What is hidden behind a phase diagram?

F. Berthier, J. Creuze, B. Legrand

So similar…

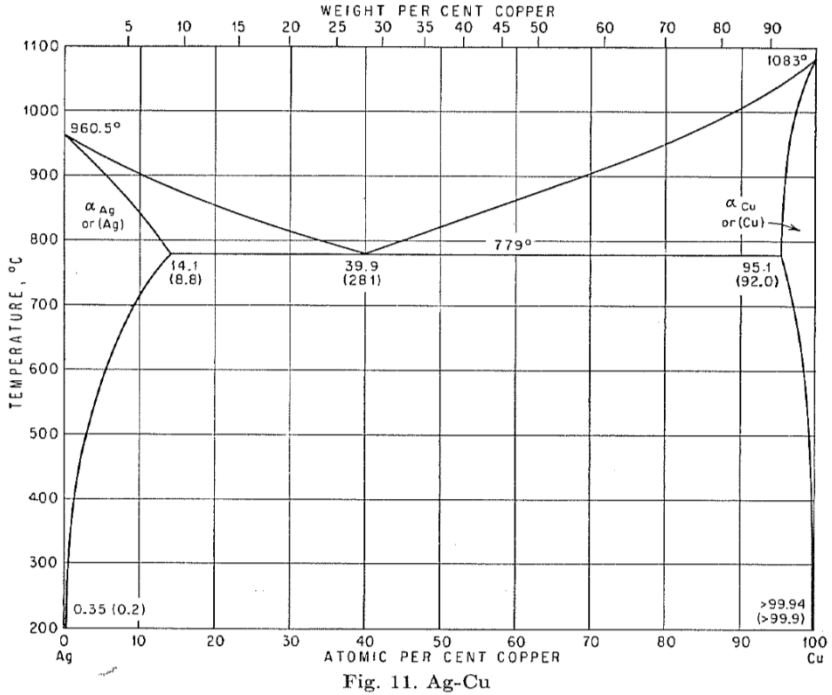
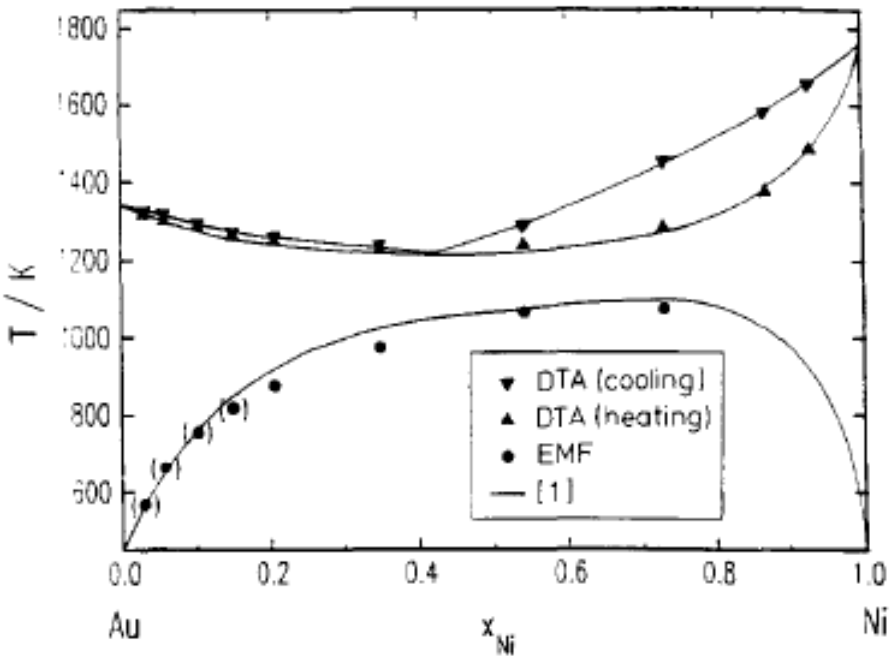


Fig. 11. Ag-Cu



$T_c = 1180\ K$

$\frac{r_{Ag}}{r_{Cu}} = 1{,}13$

LRO : homo

SRO : homo

$T_c = 1083\ K$

$\frac{r_{Au}}{r_{Ni}} = 1{,}16$

LRO : homo

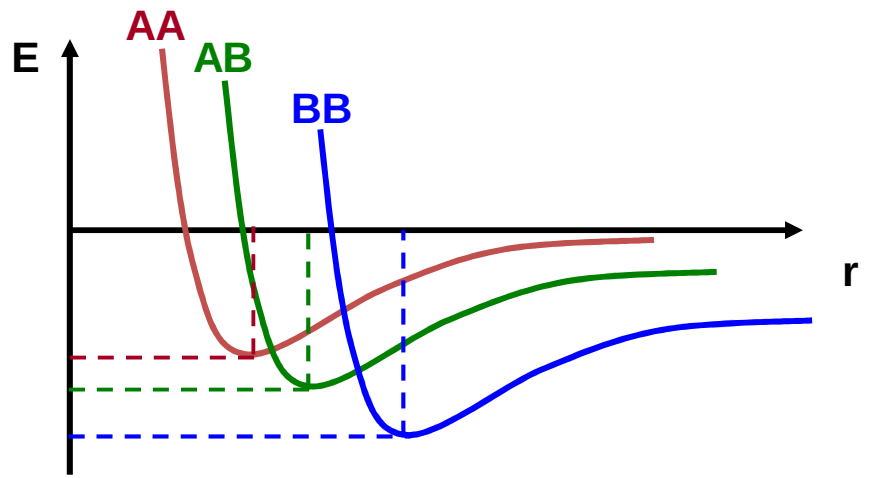
SRO : hetero or homo

… but different, why ?

From binding energies ….

Realistic energy

$$\begin{cases} E_{coh} \\ r_0 \\ B \end{cases}$$



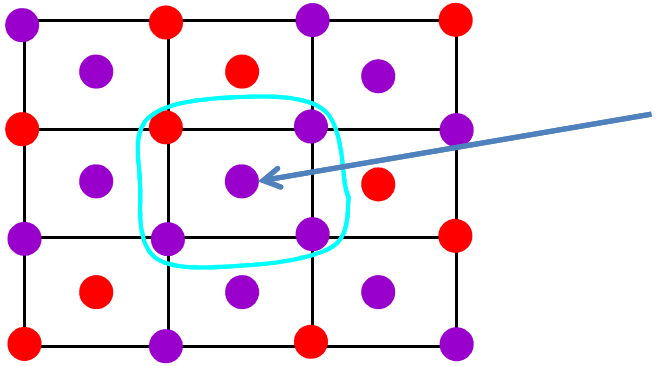
What is the respective role of chemistry and of elasticity in phase diagrams, in segregation phenomenon, ...?

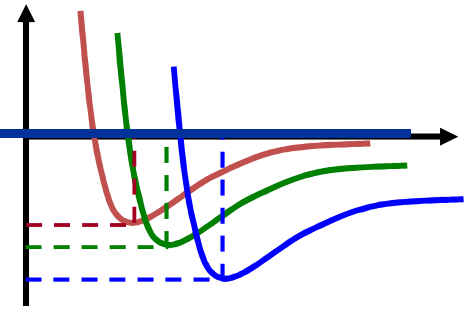
How to pass from (long) simulations with atomic displacements … to (short) simulations on rigid lattice?

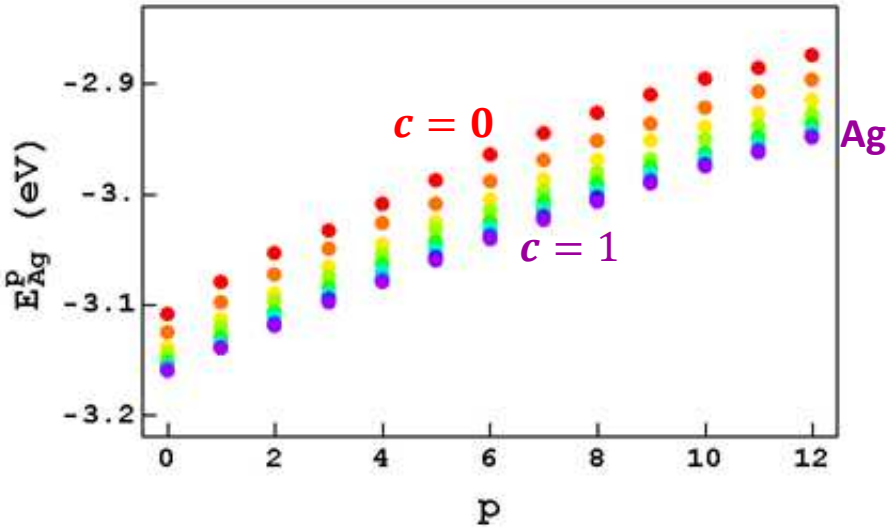
How to pass from ab initio calculations... to the thermodynamics of defects ?

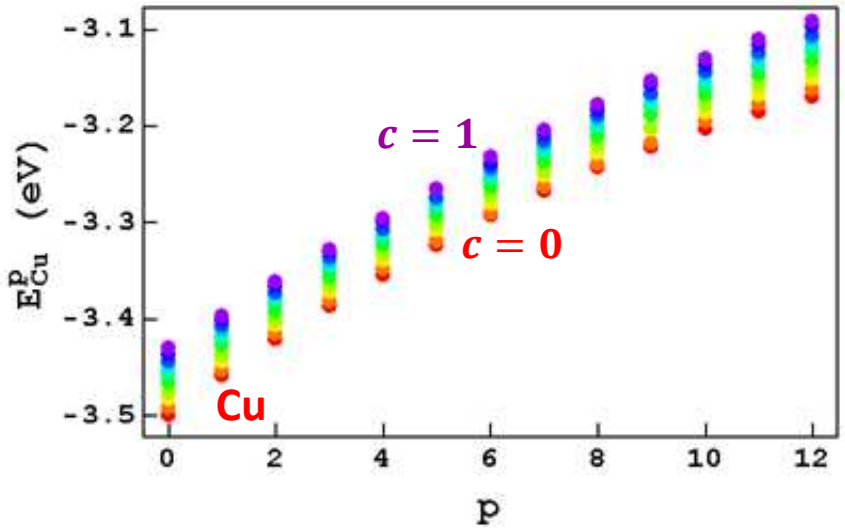
… to site energies

Ag_cCu_{1-c}



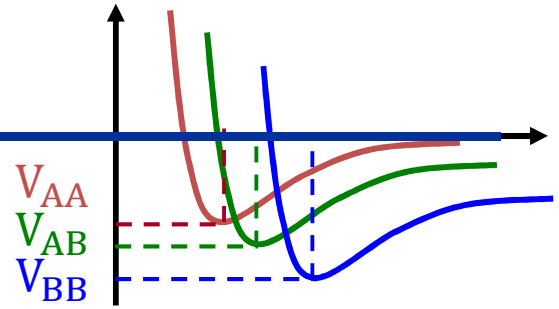


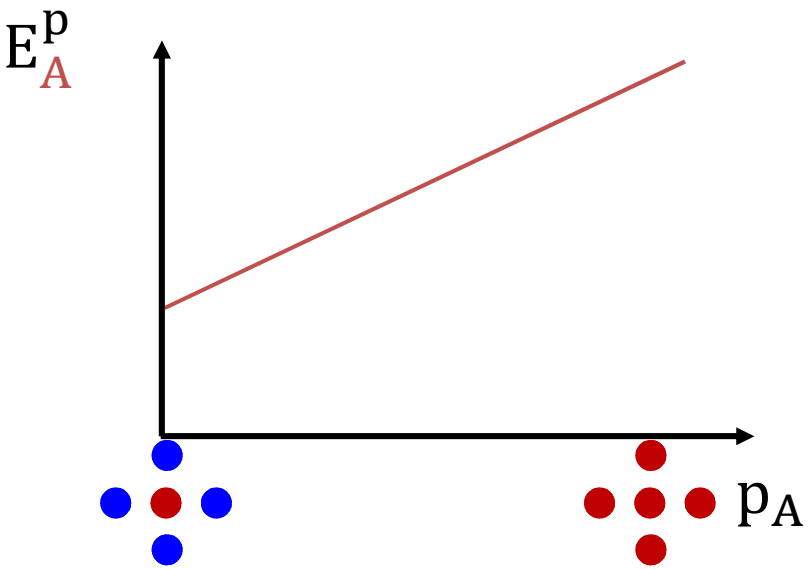




Non-linearity in p: local chemistry
c-dependency : elasticity

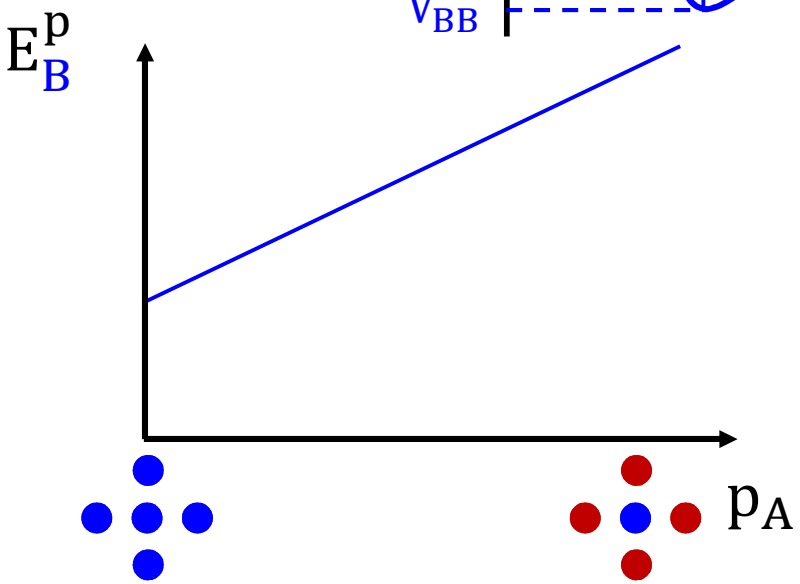
From linear Ising model…





$$E_A^0 = \frac{Z}{2} V_{AB} \qquad E_A^Z = \frac{Z}{2} V_{AA}$$

slope = $V_{AA} - V_{AB}$

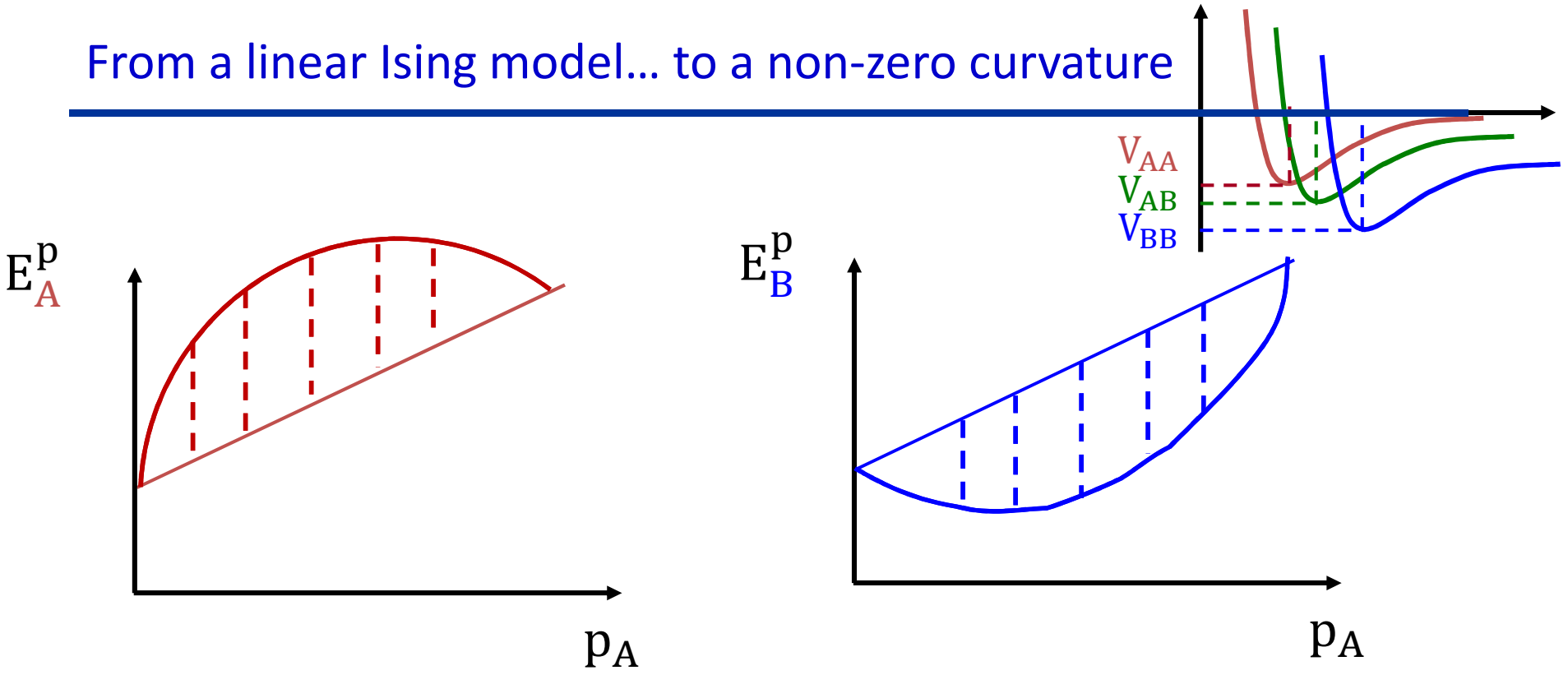


$$E_B^0 = \frac{Z}{2} V_{BB} \qquad E_B^Z = \frac{Z}{2} V_{BA}$$

slope = $V_{AB} - V_{BB}$

Slope difference : $V = (V_{AA} + V_{BB} - 2V_{AB})/2$

From a linear Ising model… to a non-zero curvature

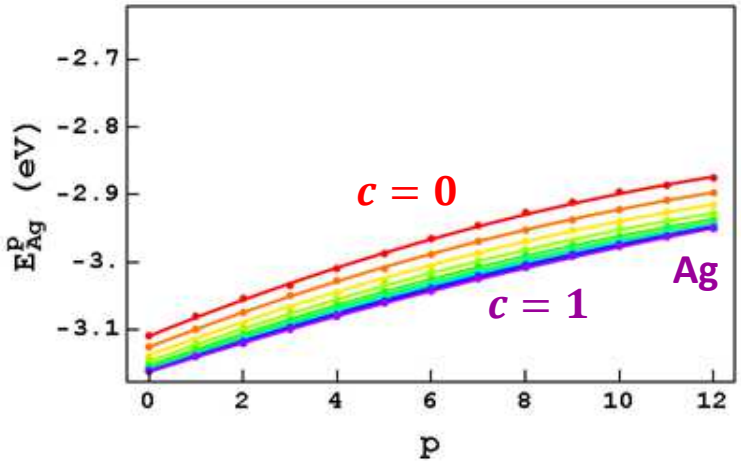


Curvature :

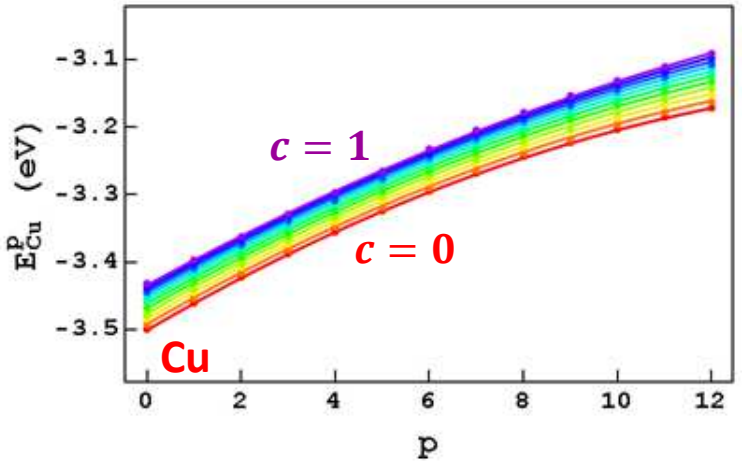
changes V_1
leads to a non-zero value of V_2, V_3, V_4 (for cfc structures)
leads to a supplementary term $c(1-c)(1-2c)\Delta\Gamma$

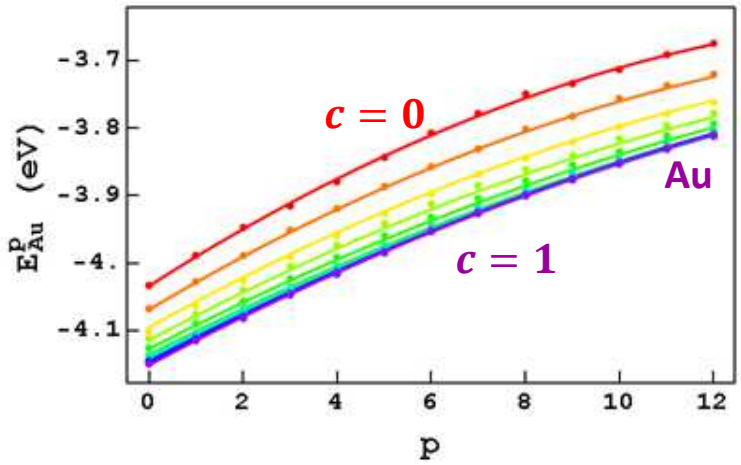
What are the consequences on order phenomenon ???

little game of finding differences between AgCu and AuNi

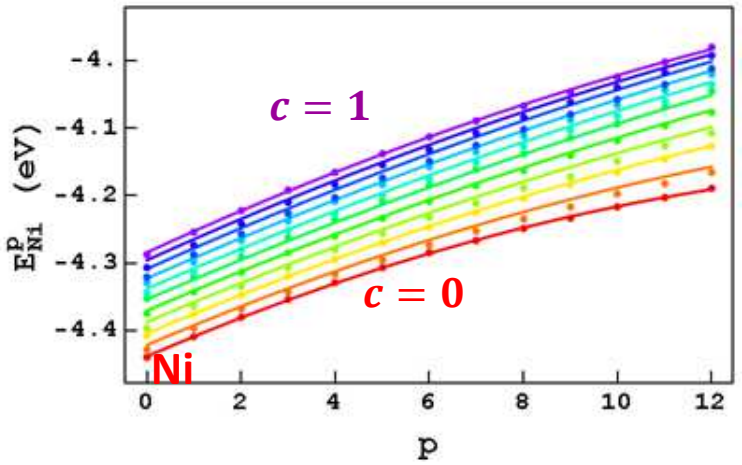


Ag_cCu_{1-c}





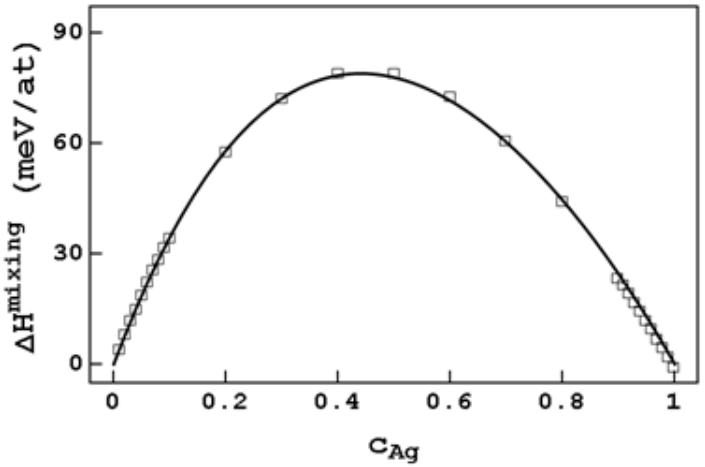
Au_cNi_{1-c}



dependency with c varies with the system

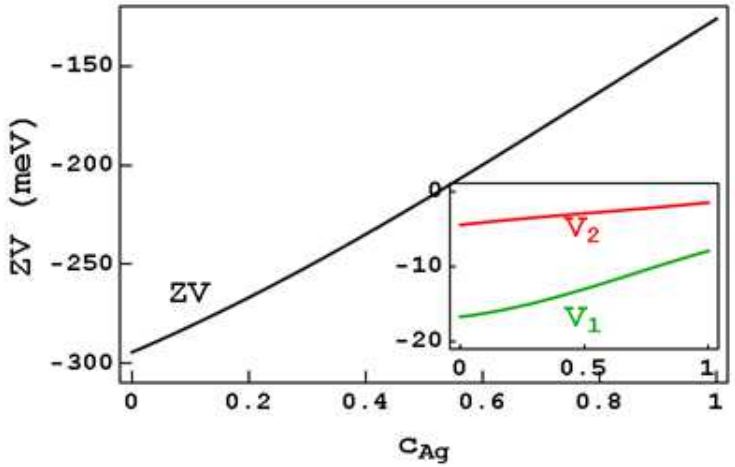
little game of finding differences between AgCu and AuNi

homo

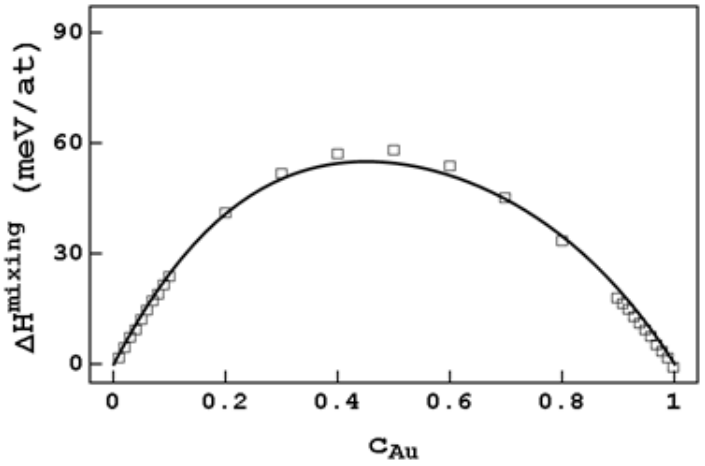


Ag_cCu_{1-c}

V_1, Z V : homo

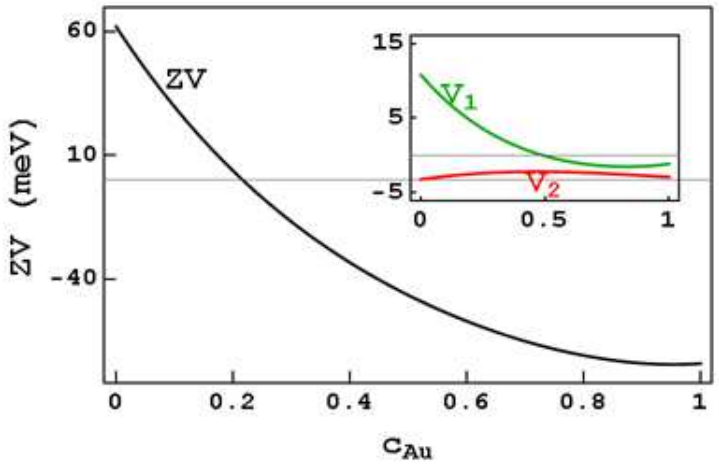


homo



Au_cNi_{1-c}

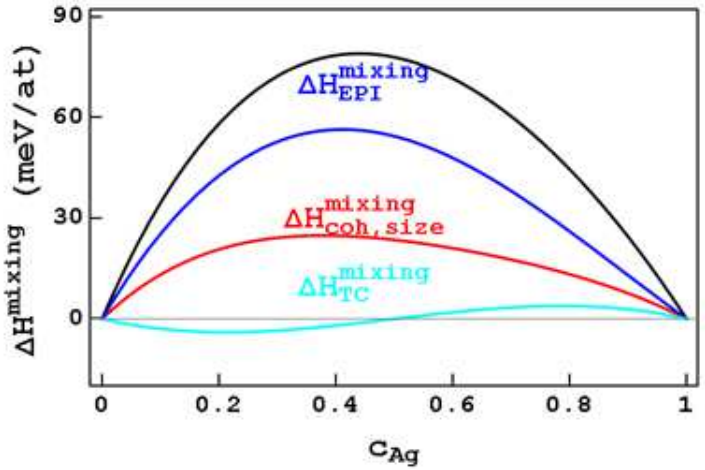
V_1, Z V : hetero / homo !!!



Identical mixing enthalpy but EPIs are different...

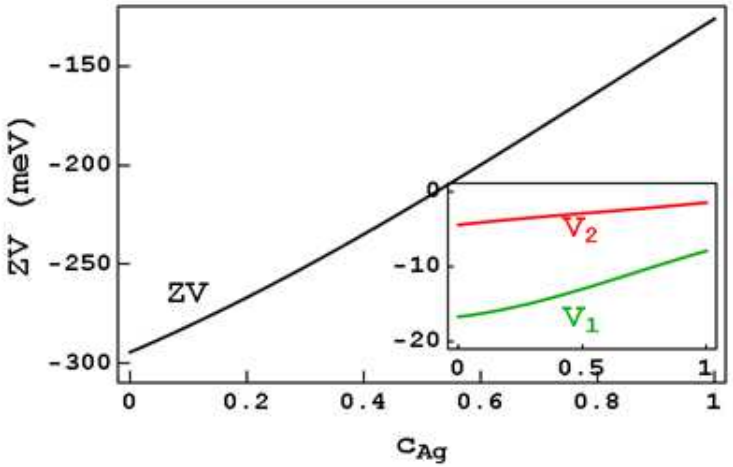
little game of finding differences between AgCu and AuNi

ΔH_{EPI} : homo

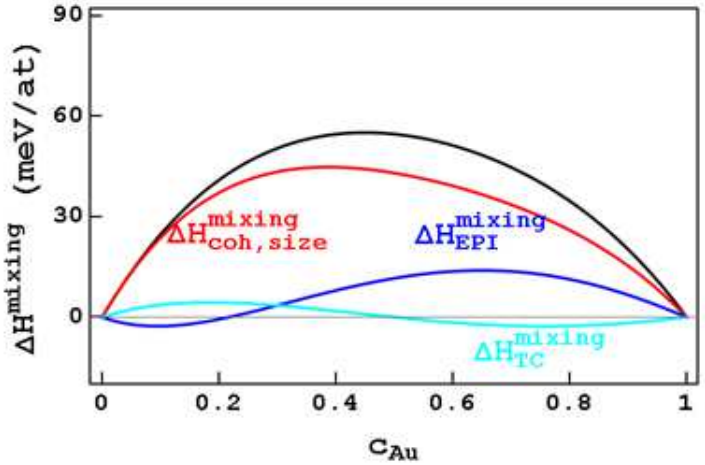


Ag_cCu_{1-c}

V_1, Z V : homo

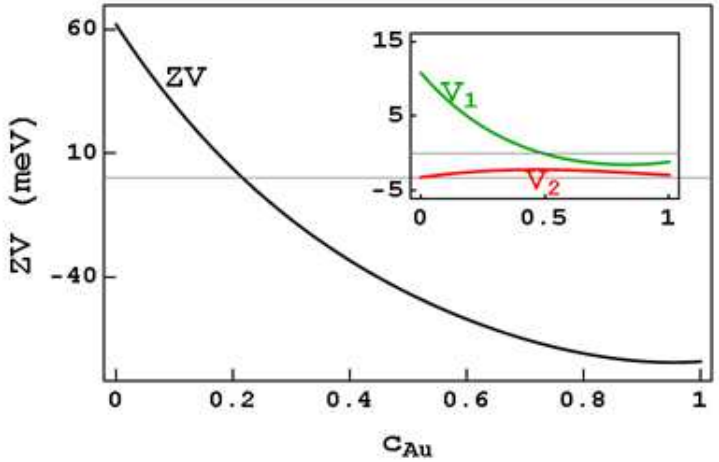


ΔH_{EPI} : hetero/homo



Au_cNi_{1-c}

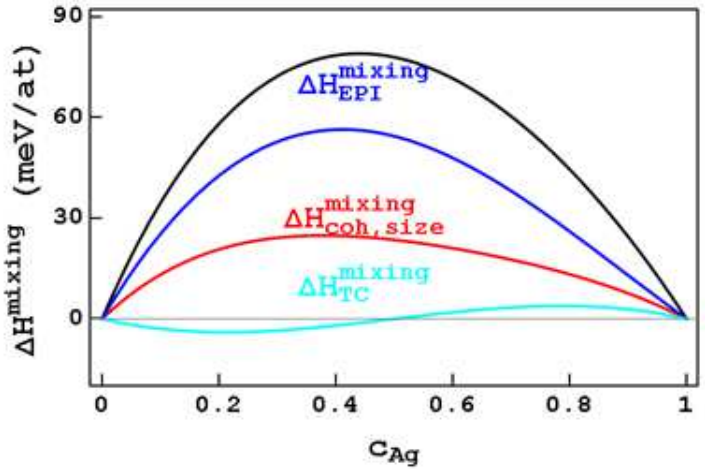
V_1, Z V : hetero / homo !!!



Mixing enthalpy displays all its complexity...

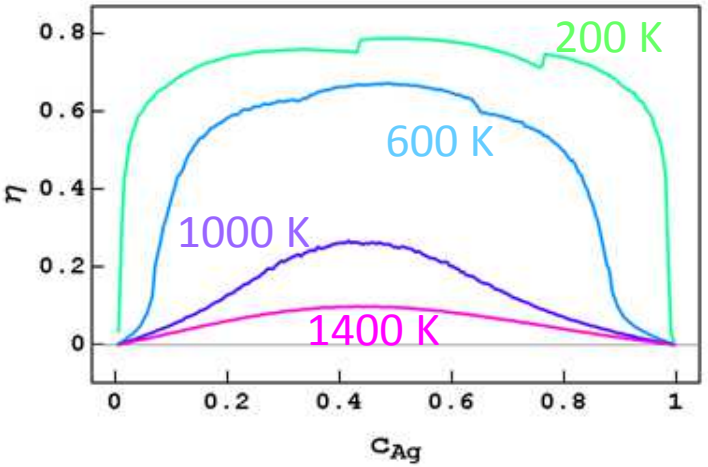
little game of finding differences between AgCu and AuNi

ΔH_{EPI} : homo

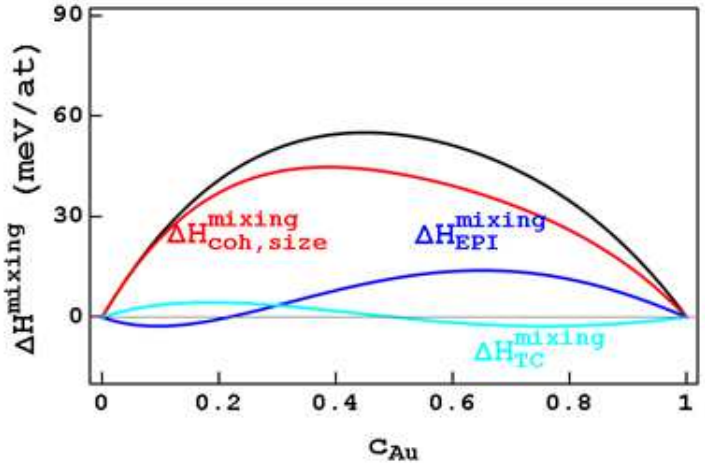


Ag_cCu_{1-c}

SRO : homo

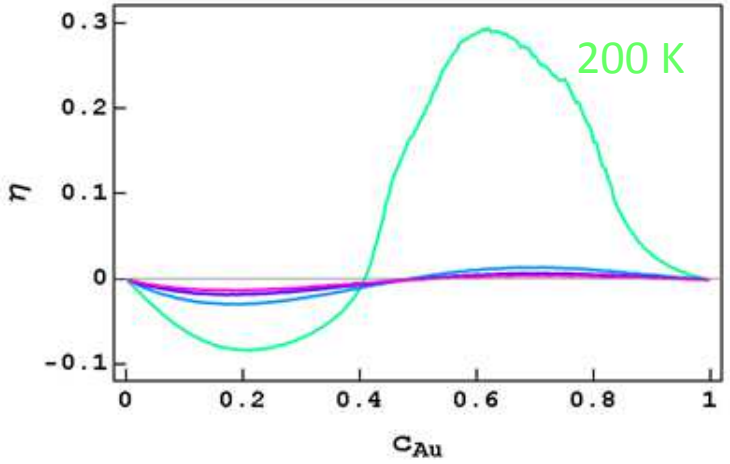


ΔH_{EPI} : hetero/homo



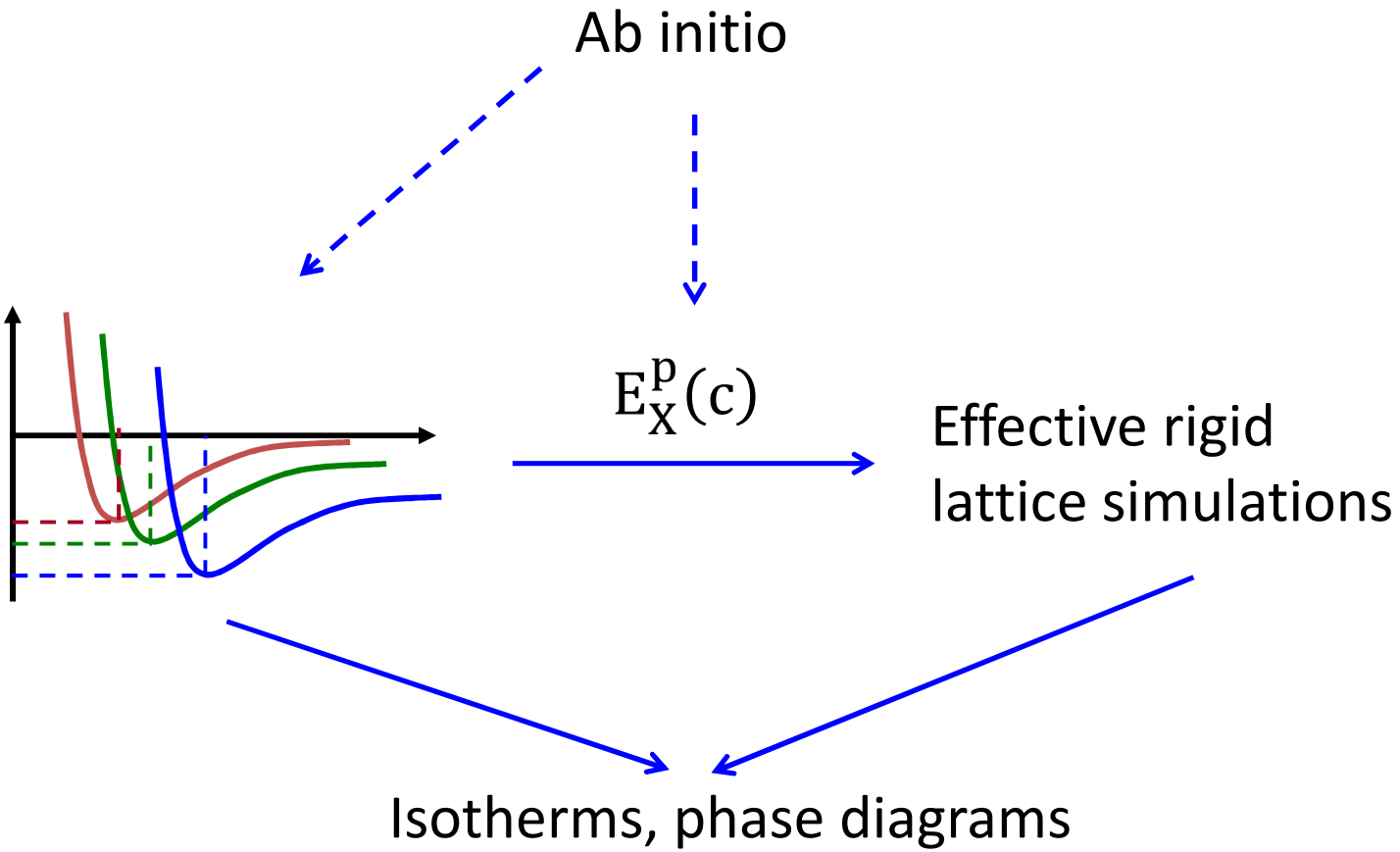
Au_cNi_{1-c}

SRO : hetero / homo !!!



ΔH_{EPI}, V, SRO have the same behavior

Summary and perspectives



Superficial segregation, thermodynamics of defects