0.58
99	mp-23066	Pb5(SI3)2	0.56

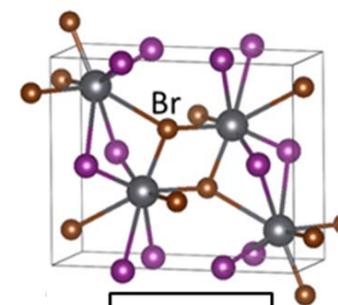
Top 10 lowest LTC compounds among 54,779

Virtual screening of 54,779 compounds in MPD library

ranking	Z-score	compound	
		formula	space group
1	1.90	PbRbI ₃	<i>Pnma</i>
2	1.76	PbI ₂ Br	<i>Pnma</i>
3	1.56	PbRb ₄ Br ₆	<i>R-3c</i>
4	1.56	PbI ₂ Cl	<i>Pnma</i>
5	1.56	PbCl ₂ Br	<i>Pnma</i>
7	1.44	PbI ₂	<i>R-3m</i>
8	1.43	PbI ₂	<i>P63mc</i>

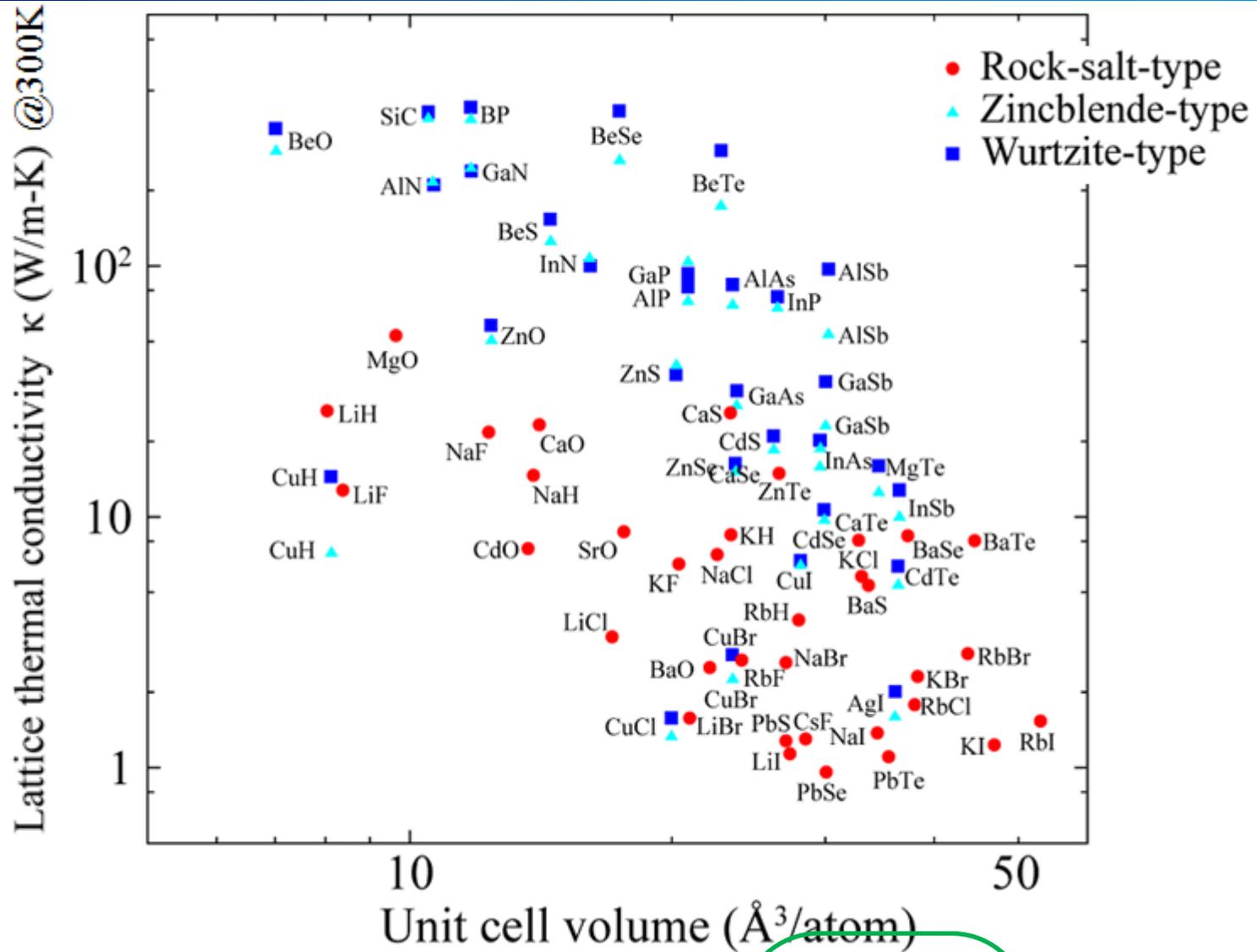


RbPbI₃

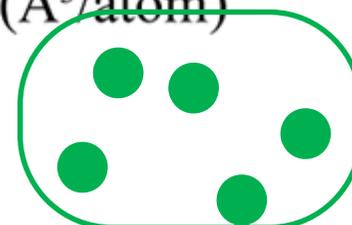


PbI₂Br

Lattice Thermal Conductivity (LTC)



Newly discovered !!



Thermoelectric materials

Essential for utilizing otherwise waste heat.

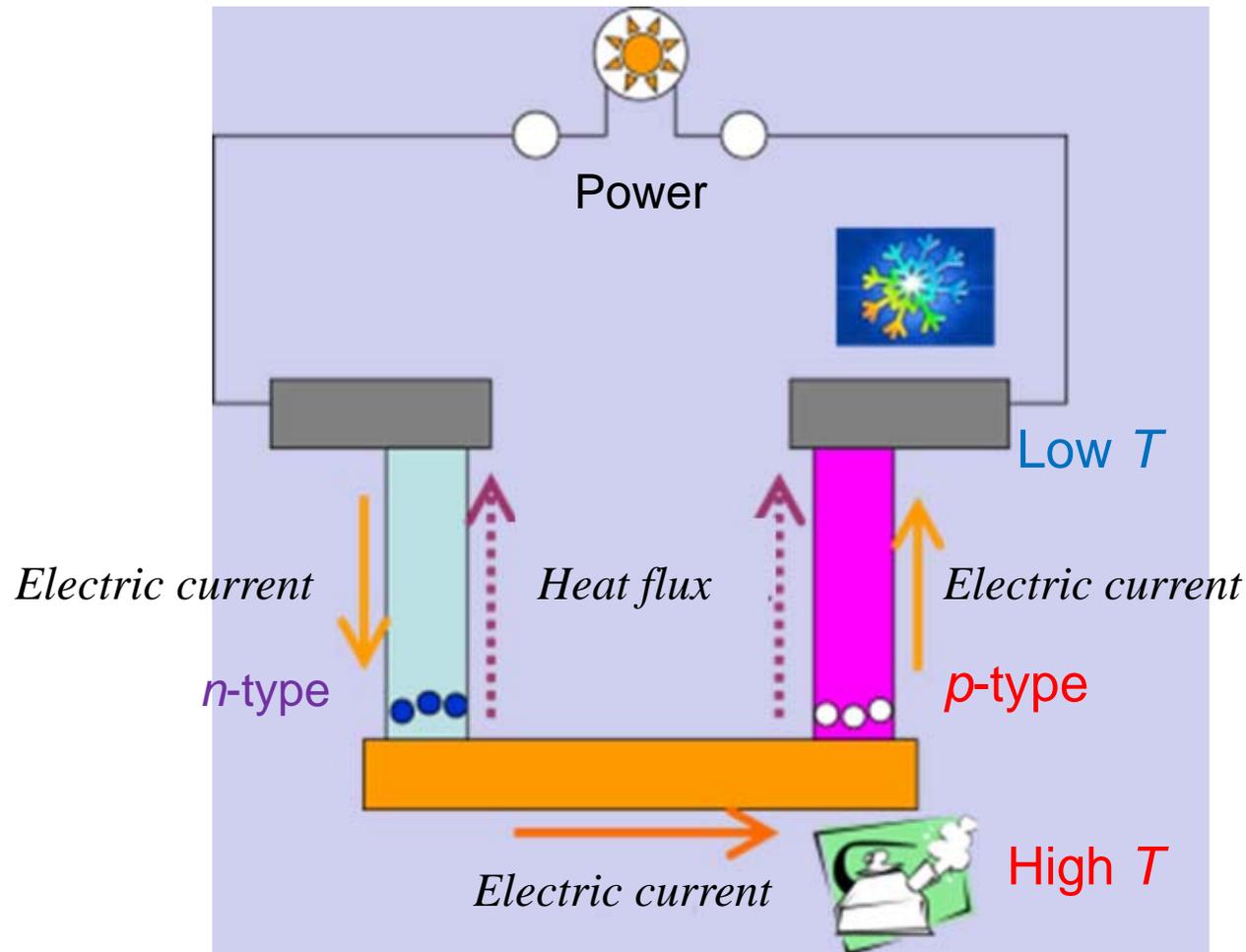


Figure of Merit

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

S : Seebeck coefficient
 σ : electrical conductivity
 κ : **thermal conductivity**

Top 10 lowest LTC compounds among 54,779

Virtual screening of 54,779 compounds in MPD library

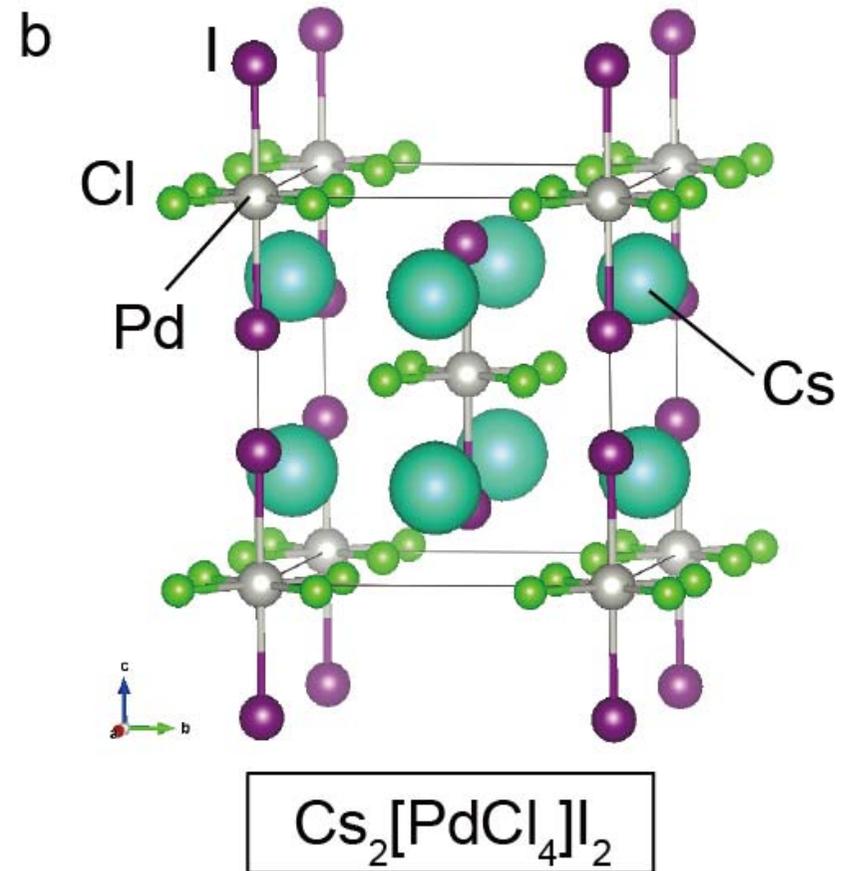
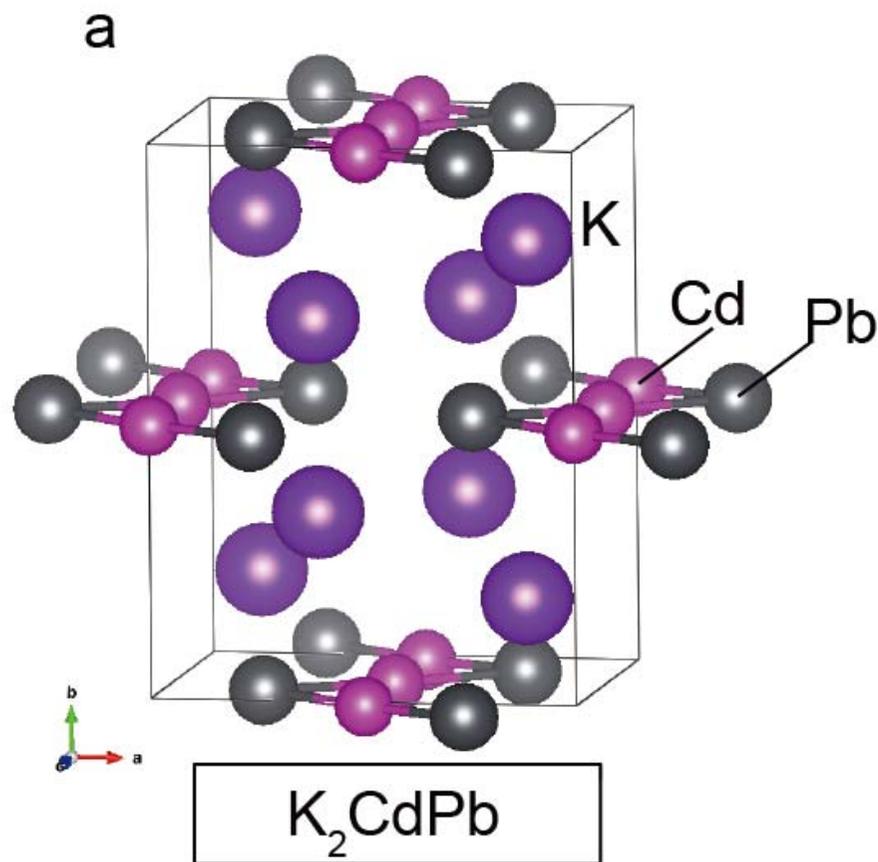
ranking	Z-score	compound		<i>ab initio</i> LTC (W/m·K)	Band Gap (eV)
		formula	space group		
1	1.90	PbRbI ₃	<i>Pnma</i>	0.10	2.46
2	1.76	PbIBr	<i>Pnma</i>	0.13	2.56
3	1.56	PbRb ₄ Br ₆	<i>R-3c</i>	0.08	3.90
4	1.56	PbICl	<i>Pnma</i>	0.18	2.72
5	1.56	PbClBr	<i>Pnma</i>	0.09	3.44
7	1.44	PbI ₂	<i>R-3m</i>	0.29	2.42
8	1.43	PbI ₂	<i>P63mc</i>	0.29	2.45

121	0.39	K ₂ CdPb	<i>Ama2</i>	0.45	0.18
144	0.29	Cs ₂ [PdCl ₄] ₂	<i>I4/mmm</i>	0.31	0.88

Newly discovered candidates for thermoelectrics

with low LTC of < 0.5 W/mK (@300 K)

and narrow band gap of < 1 eV.





Fin