Quantum Matter: Computation Meets Experiments
8-14 March, 2020
Aspen Center for Physics

Computational Material Designs

– Material design methodology & examples:

I. Tl & In compounds

II. 112-family Fe-based superconductor

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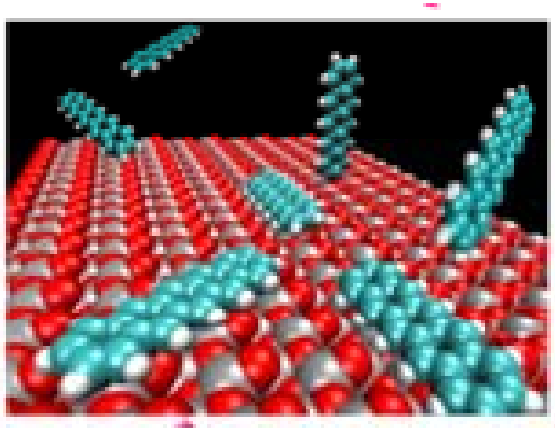
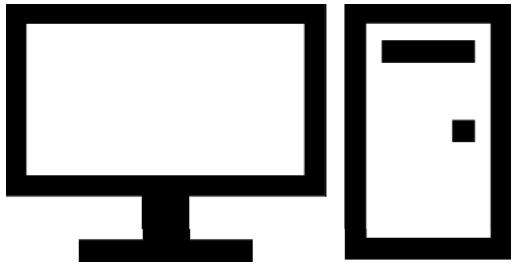
Chang-Jong Kang

Conventional Approach in Correlated Material Designs

Experiments lead Material Designs.

Experiment → Material Design → Theory





Materials discovery has historically proceeded via trial and error, or by accident.

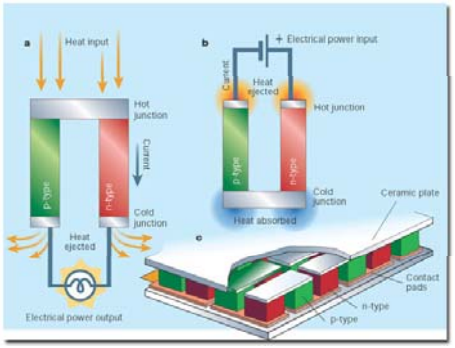
(ex) Hg SC, heavy fermions, cuprates, Fe-based SC

New Paradigm in Material Designs

Superconductor

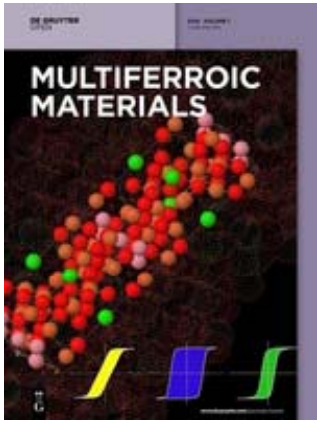
Theory-guided

Thermoelectric materials

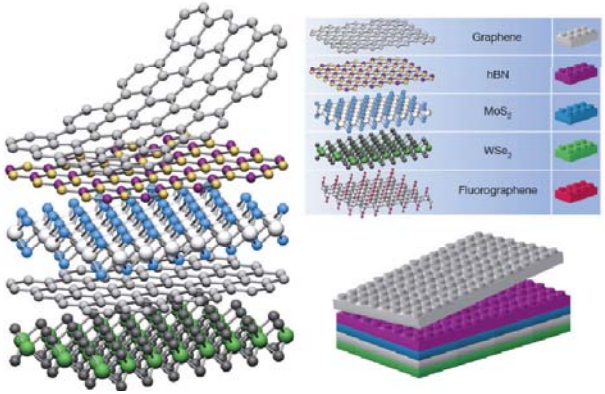


Material Design

Multiferroic materials



Van der Waals materials



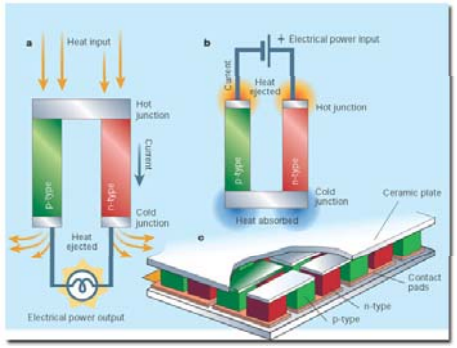
Topological materials

New Paradigm in Material Designs

Superconductor

Theory-guided

Thermoelectric materials



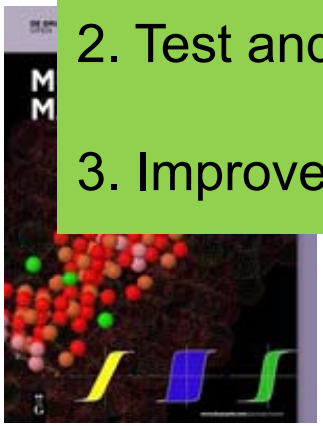
Material Design

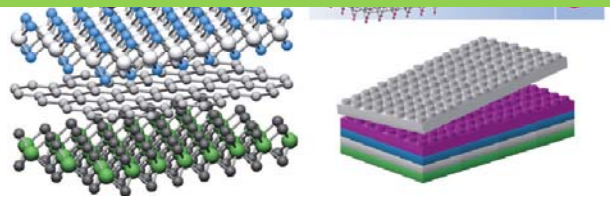
1. Find new interesting materials.

2. Test and develop a material design methodology.

3. Improve our physical understanding from material discovery.

Multif



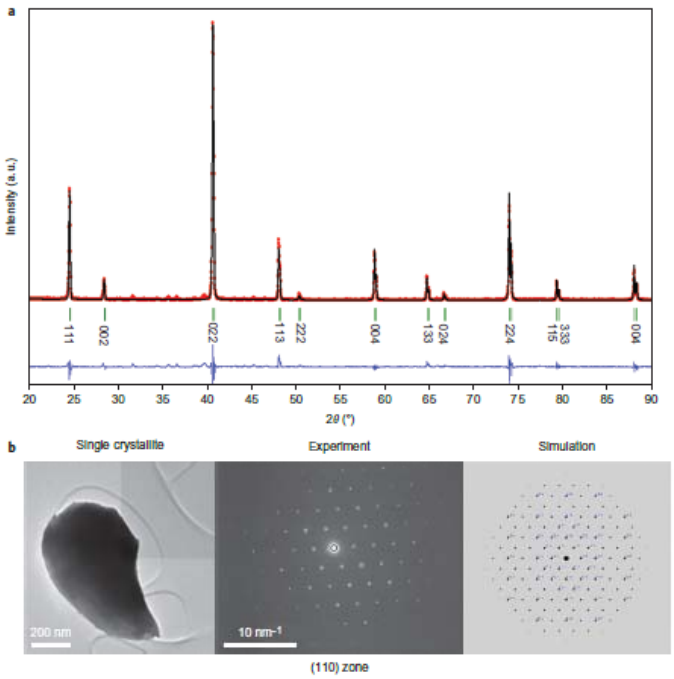


terials

Examples: Theory-guided material search

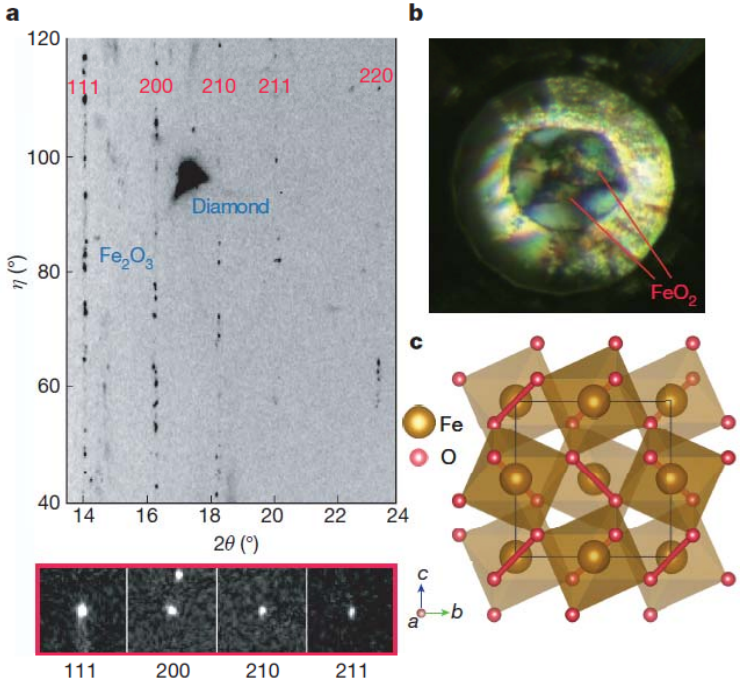
Many accomplishments in theory-guided material search

HfIrSb



R. Gautier *et al.*, Nat. Chem. **7**, 308 (2015)

FeO_2 (high pressure phase)



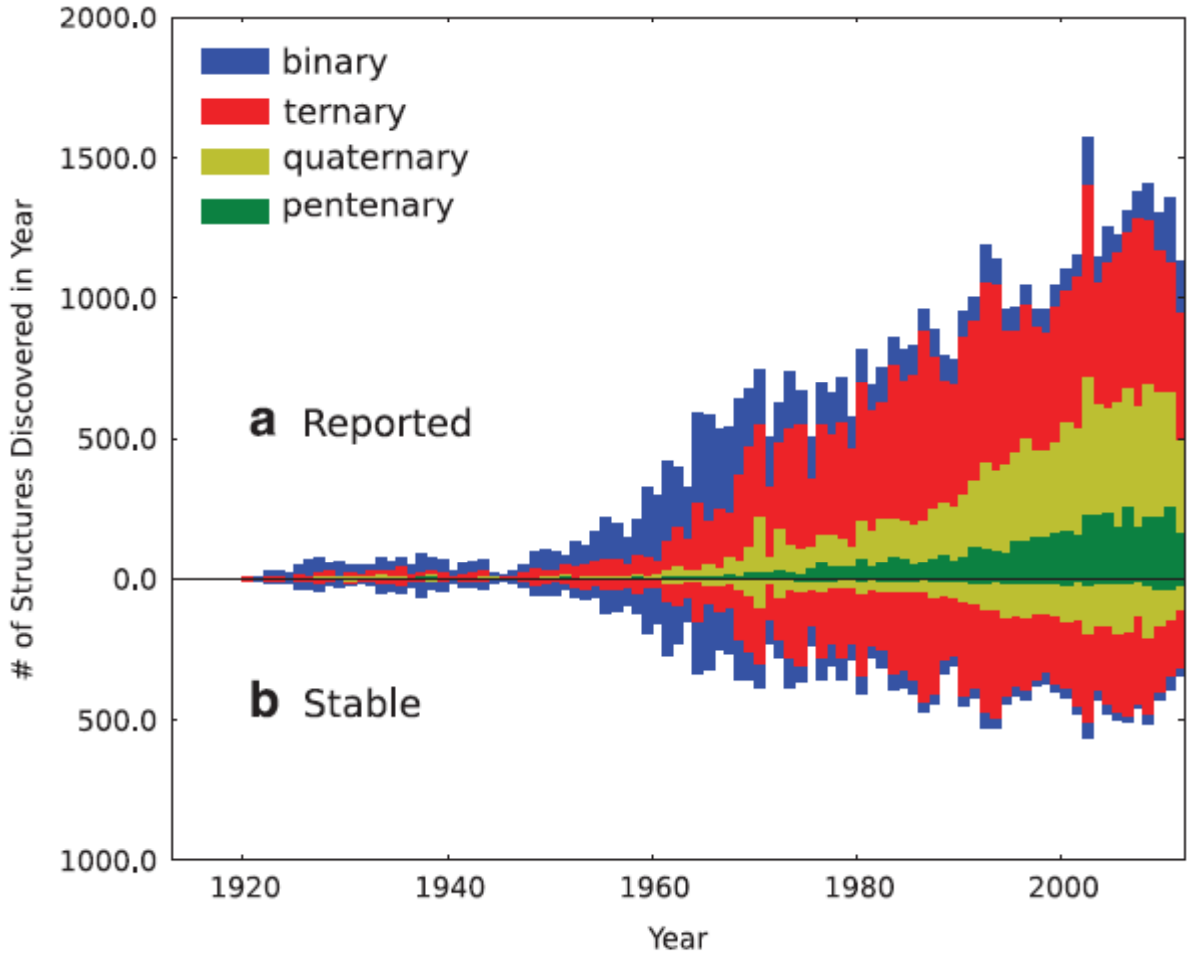
Q. Hu *et al.*, Nature **534**, 241 (2016)

Na_2He – X. Dong *et al.*, Nat. Chem. **9**, 440 (2017)

Ca_2C – Y.-L. Li *et al.*, Nat. Commun. **6**, 6974 (2015)

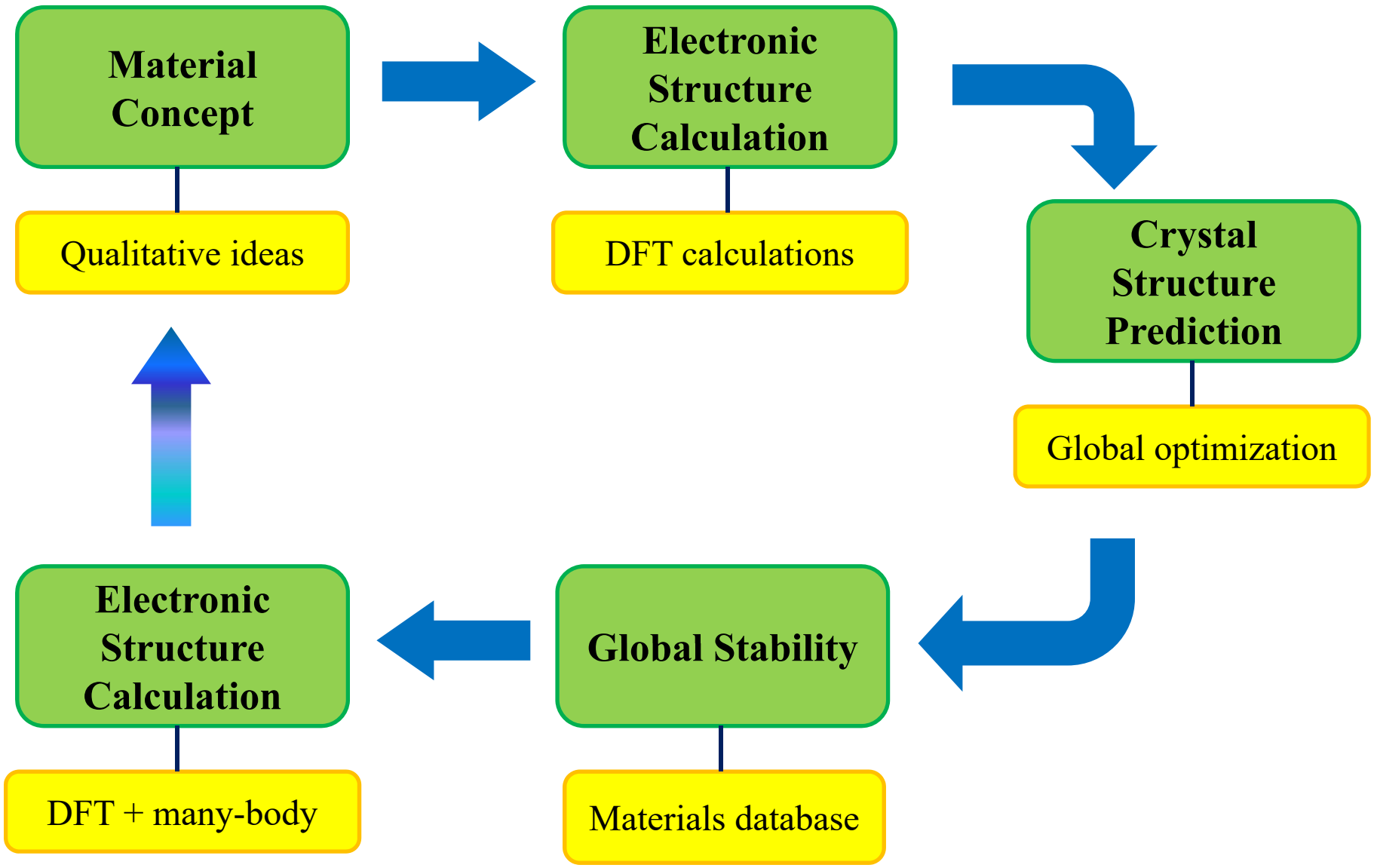
Current Situation in Material Designs

There has been increasing interest in material designs.

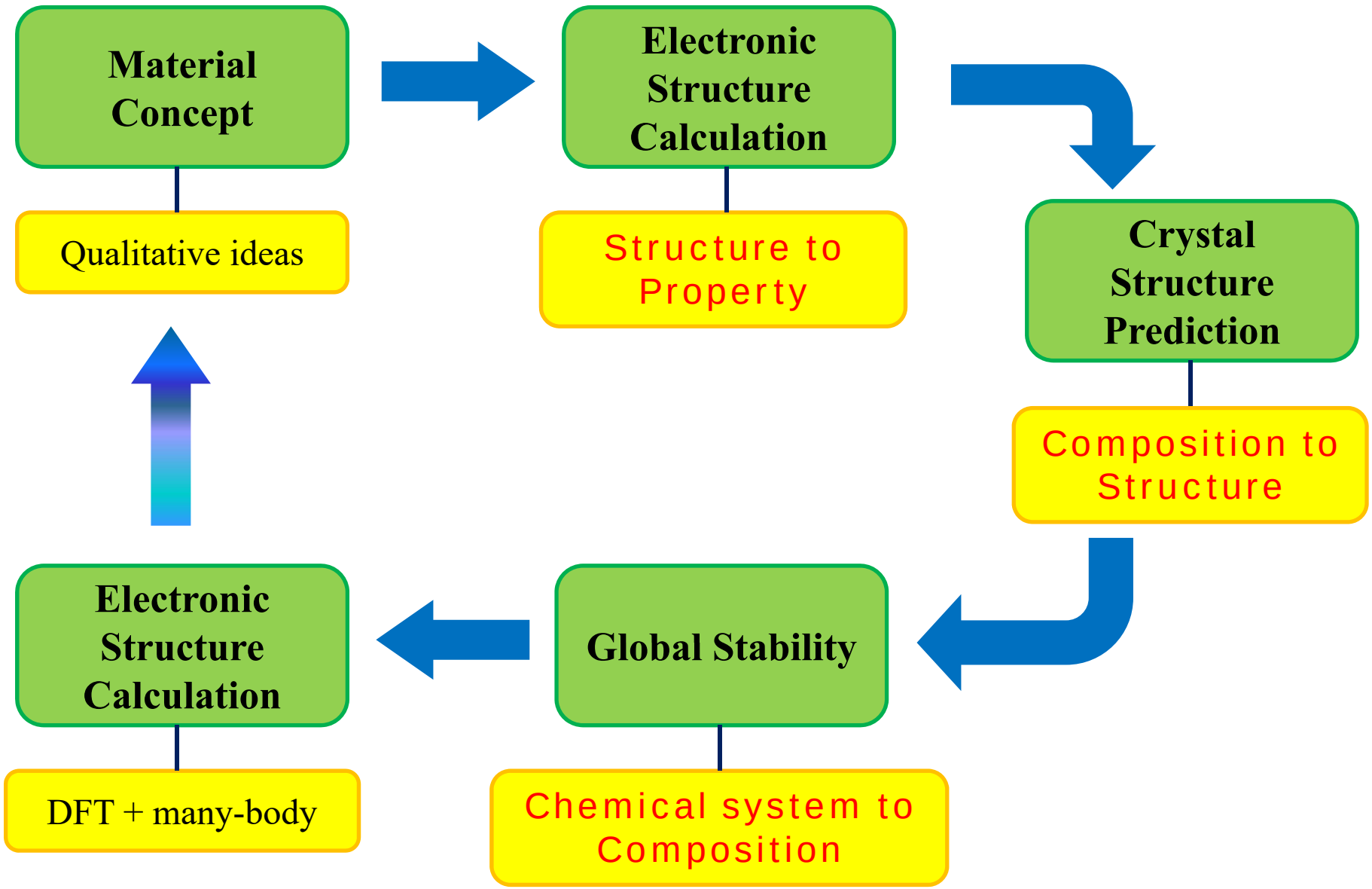


S. Kirklin *et al.*, npj Comput. Mater. **1**, 15010 (2015)

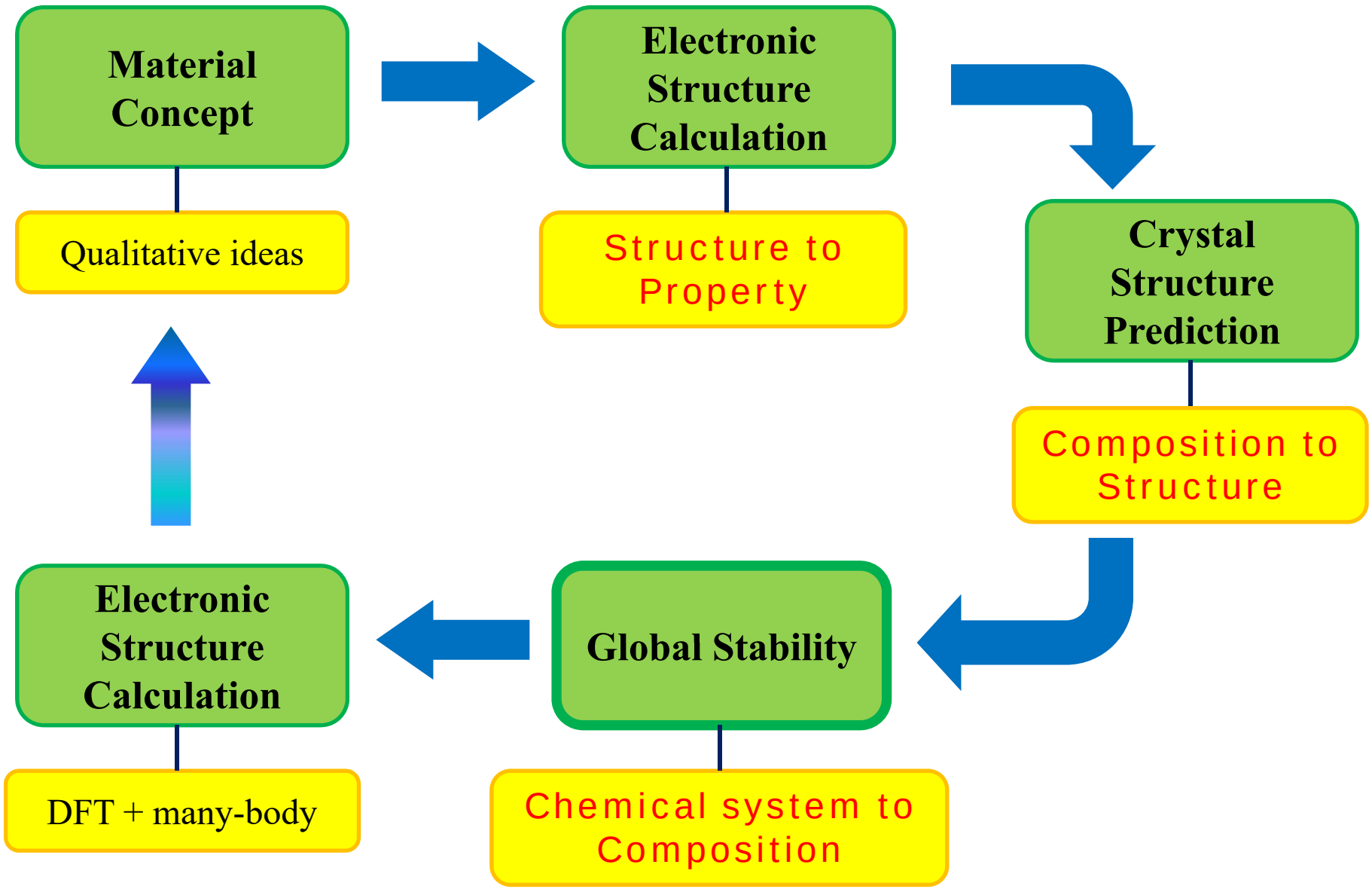
Computational Material Design Workflow



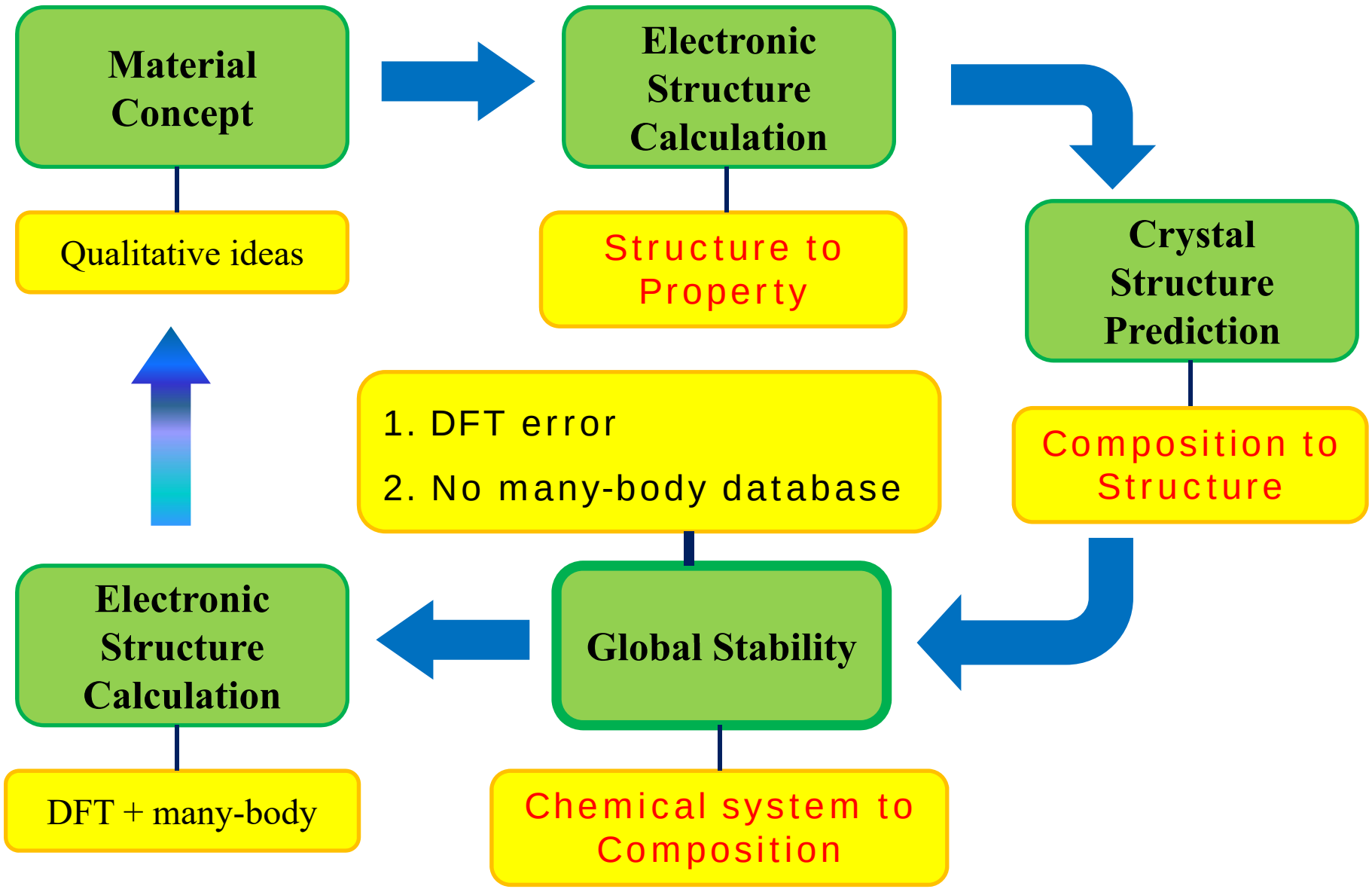
Computational Material Design Workflow



Computational Material Design Workflow



Computational Material Design Workflow



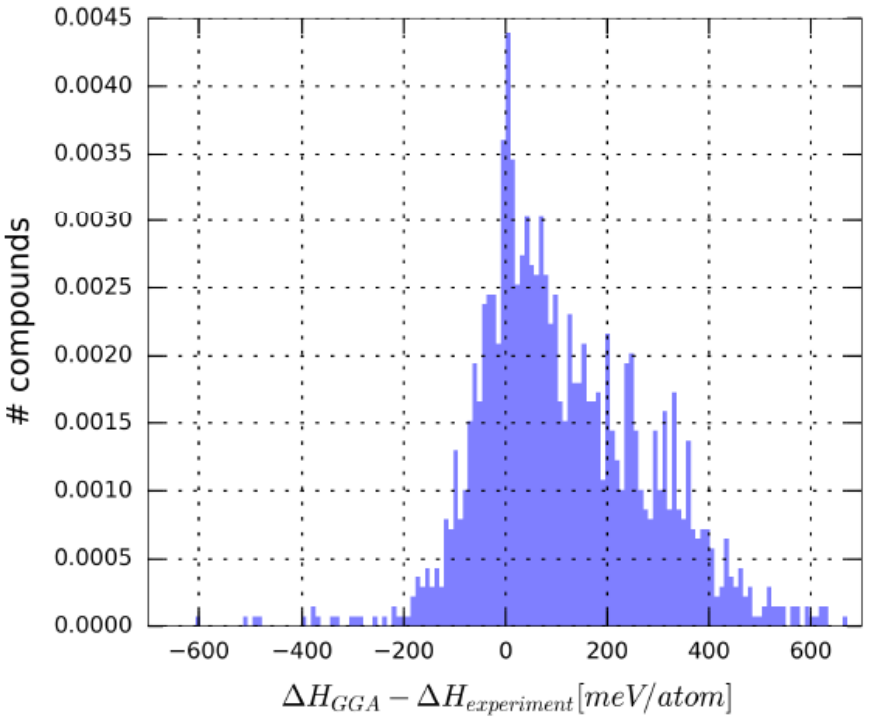
Current Challenges in Material Designs

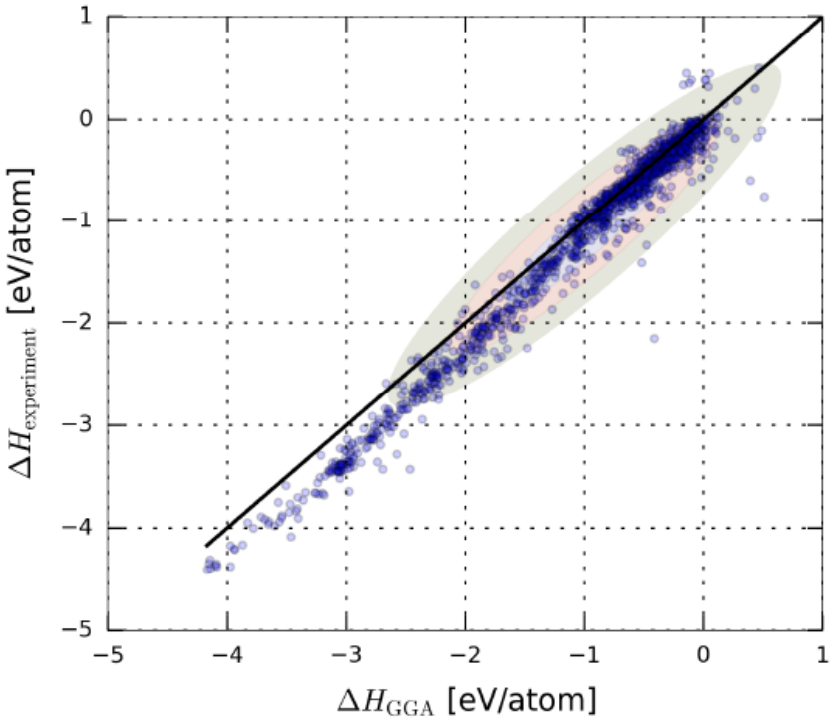
1. Computational error in DFT total energy calculations.

→ **Empirical corrections** are needed.

Material Designs – Computational Error

ΔH: comparison between DFT-GGA and experiment





DFT-GGA formation energies are overestimated.

→ **Need corrections !!!**

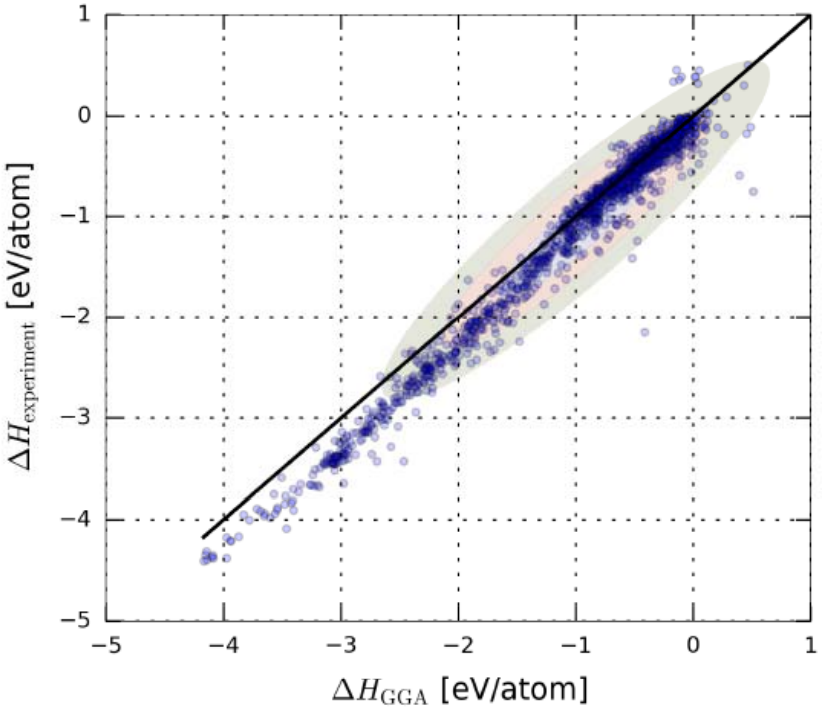
G. Hautier *et al.*, PRB **85**, 155208 (2012); S. Kirklin *et al.*, npj Comput Mater. **1**, 15010 (2015)

R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

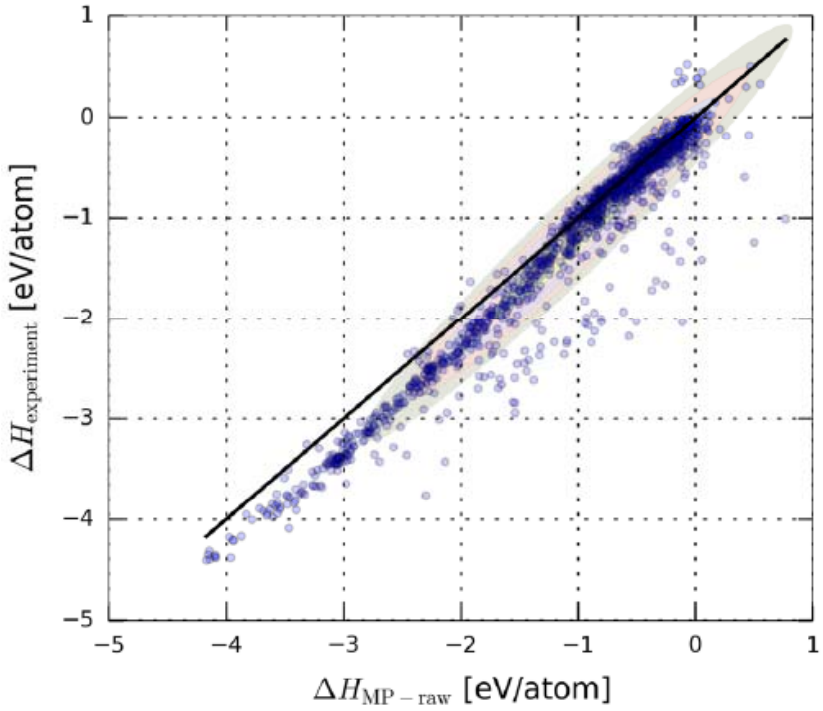
Material Designs – Computational Error

Does inclusion of U (GGA + U) improve the DFT error ?

GGA calculations



GGA + U calculations



Inclusion of U (GGA + U) is not enough.

V. Stevanović *et al.*, PRB **85**, 115104 (2012); G. Hautier *et al.*, PRB **85**, 155208 (2012)

R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

Material Designs – Empirical Corrections

Three broadly used empirical schemes for corrections

1. FERE (Fitted Elemental-phase Reference Energy)

   V. Stevanović *et al.*, PRB **85**, 115104 (2012)

2. MP (Materials Project)

   A. Jain *et al.*, APL Materials **1**, 011002 (2013)

3. OQMD (Open Quantum Materials Database)

   S. Kirklin *et al.*, npj Comput Mater. **1**, 15010 (2015)

1. FERE

All elements

$$\Delta H^{exp}(A_mB_n) = E^{GGA+U}(A_mB_n) - m\,\mathbf{E^{Fitted}(A)} - n\,\mathbf{E^{Fitted}(B)}$$

2. MP / OQMD

A = **Selected TM**

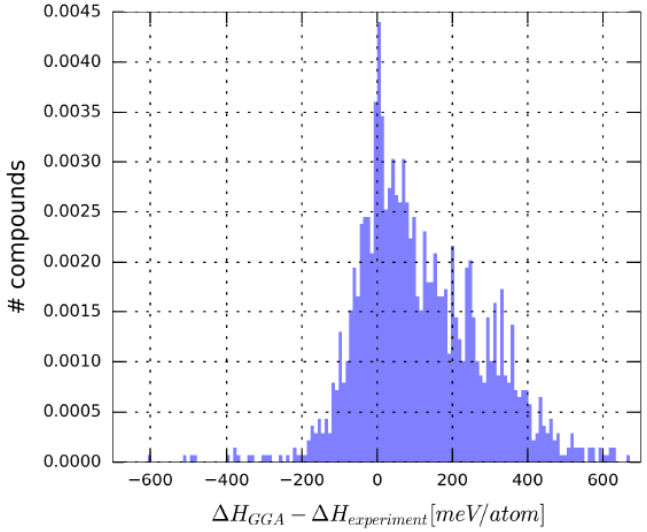
B = **O** or **F**

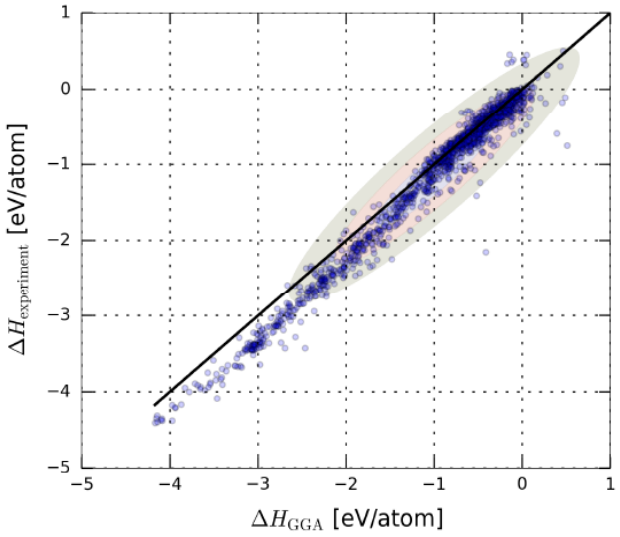
$$\Delta H^{exp}(A_mB_n) = E^{GGA+U}(A_mB_n) - m\,E^{GGA}(A) - n\,E^{GGA}(B) - \boldsymbol{\Sigma\, m\,\Delta E}$$

ΔE: GGA versus GGA + U compatibility correction

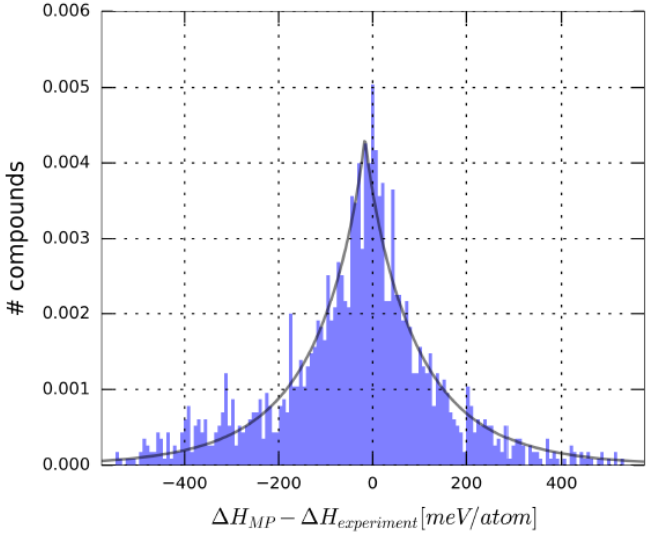
Material Designs – Empirical Corrections

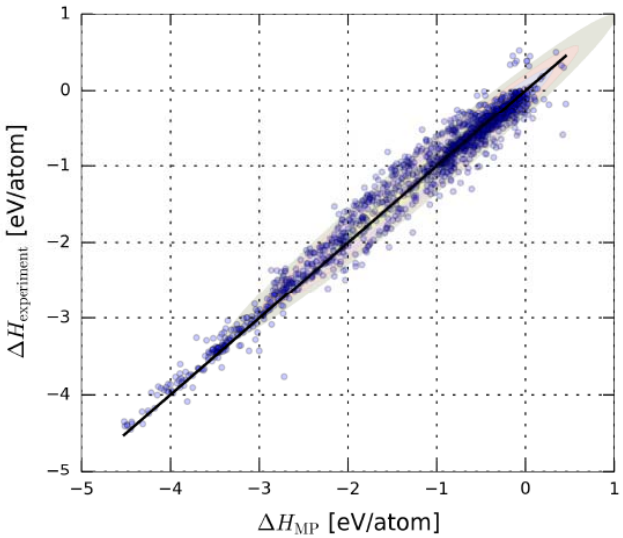
Without corrections





With MP corrections

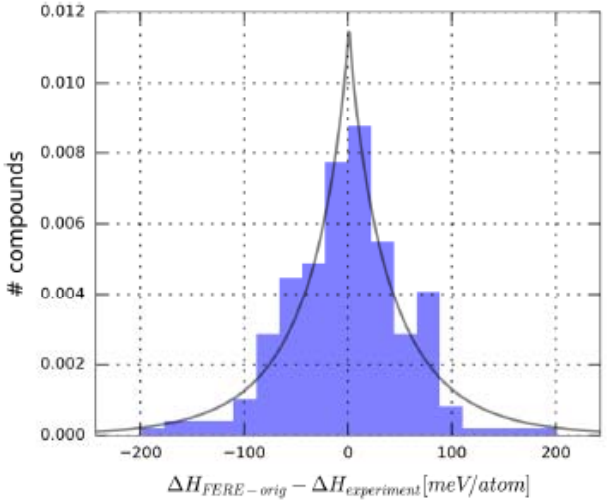


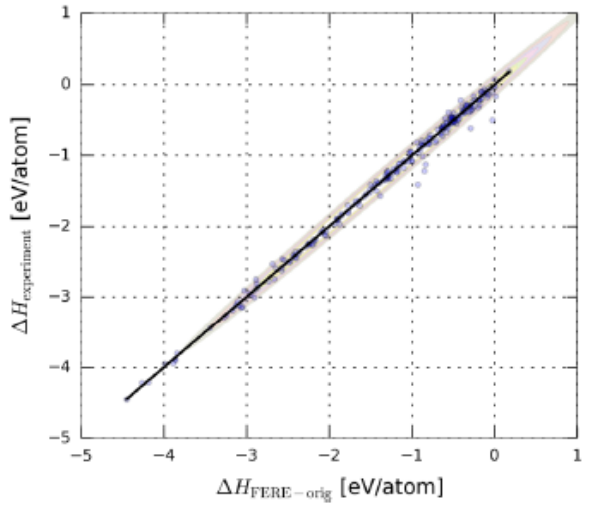


R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

Material Designs – Empirical Corrections

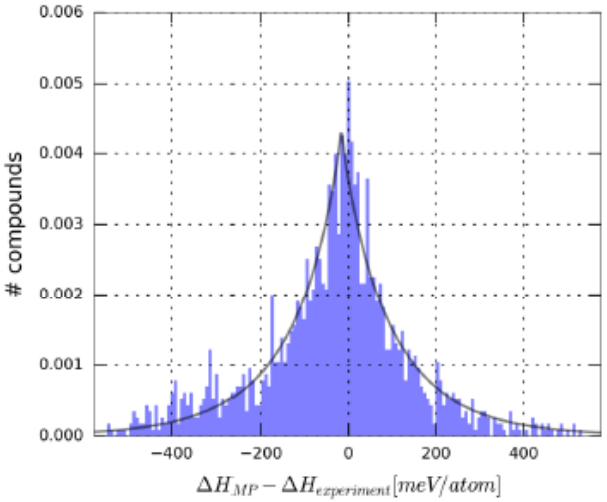
FERE

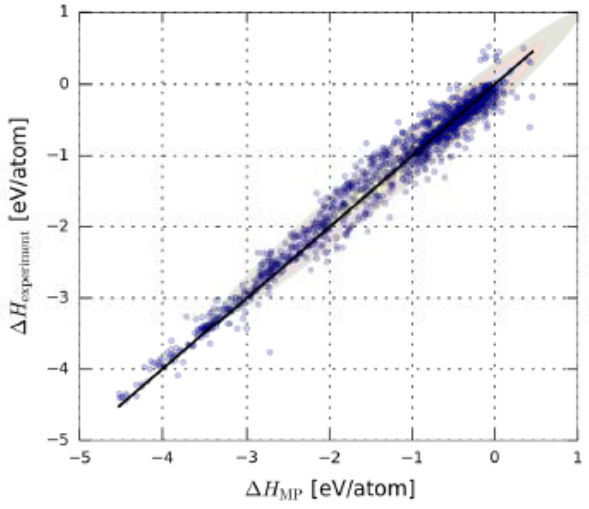




V. Stevanović *et al.*, PRB **85**, 115104 (2012)

Materials Project





G. Hautier *et al.*, PRB **85**, 155208 (2012)

R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

Material Designs – Existence Probability

Chemical reaction for a new compound

$$A + B \leftrightarrow AB$$

Theory
- ΔH_{exact} "exact" formation energy
- ΔH_{calc} DFT formation energy with empirical corrections

Experiment
- ΔH_{exp} (unknown) experimental formation energy

$\Delta H_{exact} < 0$ guarantees that $\Delta H_{exp} < 0$

$\therefore$ The material will be synthesized in experiment.

However, we do not have the exact method.

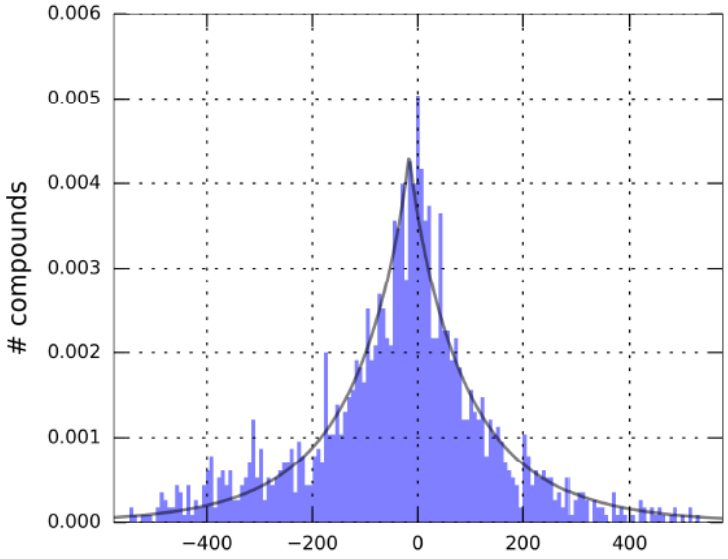
$\Delta H_{calc} < 0$ does not guarantee that $\Delta H_{exp} < 0$ due to DFT errors

Q) What is probability of $\Delta H_{exp} < 0$ given that $\Delta H_{calc} = x$?

Material Designs – Existence Probability

Probability density function

$$F_{\alpha\beta\mu}(d) = \frac{\beta}{2\alpha\Gamma(1/\beta)}\, e^{-(|d-\mu|/\alpha)^{\beta}}$$



1. Merge all databases and obtain PDF

$$P\left(\Delta H_{\text{calc}} - \Delta H_{\text{exp}} = d\right) = F_{\alpha\beta\mu}(d)$$

2. Estimate probability that $\Delta H_{\text{exp}} < 0$

$$P(x) = P\left(\Delta H_{\text{exp}} < 0 \,\middle|\, \Delta H_{\text{calc}} = x\right)$$

$$= \int_{-\infty}^{0} P\left(\Delta H_{\text{exp}} = y \,\middle|\, \Delta H_{\text{calc}} = x\right) dy$$

$$= \int_{-\infty}^{0} F_{\alpha\beta\mu}\left(x - y\right) dy$$

3. Test with experiments

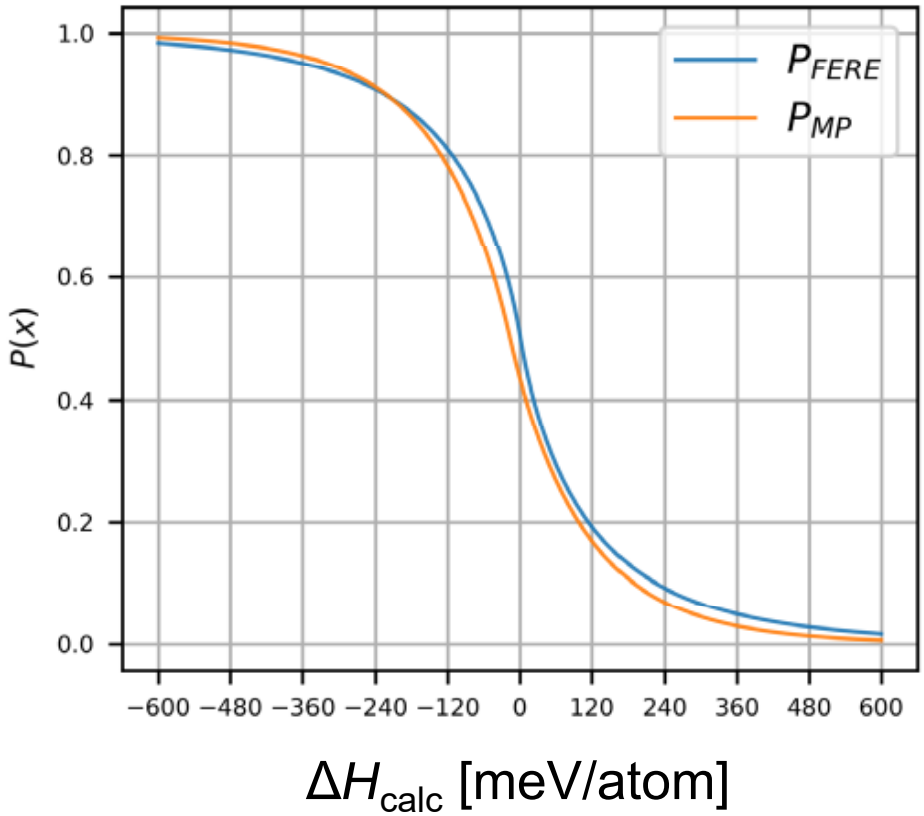
Adler, **Kang**, Yee, and Kotliar,
Reports on Progress in Physics **82**, 012504 (2019)

Material Designs – Existence Probability

Existence probability

P(x): probability for a compound to exist

"Good indicator for Material Designs"



R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

Current Challenges in Material Designs

2. Currently, DFT formation energies (with empirical corrections) are only available in material databases.

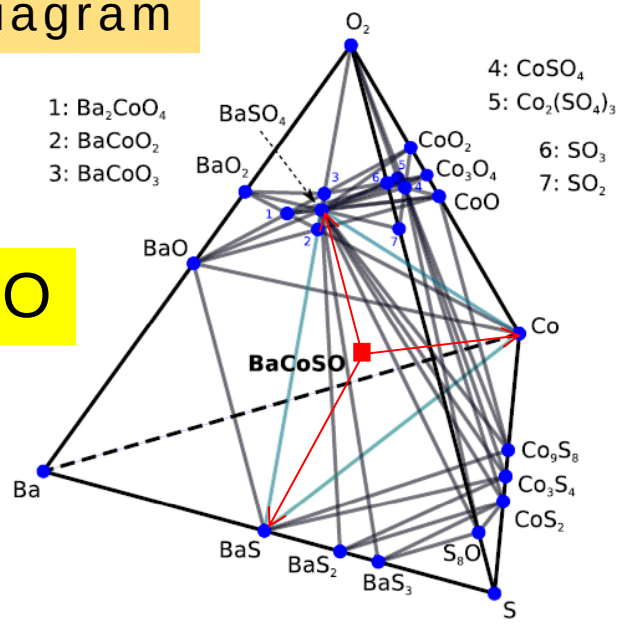
(DFT database) Materials Project, AFLOW, OQMD, …

→ **DFT+Gutzwiller / DFT+DMFT database** is necessary for strongly correlated material designs.

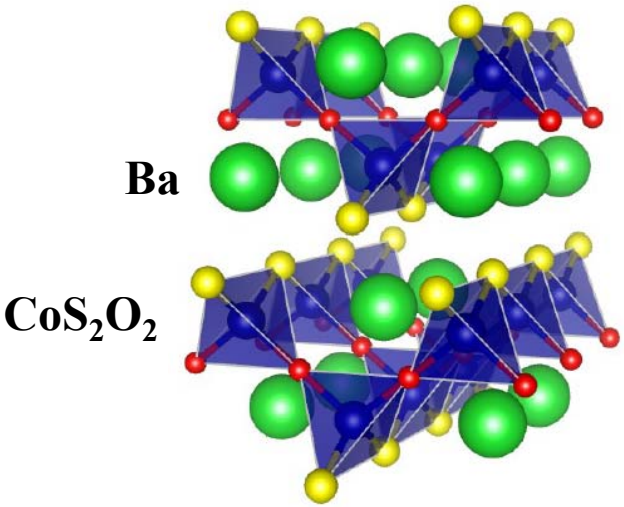
Why Many-body Database is Necessary

Phase diagram

BaCoSO



Crystal structure



Material	Determinant reaction	$\Delta H_{\text{Materials proj.}}$ (eV/atom)	$\mathcal{P}(x)$	$\Delta H_{\text{Gutzwiller}}$ (eV/atom)
BaCoSO	$4\,\text{Co} + 3\,\text{BaS} + \text{BaSO}_4 \rightarrow 4\,\text{BaCoSO}$	0.102	0.17	−0.209

BaCoSO was synthesized experimentally in Oxford chemistry group.

(Ref.) Edward J. T. Salter *et al.*, Inorg. Chem. **55**, 1697 (2016)

R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

Why Many-body Database is Necessary

Material	Determinant reaction	$\Delta H_{\text{Materials proj.}}$ (eV/atom)	$\mathcal{P}(x)$	$\Delta H_{\text{Gutzwiller}}$ (eV/atom)
$La_2CuS_2O_2$	$La_2SO_2 + CuS \rightarrow La_2CuS_2O_2$	0.232	0.06	0.214
La_2CuSO_3	$3\,La_2SO_2 + 4\,Cu + La_2SO_6 \rightarrow 4\,La_2CuSO_3$	0.324	0.02	0.286
$Hg(CaS)_2CuO_2$	$HgO + 2\,CaS + CuO \rightarrow Hg(CaS)_2CuO_2$	0.170	0.09	−0.151
$CsTlCl_3$	$TlCl + Cs_2TlCl_5 \rightarrow 2\,CsTlCl_3$	0.003	0.41	—
$CaFeAs_2$	$CaAs + FeAs \rightarrow CaFeAs_2$	0.013	0.37	0.007
BaCoSO	$4\,Co + 3\,BaS + BaSO_4 \rightarrow 4\,BaCoSO$	0.102	0.17	−0.209

DFT+Gutzwiller / DFT+DMFT database would provide better statistics and more reliable computational results in strongly correlated electron systems.

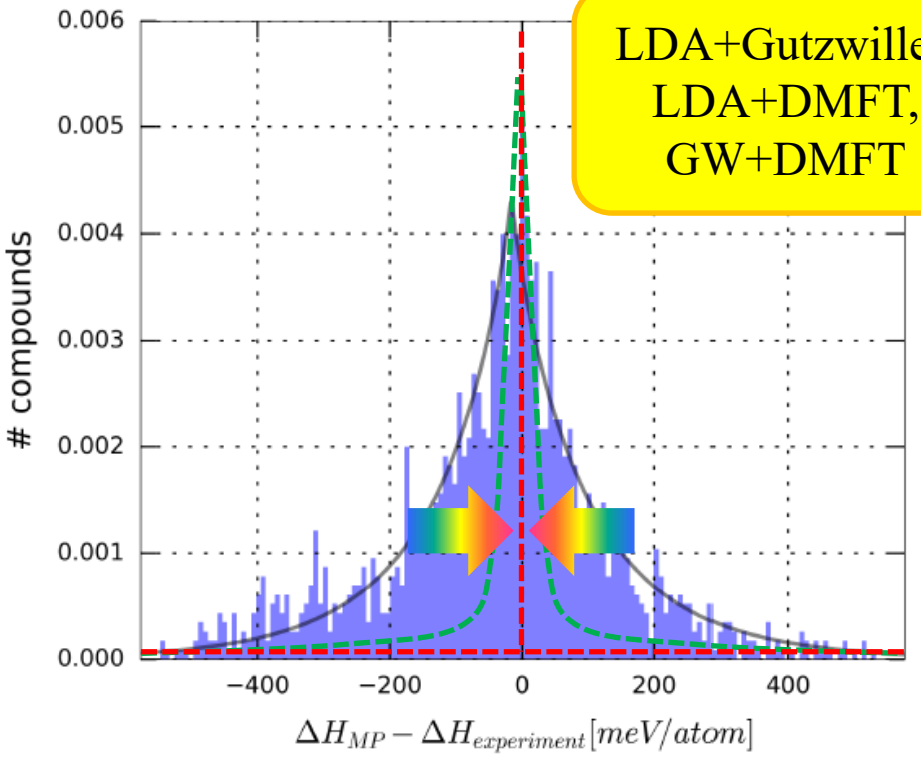
H. He, C.-H. Yee *et al.*, PNAS **115**, 7890 (2018)

C.-H. Yee, T. Birol, and G. Kotliar, EPL **111**, 17002 (2015)

R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

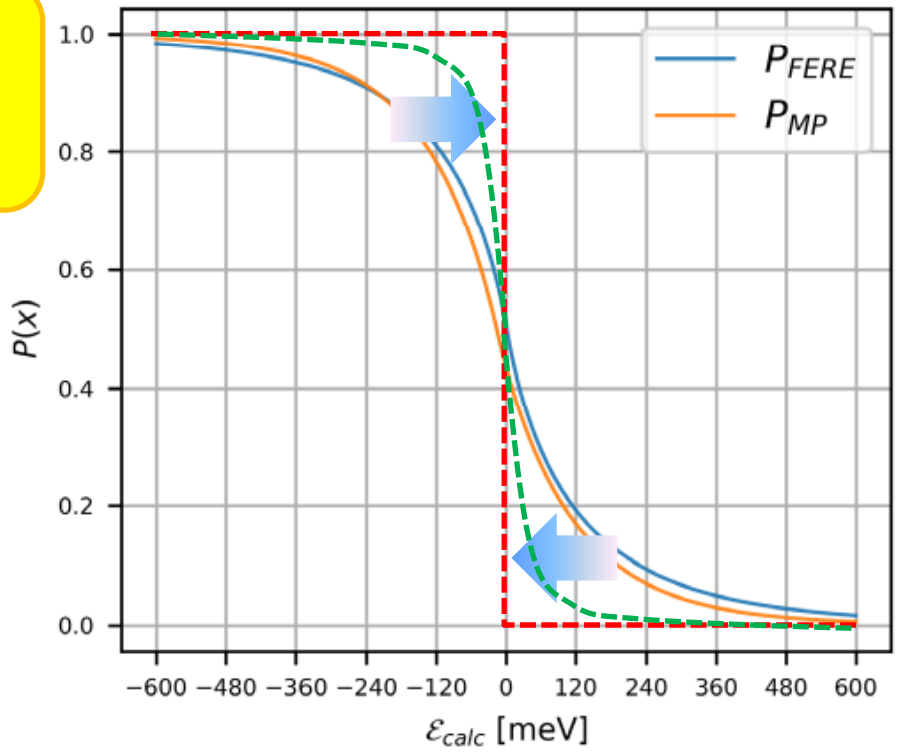
Material Designs with Advanced Methods

Probability distribution function



LDA+Gutzwiller,
LDA+DMFT,
GW+DMFT

Existence probability



DFT+Gutzwiller / DFT+DMFT database would provide better statistics and more reliable computational results.

Example of Materials Design

I. Tl & In compounds

(Impact of static correlation)

New Type of Superconductor, $Ba_{1-x}K_xBiO_3$

$Ba_{1-x}K_xBiO_3$ (cubic perovskite)

$T_C \sim 30$ K

R. J. Cava *et al.*, Nature **332**, 814 (1988)

(LDA) $\lambda_{el\text{-}ph} = 0.33 \rightarrow T_C \sim 1$ K

Meregalli and Savrasov, PRB **57**, 14453 (1998)

(HSE06 / GW)

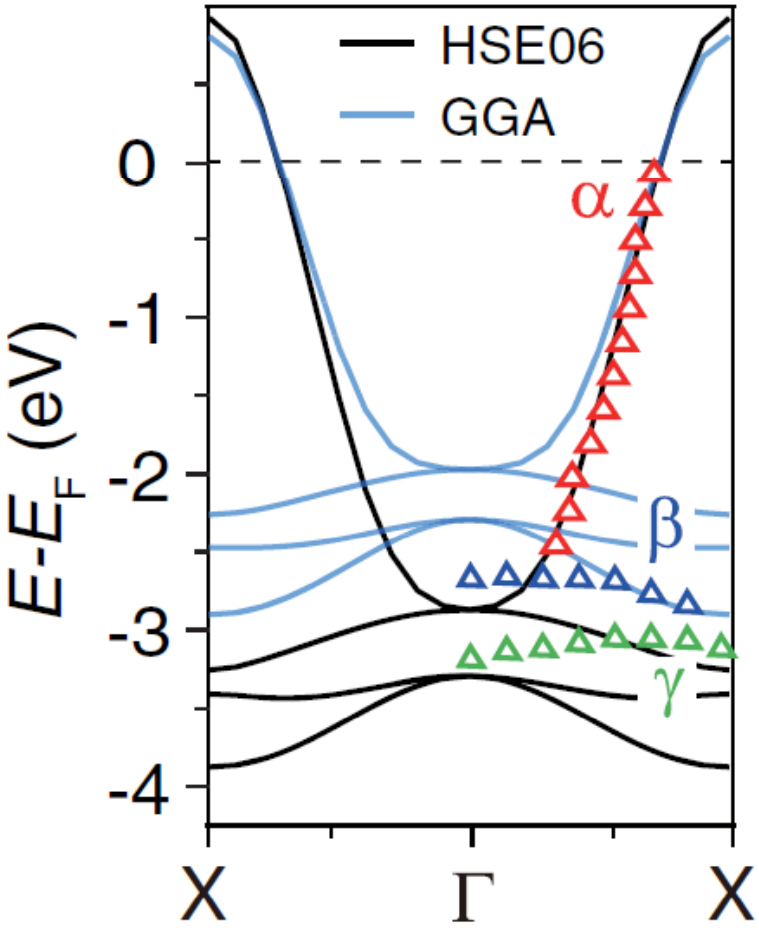
$\lambda_{el\text{-}ph} \sim 1 \rightarrow T_C \sim 30$ K

Yin, Kutepov, and Kotliar, PRX **3**, 021011 (2013)

Z. Li *et al.*, PRL **122**, 186402 (2019)

Static correlation enhances $\lambda_{el\text{-}ph}$!

ARPES ($Ba_{0.51}K_{0.49}BiO_3$)



C. H. P. Wen *et al.*, PRL **121**, 117002 (2018)

New Type of Superconductor, $CsTlX_3$ (X = F, Cl)

Theory

$CsTlF_3$, $CsTlCl_3$

Not reported in ICSD

0.35 hole-doped compounds

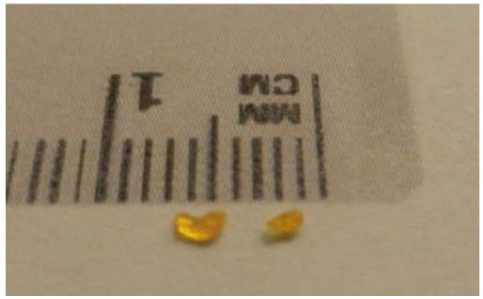
$CsTlF_3$	$\lambda_{el\text{-}ph}$	T_C
LDA	0.55	5.2
HSE06	1.51	30

$CsTlCl_3$	$\lambda_{el\text{-}ph}$	T_C
LDA	0.91	9.0
HSE06	2.32	21

Yin and Kotliar, EPL **101**, 27002 (2013)

Experiment

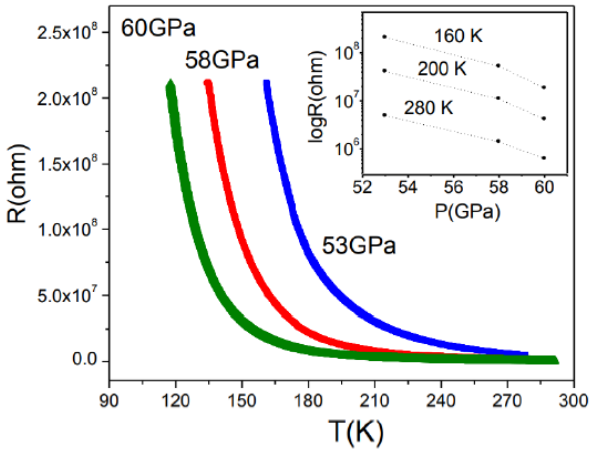
$CsTlF_3$, $CsTlCl_3$



$CsTlF_3$: Fm-3m (cubic)

$CsTlCl_3$: two polymorphs,

I4/m (tetra) and Fm-3m



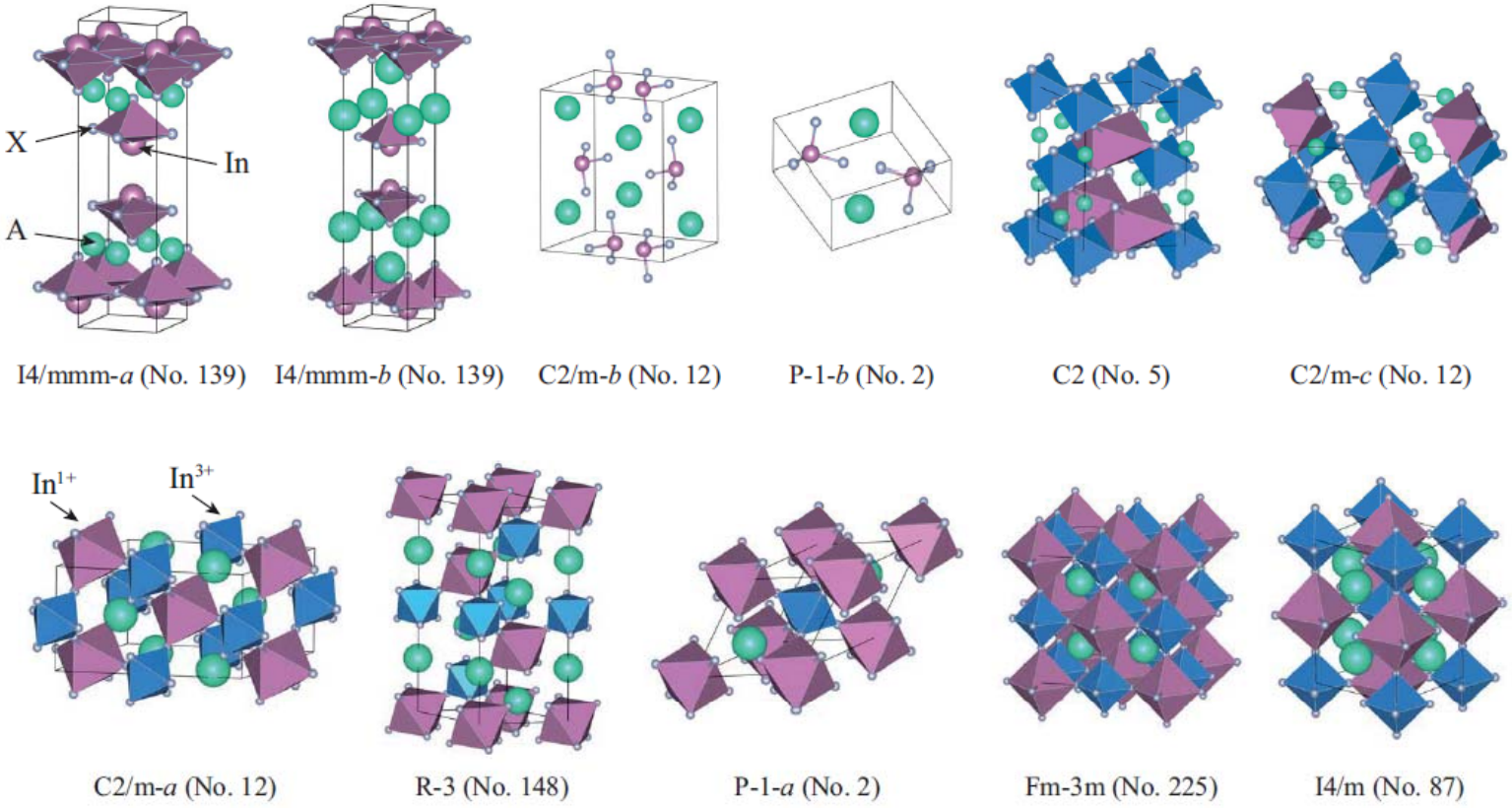
Band gap is reduced upon pressure.

Attempts to dope were unsuccessful.

M. Retuerto *et al.*, Chem. Mater. **25**, 4071 (2013)

Material Design of Indium Compounds

Indium compounds do not have the toxicity problems associated with Thallium and are expected to be synthesized more easily.



1. Predict new materials with high confidence
2. Predict crystal structures with less confidence

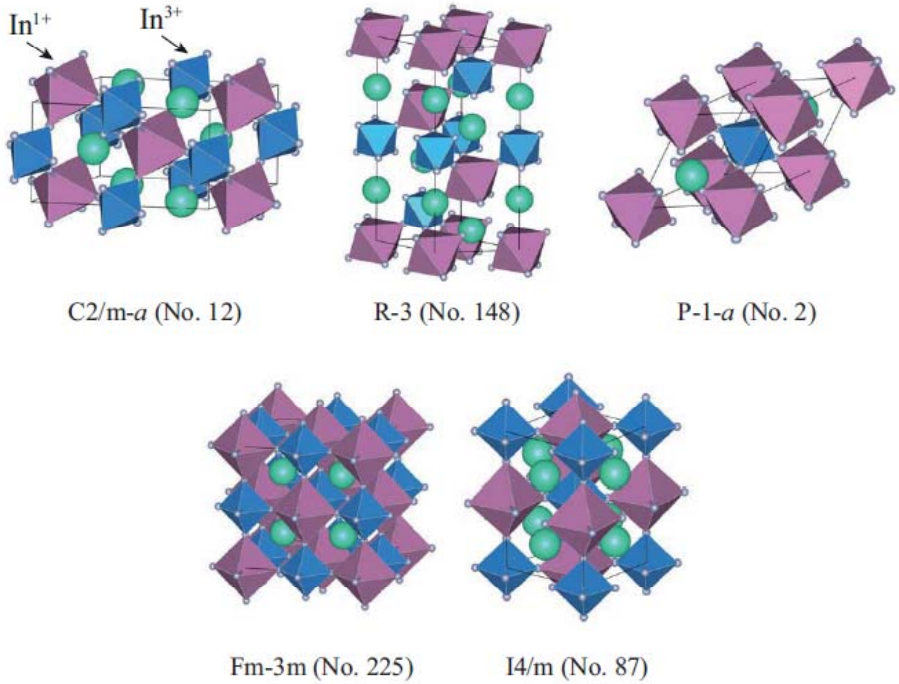
C.-J. Kang and G. Kotliar, PRM **3**, 015001 (2019)

Material Design of Indium Compounds

Theory

$CsInCl_3$

Not reported in ICSD



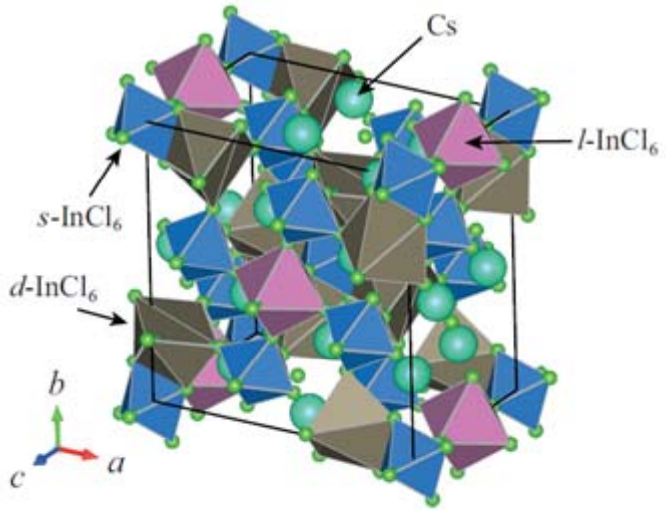
Existence probability: 0.52

C.-J. Kang and G. Kotliar, PRM **3**, 015001 (2019)

Experiment

$CsInCl_3$

Material synthesis at Rutgers (Martha Greenblatt's group)



Space group: I4/m (No. 87)

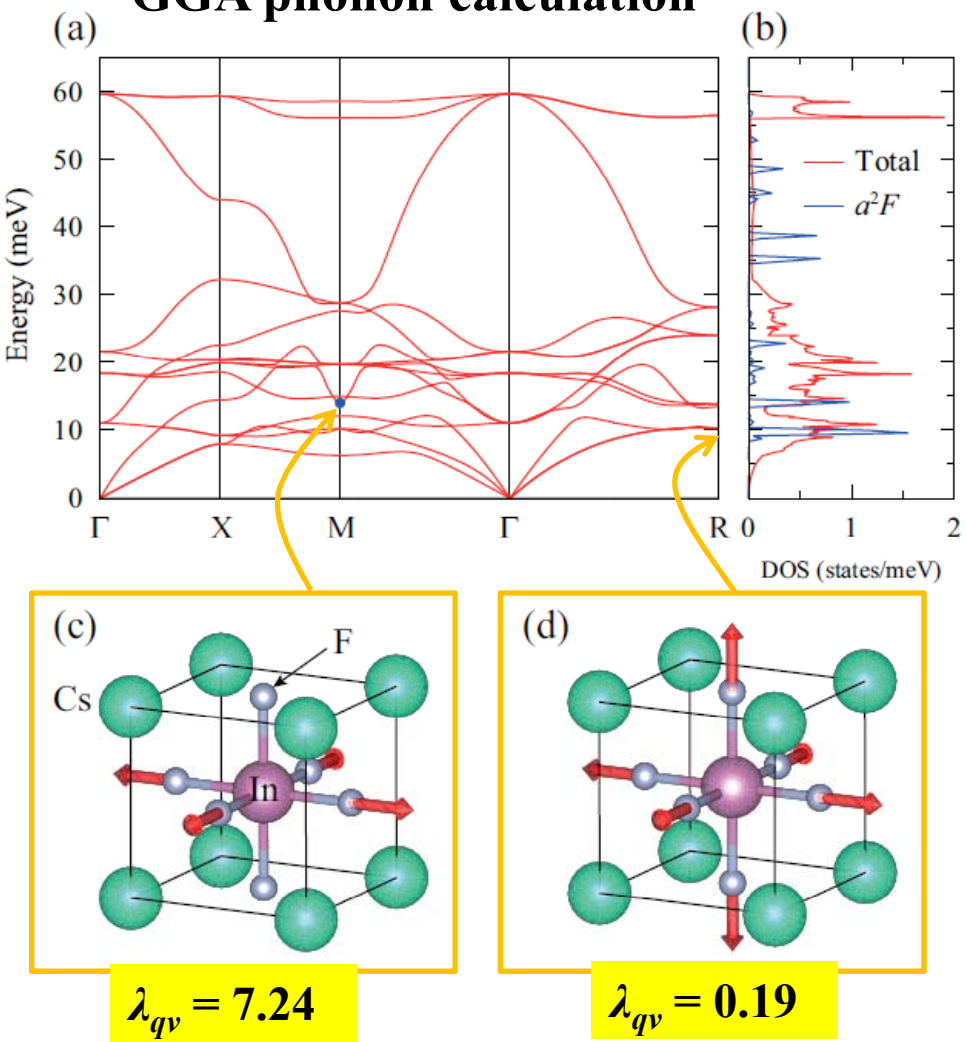
Meta-stable phase

(EXP) X. Tan *et al.*,
Chemistry of Materials **31**, 1981 (2019)

Superconductivity of Indium Compounds

0.5 hole-doped $CsInF_3$ (cubic perovskite)

GGA phonon calculation



$\lambda_{qv} = 7.24$

$\lambda_{qv} = 0.19$

Existence probability: 0.78

How to prepare the hope-doped $CsInF_3$
1. O substitution for F: $CsIn(F_{1-x}O_x)_3$
2. Cs vacancy: $Cs_{1-\delta}InF_3$

	GGA	HSE06
REPME (eV/Å)	5.00	6.95
λ	1.80	3.48
ω_{log} (K)	157	124
T_c (K)	21 (18)	24 (22)

Hope-doped $CsInF_3$ under pressure shows superconductivity with $T_C \sim$ 24 K.

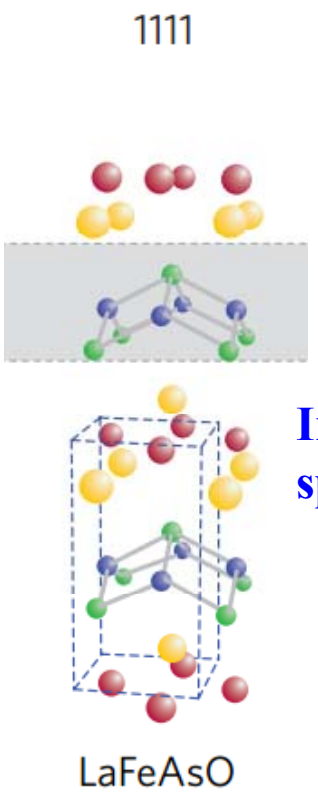
C.-J. Kang and G. Kotliar, PRM **3**, 015001 (2019)

Example of Material Design

II. 112-family Fe-based superconductor

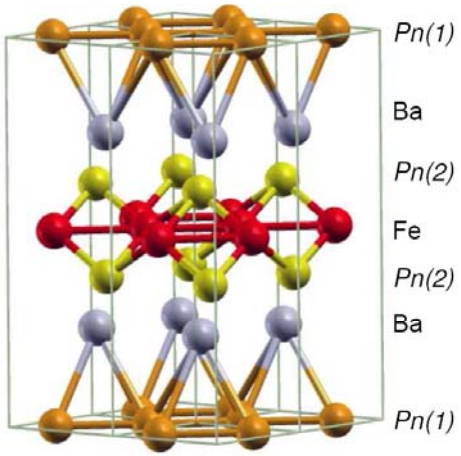
(Impact of dynamic correlation)

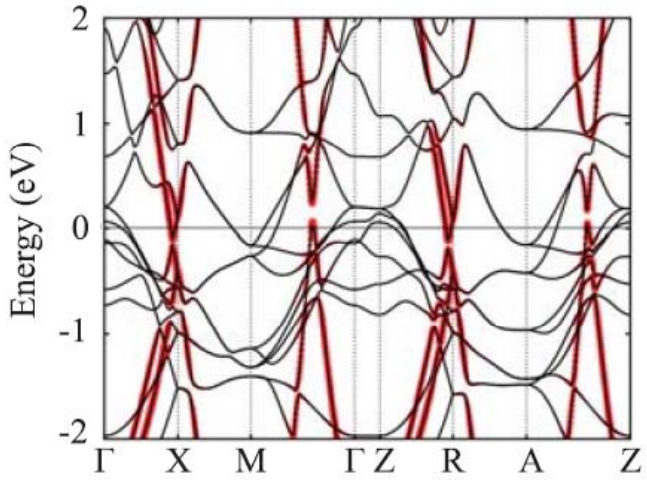
1st & 2nd Steps: Qualitative Idea & Electronic Structure Calculations



The simple substitution of As for O leads to a 112-family Fe-based superconductor.

DFT – metallic spacer layers





Hypothetical BaFePn_2 (Pn = As, Sb)

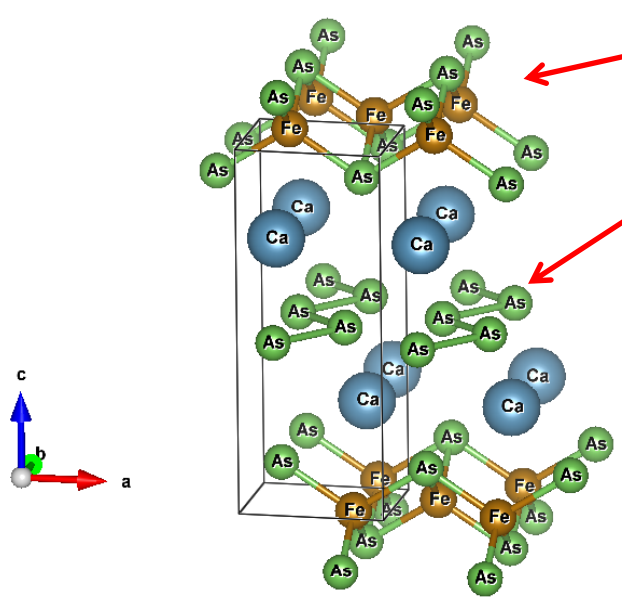
Tetragonal structure (space group: P4/nmm, No. 129)

J. H, Shim, K. Haule, and G. Kotliar, PRB **79**, 060501 (R) (2009)

3rd Step: Crystal Structure Prediction

Theory

$CaFeAs_2$



FeAs layer

Zigzag As chain

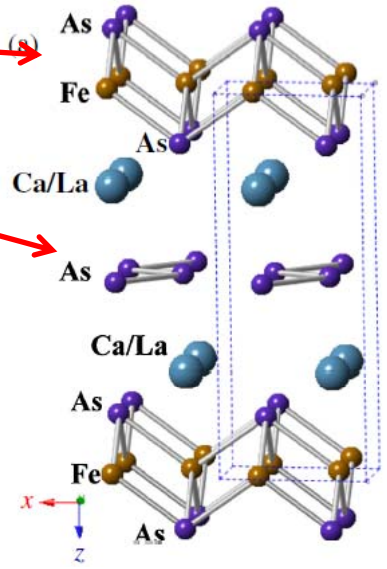
It has inversion symmetry.

Space group: $P2_1/m$ (# 11)
Monoclinic structure
a **= 3.962 Å,** ***b*** **= 3.896 Å,** ***c*** **= 10.057 Å**
β **= 91.135° (*α* = *γ* = 90°)**

C.-J. Kang *et al.*, PRB **95**, 014511 (2017)

Experiment

$Ca_{1-x}La_xFeAs_2$

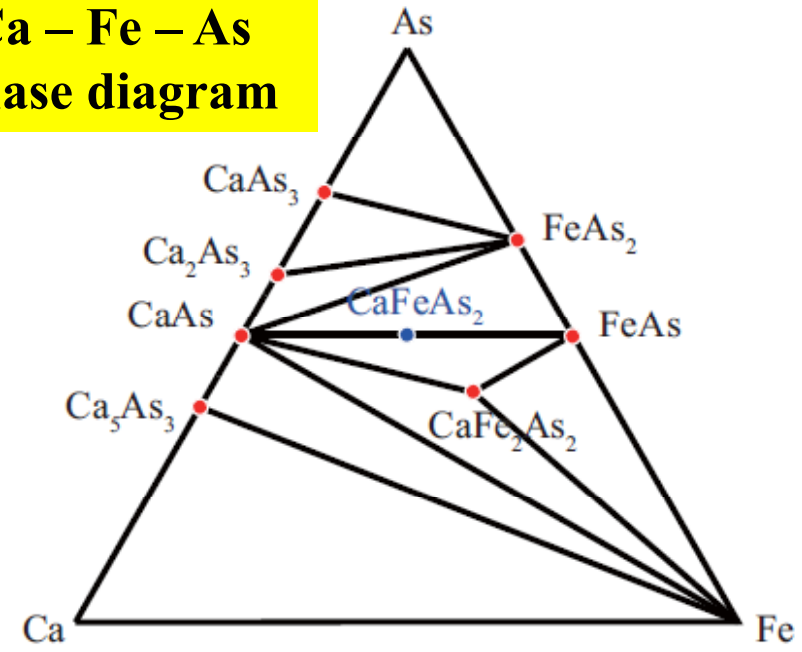


At T = 100 K,
Space group: $P2_1$ (# 4)
Monoclinic structure
a **= 3.94710 Å,** ***b*** **= 3.87240 Å,**
c **= 10.3210 Å**
β **= 91.415° (*α* = *γ* = 90°)**

Katayama *et al.*, JPSJ **82**, 123702 (2013)

4th Step: Global Stability of $CaFeAs_2$

Ca – Fe – As Phase diagram



Determinant reaction

$CaAs + FeAs \rightarrow CaFeAs_2$

DFT w/ empirical corrections

$\Delta H_{DFT\text{-}MP} = +13$ meV/atom

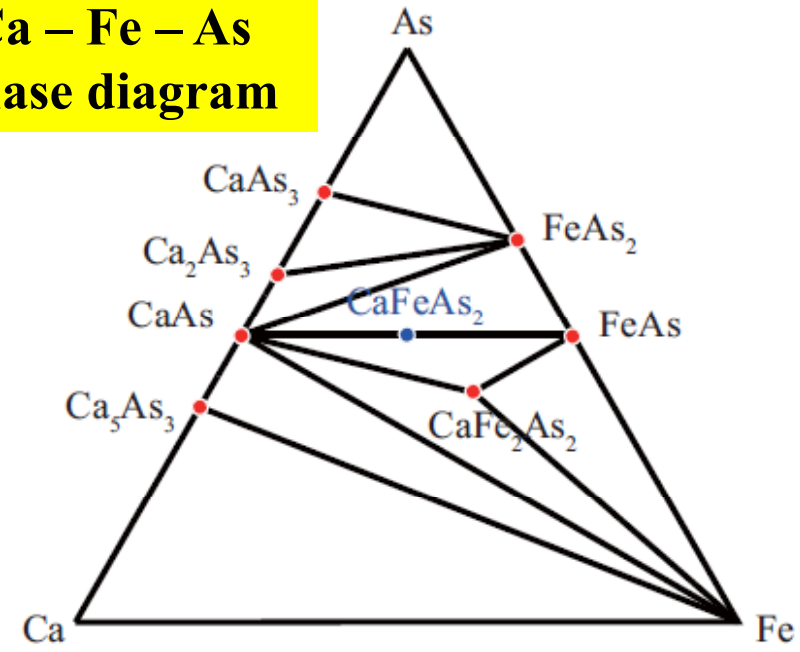
Existence probability: 0.39

DFT + Gutzwiller

$\Delta H_{Gutz} = +7$ meV/atom

4th Step: Global Stability of $CaFeAs_2$

Ca – Fe – As Phase diagram



Determinant reaction

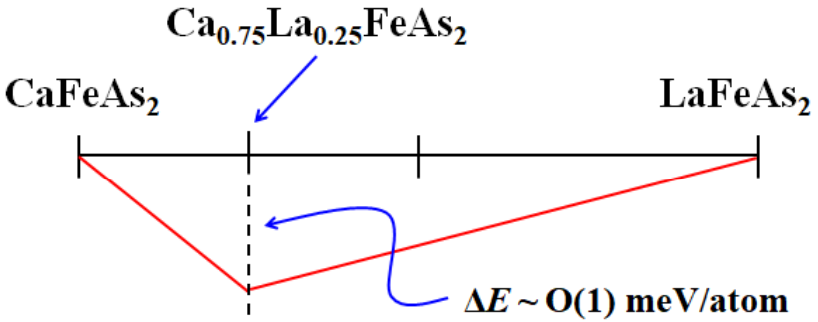
$CaAs + FeAs \rightarrow CaFeAs_2$

DFT w/ empirical corrections

$\Delta H_{DFT\text{-}MP} = +13$ meV/atom

Existence probability: 0.39

Further stabilization induced by rare-earth doping



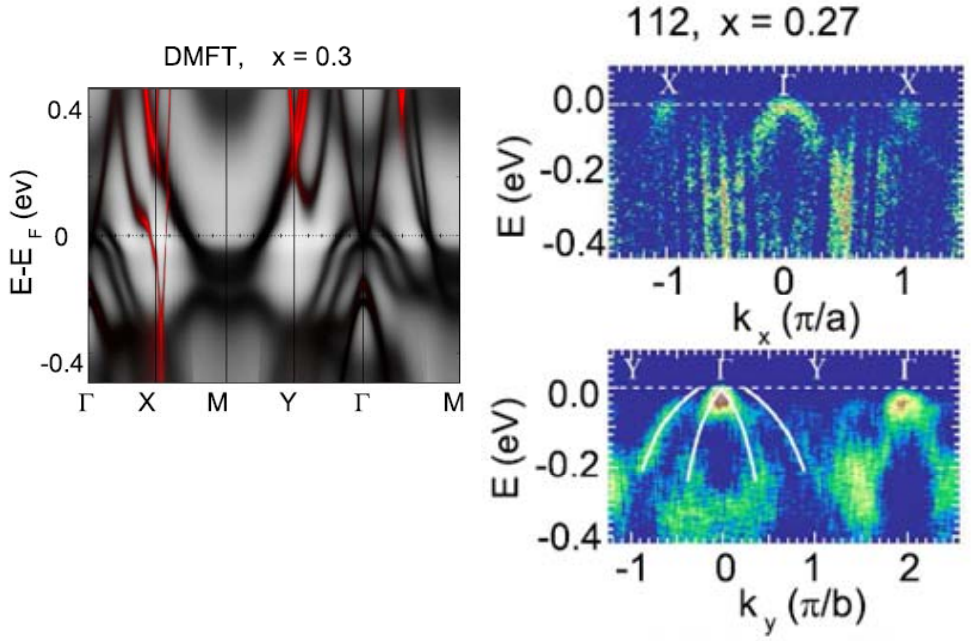
DFT + Gutzwiller

$\Delta H_{Gutz} = +7$ meV/atom

Superconducting mechanism in Fe112 family

$Ca_{1-x}La_xFeAs_2$

DMFT **ARPES**



As spacer layer: metallic Dirac cone

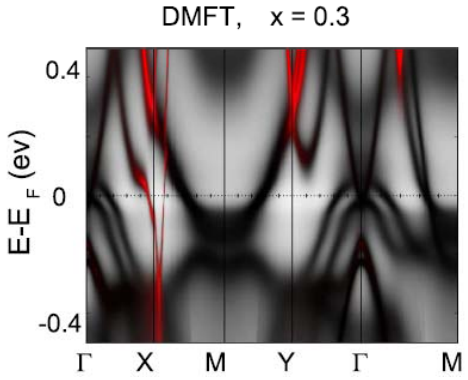
S. Jiang *et al.*, PRB **93**, 054522 (2016)

C.-J. Kang, T. Birol, and G. Kotliar,
PRB **95**, 014511 (2017)

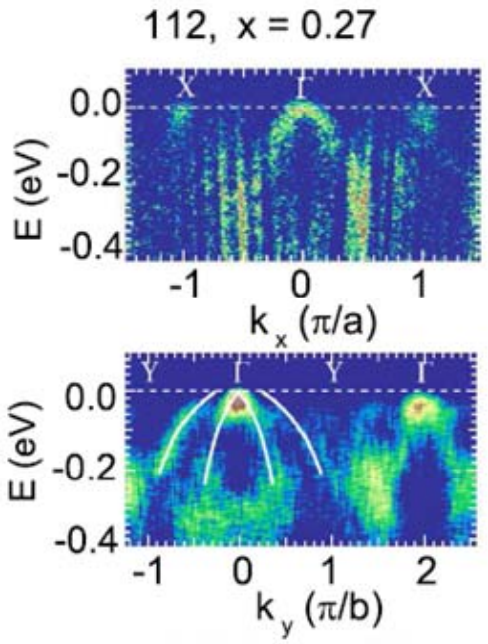
Superconducting mechanism in Fe112 family

$Ca_{1-x}La_xFeAs_2$

DMFT



ARPES

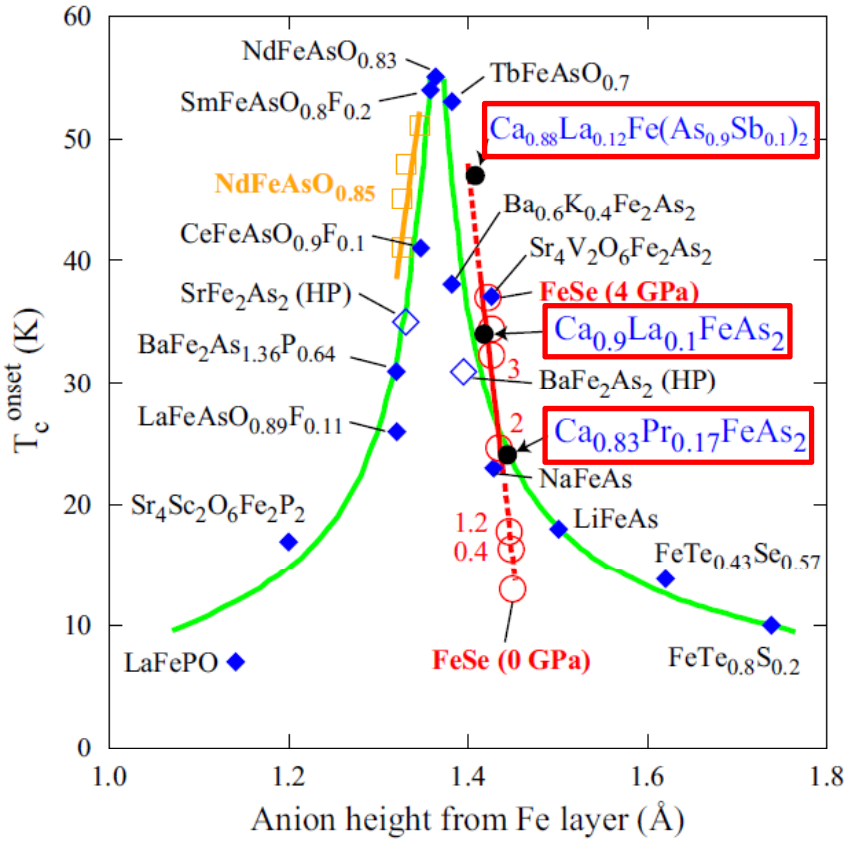


As spacer layer: metallic Dirac cone

S. Jiang *et al.*, PRB **93**, 054522 (2016)

C.-J. Kang, T. Birol, and G. Kotliar, PRB **95**, 014511 (2017)

Superconducting T_c vs. Anion height



It supports the spin fluctuation mediated superconductivity.

Acknowledgement

- **Theory**

Gabriel Kotliar **(Rutgers)**

Ran Adler **(Rutgers)**

Turan Birol **(U. Minnesota)**

Chuck-Hou Yee **(Rutgers / Bloomberg)**

- **Experiment**

- Material synthesis

Martha Greenblatt **(Rutgers)**

Xiaoyan Tan **(George Mason)**

Thank you for your attention!

Supplementary

Global Stability of La_2CuO_4

ΔE	ΔV	Synthesis pathway	
232	−1.92	$La_2SO_2 + CuS$	$\rightarrow La_2CuS_2O_2$
362	−1.45	$Y_2SO_2 + CuS$	$\rightarrow Y_2CuS_2O_2$
415	−1.36	$Lu_2SO_2 + CuS$	$\rightarrow Lu_2CuS_2O_2$
542	−1.04	$Sc_2SO_2 + CuS$	$\rightarrow Sc_2CuS_2O_2$
304	−2.00	$La_2O_3 + CuS$	$\rightarrow La_2CuSO_3$
780	−1.11	$Sc_2O_3 + CuS$	$\rightarrow Sc_2CuSO_3$
217	−1.28	$La_2SO_2 + CuO$	$\rightarrow La_2CuSO_3$
519	−0.54	$Sc_2SO_2 + CuO$	$\rightarrow Sc_2CuSO_3$
65	−2.71	$LaCuO_2 + 2\,La_2O_3 + La(CuO_2)_2$	$\rightarrow 3\,La_2CuO_4$

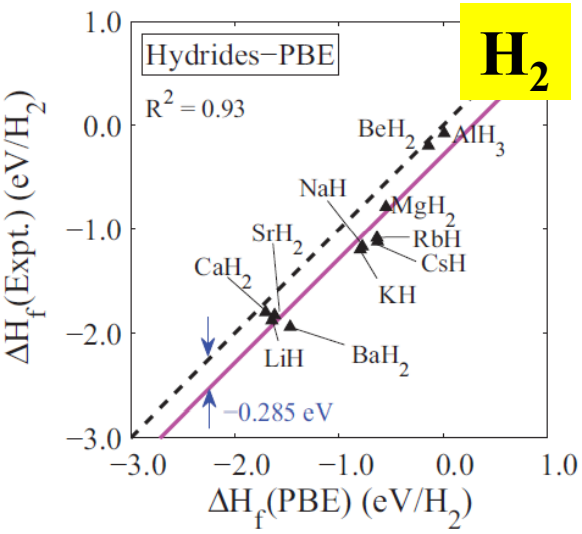
La_2CuO_4: $\mathbf{\Delta H_{DFT\text{-}MP}}$ = +65 meV/atom

(Existence probability = 0.26)

R. Adler, **C.-J. Kang**, C.-H. Yee, and G. Kotliar, Reports on Progress in Physics **82**, 012504 (2019)

Material Designs – Empirical Corrections

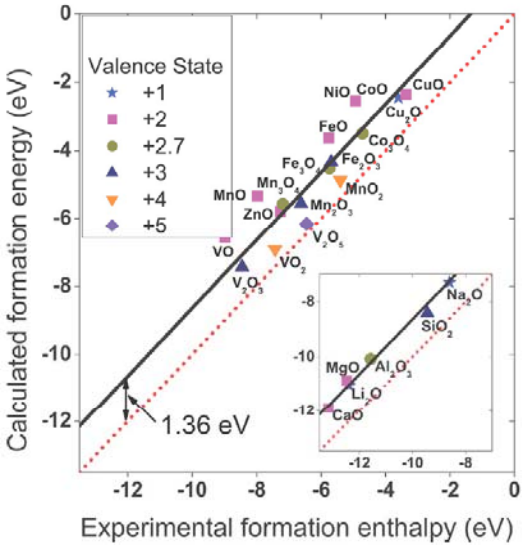
1. Gas Correction



$$\Delta H^{Expt} = \Delta H^{DFT} + C$$

S. Grindy *et al.*,
PRB **87**, 075150 (2013)

2. Anion Correction



- oxide (O^{2-}): -0.702 eV
- peroxide (O_2^{2-}): -0.466 eV
- superoxide (O_2^{1-}): -0.146 eV
- ozonide (O_3^{1-}): 0.00 eV
- sulfide (S^{2-}): -0.663 eV

L. Wang *et al.*,
PRB **73**, 195107 (2006)

3. Coulomb-*U* Correction

TABLE I. *U* values used in this work for all oxide systems. Multiple values for Wang *et al.* indicate fits to different reactions; for details see Ref. 15. We also present in the last column the energy adjustments that are used to adjust GGA + *U* energies (derived in Sec. III B).

Element	*U* value used in this work (oxides, eV)	*U* values fit by Wang *et al.*[15]	Average ΔE_M (eV)
V	3.1	3.0, 3.1, 3.3	1.764
Cr	3.5	3.5	2.067
Mn	3.9	3.5, 3.8, 4.0	1.687
Fe	4.0	3.9, 4.1	1.723
Co	3.4	3.3	1.751
Ni	6.0	6.4	2.164
Cu	4.0	4.0	1.156
Mo	3.5	N/A	2.668

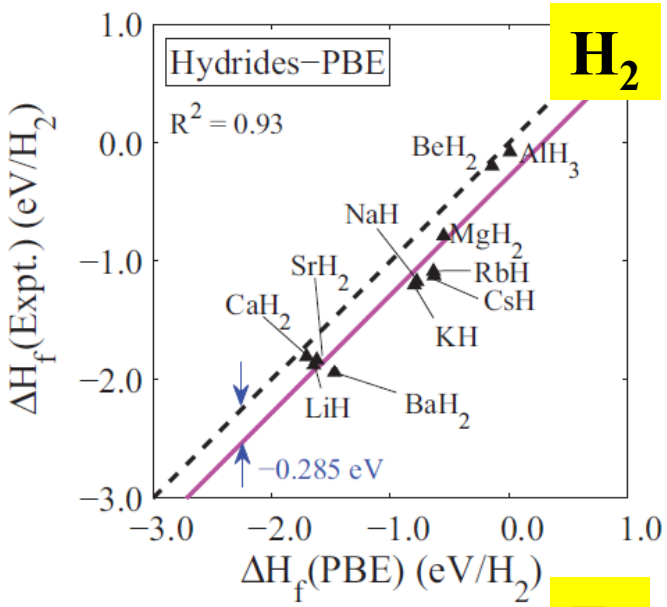
$$\Delta H^{\text{Expt}} = \Delta H^{\text{GGA+U}} - \sum_M n_M \Delta E_M$$

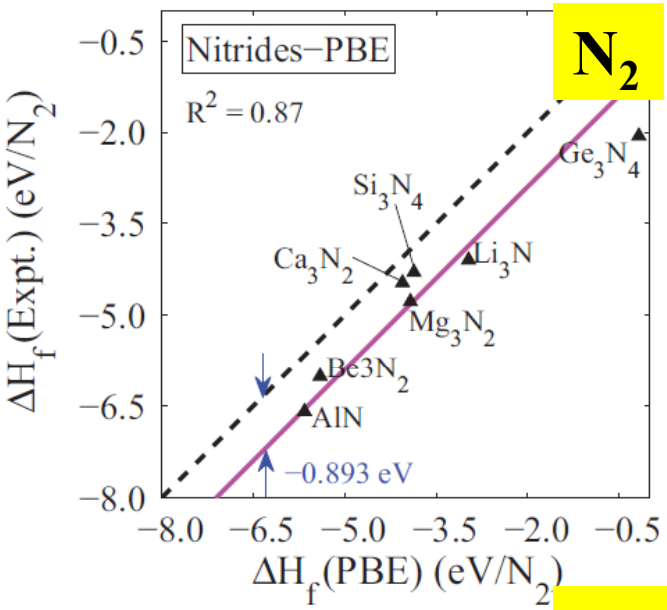
A. Jain *et al.*,
PRB **84**, 045115 (2011)

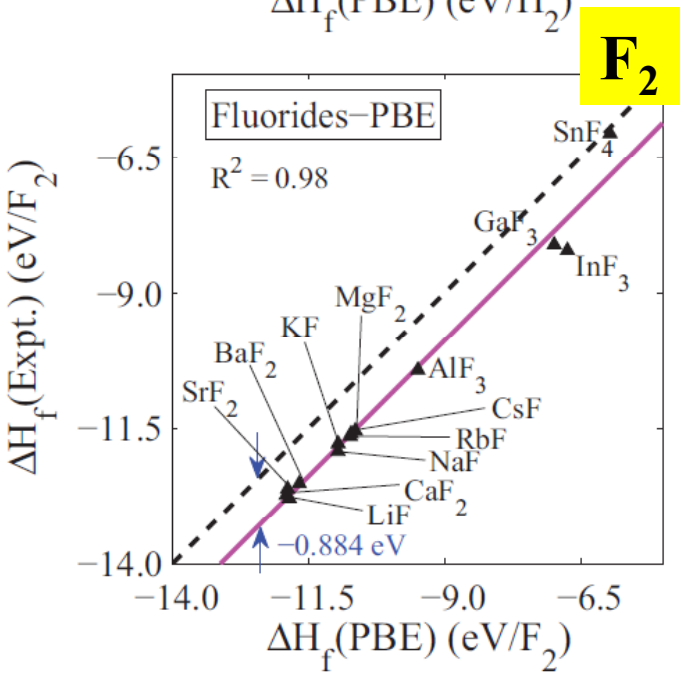
Material Designs – Empirical Corrections

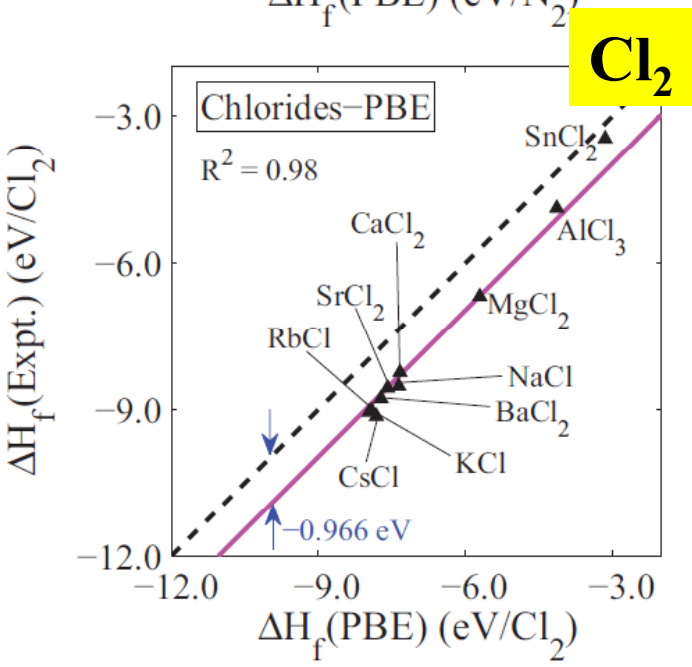
1. Gas Correction

$$\Delta H^{Expt} = \Delta H^{DFT} + C$$







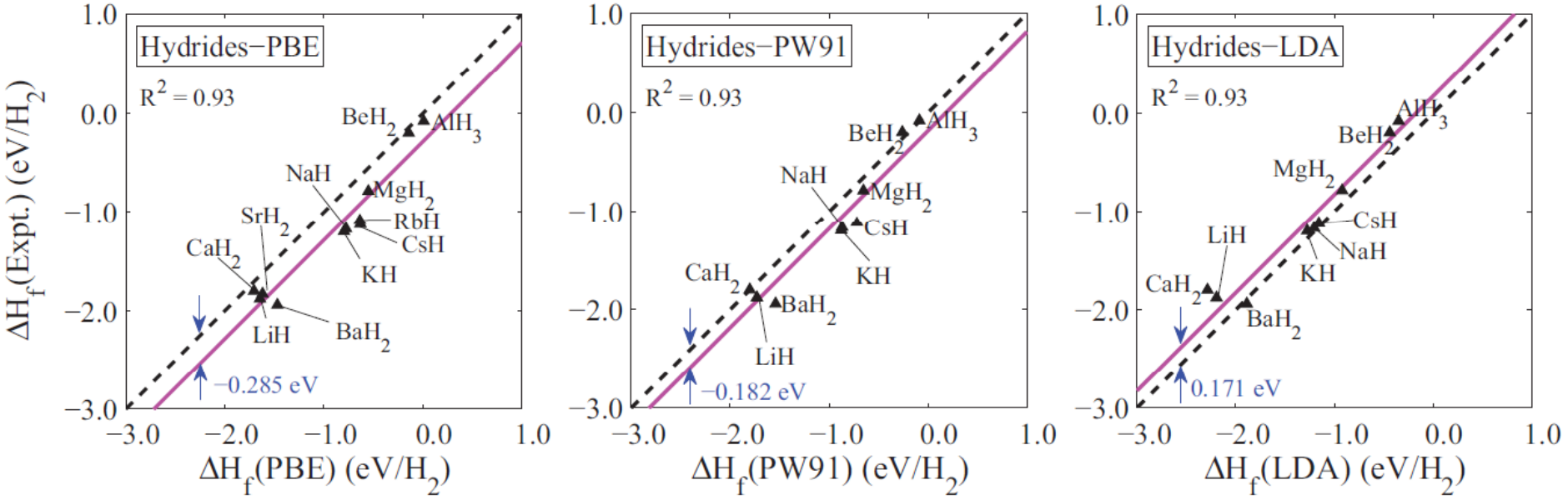


S. Grindy *et al.*,
PRB **87**, 075150 (2013)

Material Designs – Empirical Corrections

1. Gas Correction

$$\Delta H^{Expt} = \Delta H^{DFT} + C$$



The constant C could be varied with the exchange-correlation functional.

S. Grindy *et al.*,
PRB **87**, 075150 (2013)

Material Designs – Empirical Corrections

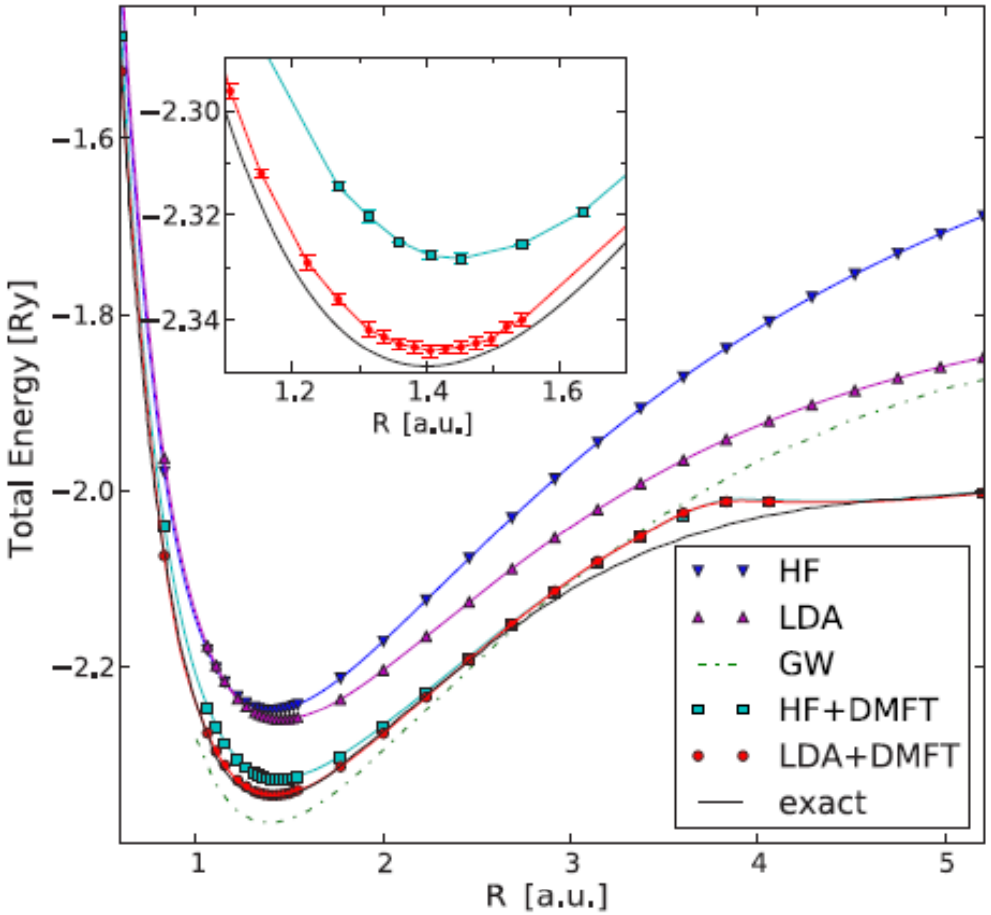


FIG. 1. (Color online) Total energy curves of the H_2 molecule versus interatomic distance R calculated by different methods: LDA+DMFT, HF+DMFT, LDA, and HF. The *GW* and exact result are also presented for comparison.

J. Lee *et al.*,
PRB **91**, 155144 (2015)

Evolutionary Algorithm

It adopts Charles Darwin's Theory of Evolution.

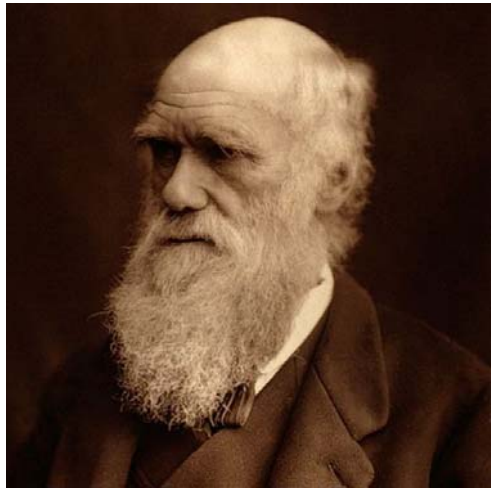
Initial Population
(Create initial population with random individuals)

Assignment
(Assign genetic information for individuals)

Fitness Evaluation
(Determine fitness using objective values)

Selection
(Select fittest individual)

Reproduction
(Create new individuals)

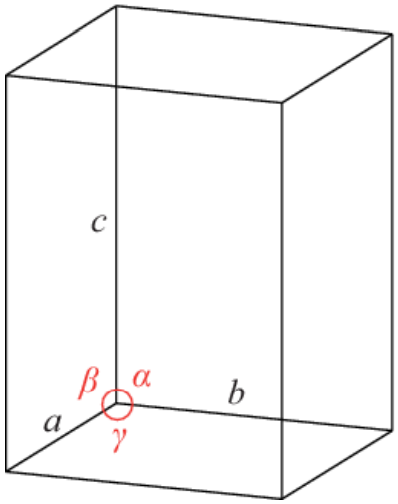


The process continues until the selected fittest does not change over a certain number of generations.

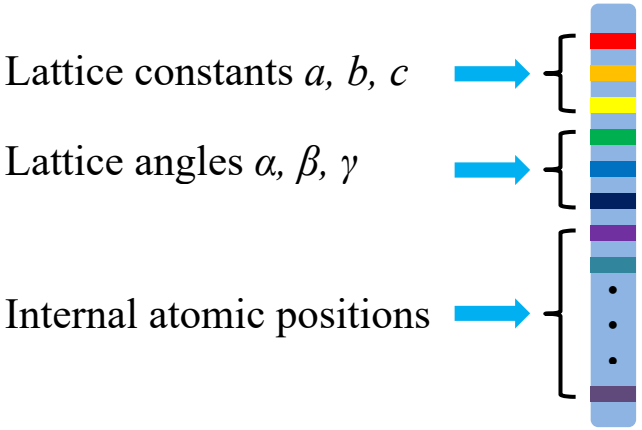
Evolutionary Algorithm in Solid State Physics

Crystal structure could be represented by genetic information.

Crystal structure



Genetic information

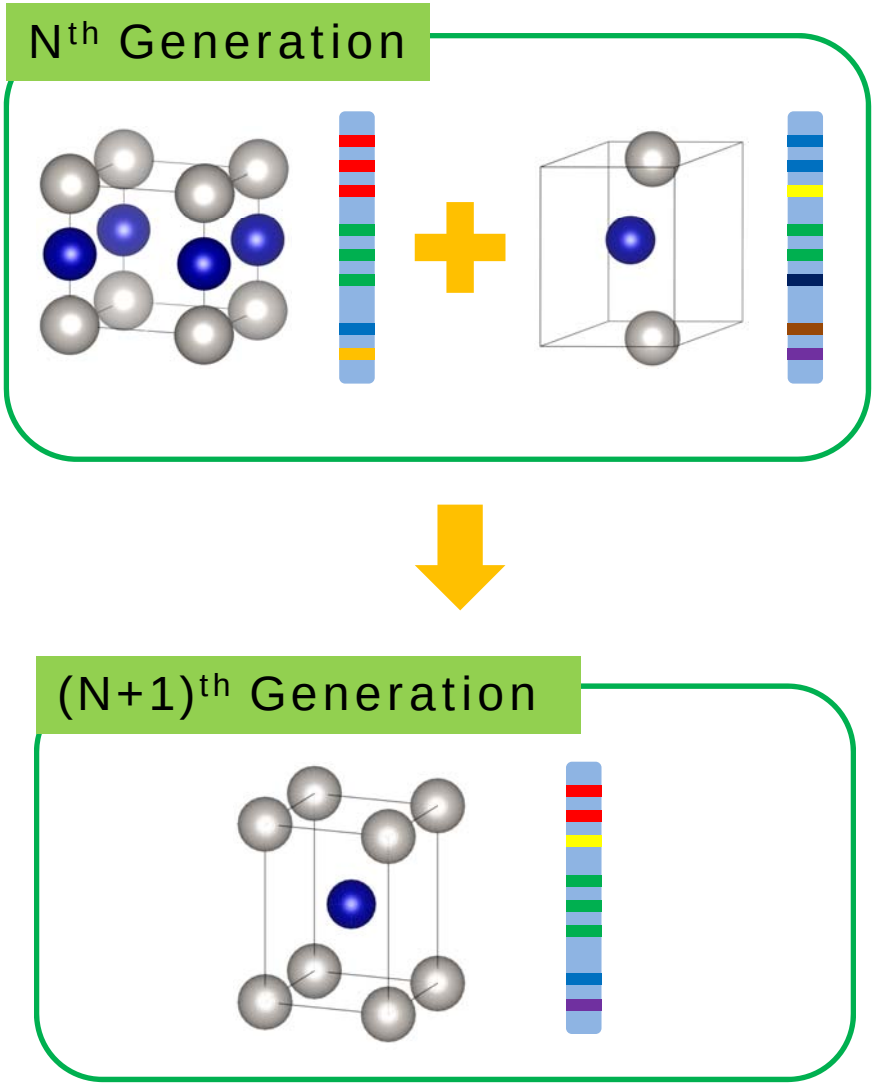


One-to-one correspondence between

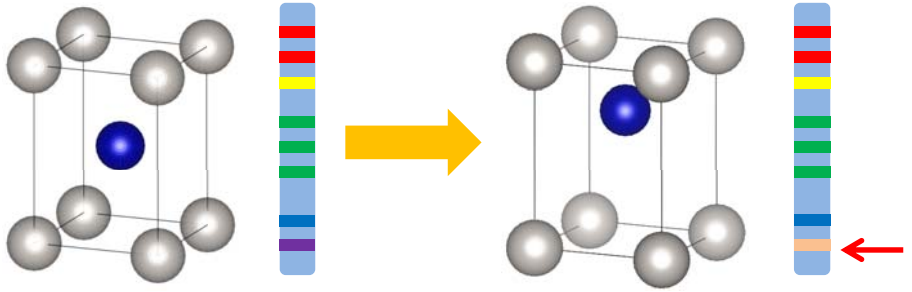
crystal structure and generic information

Evolutionary Algorithm in Solid State Physics

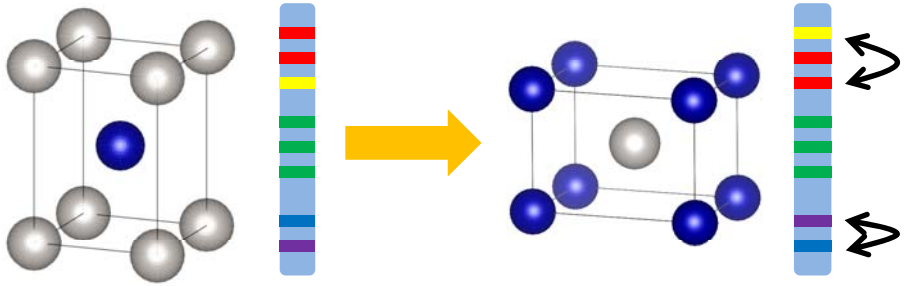
1. Heredity



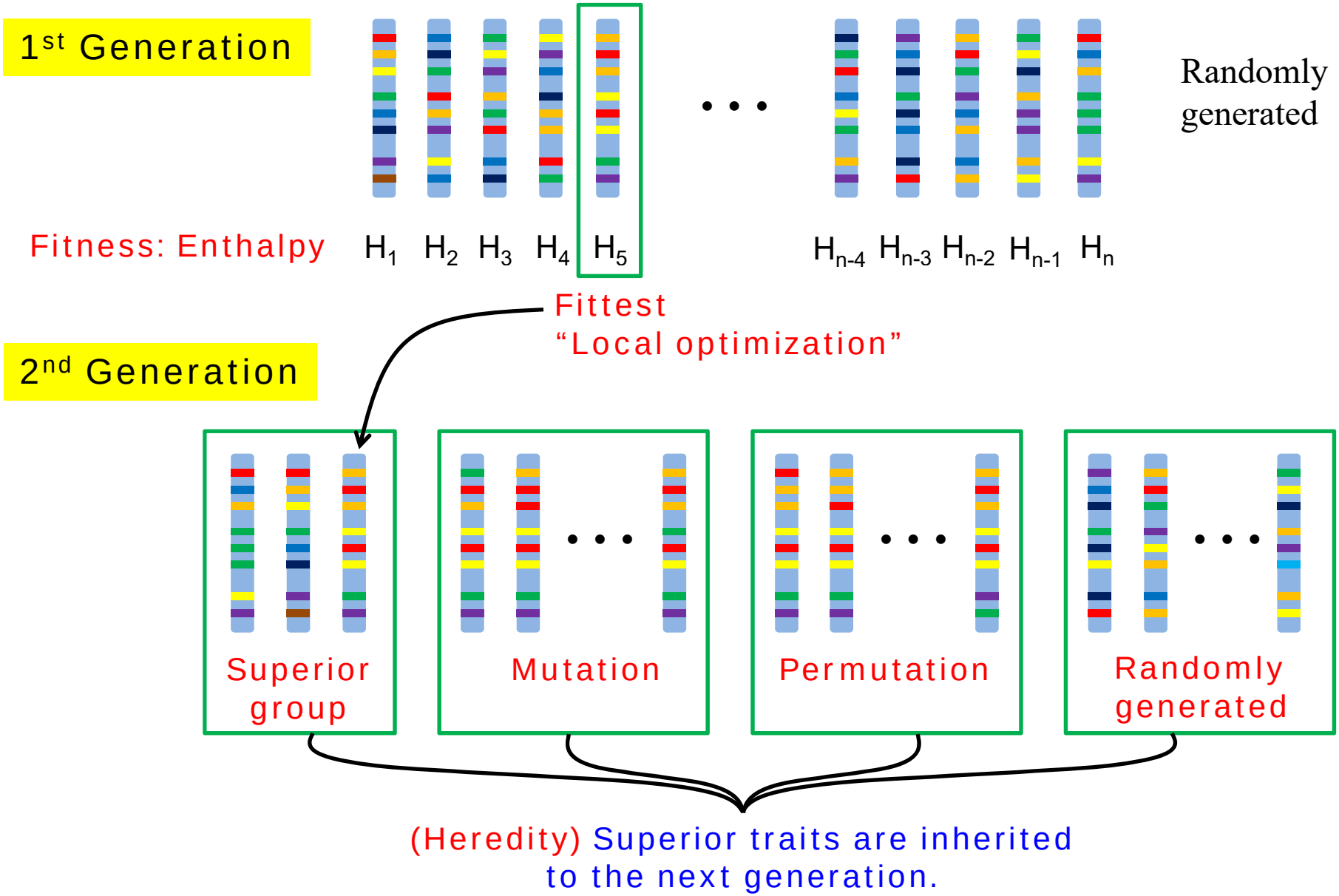
2. Mutation



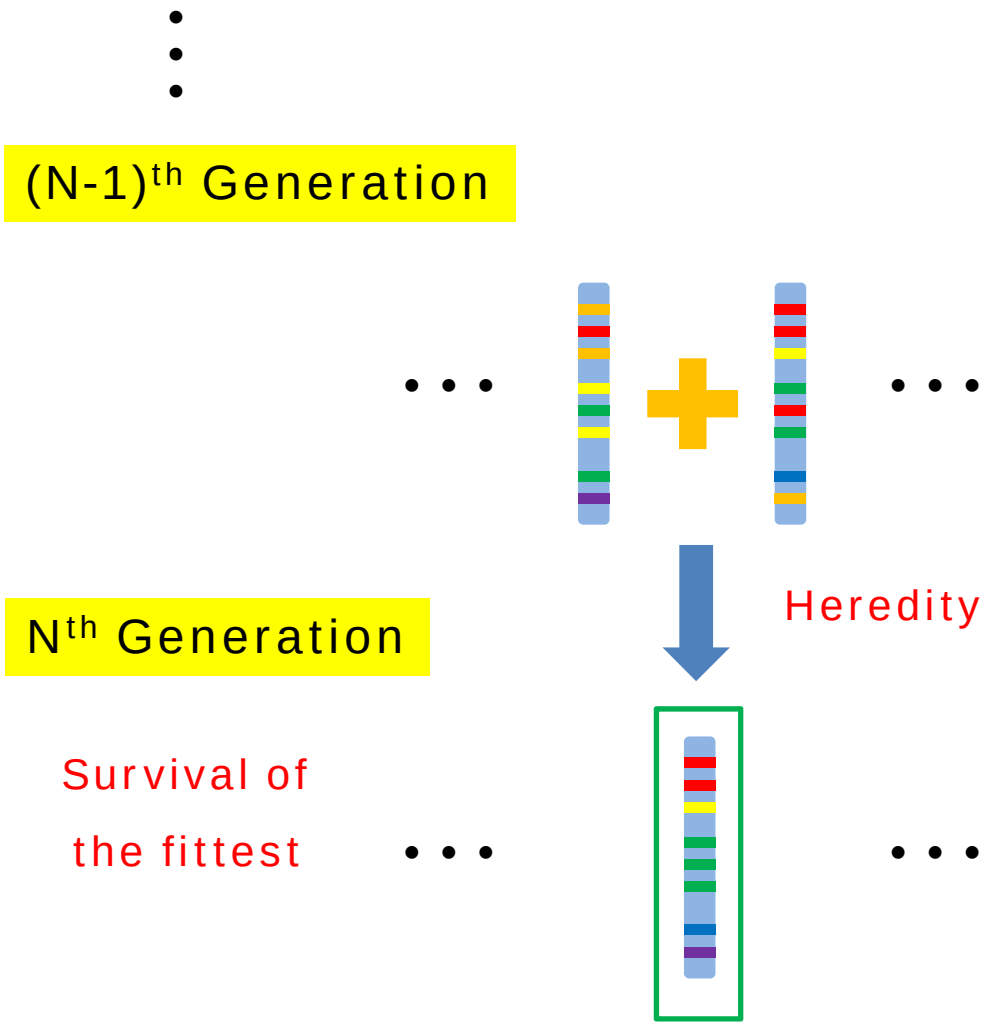
3. Permutation

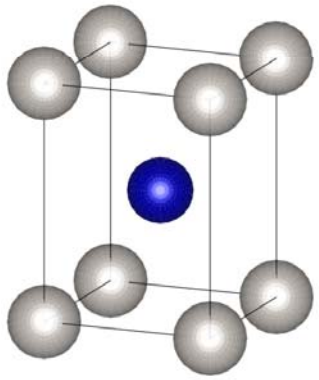


Evolutionary Algorithm in Solid State Physics



Evolutionary Algorithm in Solid State Physics



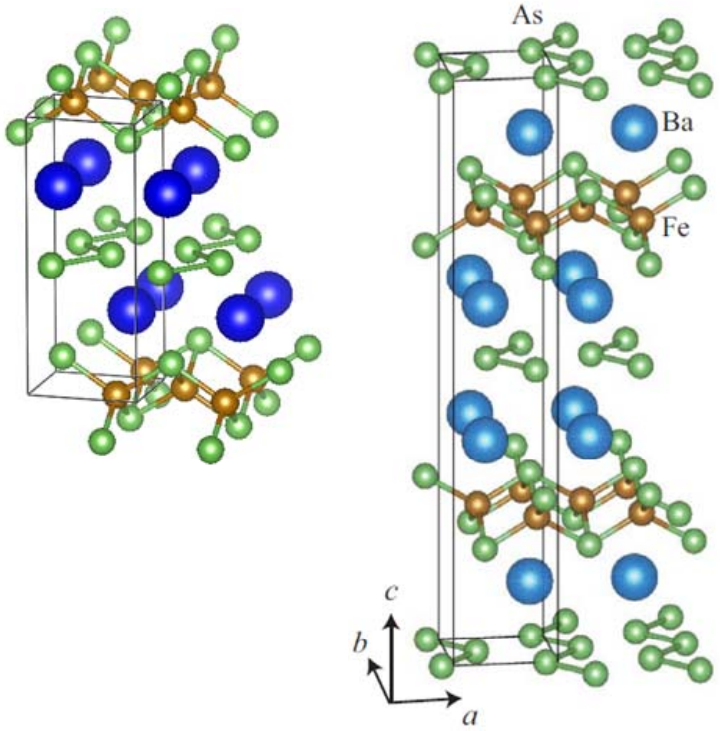


Ground-state crystal structure

Applications of Evolutionary Algorithm

112 family Fe-based superconductors

$(Ca,Sr)FeAs_2$ **$BaFeAs_2$**

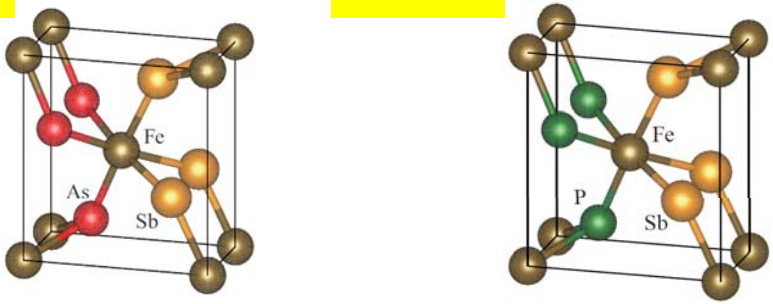


C.-J. Kang *et al.*, PRB **95**, 014511 (2017)

(EXP) N. Katayama *et al.*,
JPSJ **82**, 123702 (2013)

New thermoelectric materials

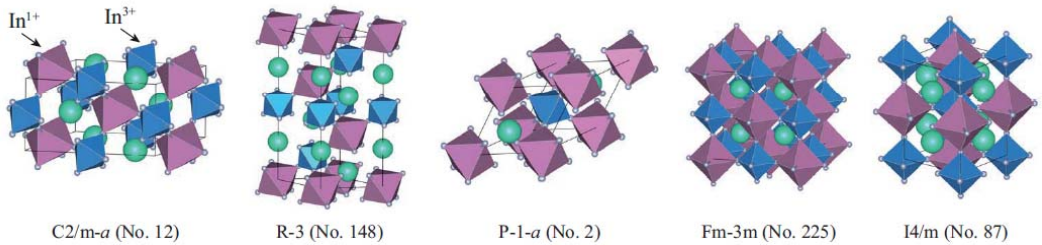
FeSbAs **FeSbP**



C.-J. Kang *et al.*, PRM **2**, 034604 (2018)

(EXP) X. Tan *et al.*, Chemistry of Materials **30**, 4207 (2018)

Bond/valence disproportionation materials

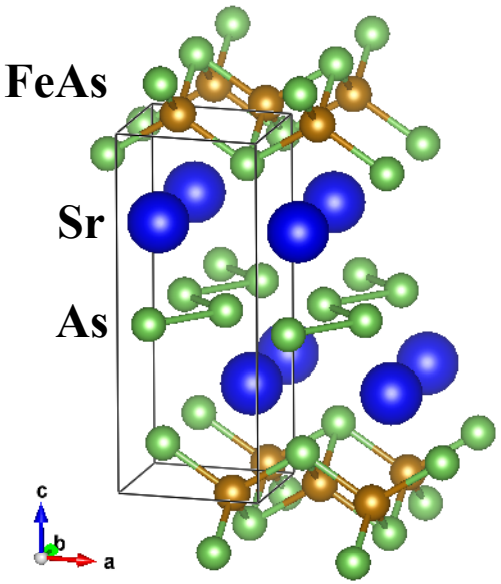


C.-J. Kang *et al.*, PRM **3**, 015001 (2019)

(EXP) X. Tan *et al.*, Chemistry of Materials **31**, 1981 (2019)

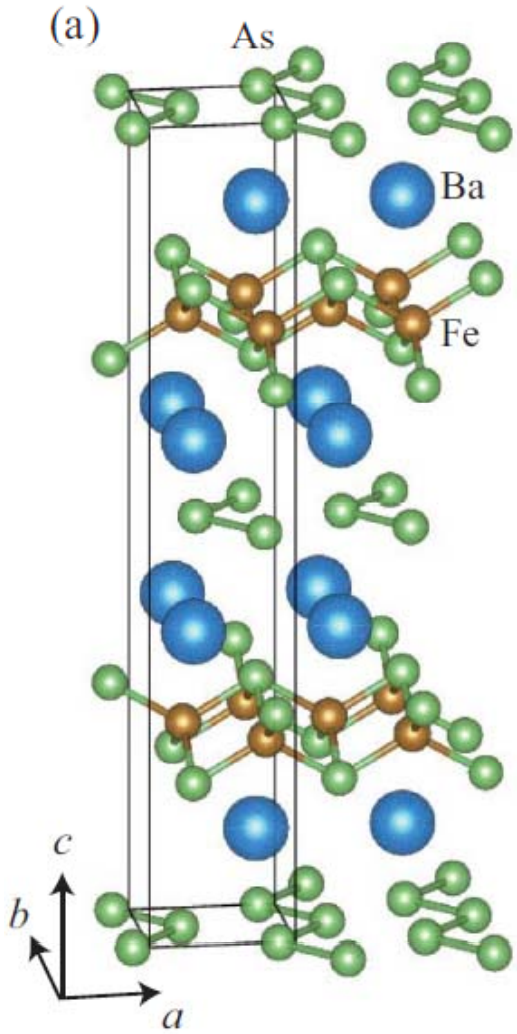
Structure predictions in (Sr, Ba)$FeAs_2$

$SrFeAs_2$



Space group: $P2_1/m$ (# 11)
Monoclinic structure
a **= 4.022 Å,** ***b*** **= 3.947 Å,**
c **= 10.786 Å**
β **= 91.416° (*α* = *γ* = 90°)**

$BaFeAs_2$



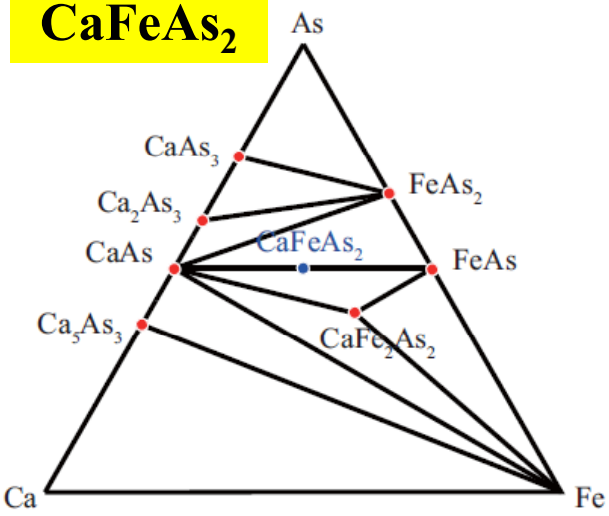
Space group: Imm2 (# 44)
Orthorhombic structure
a **= 4.059 Å,** ***b*** **= 3.984 Å,**
c **= 23.161 Å**
(*α* = *β* = *γ* = 90°)

Lack of inversion symmetry

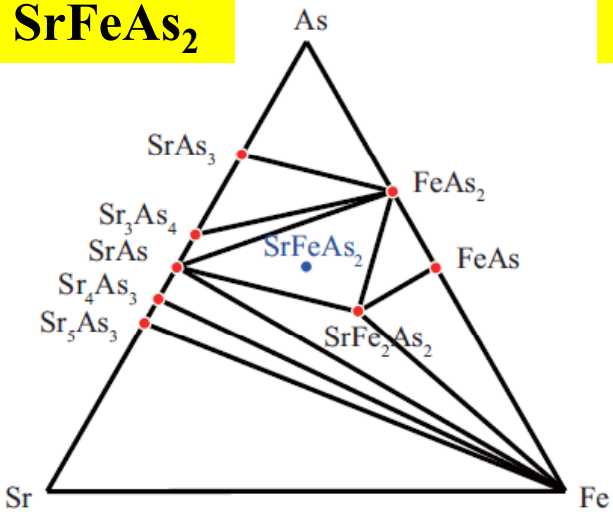
C.-J. Kang *et al.*, PRB **95**, 014511 (2017)

Global stability of Fe 112 phase materials

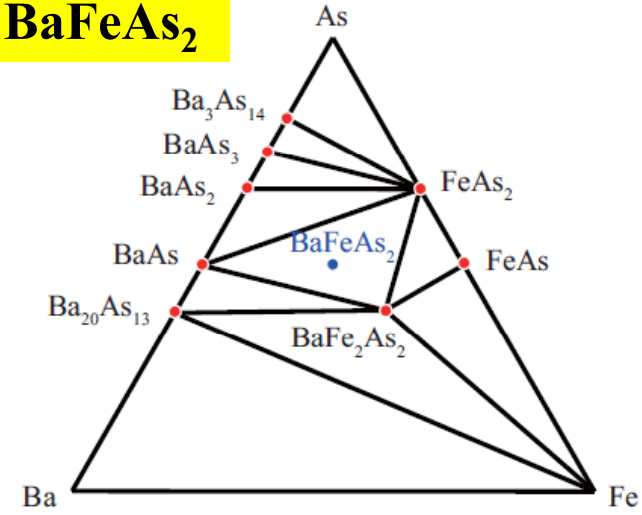
$CaFeAs_2$



$SrFeAs_2$



$BaFeAs_2$



Determinant reaction

$CaAs + FeAs \rightarrow CaFeAs_2$	$2\ SrAs + FeAs_2 + SrFe_2As_2 \rightarrow 3\ SrFeAs_2$	$2\ BaAs + FeAs_2 + BaFe_2As_2 \rightarrow 3\ BaFeAs_2$
E_{hull} = +13 meV/atom	**E_{hull} = +24 meV/atom**	**E_{hull} = +17 meV/atom**
Prob. = 0.39	**Prob. = 0.36**	**Prob. = 0.38**

DFT + Gutzwiller

E_{hull} = +7 meV/atom