Rencontre CINES–chercheurs en chimie

Thermodynamic modeling assisted by massive first principles calculations

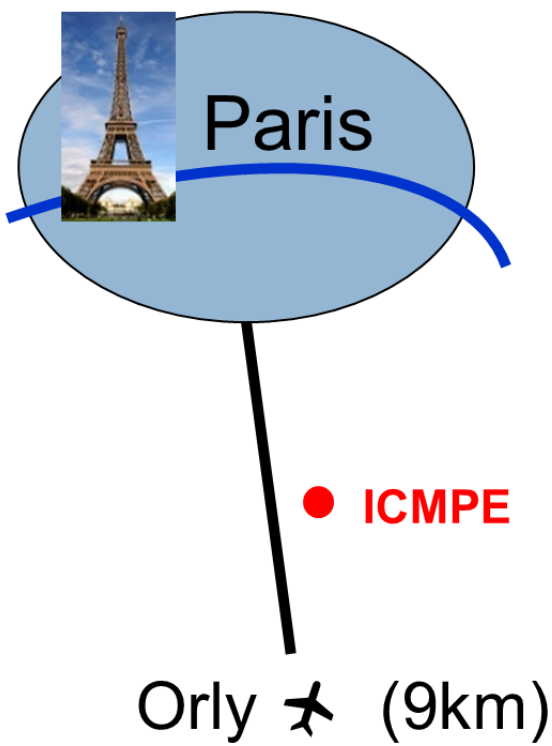
J.-C. Crivello[1], DARI A0020906175

[1] CMTR ICMPE UMR7182, UPE CNRS, Thiais, France

CINES, Montpellier, Septembre 2018

ICMPE: Institute of Chemistry & Materials Science, Paris-East

$\simeq$ 120 permanents + 50 non-permanents

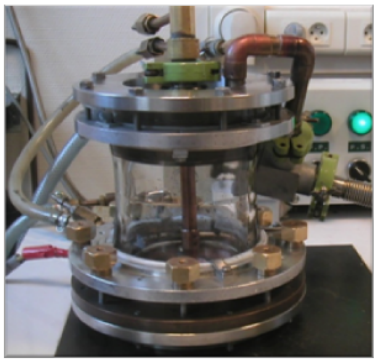


ICMPE: research on materials science

Synthesis, Structural and chemical characterization
XRD, EPMA, SEM-FEG-EBSD, ICP-OES, TDS, ATG, PPMS,...

Ball-milling, SPS, melt spinning, induction and arc melting...




Multi-scale calculations

5 reseachers, 3 PhDs, 4 workstations, no assist

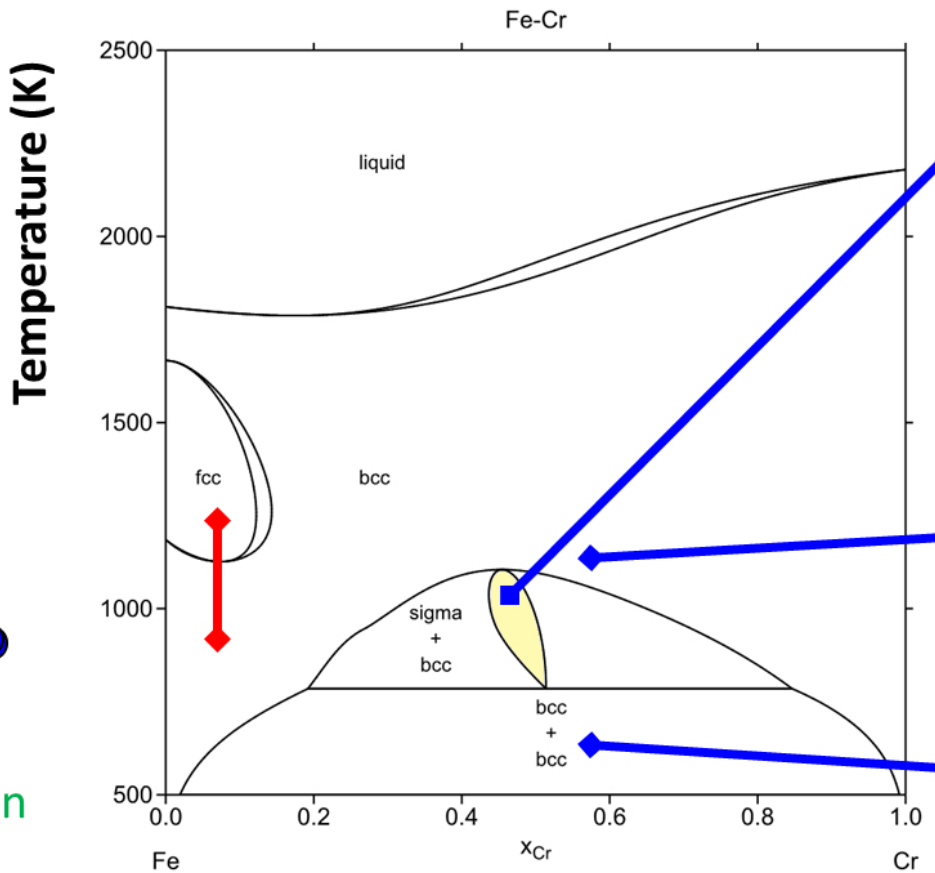
GENCI since 2009: 1.400.000 h/year in 2018

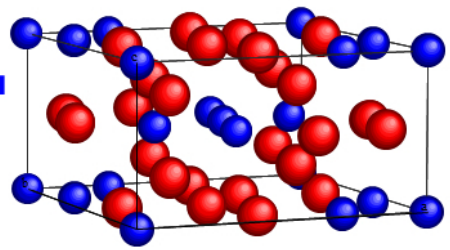
Multi-scale calculations

computation of phase diagram?

Calphad

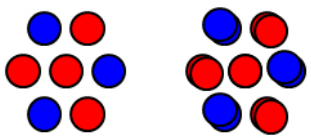
Enthalpy?





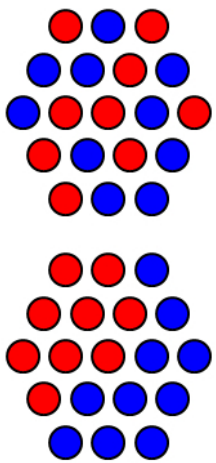
DFT, CEF

Entropy?



BWA, CVM

Phonon

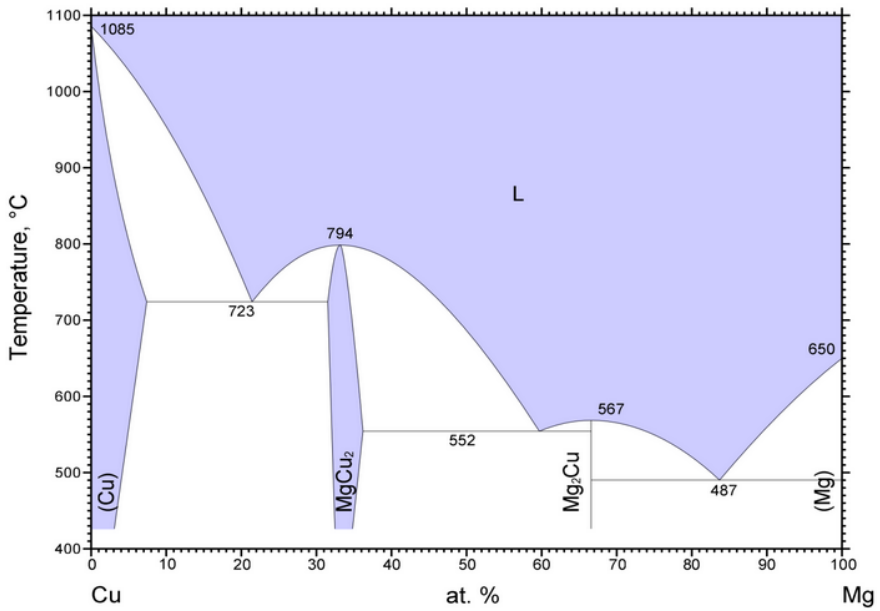


CEM, SQS

Enthalpy of formation

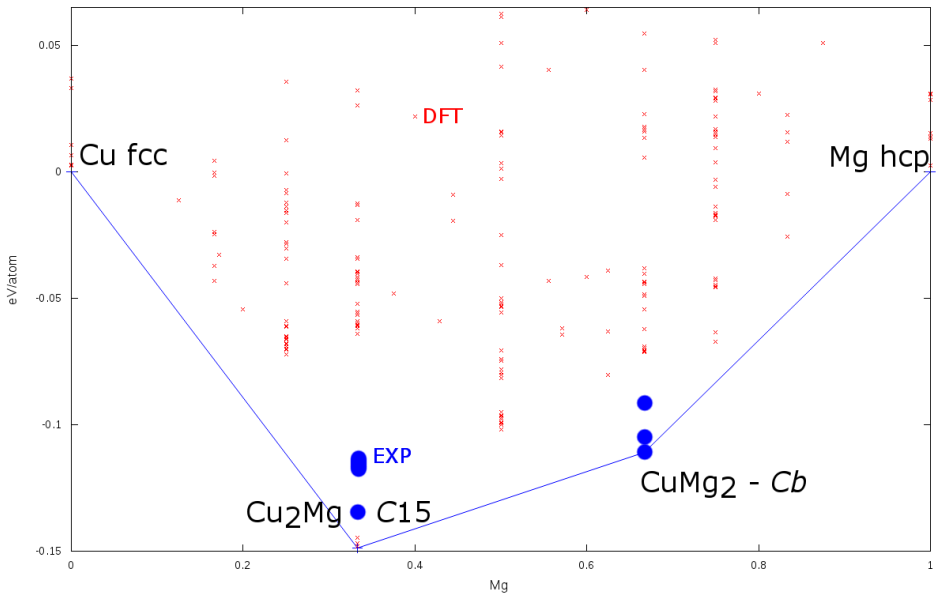
Ex: Cu–Mg system

phase diagram



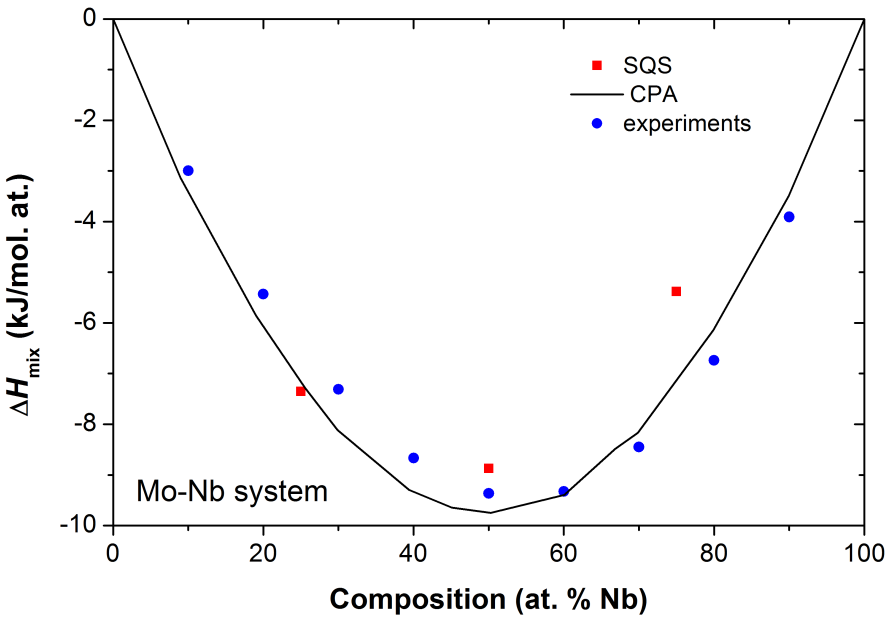
[1] DFT from AFLOW database

calculation of heats of formation



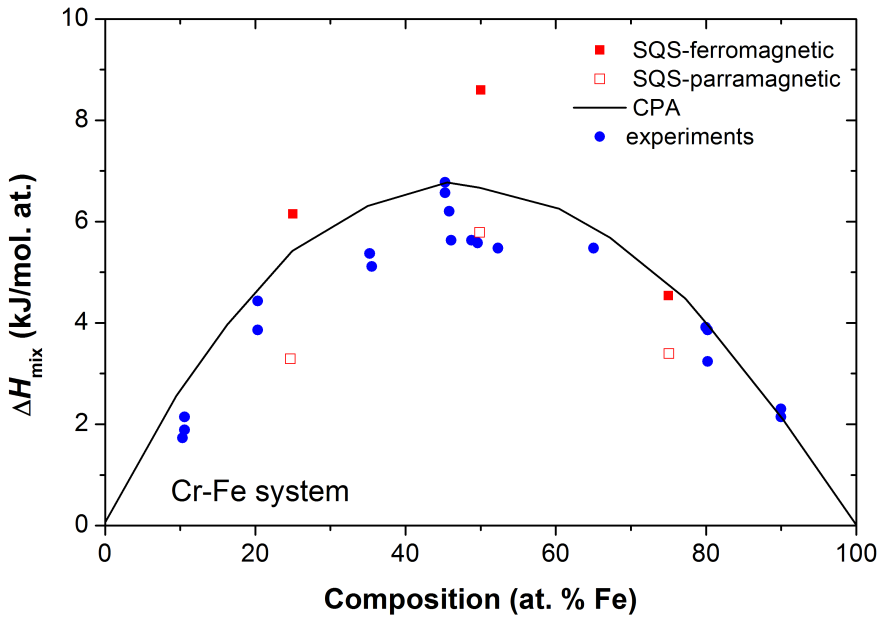
Enthalpy of mixing

Ex: Mo–Nb (bcc):



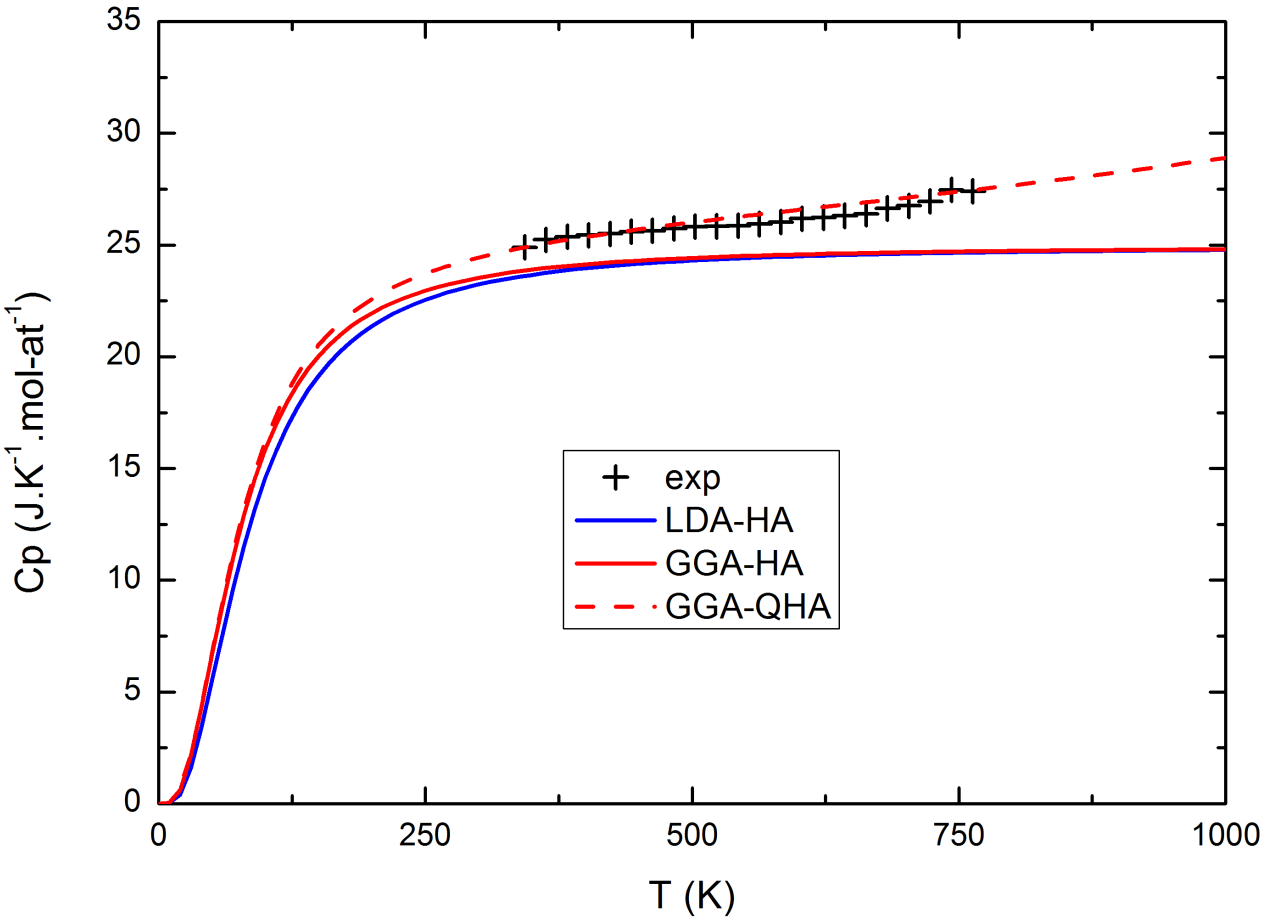
[2] Jiang *et al.*, Phys Rev B 69 (2004)

Ex: Cr–Fe (bcc):



$F(T \neq 0)$

Ex: Laves $C15-Cu_2Mg$
Phonon calculation in harmonic, quasi-harmonic approximation:



Calculation methods

- DFT PAW : VASP 5.4 (GGA, meta-GGA, mBJ)
- Phonopy 1.13 (Supercell approach)
- ATAT / MCSQS (CEM, SQS)

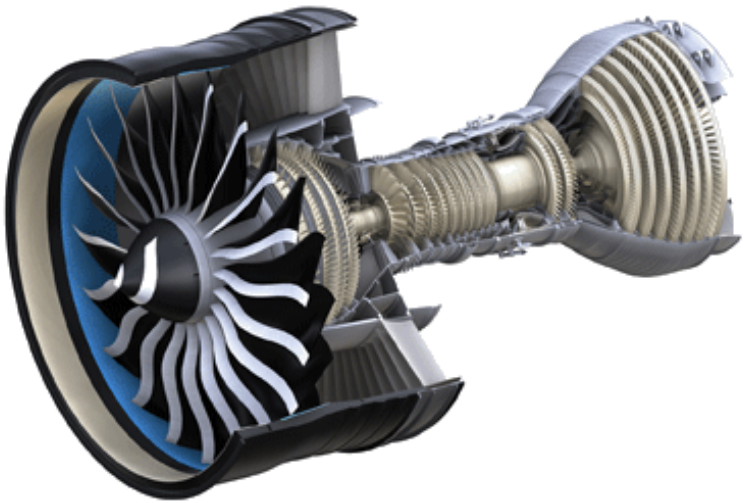
Contents

Contents

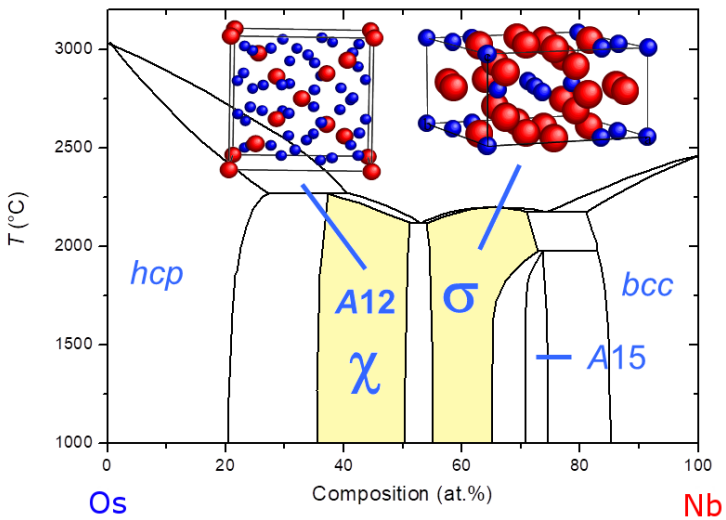
Non-stoichiometry of complex intermetallics

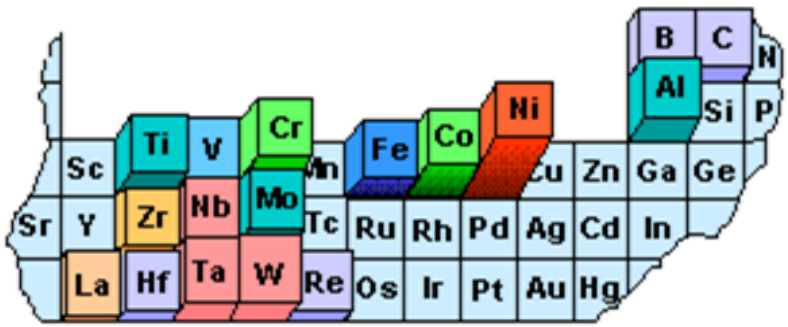
In **superalloys**, (*e.g.* Ni-based) refractory bcc element is added:

- improve the creep resistance at high temperature
- precipitation of brittle IMC phases



Ex: Os–Nb phase diagram



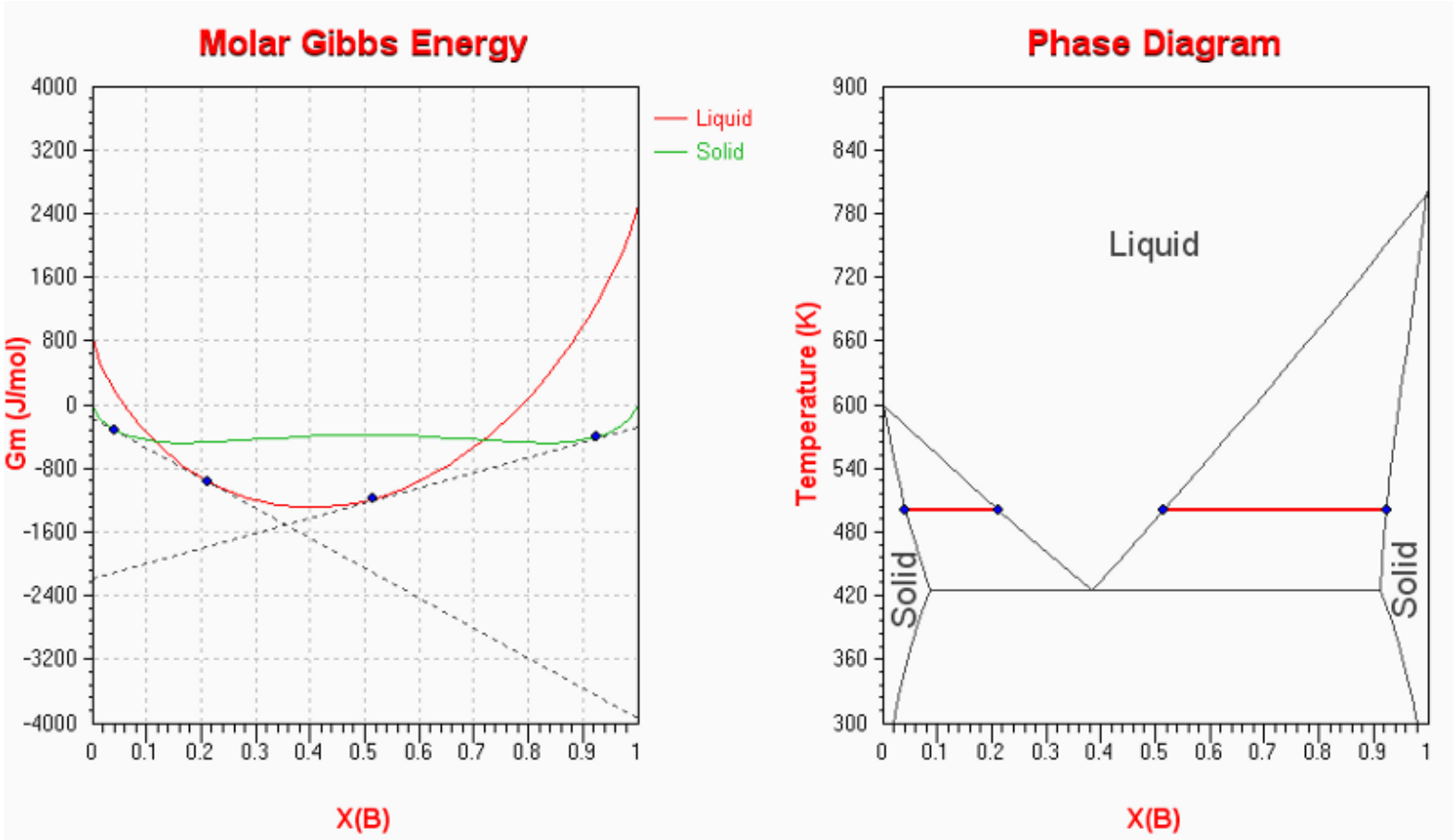


How can we predict IMC precipitation?

Modeling of phase diagram

The **Calphad** method (*CALculation of PHAse Diagram*) :

- based on Gibbs energies $G^{\varphi}(x,T,P) = H - T \cdot S$
- phases φ_i in equilibrium if $\mu_i = \left(\frac{\partial G}{\partial x_i}\right)_{P,T}$



Thermodynamic modeling with Calphad

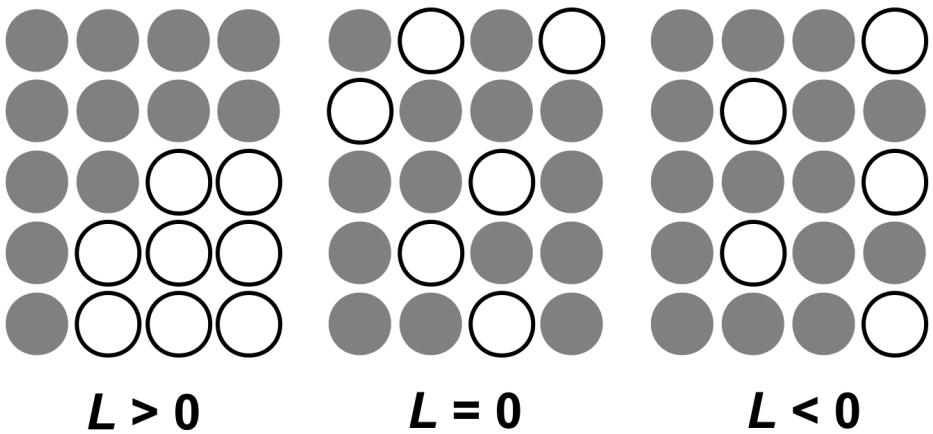
Using the **Compound Energy Formalism** (CEF):

$$G^{\varphi} = {}^{\mathrm{srf}}G^{\varphi} + {}^{\mathrm{cnf}}G^{\varphi} + {}^{\mathrm{ex}}G^{\varphi} + {}^{\mathrm{phy}}G^{\varphi}$$

[3] B. Sundman and B. J. Ågren, J. Phys. Chem. Solids 42 (1981) 297.

(i) description of a solid solution (ex: $A-B$) :

- ${}^{\mathrm{srf}}G^{\varphi} = x_A G^{\varphi}_A + x_B G^{\varphi}_B$
- ${}^{\mathrm{cnf}}G^{\varphi} = -T \cdot {}^{\mathrm{cnf}}S^{\varphi} = -RT(x_A \ln x_A + x_B \ln x_B)$
- ${}^{\mathrm{ex}}G^{\varphi} = x_A x_B L_{AB}$, où $L_{AB} = \sum_{i=0}^{n} {}^{i}L^{\varphi}_{A,B}(x_A - x_B)^i$

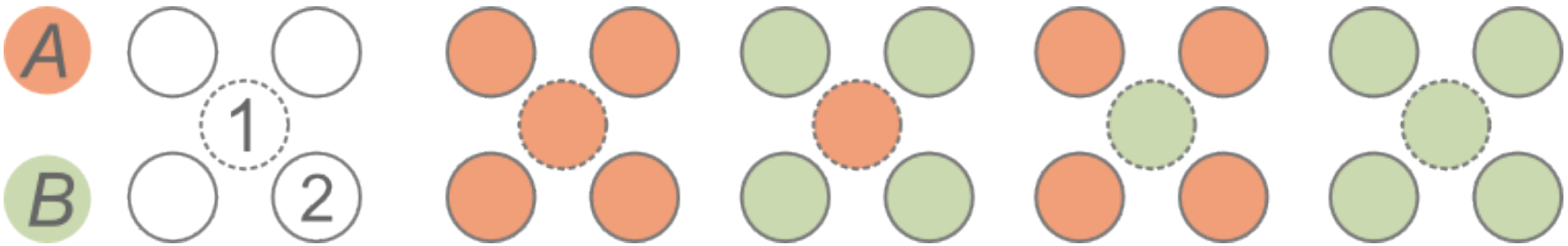


Thermodynamic modeling with Calphad

(ii) description of a non-stoichiometric compounds in (CEF)

The ${}^{\mathrm{srf}}G^{\varphi}$ is expressed regarding the crystallography of the φ phase.

As an example, the compound AB described by a full substitution model $(A,B) : (A,B)_1$



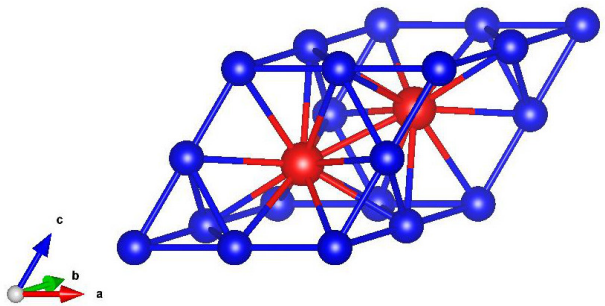
$$ {}^{\mathrm{srf}}G = y_A^1 y_A^2 G^0_{A:A} + y_A^1 y_B^2 G^0_{A:B} + y_B^1 y_A^2 G^0_{B:A} + y_B^1 y_B^2 G^0_{B:B} $$

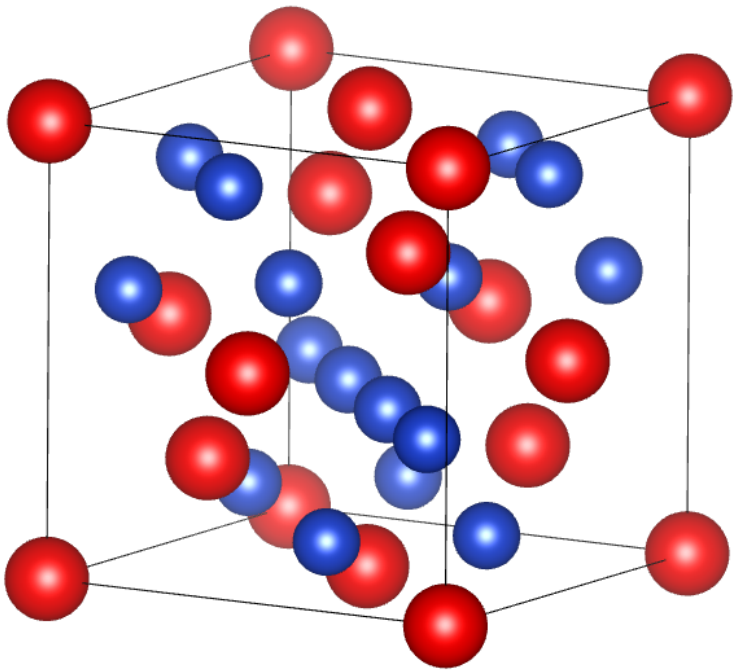
Where each $G^0 \simeq \Delta H_f$ could be expressed by DFT.

An example: the Laves phase Cu_2Mg

Crystal structure:

Strukturbericht: $C15$, Pearson: cF24
Space group: $Fd\bar{3}m$ (227, o1)
$a \simeq 7.05$ Å, 6 atoms in the primitive cell





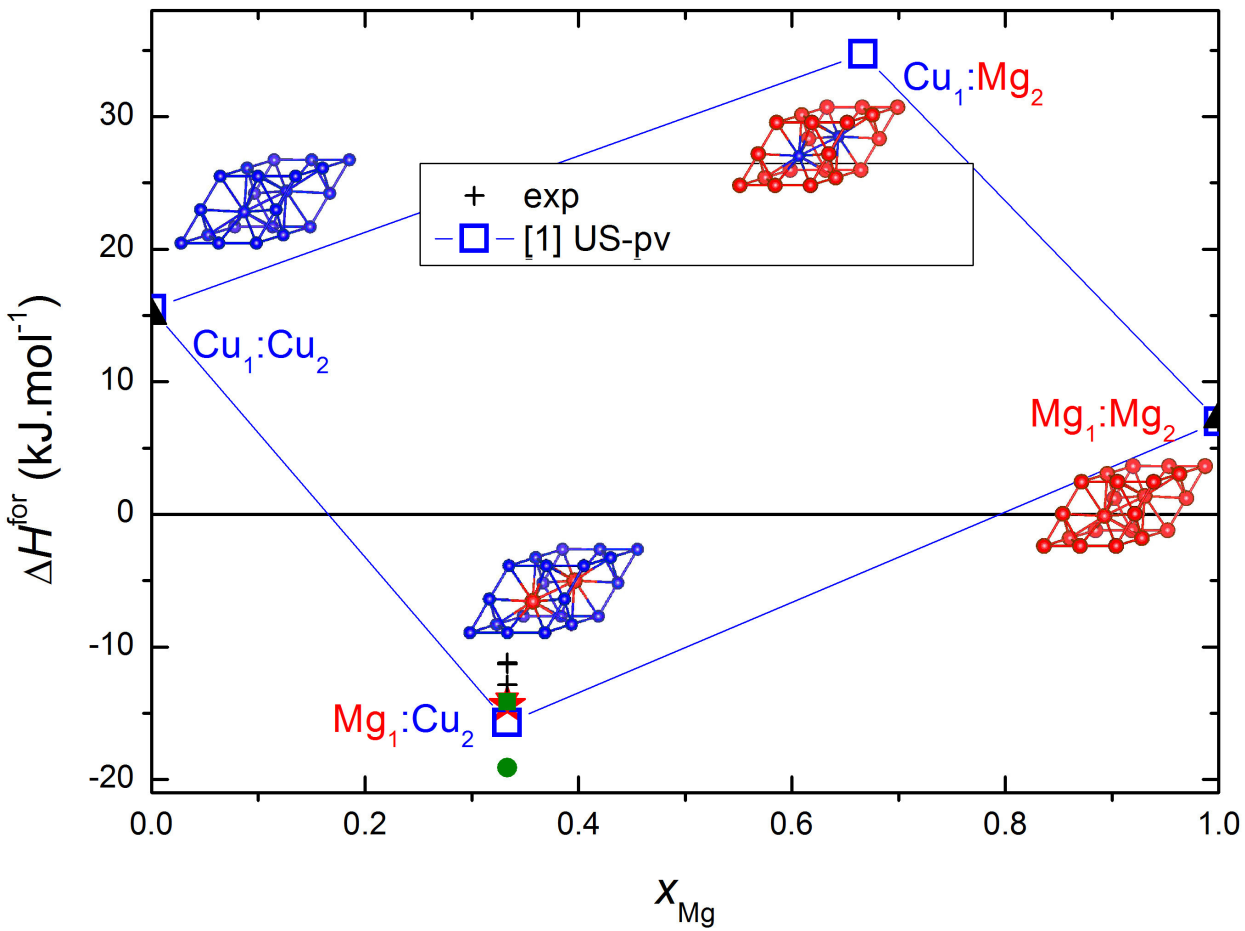
Site	Wyc	x	y	z	CN
Cu	$16d$	5/8	5/8	5/8	12
Mg	$8a$	0	0	0	16

$\Rightarrow$ **DFT calculation of every end-members**

$C15$: 2 sites, 2^2=4 ordered binary configurations in the CEF

The Laves phase described by the $(Cu,Mg)_1:(Cu,Mg)_2$ model

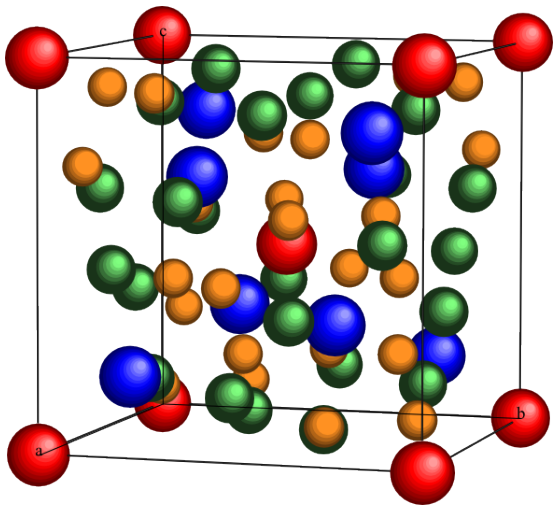
Heat of formation of 2^2=4 end-members at 0 K



More complex structures: the $\chi-$ and $\sigma-$phase

Crystal structure of the $\chi-$phase

α-Mn, $A12$, $I\bar{4}3m$, (217)
$a \simeq 9$ Å, 58(29) atoms in 4 sites

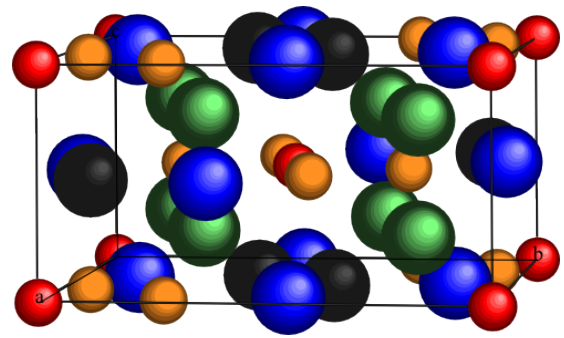


Site	Wyc	x	y	z	CN
$\mathcal{A}$	$2a$	0	0	0	16
$\mathcal{B}$	$8c$	$\sim$0.32	x	x	16
$\mathcal{C}$	$24g_1$	$\sim$0.36	x	$\sim$0.03	13
$\mathcal{D}$	$24g_2$	$\sim$0.09	x	$\sim$0.28	12

In a binary system:
2^4=16 different ordered configurations

Crystal structure of the $\sigma-$phases

σ-CrFe, $D8_b$, $P4_2/mnm$ (136)
$a \simeq$9Å, $c \simeq$5Å, 30 atoms in 5 sites



Site	Wyc	x	y	z	CN
$\mathcal{A}$	$2a$	0	0	0	12
$\mathcal{B}$	$4f$	$\sim$0.39	x	0	15
$\mathcal{C}$	$8i_1$	$\sim$0.46	$\sim$0.13	0	14
$\mathcal{D}$	$8i_2$	$\sim$0.74	$\sim$0.07	0	12
$\mathcal{E}$	$8j$	$\sim$0.18	x	$\sim$0.25	14

In a binary system:
2^5=32 different ordered configurations

[4] Joubert *et al.*, Prog. Mater. Sci. 54 (2009)
[5] Joubert, Prog. Mater. Sci. 53 (2008)

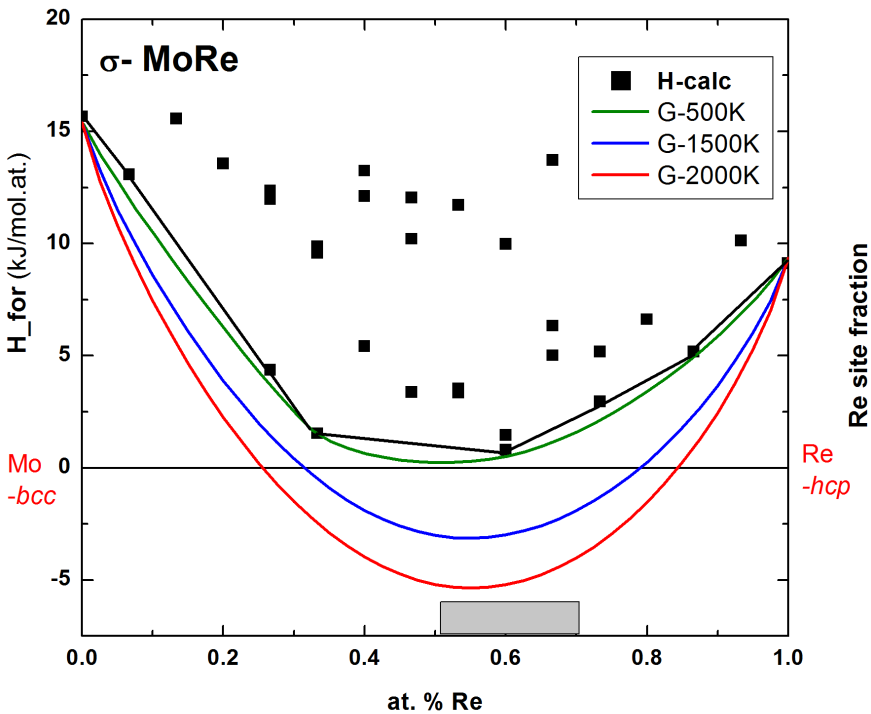
The $\sigma-$phase in a binary system, *e.g.* Mo–Re

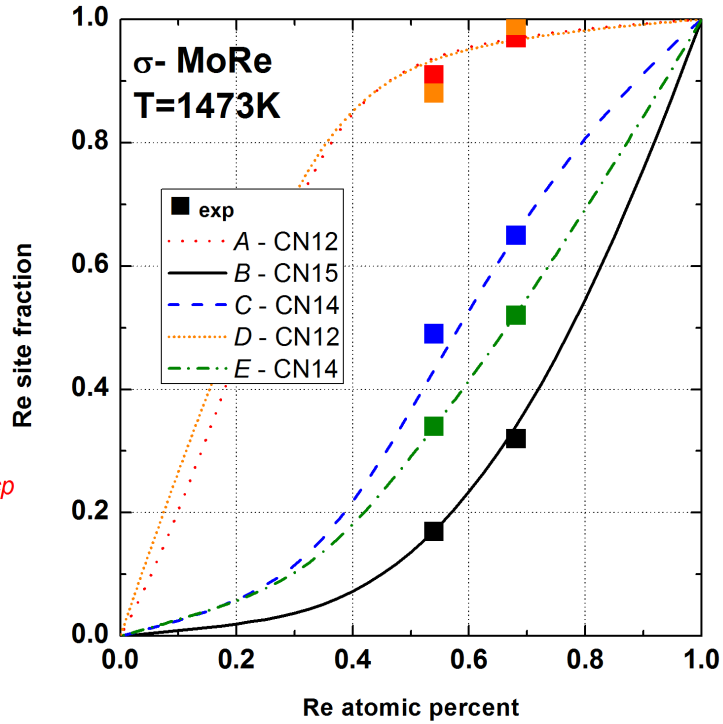
(1) ΔH_{for} of every ordered compound: $2^5 = 32$ configurations
(2) Estimation of the Gibbs energy neglecting the interaction between atoms of same lattice (Bragg Williams – Gorsky approximation):

$$G^{\sigma} = {}^{\text{srf}}G^{\sigma} + {}^{\text{cnf}}G^{\sigma} + \cancel{{}^{\text{ex}}G^{\sigma}} + \cancel{{}^{\text{phy}}G^{\sigma}}$$

with $${}^{\text{srf}}G^{\sigma} = \sum_{ijklm=\text{Mo,Re}} \left[y_i^{(\mathcal{A})} y_j^{(\mathcal{B})} y_k^{(\mathcal{C})} y_l^{(\mathcal{D})} y_m^{(\mathcal{E})} \right] \times \Delta\, {}^{\text{for}}H^{0,\sigma}_{ijklm}$$

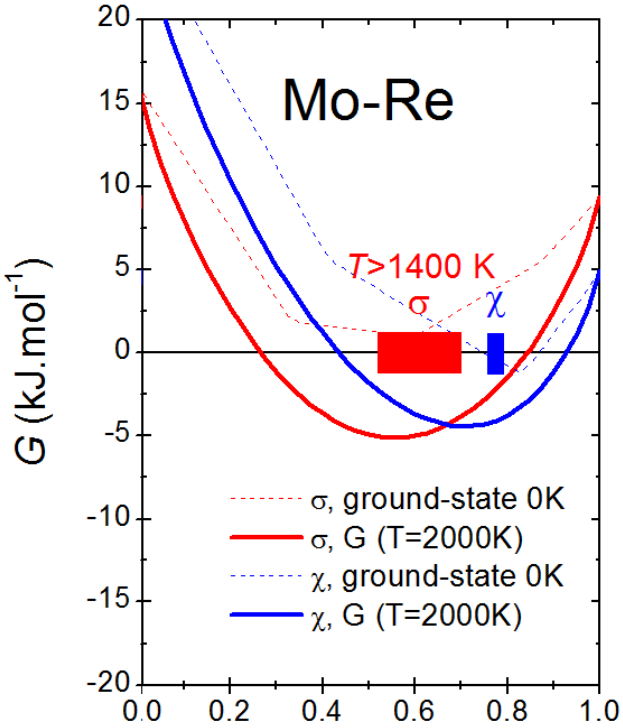
and $${}^{\text{cnf}}G^{\sigma} = -R \times T \sum_s a^{(s)} \sum_{i=\text{Mo,Re}} y_i^{(s)} \times \ln(y_i^{(s)})$$

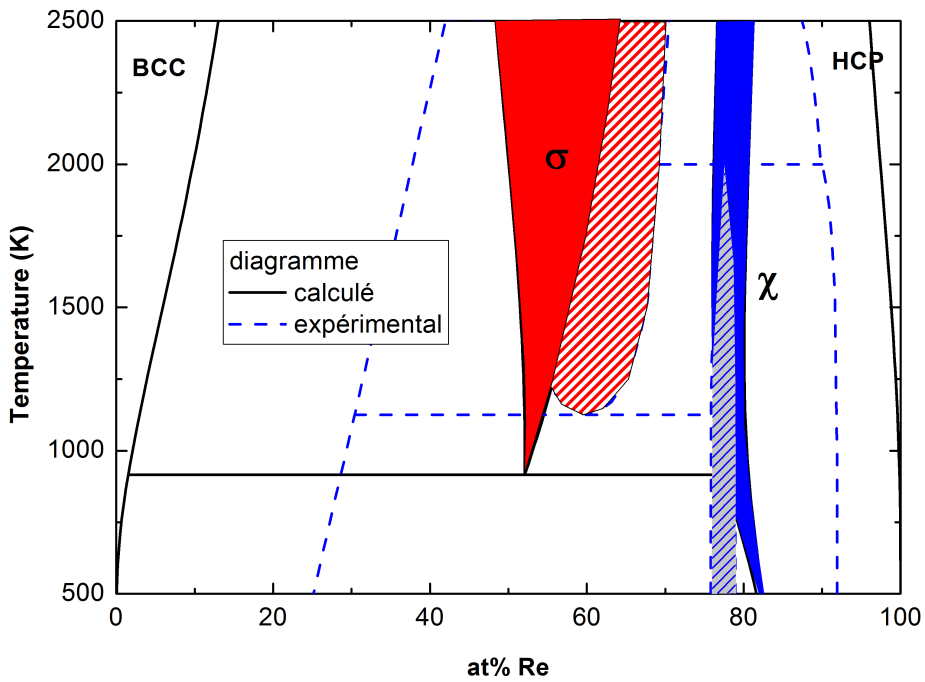




An *ab initio* binary phase diagram

(1) ΔH_{for} of every ordered compound of both χ and $\sigma-$phase
(2) Estimation of the Gibbs energy in BWG approximation
(3) phases diagram build from the common tangent rule





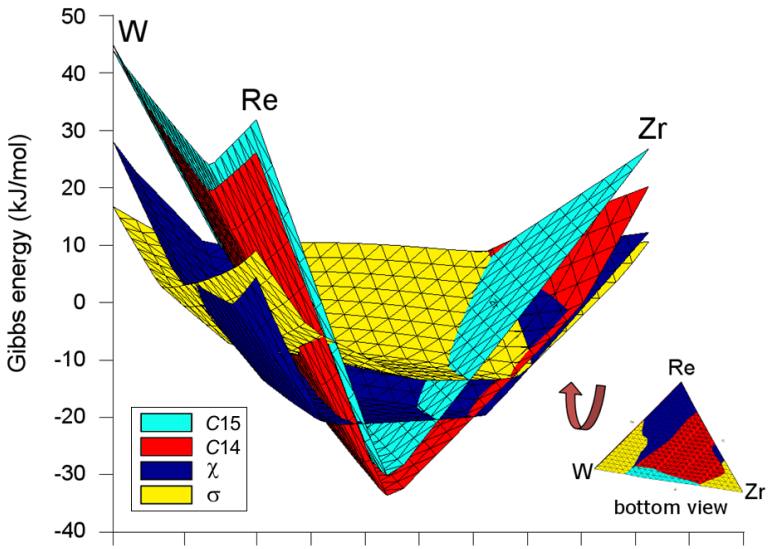
[6] Crivello *et al.* Inorg. Chem. (2013)

[7] Crivello *et al.* J. Phys.: Condens. Matter (2010)

An ternary system? *e.g.* Re–W–Zr

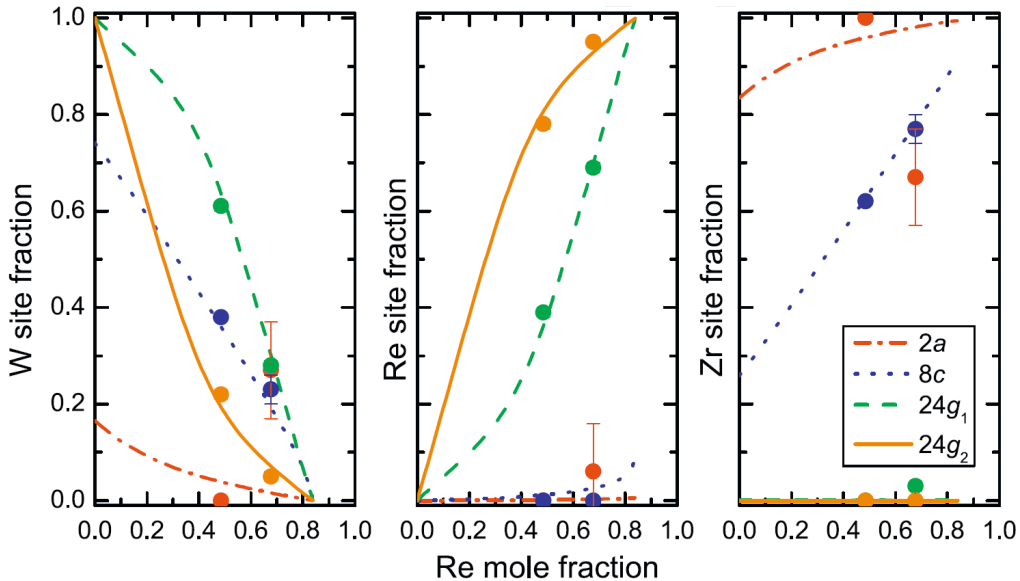
Systematic calculations

- 4 phases: χ ($3^4 = 81$), σ ($3^5 = 243$), $C15$, $C14$
- 3 solid solutions (fcc, bcc, hcp by SQS)



[8] Joubert, Crivello *et al.*, Acta. Mater (2014)

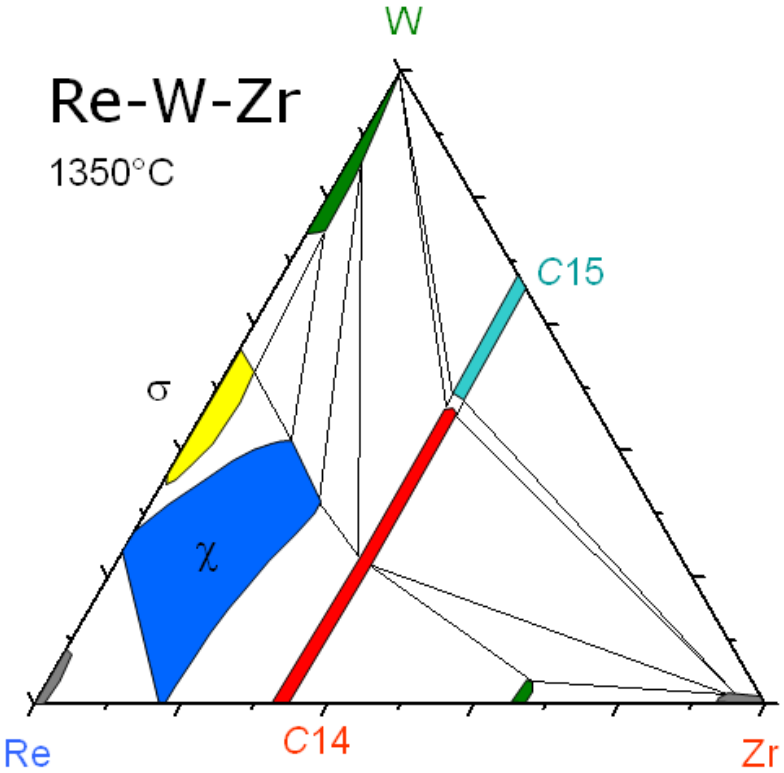
Sites occupation in the $\chi-$phase:



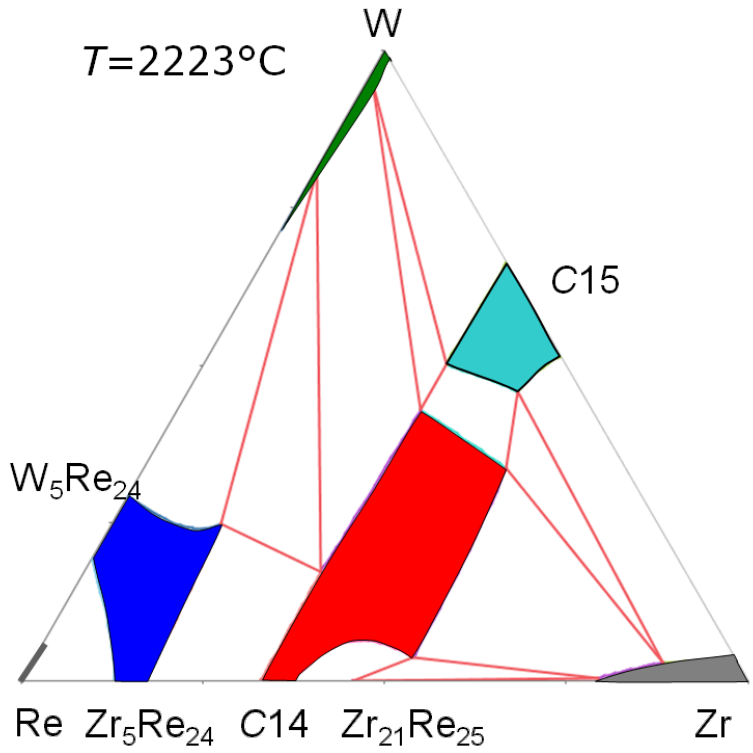
Experiment occupancies obtained by joint refinement on 2 diffraction sets of different contrast

An *ab initio* ternary phase diagram

Experimental:



Computed with BWG approximation:



Similar agreement in other system: Mo-Ni-Re, Cr-Co-Re,...

[9] K. Yaqoob *et al.*, Inorg. Chem. (2012)

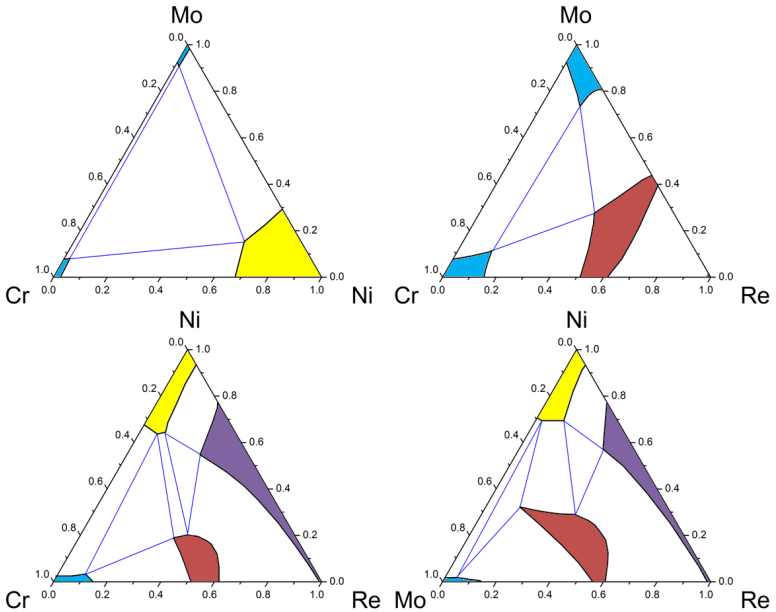
[10] Joubert, Crivello *et al.*, Applied Sciences (2015)

Study of a quaternary system: Cr–Mo–Ni–Re

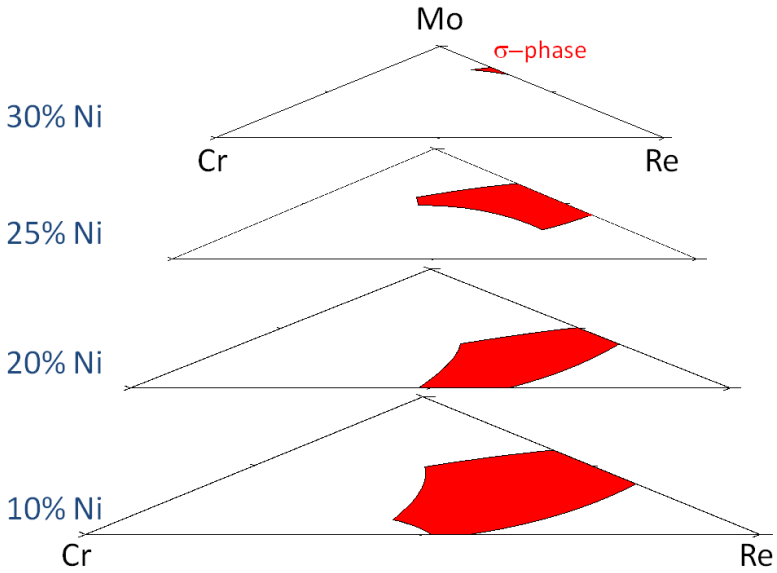
$4^5 = 1024$ configurations ordered in σ phase

Use of **ZenGen** code [11] Crivello *et al.*, Calphad (2015)

Experimental:



Computed with BWG approximation:



prediction of TCP phases precipitation

- BWA may works for complex IMC such as TCP (χ, σ,...)
- not sufficient for more simple IMC such as Laves phases

Contents

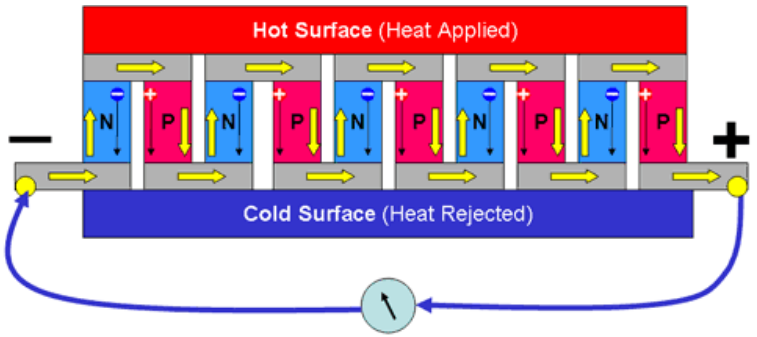
Temperature phase transition for thermoelectric applications

The **thermoelectric effect** is the conversion of temperature differences to electric voltage (and vice versa)

Evaluation of material with the **figure of merit**: $ZT = \frac{\alpha^2 T}{\rho\lambda}$

Heusler type Fe_2VAl: potential candidate

- semi-metal, Pauli paramagnetic
- good electronic transport properties: $\frac{\alpha^2}{\rho} = 5\,\mathrm{mW\,m^{-1}\,K^{-2}}$
- but thermal conductivity (λ) is too large



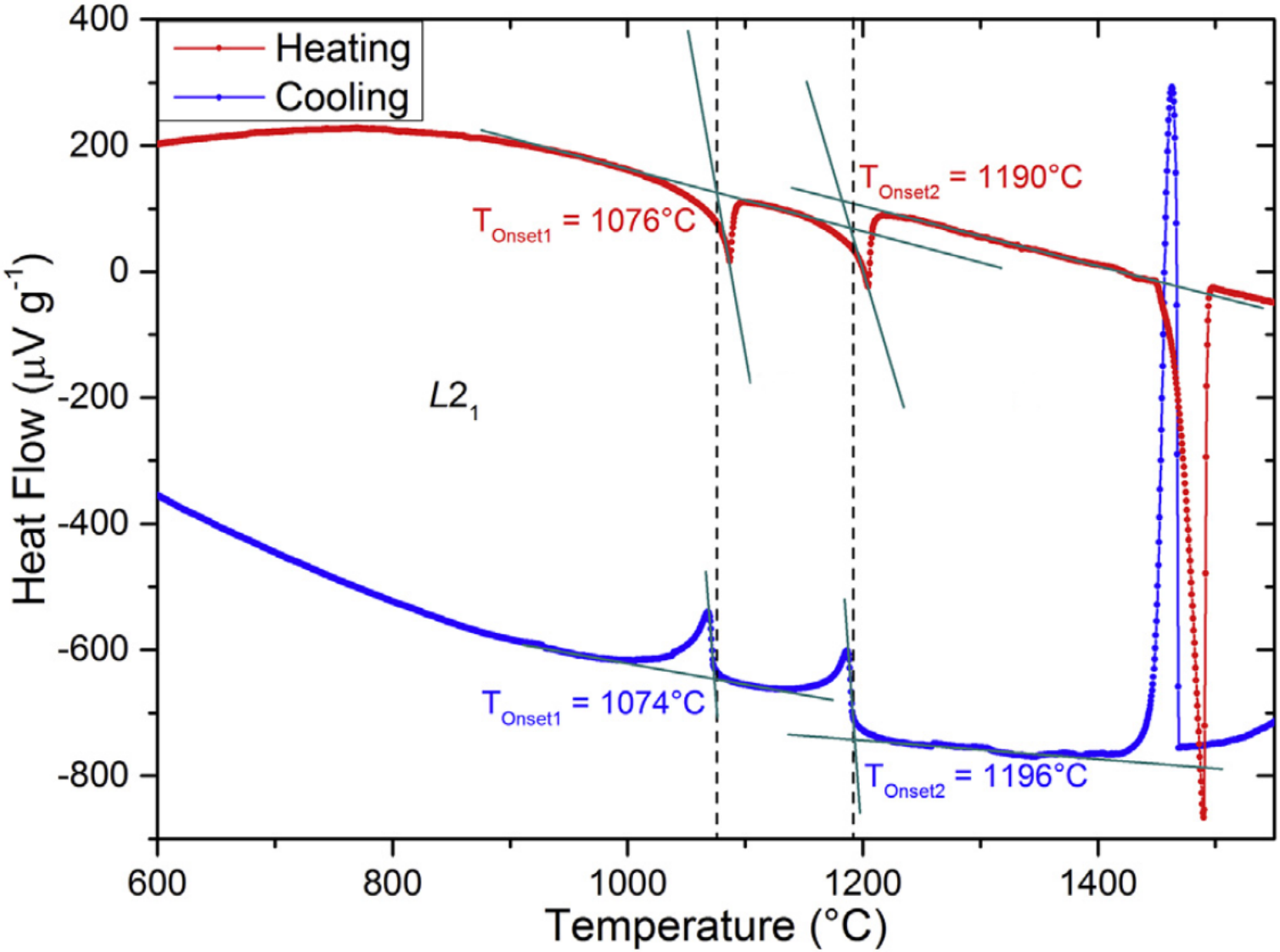
Thermoelectric Generator (TEG)

Effect of temperature?

Fe_2VAl

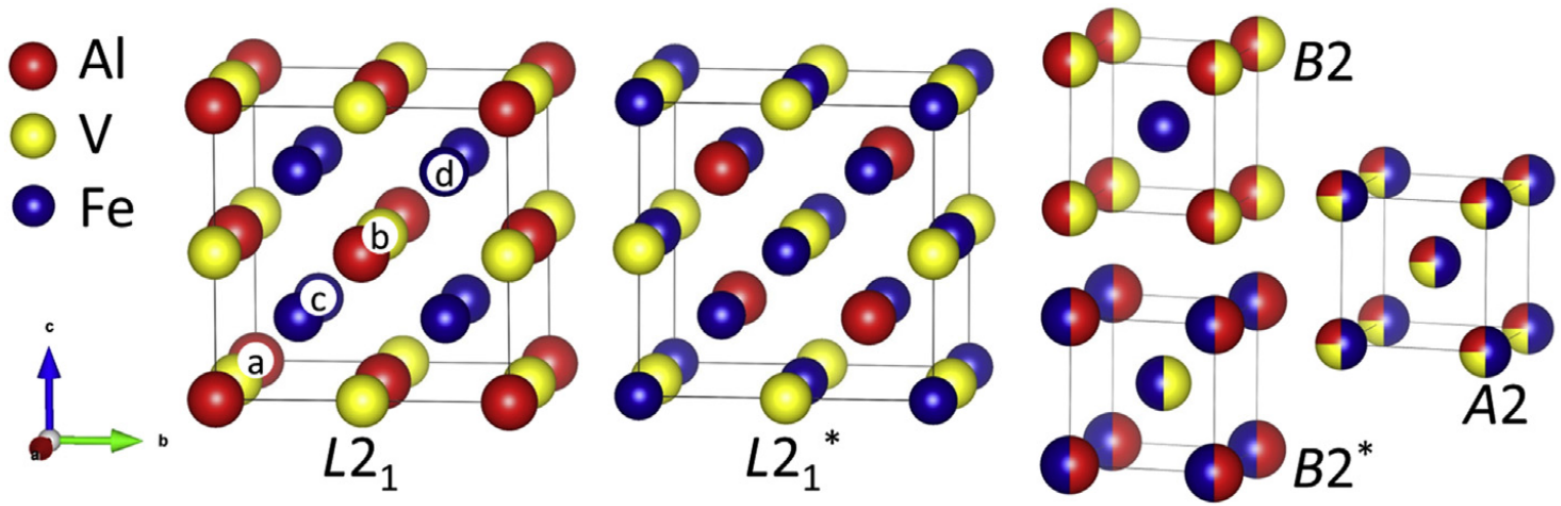
Fe_2VAl: phase transition

experimental: DTA heating and cooling scan



Fe_2VAl: phase transition

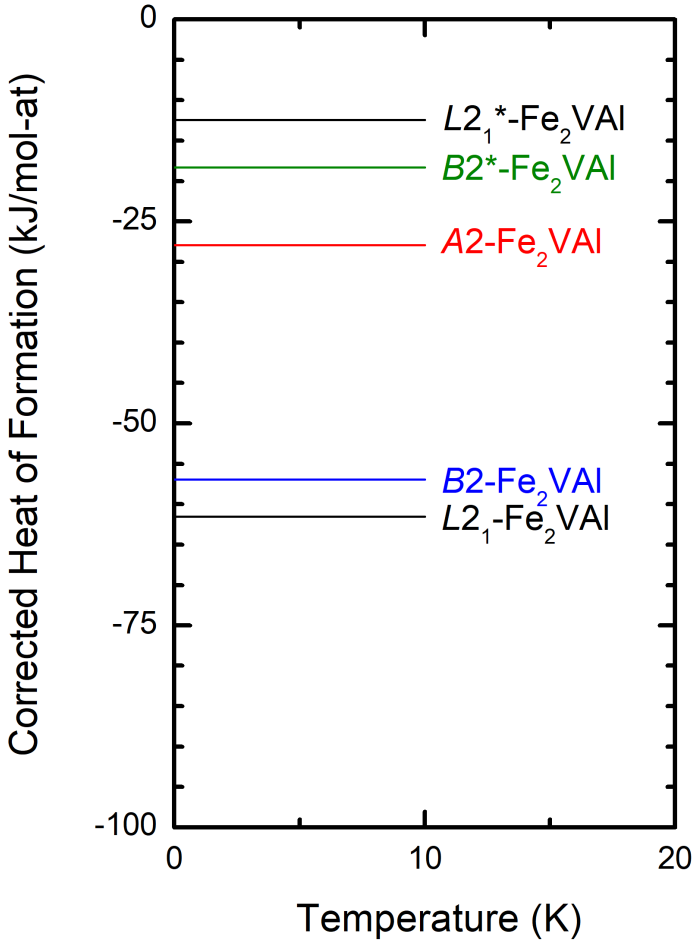
theoritical work: what is the most stable phase?
with temperature dependance?

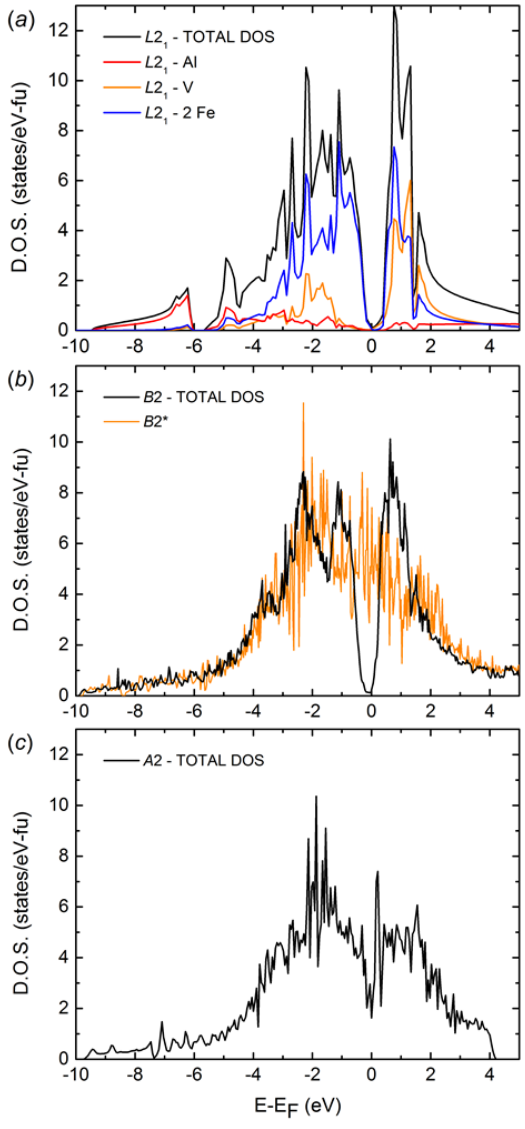


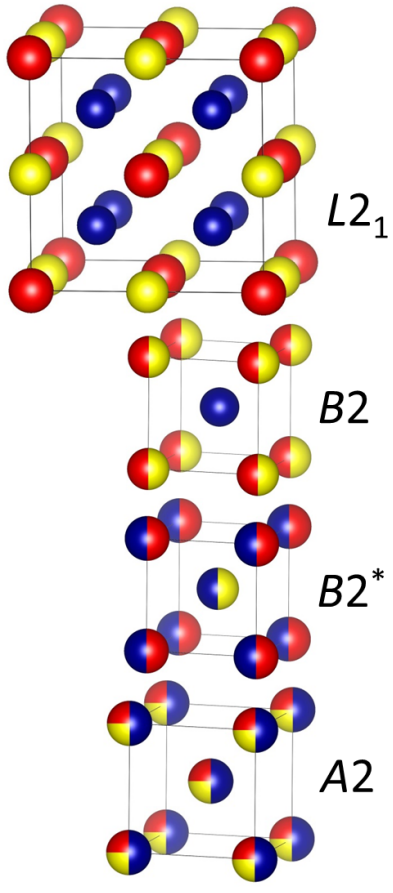
two combined calculations

- SQS
- phonon

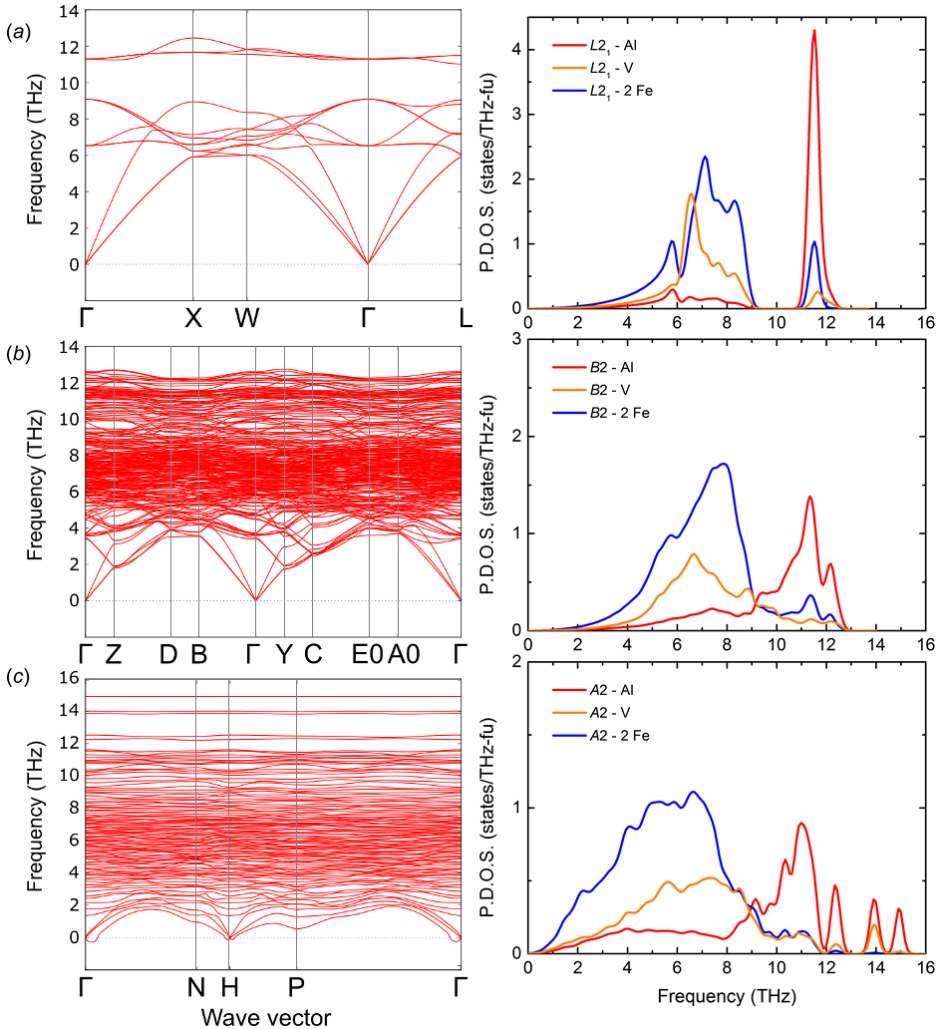
Fe_2VAl: SQS+DFT results at 0 K







Fe_2VAl: phonon calculations



Calculations done with Phonopy code in harmonic approximation [12] Togo, Oba, Tanaka, PRB 78 (2008)

- SQS-$B2$: 64 atoms, 112 displ.
- SQS-$A2$: 32 atoms, 191 displ.

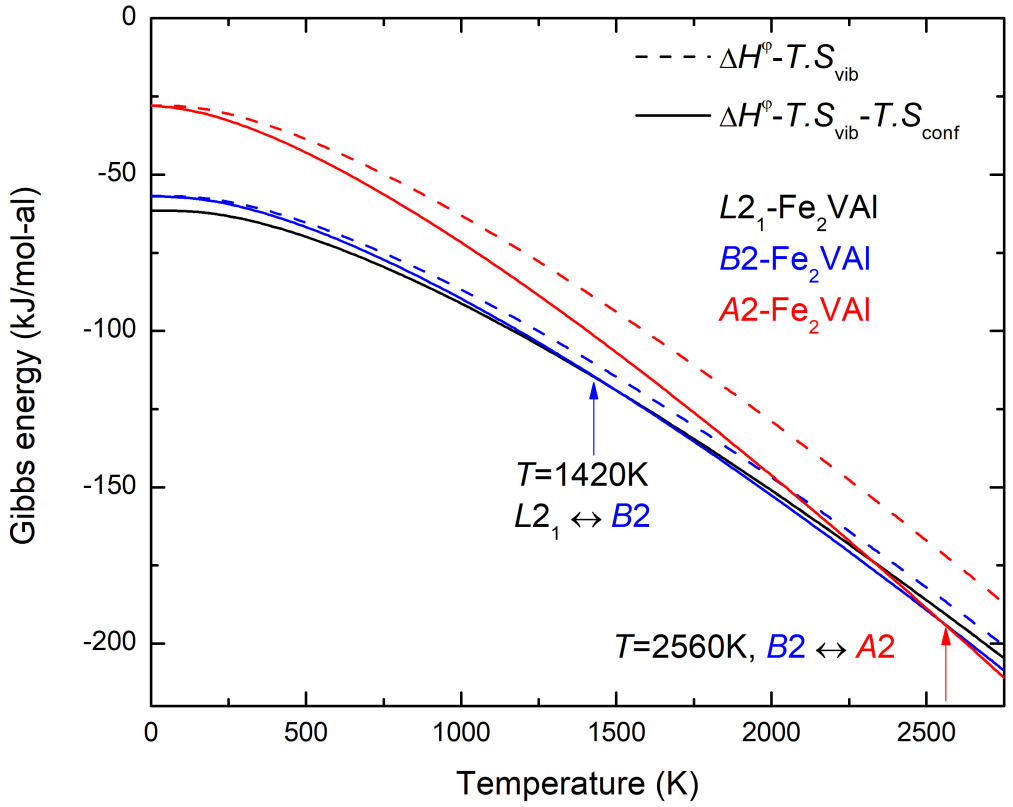
From the phonon dispersion curves, Helmholtz free energy:

$$F(T) = \frac{1}{2}\sum_{\mathrm{q},s}\hbar\omega(\mathrm{q},s) + k_B T \sum_{\mathrm{q},s}\ln\left[1-\exp\left(-\frac{\hbar\omega(\mathrm{q},s)}{k_B T}\right)\right]$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V ; \quad C_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V$$

Fe_2VAl: thermodynamic modeling

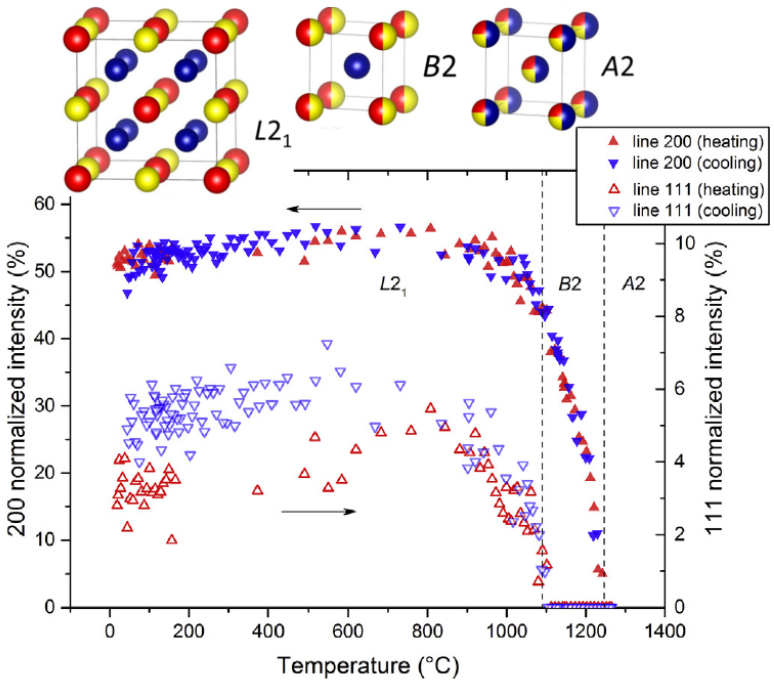
$$\Delta G^{\varphi}(x,T,P) = \Delta H - T \cdot \Delta S$$

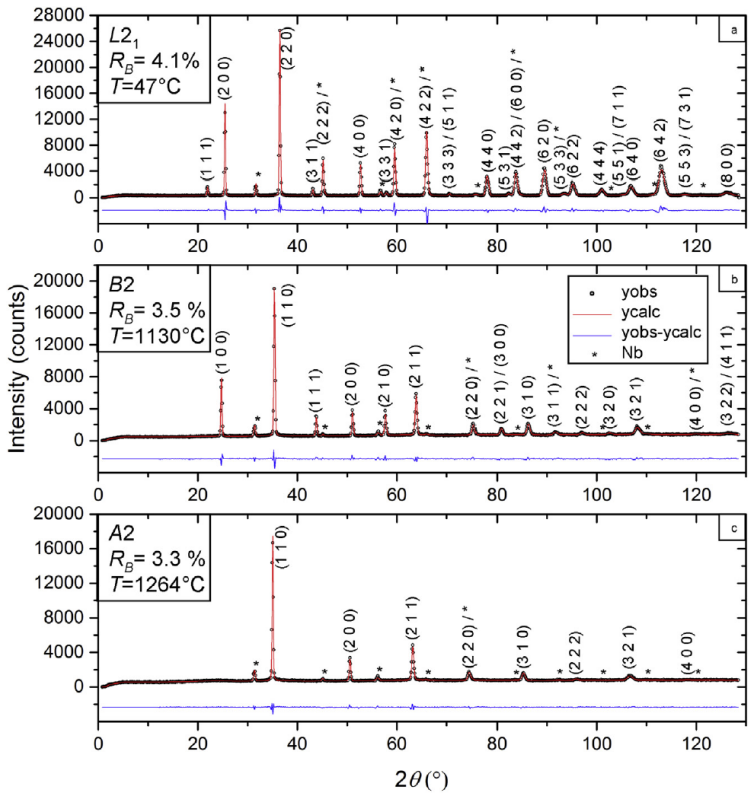


$\Rightarrow$ Prediction of the phase transitions $L2_1 \rightarrow B2 \rightarrow A2$

[13] Maier, Acta Mater. (2015)

Fe_2VAl: agreements





Neutron diffraction with temperature: order/disorder transitions

[14] Maier, Acta Mater. (2015)

Contents

The hydrogen economy

Why hydrogen ?

- H is a renewable resource, very abundant (15% at. on Earth)
- H is a zero-emission fuel (when burned with oxygen)
- H is associated to a high exothermic reaction (in mass unit)

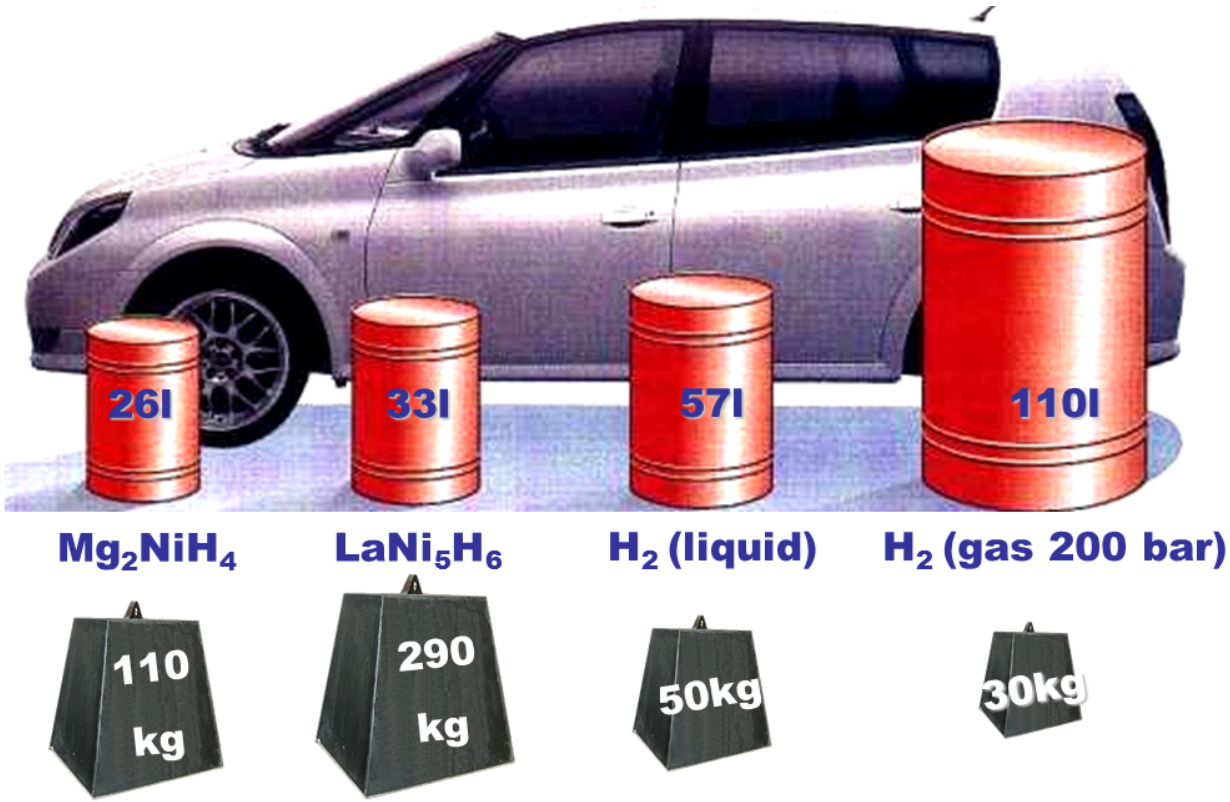
$$\mathrm{H_2} + \frac{1}{2}\mathrm{O_2} \Leftrightarrow \mathrm{H_2O}, \quad +142\mathrm{MJ/kg}$$

What are its limitations?

- H needs to be produced
- H needs to be stored

Hydrogen in the solid stored-state

4 liters of H is need to fed a fuel-cell for driving 400 km by car:



Metallic hydride

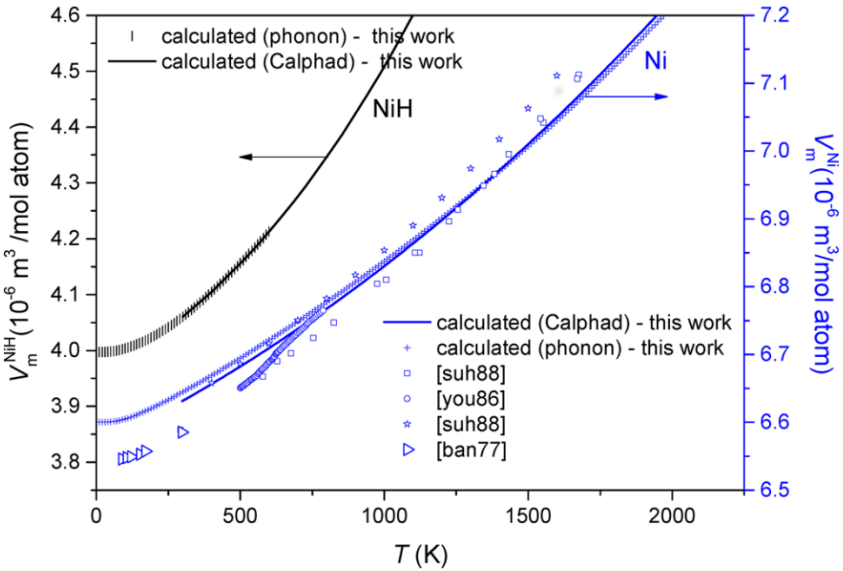
- presents high volumic density
- is safe (in opposition to the liquid or gas state)
- drives H with a tunable and reversible reaction

A complete investigation: Ni–H system

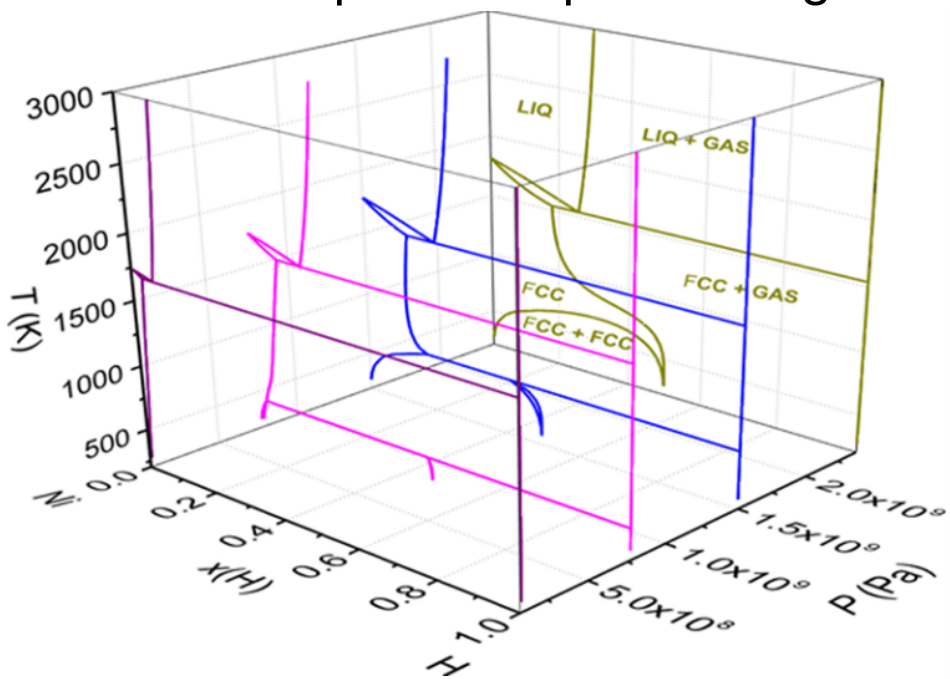
A combined methodologies approaches based on Calphad modelling:

- DFT + CEM : ${}^{\mathrm{ex}}G^{\varphi}$
- DFT + phonon QHA : $V(T,P)$
- high pressure model: $V(T,P) = x + y \ln\left(\frac{B}{P^0}\right)$

consistent set of volume equilibrium

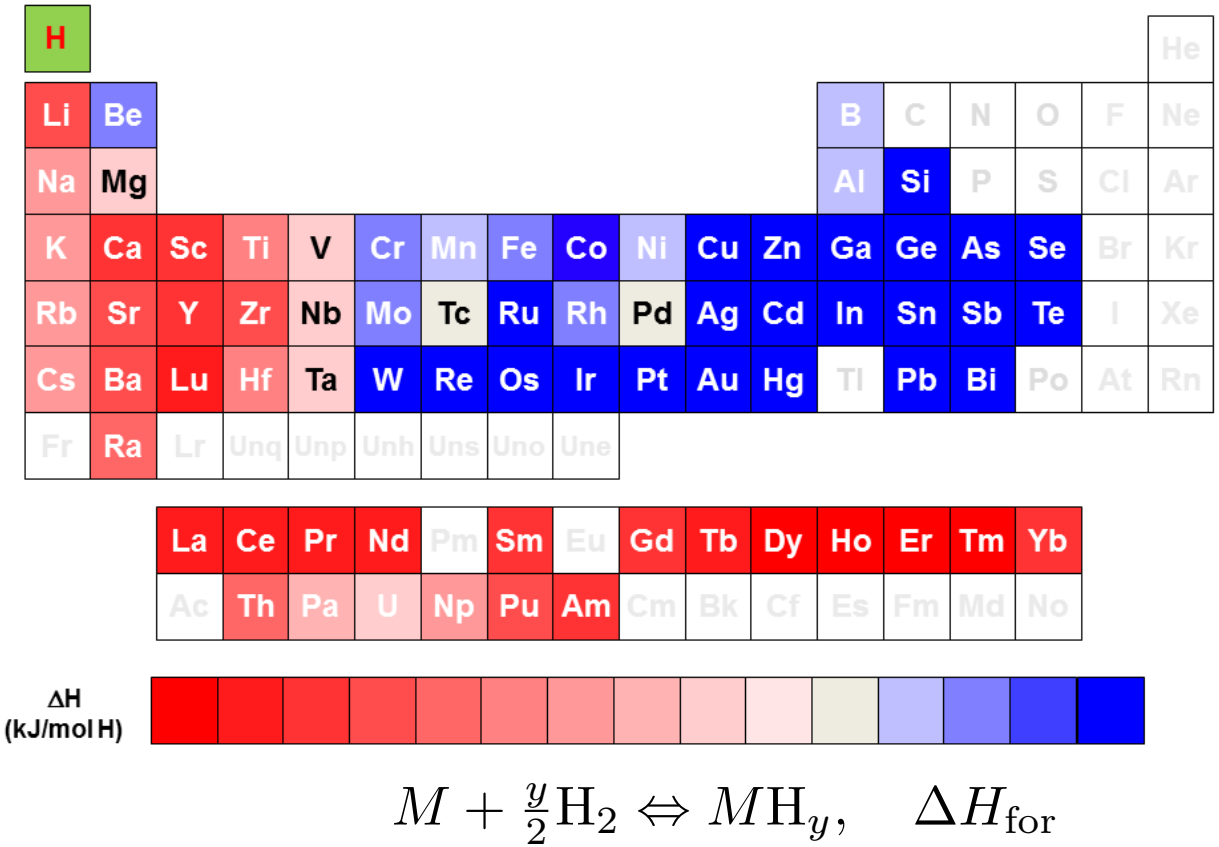


estimation of pressure phase diagram



[15] Bourgeois *et al.*, J Phys Chem C, 119 (2015)

Binary metal hydrogen $M-$H systems



$$M + \frac{y}{2}\mathrm{H}_2 \Leftrightarrow M\mathrm{H}_y, \quad \Delta H_{\mathrm{for}}$$

Heat of formation of metallic hydride is governed by :

- the chemical nature of the host M element
- the crystal structure

Ground state map of $M-$H

A systematic/screening investigation by calculation

- 31 binary metal hydrogen $M-$H systems
- 30 crystal structures of hydrides

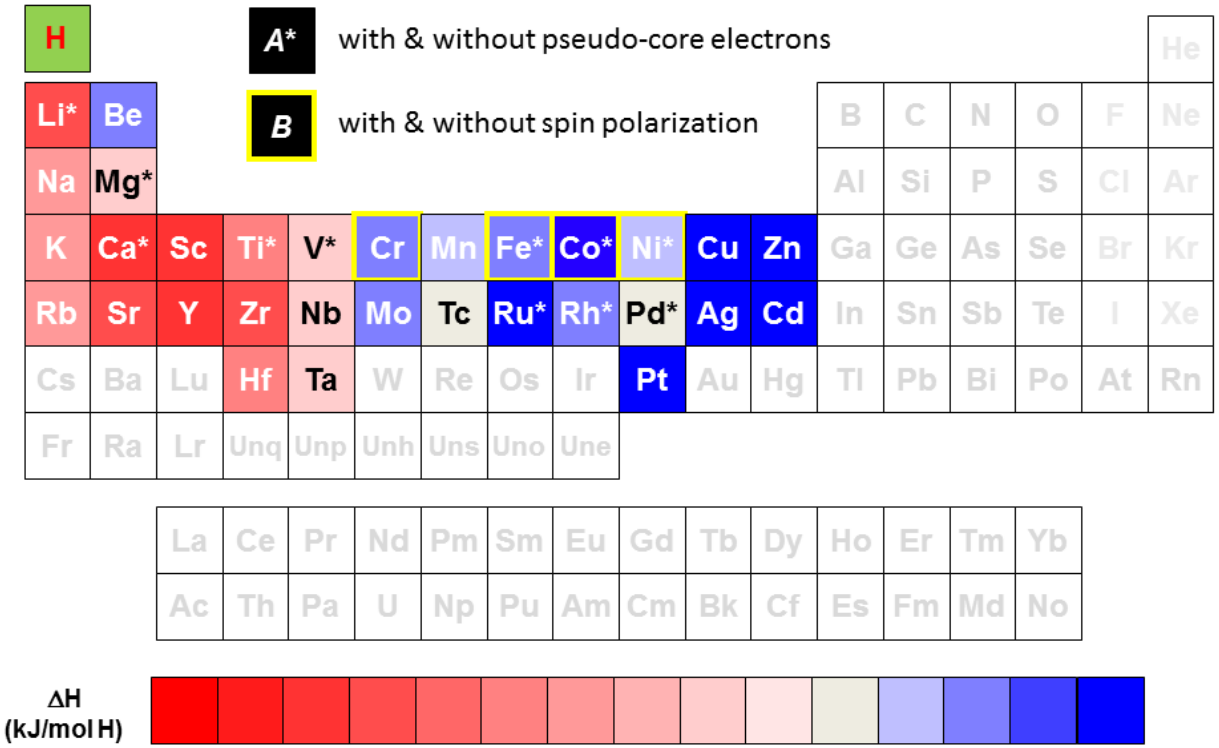
Questions

- Can we build a trustful thermodynamic database?
- May we can predict new hydride structure?
- What is the effect of the vibration?
  Application to the isotopic effect

Methodology

- DFT at 0 K (PAW, VASP, GGA-PBE, $E_{\text{cutoff}} = 800\,\text{eV}$
  $\Rightarrow \Delta H_{\text{for}}(M\text{H})^{\varphi} = E(M\text{H})^{\varphi} - E(M)^{\text{SER}} - \frac{1}{2}E(\text{H}_2)^{\text{dimer}}$
- harmonic phonon calculation $\Rightarrow \text{ZPE}, S_{\text{vib}}$

31 binary metal hydrogen $M-$H systems



Selection of $s-$ and $d-$elements

covers a large variety of

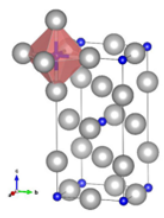
- crystal structures
- electronic structure types

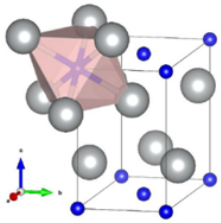
30 crystal structures of binary hydrides

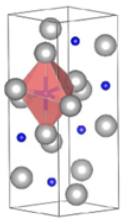
H/M	Proto.	P.S.	S.G.	Wyckoff P.	Site	M–H sys.
0.25	$PdH_{0.25}$	tI8	$I4/mmm$ (139)	M: $4c$, $4e$, H : $2a$	o	-
0.5	$AuTe_2$	mC6	$C2/m$ (12)	M: $4i$, H : $2a$	o	V
0.5	TiO_2-ana	tI12	$I4_1/amd$ (141)	M: $8e$, H : $4a$	o	Pd
0.5	CdI_2	hP3	$P\bar{3}m1$ (164)	M: $2d$, H : $1a$	o	Tc
0.5	Ta_2H	oS6	$C222$ (21)	M: $4k$, H : $2a$	o	Ta
0.75	$PdH_{0.75}$	tI8	$I4/mmm$ (139)	M: $4c$, $4e$, H : $4d$, $2b$	o	-
0.8	$PdH_{0.8}$	tI10	$I4/m$ (87)	M: $8h$, $2a$, H : $8h$	o	Pd
1	$NbH_{0.95}$	oP8	$Pnnn$ (48)	M: $4f$, H : $2a$, $2b$	te	Nb, Ti
1	PtS	tP4	$P4_2/mmc$ (131)	M: $4c$, H : $2a$, $2b$	te	Zr, Ti
1	CsCl	cP2	$Pm\bar{3}m$ (221)	M: $1a$, H : $1b$	CN=4	Na, K, Rb
1	NaCl	cF8	$Fm\bar{3}m$ (225)	M: $1a$, H : $1b$	o	Li, Na, K, Rb, Ru, Co, Rh, Ni, Pd
1	ZnO	hP4	$P6_3mc$ (186)	M: $2b$, H : $2b$	te	Cu
1	CrB	oS8	$Cmcm$ (63)	M: $4c$, H : $4c$	CN=7	Cs
1	NiAs	hP2	$P6_3/mmc$ (194)	M: $2c$, H : $2a$	o	Cr, Mn, Co
1	anti-NiAs	hP2	$P6_3/mmc$ (194)	M: $2a$, H : $2c$	CN=6	-
1	FeH	hP14	$P6_3/mmc$ (194)	M: $2c$,$2a$ H : $4f$	o	Fe
1	BN-b	hP2	$P6_3/mmc$ (194)	M: $2c$, H : $2d$	tr	-
2	ReB_2	hP6	$P6_3/mmc$ (194)	M: $2c$, H : $4f$	te	-
2	TiO_2	tP6	$P4_2/mnm$ (136)	M: $2a$, H : $4f$	tr	Mg
2	CaF_2	cF12	$Fm\bar{3}m$ (225)	M: $4a$, H : $8c$	te	Sc, Y, Ti, Zr, Hf, V, Nb, Ta, Cr, Rh
2	PdF_2	cP12	$Pa\bar{3}$ (205)	M: $4a$, H : $8c$	te	Mg
2	PbO_2	oP12	$Pbcn$ (60)	M: $4c$, H : $8d$	tr	Mg
2	ThH_2	tI6	$I4/mmm$ (139)	M: $2a$, H : $4d$	te	Ti, Zr, Hf
2	Co_2Si	oP12	$Pnma$ (62)	M: $4c$, H : $4c$	te/CN=5	Ca, Sr
3	$AuSb_3$	cI8	$Im\bar{3}m$ (229)	M: $2a$, H : $6b$	CN=2	-
3	BiF_3	cF16	$Fm\bar{3}m$ (225)	M: $4a$, H : $4b$, $8c$	o, te	-
3	ReB_3	hP8	$P6_3/mmc$ (194)	M: $2c$, H : $2a$, $4f$	o, te	-
3	HoD_3	hP24	$P\bar{3}c1$ (165)	M: $6f$, H : $12g$, $4d$, $2a$	tri/CN=3	Y
3	NaH_3	hP8	$P6_3/mmc$ (194)	M: $2c$, H : $2d$, $4f$	tr, te	-
3	Na_3As	hP8	$P6_3/mmc$ (194)	M: $2c$, H : $2b$, $4f$	tr, te	Gd

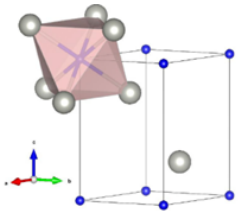
30 crystal structures of binary hydrides

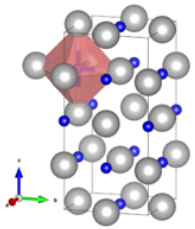
$H/M < 1$

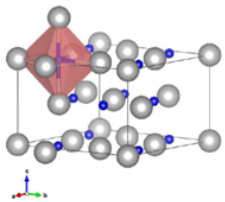

$MoNi_3$


$AuTe_2$

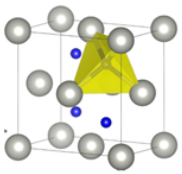

TiO_2-ana

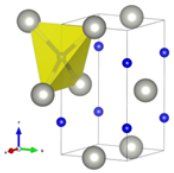

CdI_2

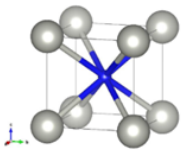

$MoNi_3$

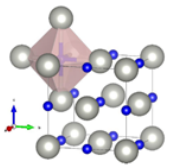

$MoNi_4$

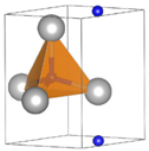
$H/M = 1$

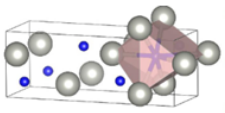

NbH

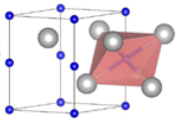

PtS

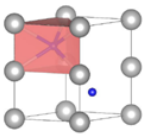

CsCl

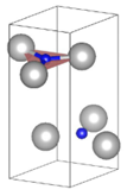

NaCl


ZnO

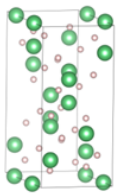

CrB

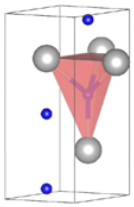

NiAs

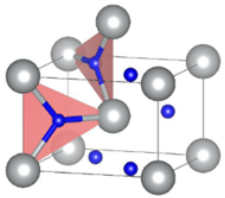

anti-NiAs

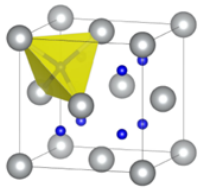

BN

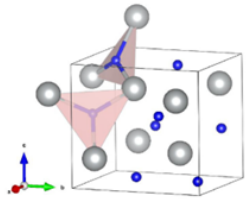
$H/M = 2$

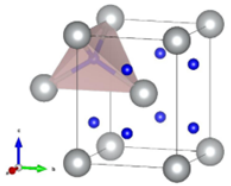

BeH_2

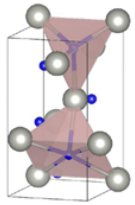

ReB_2


TiO_2

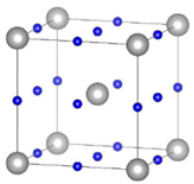

CaF_2

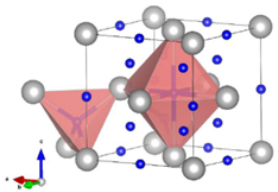

PbO_2

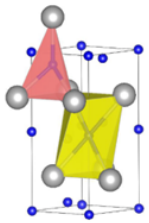

ThH_2

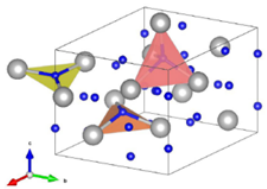

$SiCo_2$

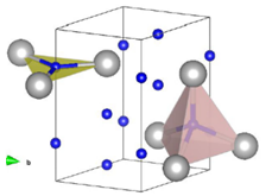
$H/M = 3$

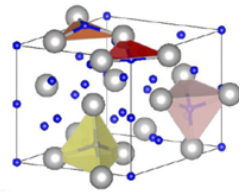

$AuSb_3$


BiF_3


ReB_3


HoD_3

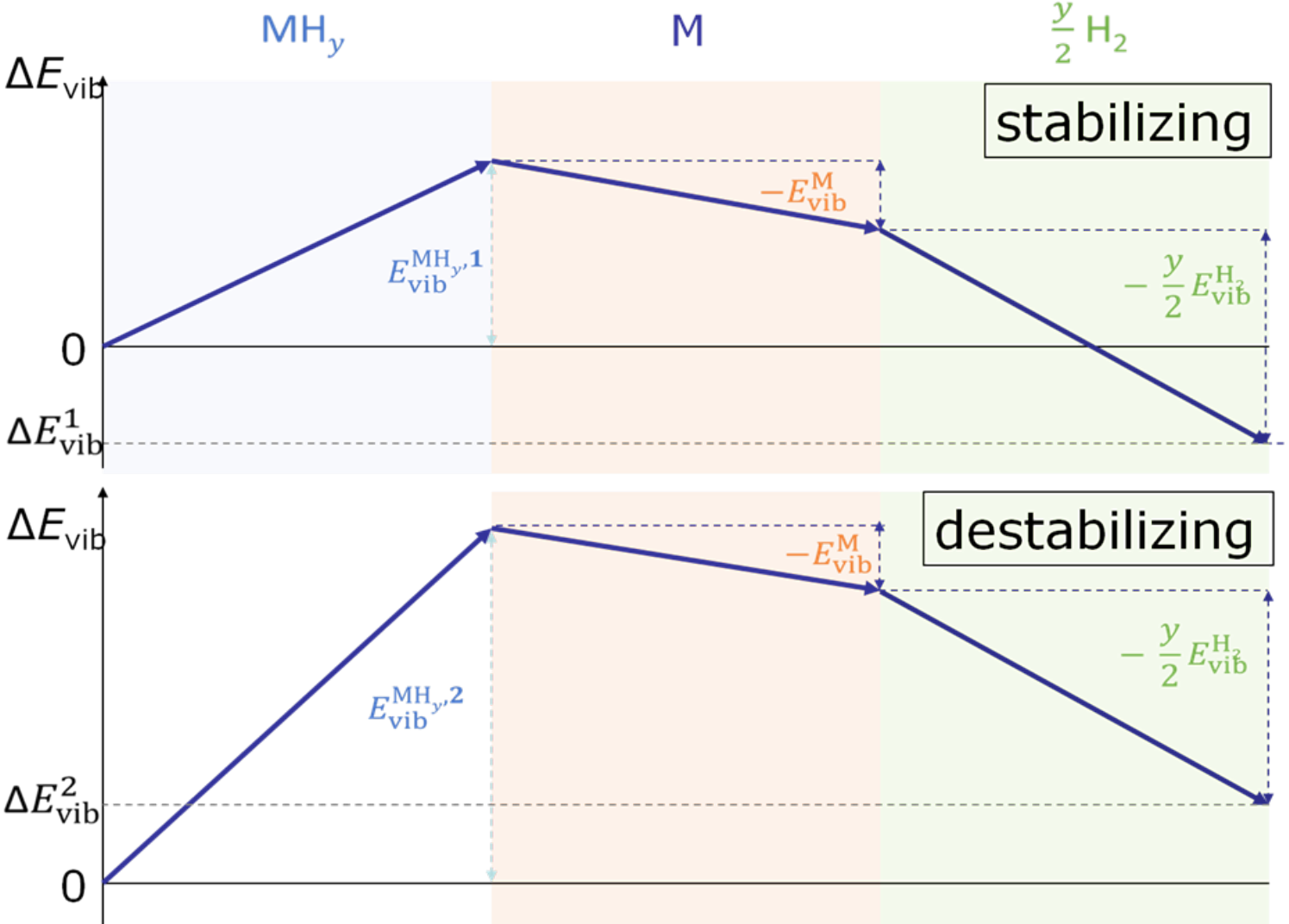

$AsNa_3$


PCu_3

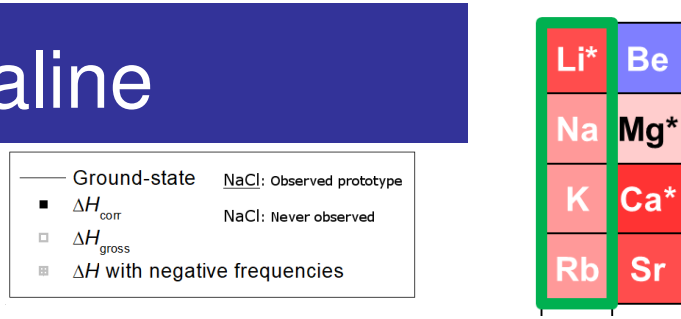
Strong importance of the ZPE contribution!

$$\Delta H^{cor}_{\text{for}}(M\text{H}_y) = \Delta H_{\text{for}}(M\text{H}_y) + \Delta E_{vib}$$

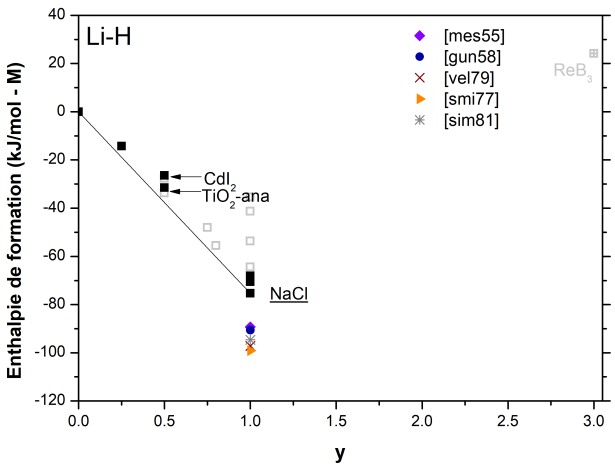
$$\Delta E_{vib} = E_{vib}(M\text{H}_y) - E_{vib}(M) - \frac{y}{2} E_{vib}(\text{H}_2^{\text{dimer}})$$



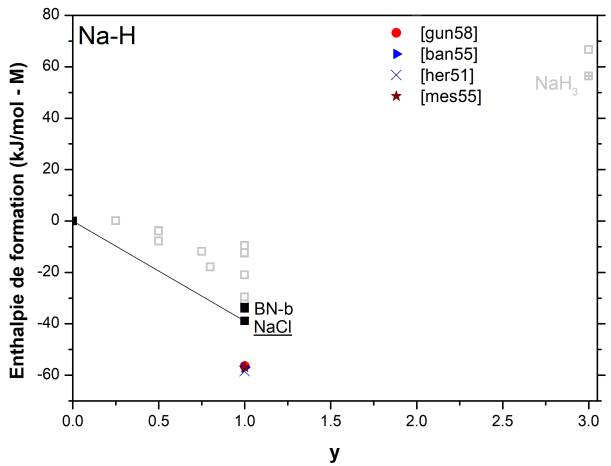
Results: column 1, alkaline



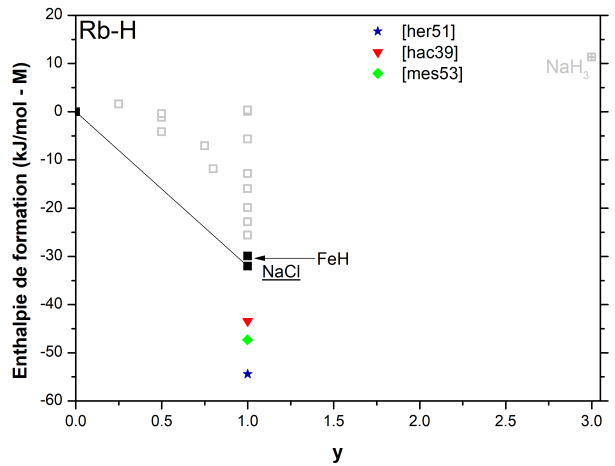
Li–H



Na–H



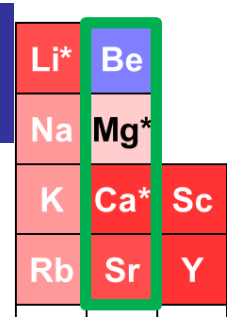
Rb–H

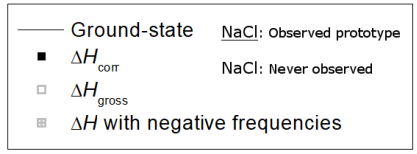


agreements: NaCl structure stable for the 4 alkali metal hydrides, with very unstable di-hydrides

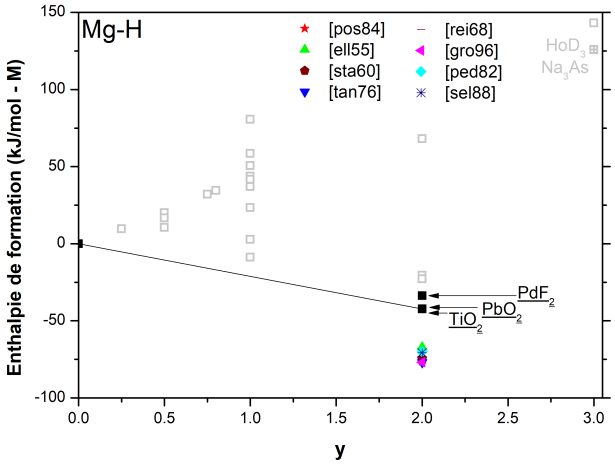
chemical bonds: ionic bond, strong charge transfer ($Li^{+0.85}$, $Na^{+0.78}$, $K^{+0.75}$, $Rb^{+0.74}$): decreasing with the increase of the period, associated with the decreased of the hydride stability

Results: column 2, alkaline earths

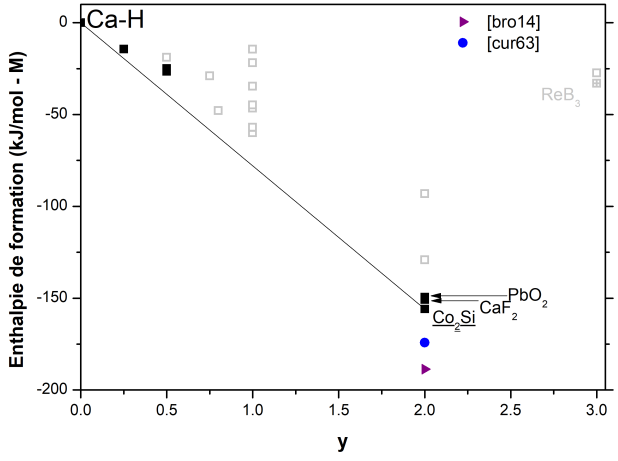




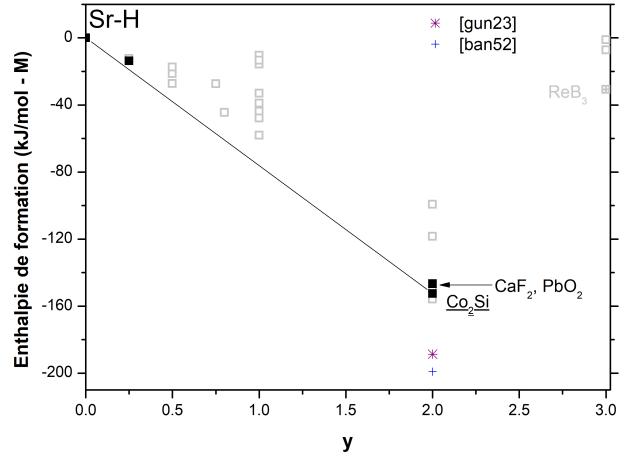
Mg–H



Ca–H



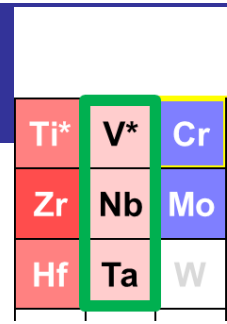
Sr–H

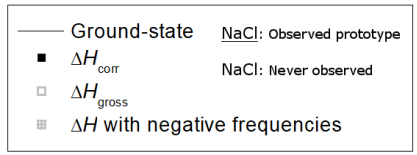


agreements: di-hydrides stable with correctly predicted structures, no-mono hydrides

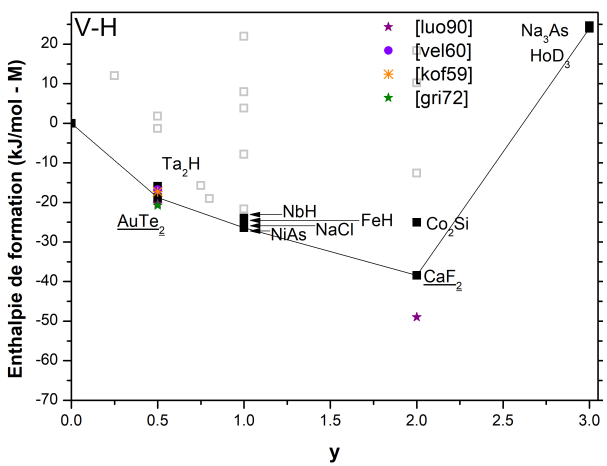
chemical bonds: important charge transfer ($Mg^{+1.6}$, $Ca^{+1.4}$, $Sr^{+1.4}$), highly exothermic formation for Ca and Sr

Results: column 5

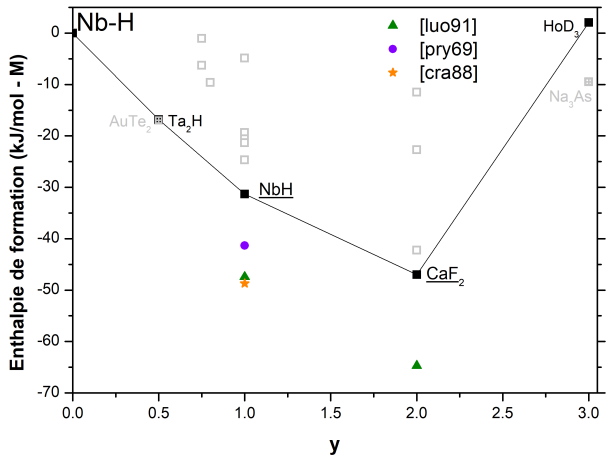




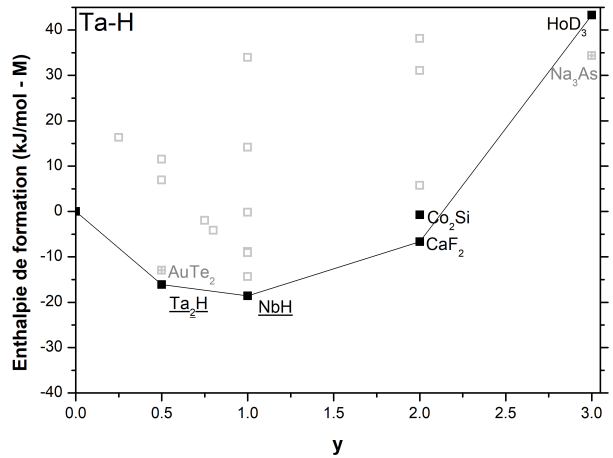
V–H



Nb–H



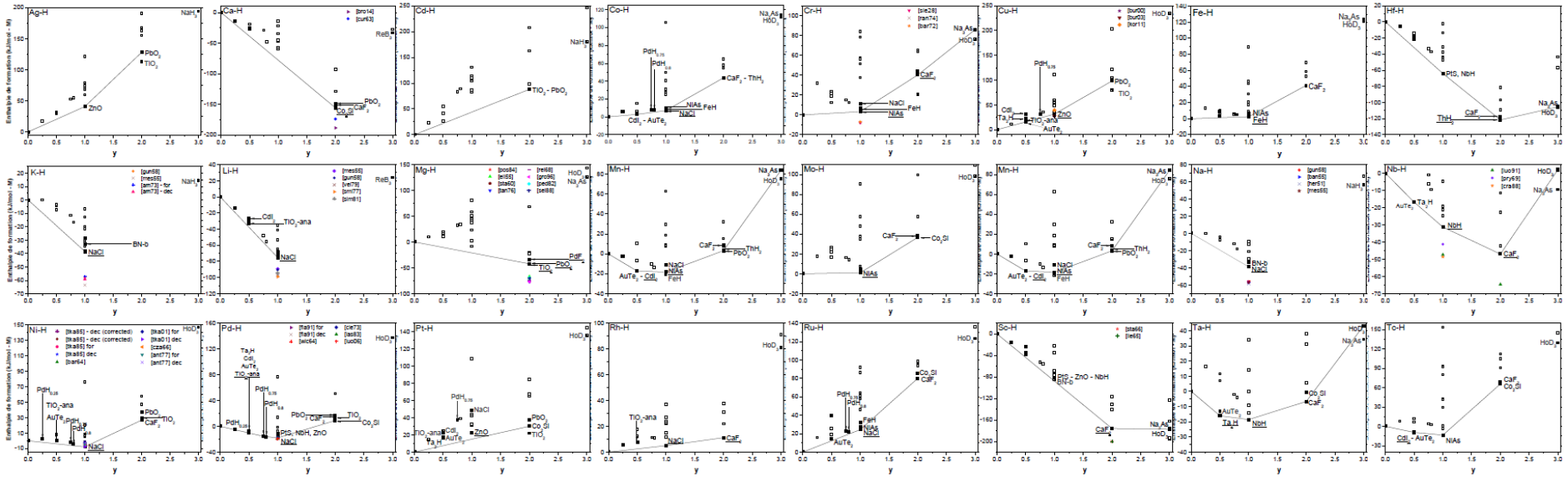
Ta–H



agreements: all hydrides stable with correctly predicted structures ($M\mathrm{H}_{0.5}$ stable only for $M = \mathrm{V}$, no TaH_2)

prediction: monohydride VH, TaH_2 at 3 GPa

A systematic/screening investigation



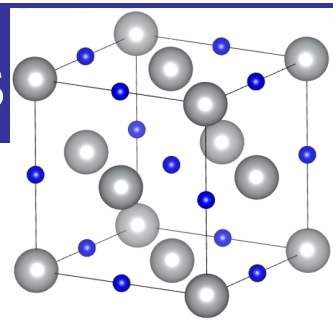
$\Rightarrow$ similar chemical properties for the hydrides formed with elements of the same column (chemical bonds, crystal structures,...)

$\Rightarrow$ obtention of the ground state and assessment of the metastability

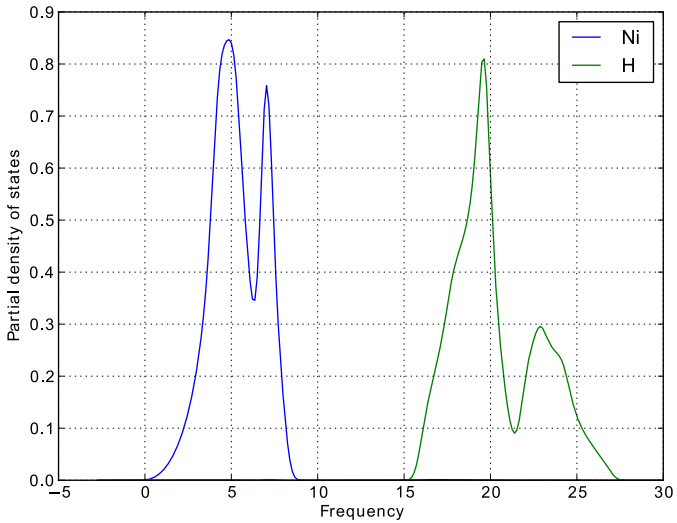
$\Rightarrow$ predicted structures in agreement with the experimental observations: prediction of higher hydrides TaH_2 (CaF_2), TcH, PdH_2 (Co_2Si), ZrH_3 (HoD_3), AgH (ZnO), TaH_2 at 3 GPa

[16] Bourgeois, Crivello *et al.* ACS Combinatorial Science (2017)

Phonon calculation & thermodynamics



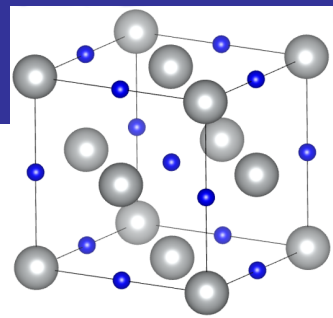
Ex: Results on NiH ($B1$, NaCl)



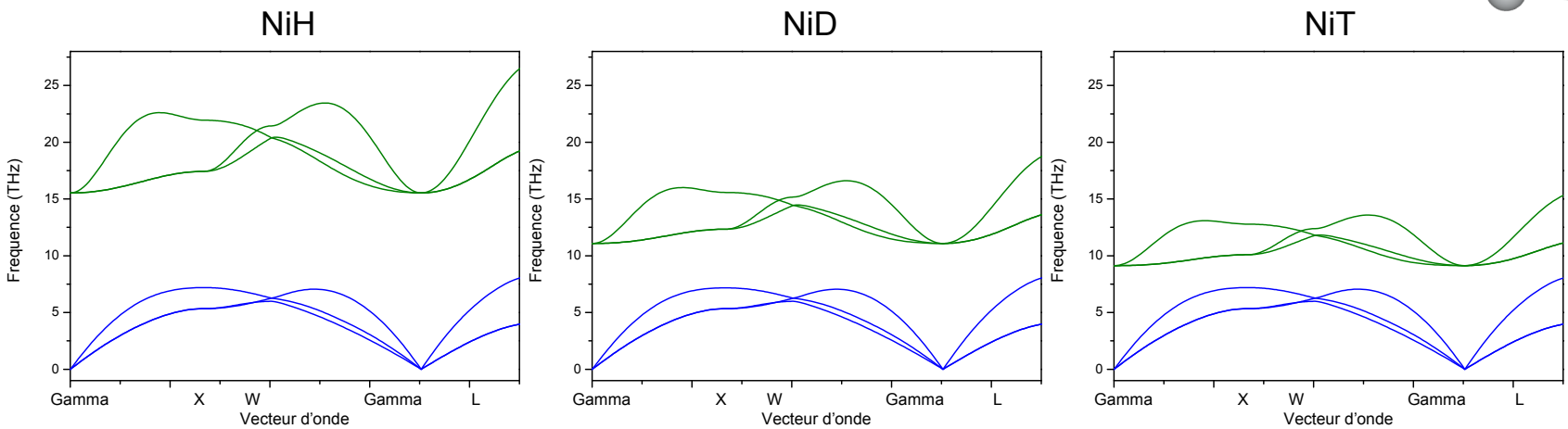
$$F(V_0,T) = \underbrace{\frac{1}{2}\sum_{\mathrm{q},s}\hbar\omega(\mathrm{q},s)}_{\text{ZPE}} + k_B T \sum_{\mathrm{q},s} \ln\left[1-\exp\left(-\frac{\hbar\omega(\mathrm{q},s)}{k_B T}\right)\right]$$

the ZPE contribution is not negligible for Metal-hydride systems!

$\omega \propto \frac{1}{\sqrt{m}} \Rightarrow$ isotope effect



Ex: Results on NiH, NiD, NiT ($B1$, NaCl)



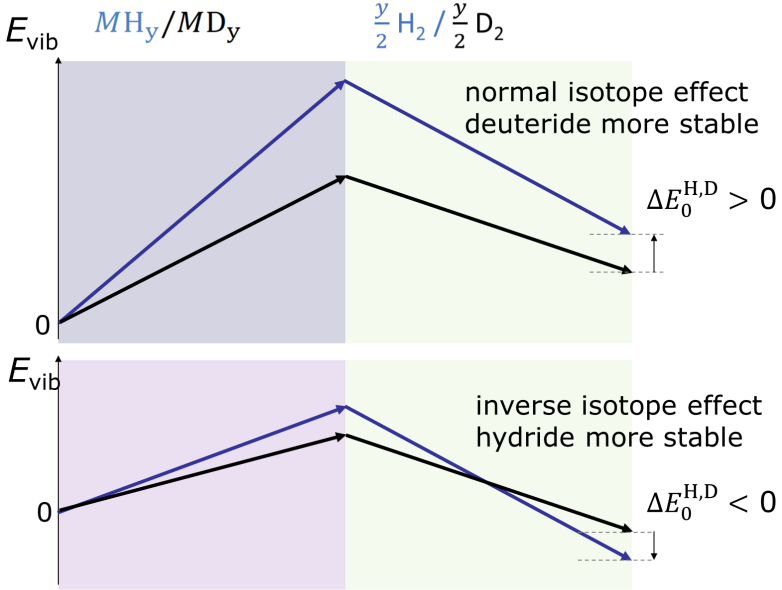
$$\Delta H^{cor}_{\text{for}}(\text{Ni}X) = \Delta H_{\text{for}}(\text{Ni}X) + \Delta E_{vib}$$

where: $\Delta E_{vib} = E_{vib}(MX_y) - E_{vib}(M) - \frac{y}{2} E_{vib}(X_2^{\text{dimer}})$

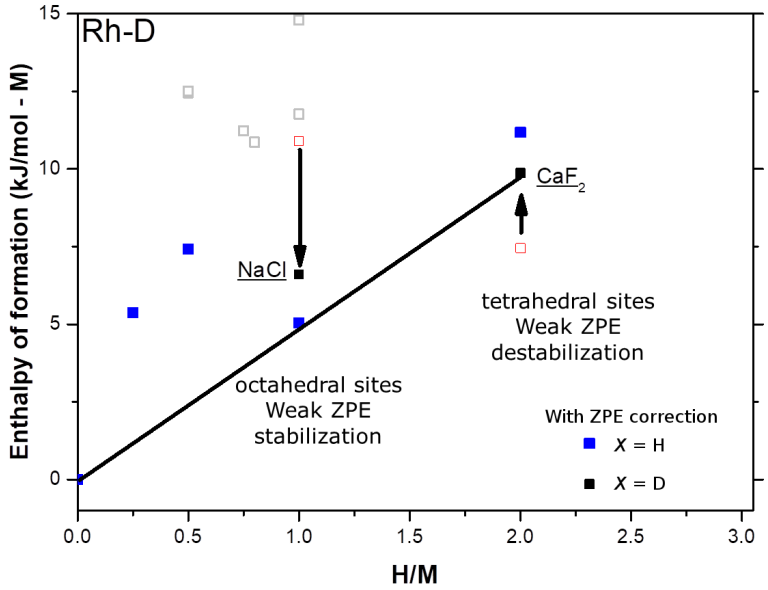
definition:

$$\Delta E^{\text{H,D}} = \left(E_{vib}(M\text{H}_y) - \frac{y}{2} E_{vib}(\text{H}_2)\right) - \left(E_{vib}(M\text{D}_y) - \frac{y}{2} E_{vib}(\text{D}_2)\right)$$

Isotope effect



$\Rightarrow$ prediction of normal or inverse stabilization

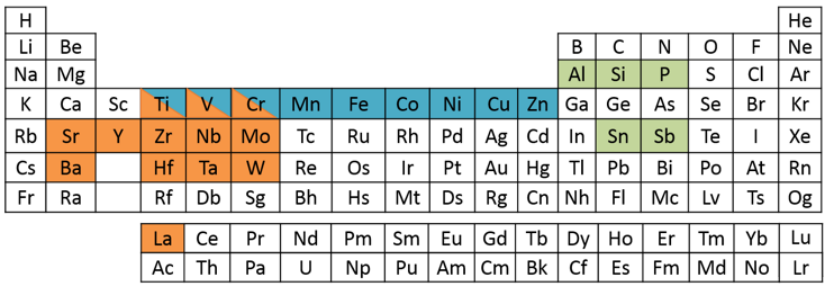


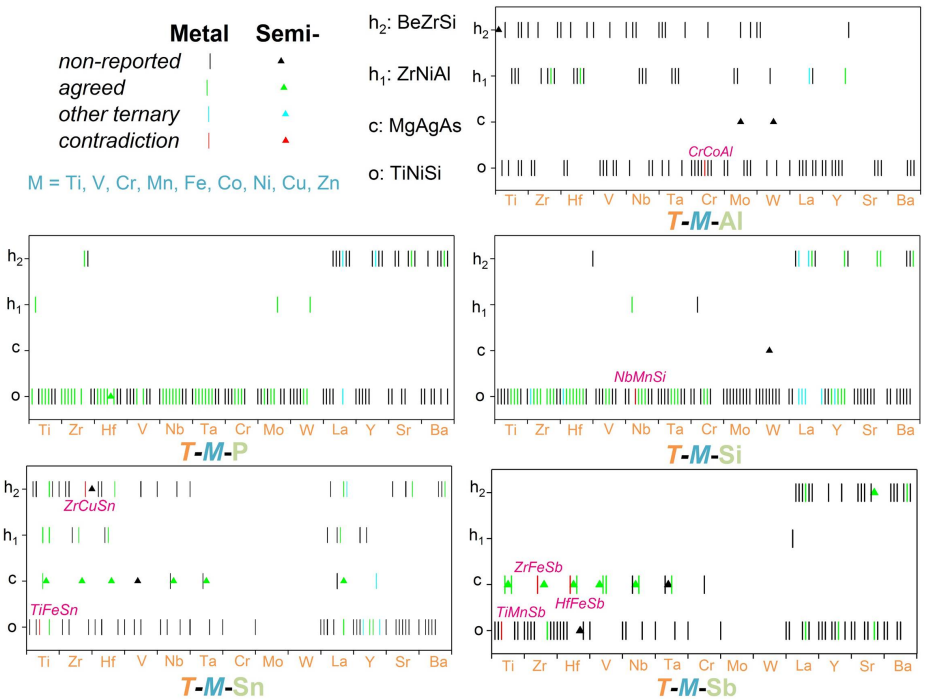
H/D: Modification of the ground state possible

$\Rightarrow$

[17] Bourgeois, Crivello *et al.*, J. Phys: Cond Mater 2018

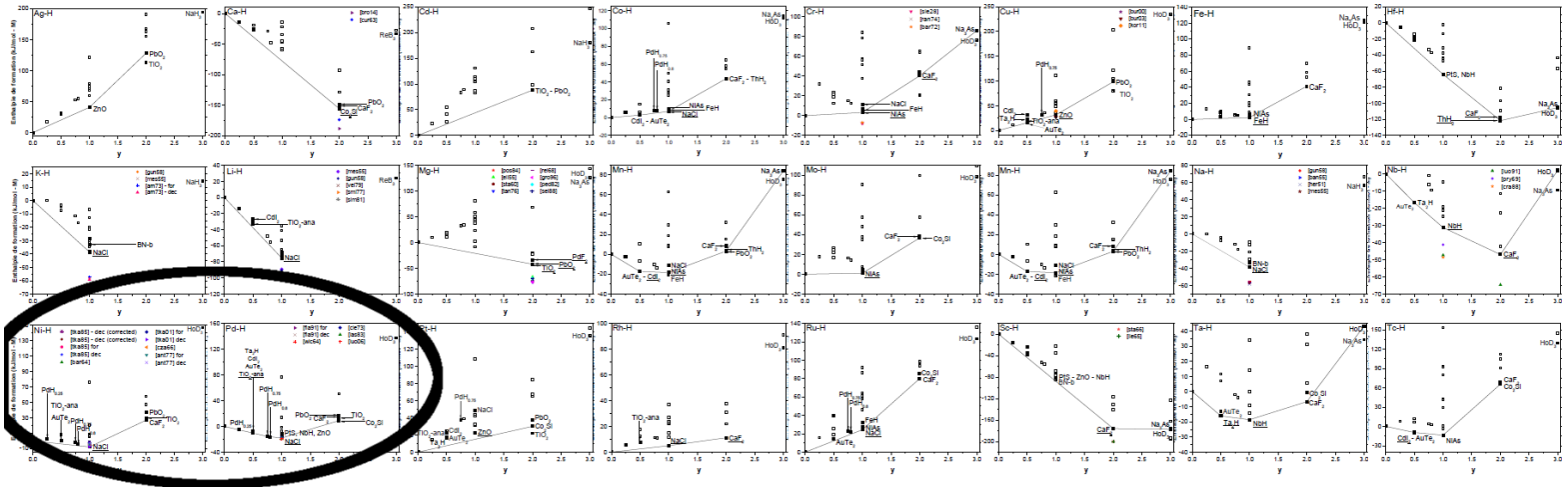
Outlook 1: Screening of new thermoelectric compounds

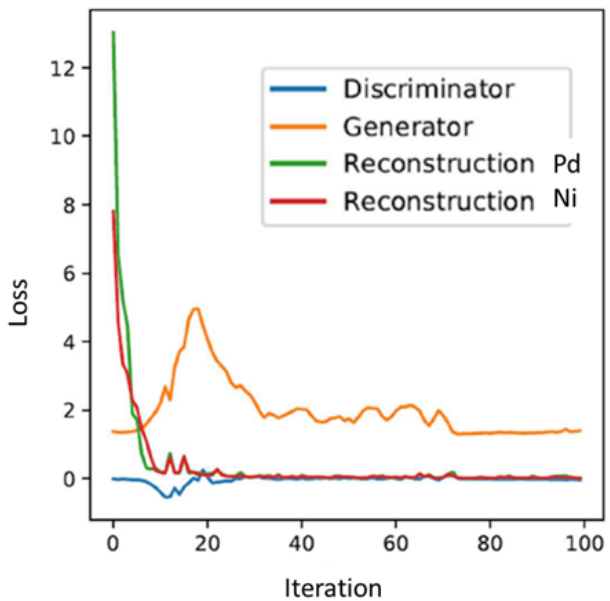


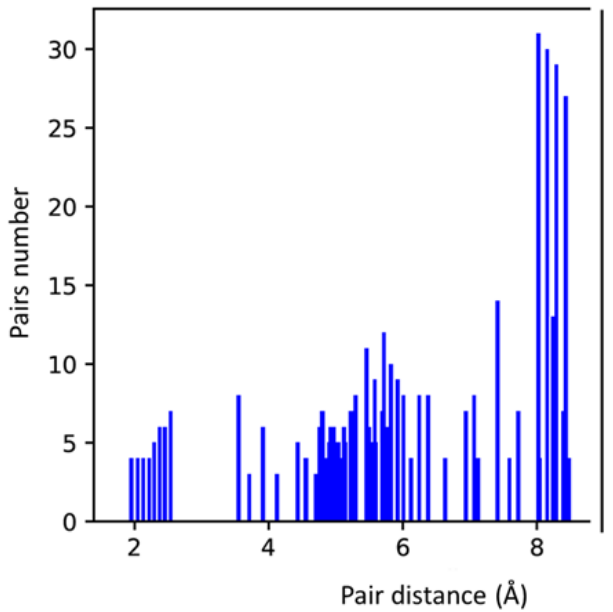


[18] Barreteau, Crivello *et al.*, J. Comput. Mater. 2019

Outlook 2: Machine learning for metal hydrides?







Conclusions

Thermodynamic modeling assisted by massive first principles calculations

Type of calculations

- large number of small DFT calculations: ~ 30 atoms/cell
- phonon calculations: large number of asymmetric supercell
- magnetism for alloys: collinear and non-collinear
- oxydes & thermoelectrics: use of meta-GGA and mBJ functionals

Continuous Help in VASP needs: thanks the CINES Support

- help for choosing the NPAR and KPAR paramaters
- help for number of nodes
- guide for typical errors

Advert & Acknowledgments

https://ai4mater-sci.sciencesconf.org/