



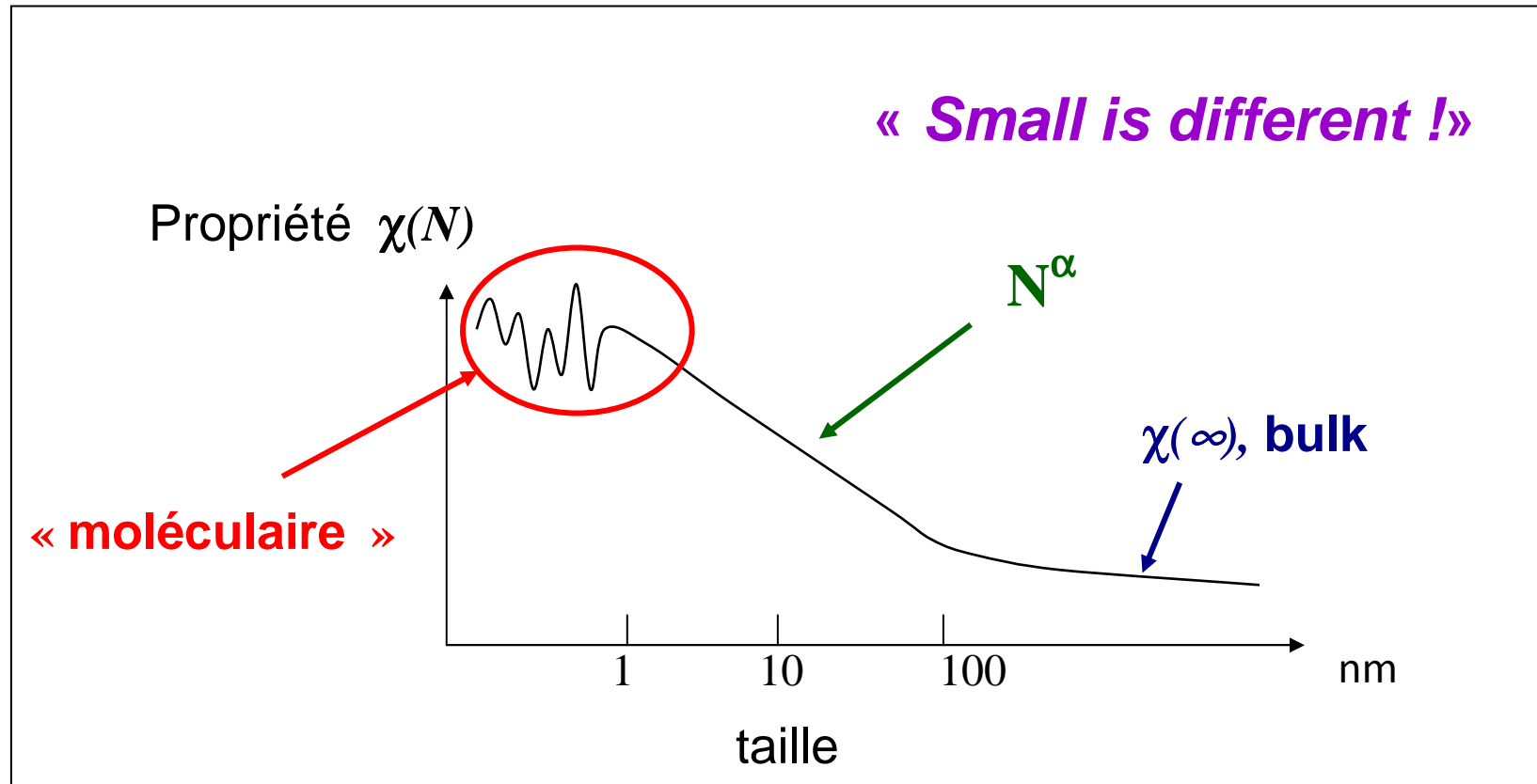
Propriétés des Nanoalliages: de la structure aux propriétés.

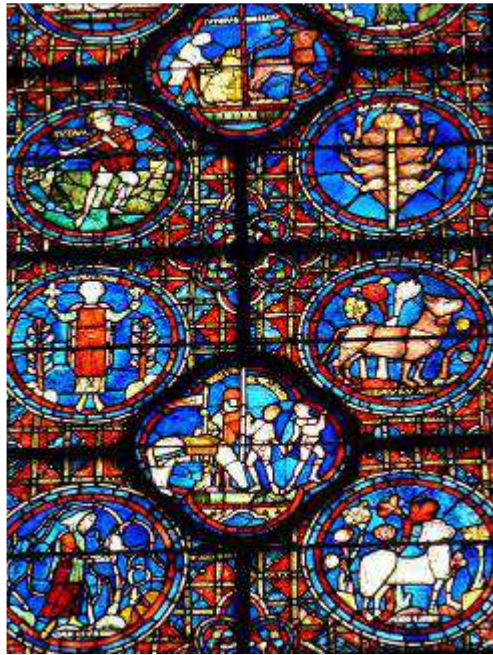
Christine Mottet, Centre Interdisciplinaire de Nanoscience de Marseille,

Jérôme Creuze, Institut de Chimie Moléculaire et des Matériaux D'Orsay,

Bernard Legrand, Section de Métallurgie Physique, CEA Saclay.

Pourquoi des agrégats ?





Moyen Âge

Une façon empirique d'utiliser les Nanoparticules:

- vitraux, arts du verre
- photographie argentique
- pétrochimie (catalyse)



20^{ème} siècle



Lycurgus Cup, art Romain, IV siècle après JC,
British Museum



Nicéphore Niépce,
1826

... **contrôle des propriétés** ⇔ **contrôle de la structure et du mode d'élaboration**

vers une étude de la **relation structure-propriétés** :

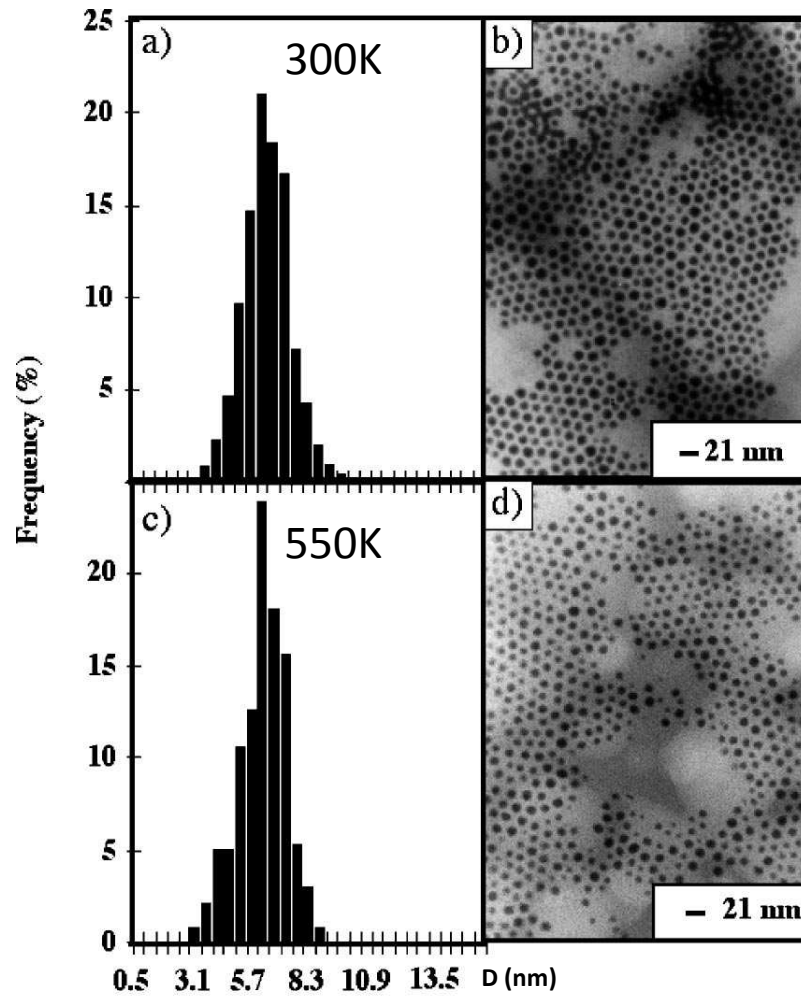
- catalyse hétérogène (activité/sélectivité/stabilité)
- propriétés optiques (plasmonique)
- magnétisme (enregistrement ultra-haute densité, hyperthermie, ...)
- piles à combustible (électrodes en Pt)



Quel environnement pour les nanoparticules métalliques ?

Chimie douce (colloïdes)

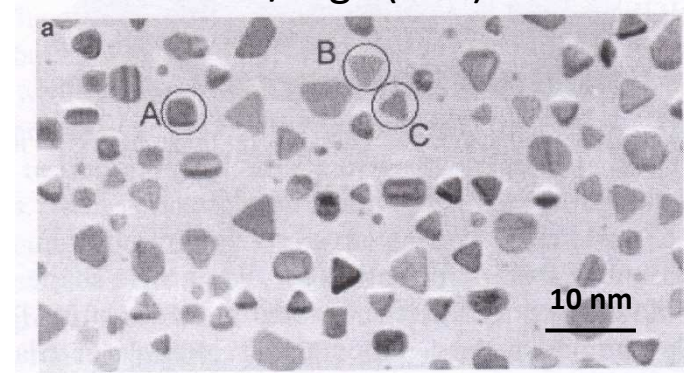
Nanoparticules de Co en solution



Petit et al., JAP 95 (2004) 4251

Physique (ultra-vide)

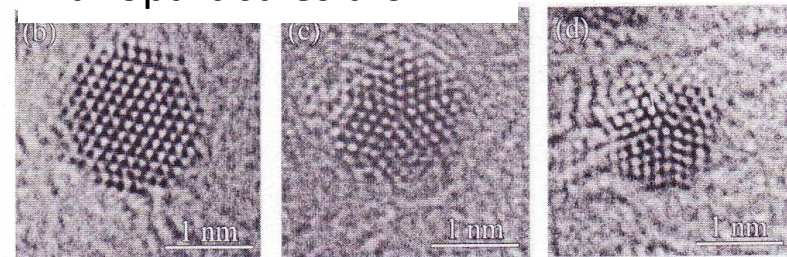
Au/MgO(100)



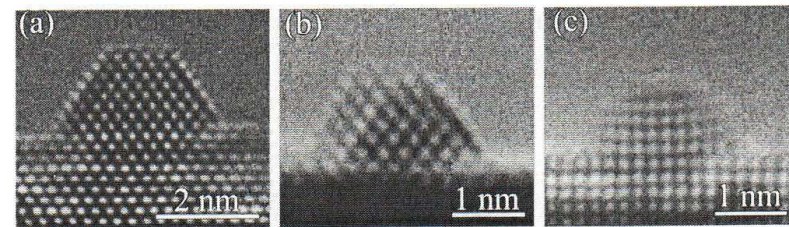
Henry, Prog. Surf. Sci. 80 (2005) 92

Nanoparticules d'or

Carbone amorphe



Substrat cristallin



Pauwels, Van Tendeloo et al., PRB 62 (2000) 10383.

Catalytic Properties of Pd-Au nanoalloys

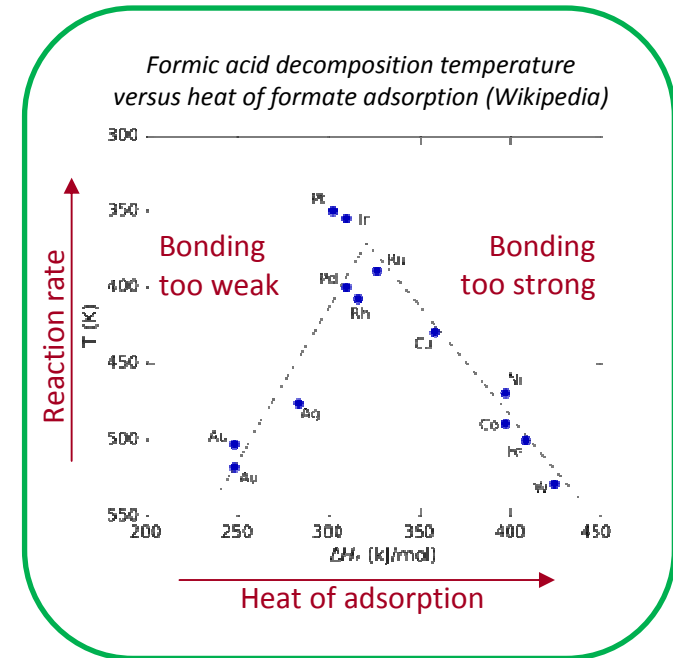
- Most of the catalysts obey to the Sabatier principle:

Pd is a good catalyst / **Au** poorly reactive in bulk

- However **Au nanoparticles supported on oxide surfaces** present high activity and/or selectivity, at low temperature, in many reactions (*Haruta*¹)

- **Pd-Au nanoalloys** improve activity/selectivity/stability

- New question: what is the **surface composition** ? in gas pressure, adsorption-induced Pd surface segregation^{2,3}



¹Haruta, *Gold as a Novel Catalyst in the 21st Century: Preparation, Working Mechanism and Applications*, **Gold Bull. 37 (2004)**

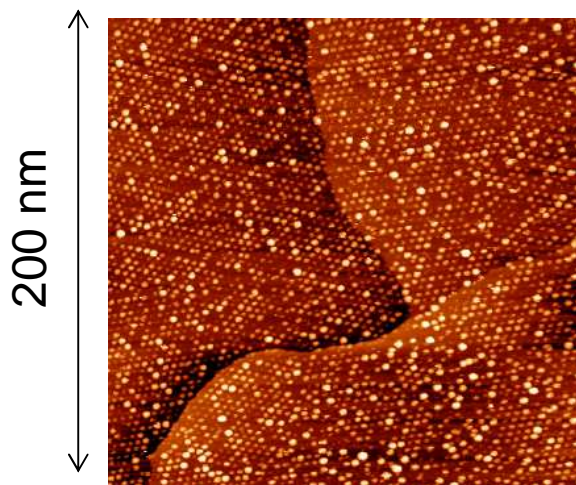
²Gao, Wang, Goodman, *CO Oxidation over AuPd(100) from Ultrahigh Vacuum to Near-Atmospheric Pressures: CO Adsorption-Induced Surface Segregation and Reaction Kinetics*, **J. Phys. Chem. C 113 (2009)**

³Delannoy, Giorgio, Mattei, Henry, Kolli, Méthivier, Louis, *Surface segregation of Pd from TiO₂-Supported AuPd Nanoalloys under CO Oxidation Conditions Observed In situ by ETEM and DRIFTS*, **ChemCatChem 5 (2013)**

Experimental studies on Pd-Au nanoalloys in vacuum

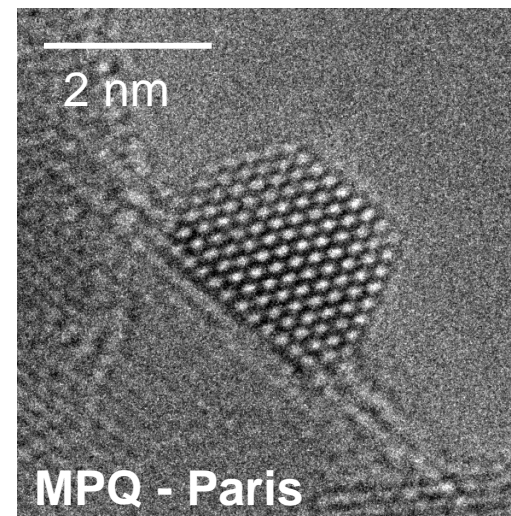
- A collection of self-organized nanoparticles with homogeneous size, shape, composition... to better link their catalytic properties with their size, structure and composition observed by STM¹.
- The characterization of a single nanoparticle of alloy observed by HRTEM².

STM: AuPd on Al₂O₃/Ni₃Al(111)



CINaM - Marseille

TEM: Au₅₀Pd₅₀ sur MgO(100)



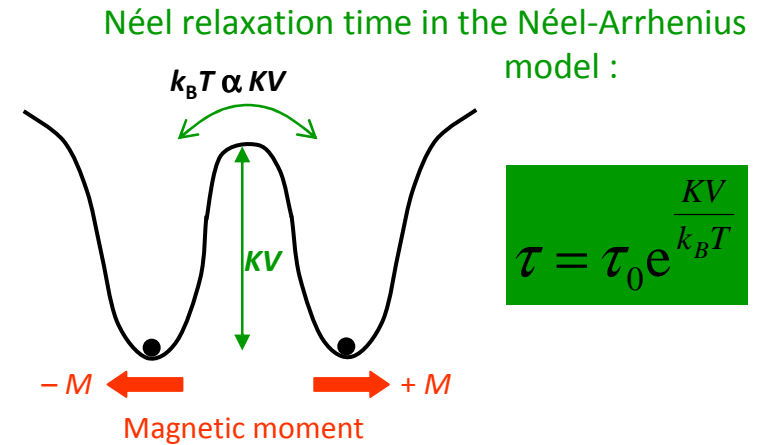
¹ M. Marsault, G. Hamm, A. Wörz, G. Sitja, C. Barth, C.R. Henry, *Preparation of regular arrays of bimetallic clusters with independent control of size and chemical composition*, *Faraday Discuss.*, **138** (2008)

²Nhat Tai NGUYEN, *Synthèse et étude des propriétés structurales, thermodynamiques et catalytiques de nanocatalyseurs Au-Pd par microscopie électronique en transmission*, *PhD Thesis, Université Paris 7* (2015)

Nanoalliages Co-Pt

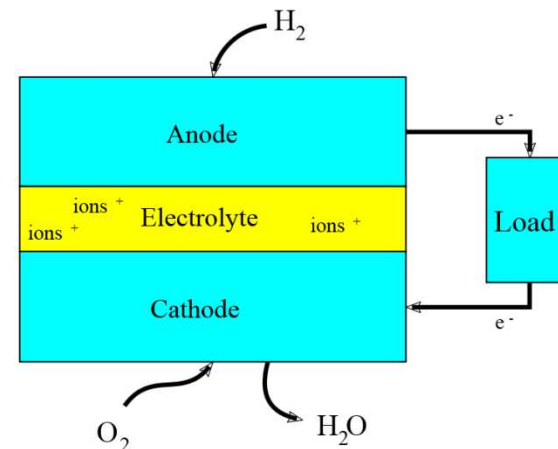
❑ Stockage magnétique haute-densité :

- Alliage de métaux 3d - 5d (FePt, CoPt, ...) augmente l'anisotropie magnétocristalline pour lutter contre le superparamagnétisme

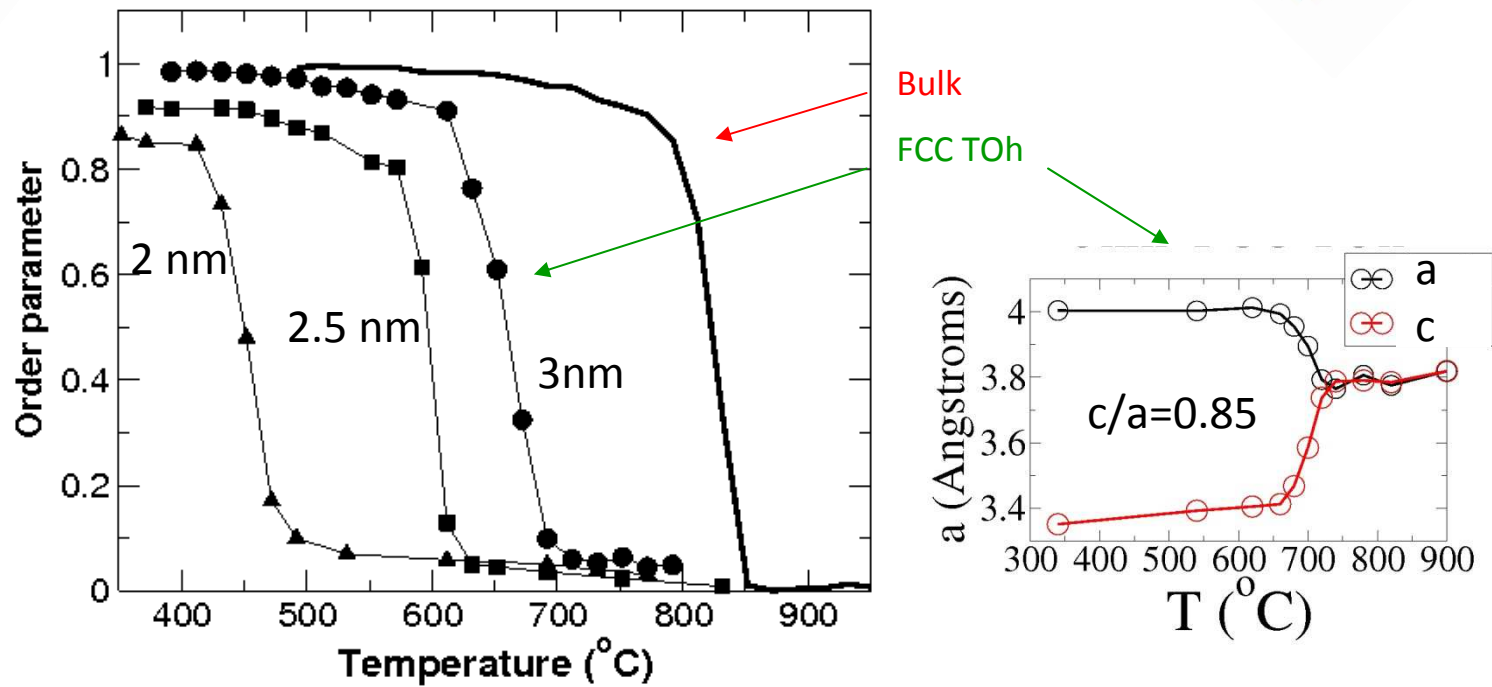
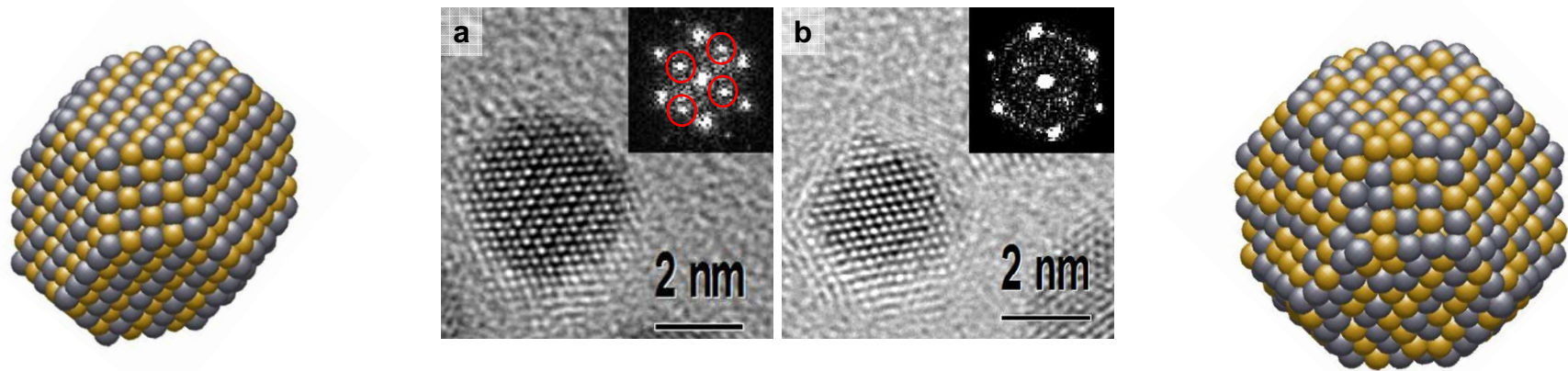


❑ Piles à combustible à membrane d'échange de protons (PEMFCs):

- Augmenter la stabilité (durabilité) de l'électrode de Pt (cathode) par des alliages de métaux de transition (catalyse).



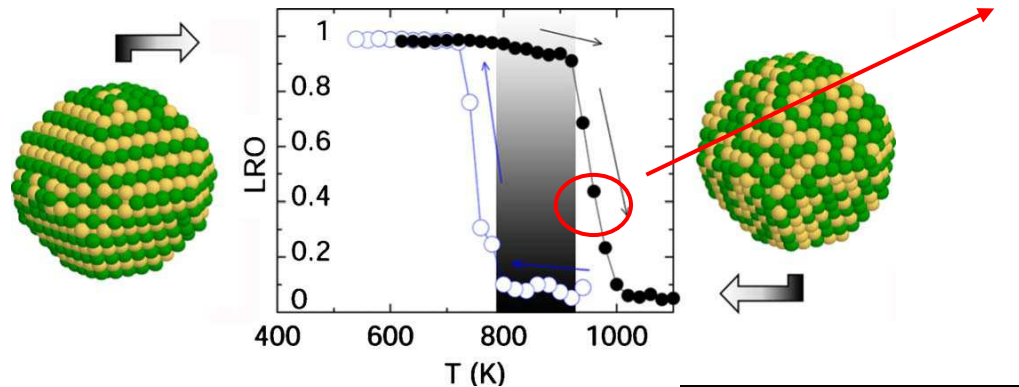
HRTEM observation / Theory of CoPt nanoalloys



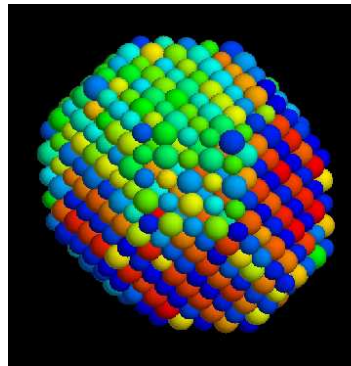
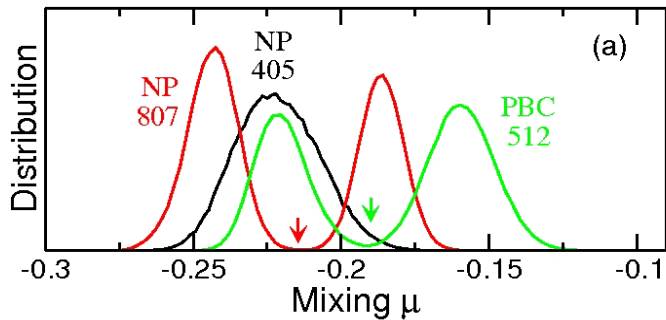
D. Alloyeau, C. Ricolleau, C. Mottet, T. Oikawa, C. Langlois, Y. Le Bouar, N. Braïdy, A. Loiseau, Nature Materials 8, 940 (2009) « Size and shape effects on the order-disorder phase transition in CoPt nanoparticles ».

Grazing Incidence X-rays Diffraction / Theory

Monte Carlo simulations



Configurational Distribution at T_c

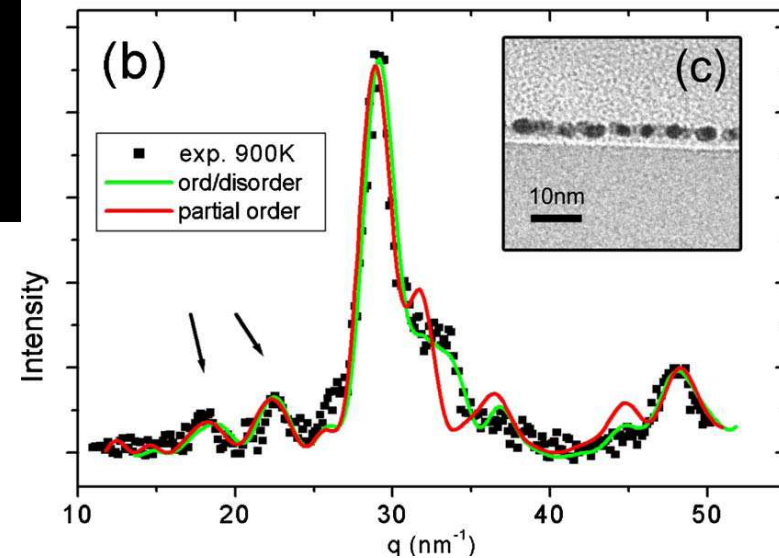
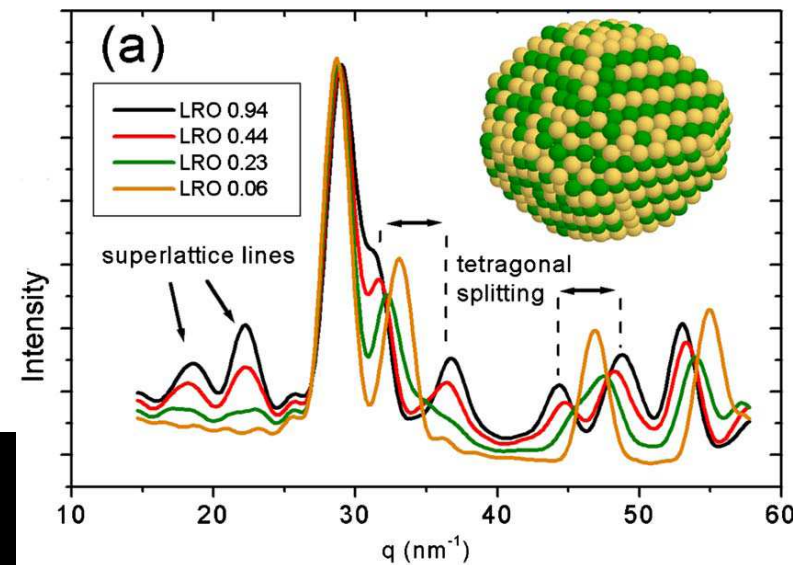


Phase coexistence : 1st order transition

P. Andrezza, et al., PRB 82, 155453 (2010)

F. Calvo, et al., PRB84, 035409 (2011)

Calculated/Exp. GIXD spectra



Problématique des Nanoalliages :

1. Effet de taille

2. Effet d'alliage

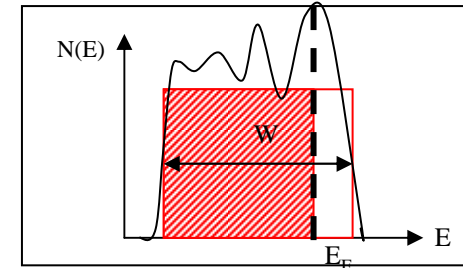
3. Effet d'environnement

... et, si possible, le couplage de tous ces effets...

Tight Binding Models for alloys

□ Semi-empirical interatomic potential : SMA

$$E = \sum_i \left(-\sqrt{\sum_j \xi^2 e^{-2q\left(\frac{r_{ij}}{r_0}-1\right)}} + \sum_j A e^{-p\left(\frac{r_{ij}}{r_0}-1\right)} \right)$$



Fitted on:

- *ab initio* calculations (lattice parameters, cohesive, surface, dissolution energies, ...)
- Experimental values (elastic constants, mixing enthalpies of alloys, ...)

□ Tight Binding Ising Model : $E = \sum P_n (\Delta h_n^{eff} - \sum V_{nm}) + \sum P_n P_m V_{nm}$

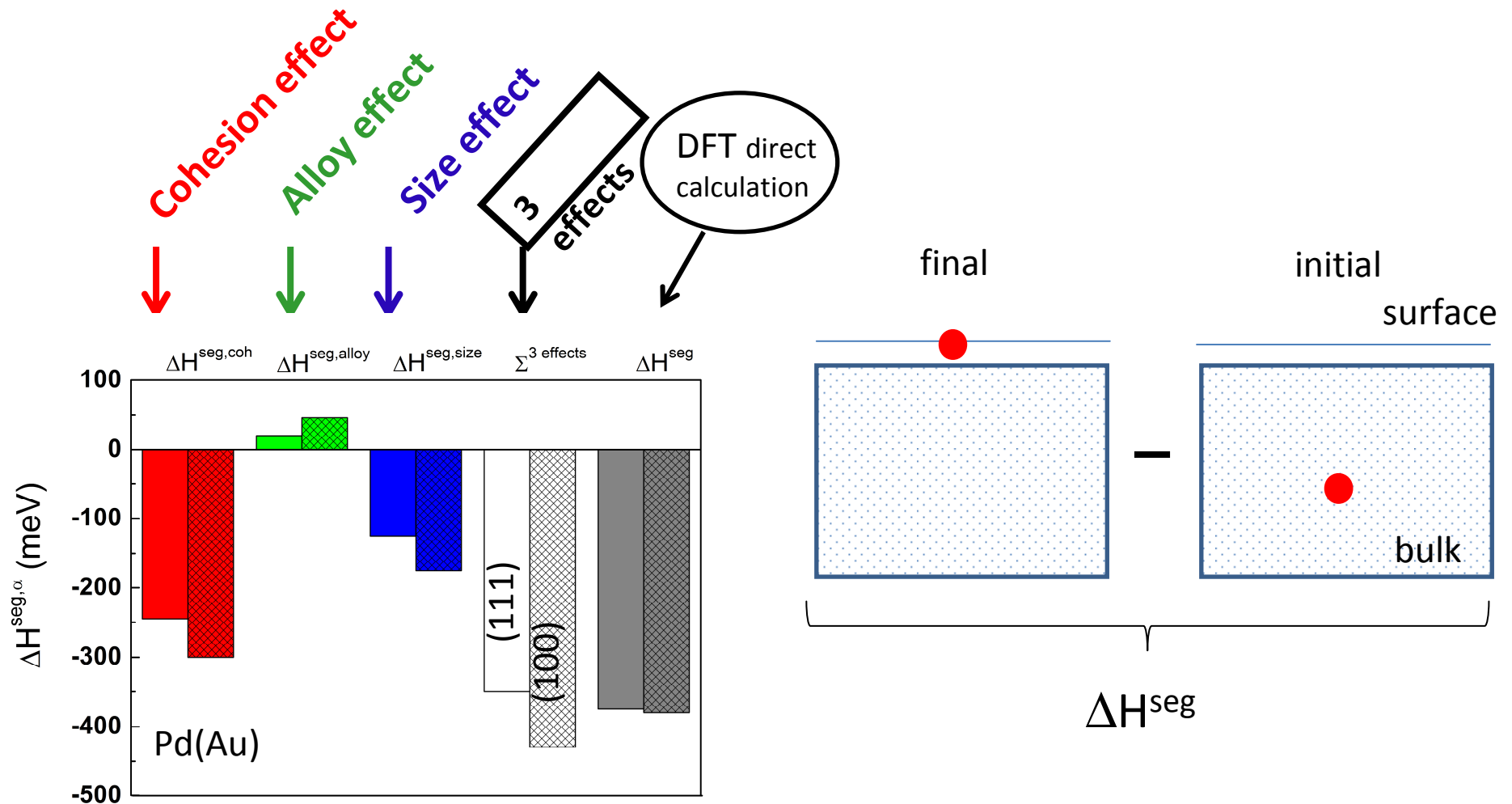
- **Cohesion effect** : $\Delta h_0^{eff} = \gamma^A - \gamma^B$

- **Alloying effect** : $V_{nm} = \frac{1}{2} \sum (V_{nm}^{AA} + V_{nm}^{BB} - 2V_{nm}^{AB})$

- **Size effect** : atomic relaxation due to size mismatch calculated with SMA

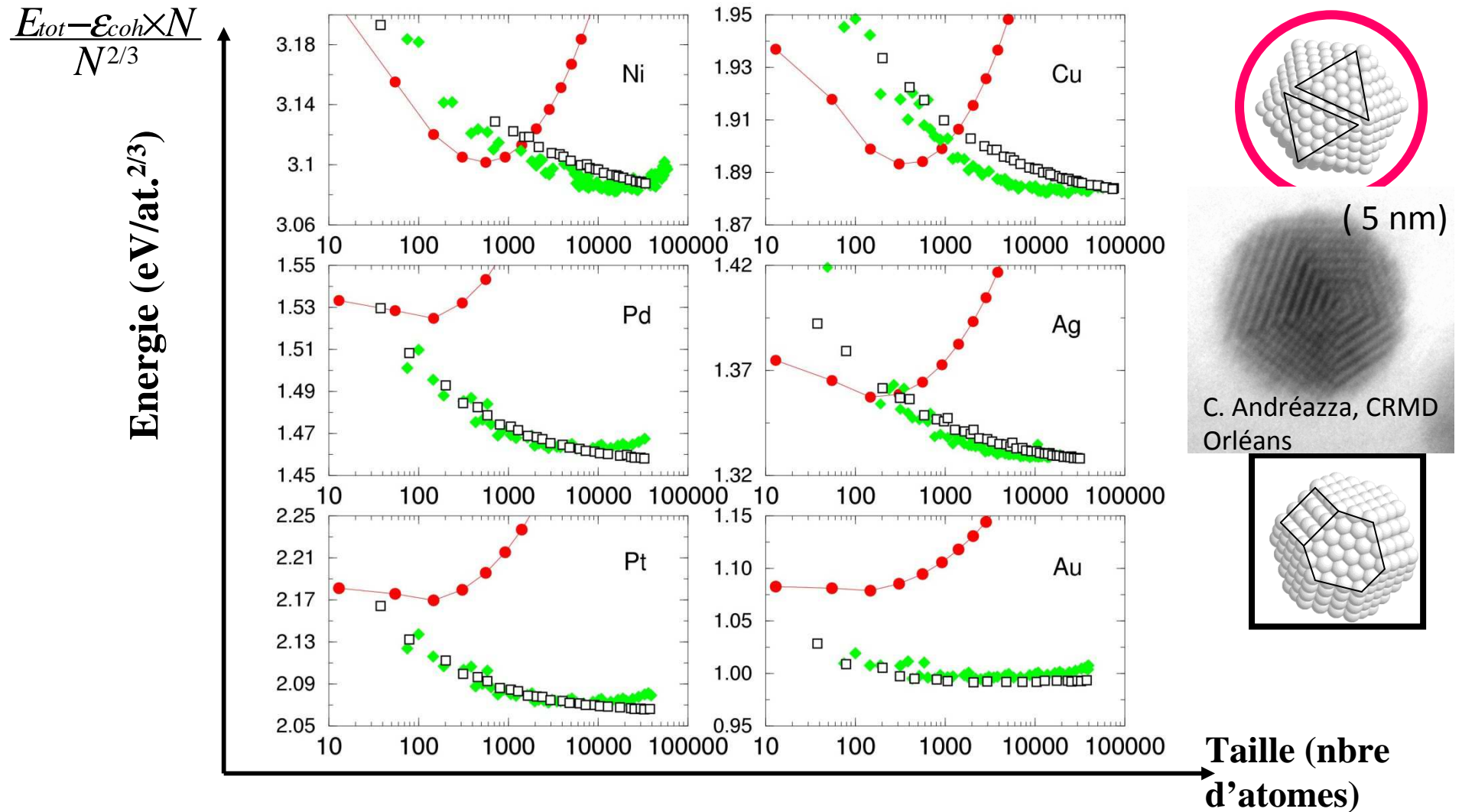
Surface segregation: TBIM analysis of the driving forces

Au impurity segregation in Pd (100) and (111) surfaces



1. Effet de taille sur la structure et la morphologie d'agrégats purs et libres

Nanoparticules libres : Quelle structure Ih, Dh, TOh (CFC) ?



Théo.: Baletto *et al.*, *J. Chem. Phys.* **116** (2002) 3856; Mottet *et al.*, *Phase Transitions* **77** (2004) 101.

Exp.: Pellarin *et al.*, *Chem. Phys. Lett.* **217** (1994) 349; Reinhard *et al.*, *Phys. Rev. Lett.* **79** (1997) 1459.

Structure d'agrégats de 13 atomes en DFT

Pt₁₃

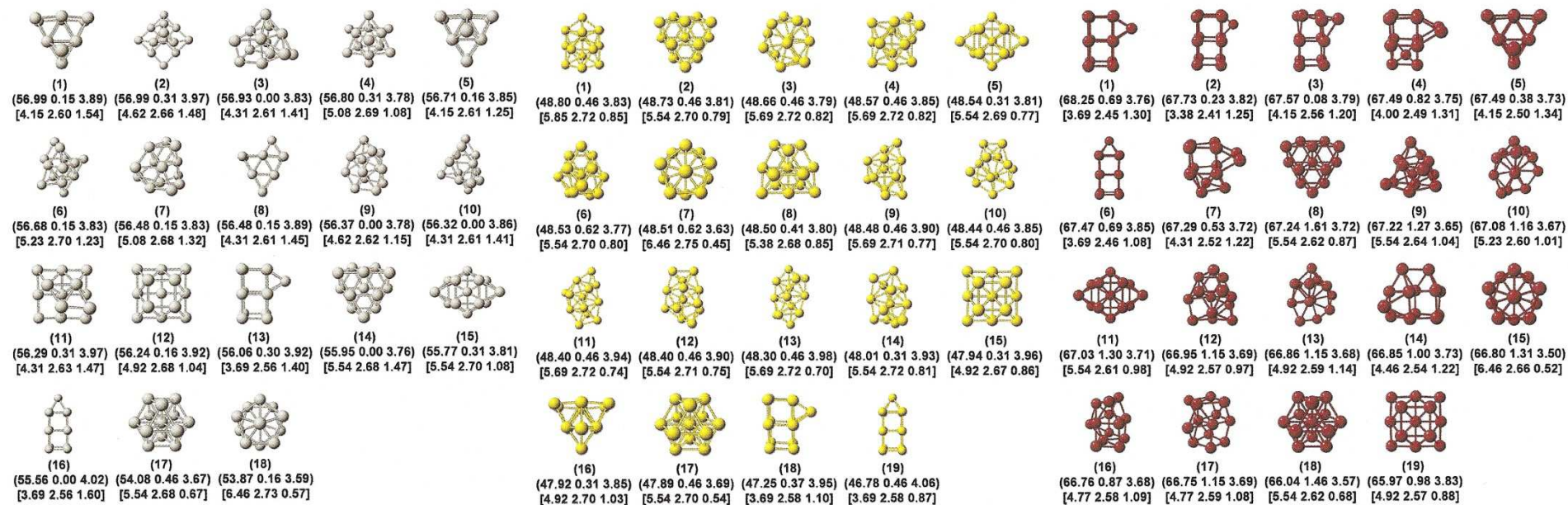
Pd₁₃

Rh₁₃

DENSITY FUNCTIONAL STUDY OF STRUCTURAL TRENDS...

L.-L. WANG AND D. D. JOHNSON

L.-L. WANG AND D. D. JOHNSON



Wang, Johnson, PRB 75, 235405 (2007).

On distingue 2 régimes:

- les tailles de 1 à 2 nm (la dizaine à la centaine d'atomes)
 - optimisation globale utilisant des potentiels semi-empiriques
 - calculs *ab initio* (DFT) sur des symétries préconçues
 - nombreuses symétries et isomères (systèmes moléculaires)

- les tailles de 2 à 10 nm (la centaine à quelques milliers d'atomes)
 - dynamique moléculaire (cas pur ou étude dynamique)
 - simulations Monte Carlo (alliages, étude à l'équilibre)
 - quelques motifs prépondérants et comparaison des stabilités entre ces motifs

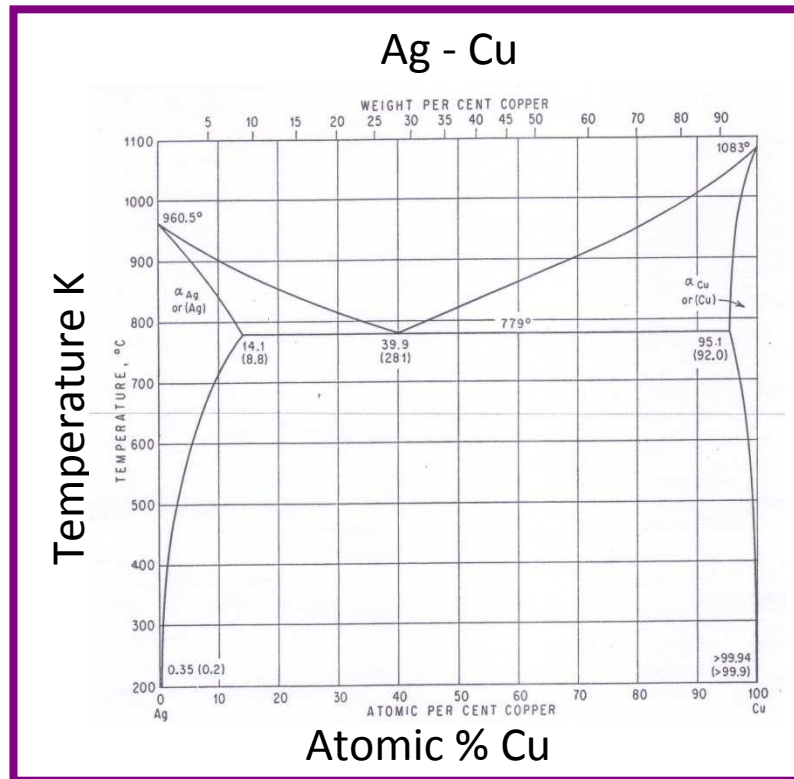
2. Effet d'alliages: Nanoalliages

*ou comment moduler les propriétés
en fonction de la taille et de la composition...*

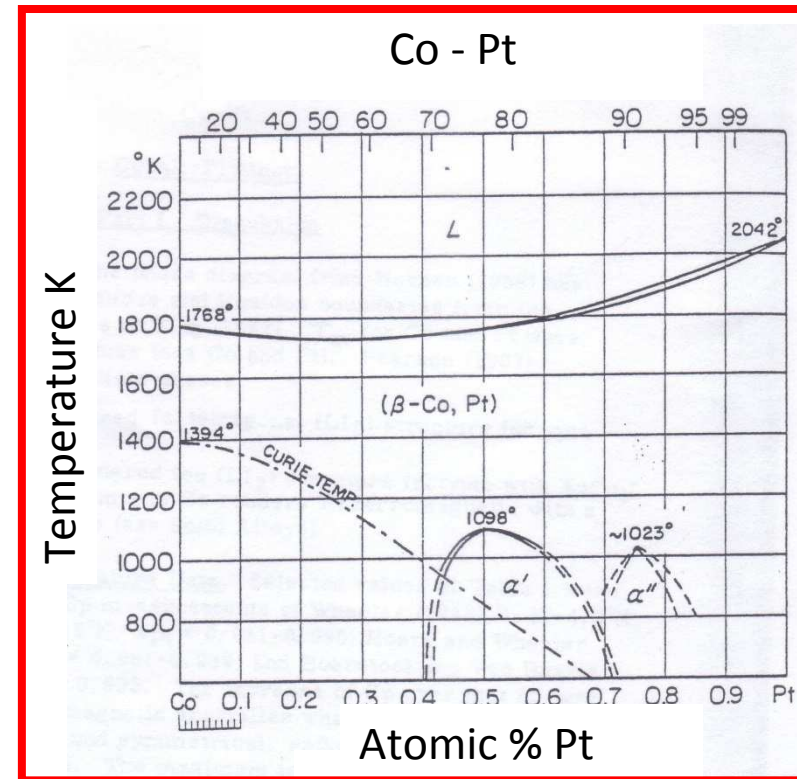
Quel ordre chimique au sein des nanoparticules ?

- coeur/coquille ?
 - mélange (solution solide) ?
 - composé ordonné ?
- } Ségrégation superficielle ?

Tendance à la démixion



Tendance à l'ordre



Hultgren et al., *Selected Values of the Thermodynamic Properties of Binary Alloys*,
American Society of Metals, Berkeley

Exemple n° 1 : Co-Pt

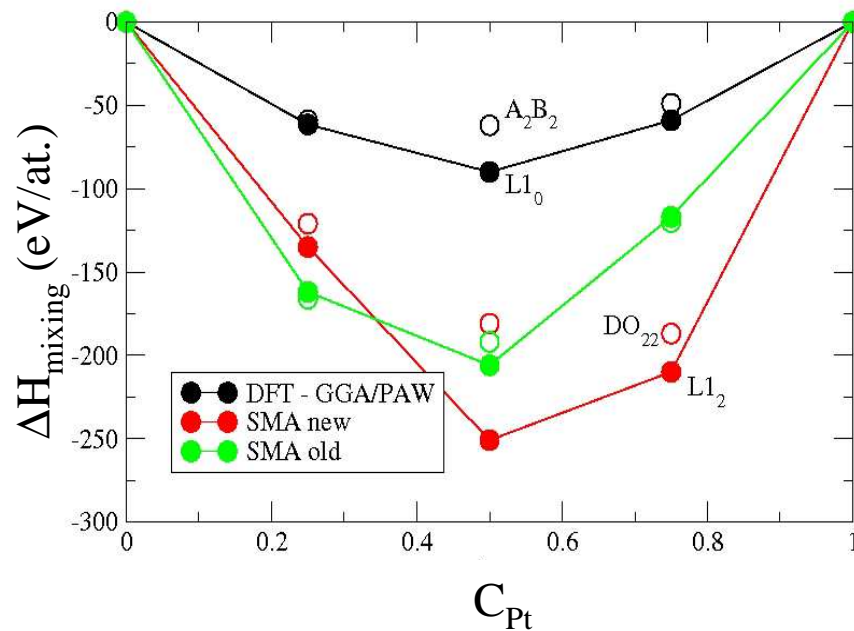
DFT Calculations on Co-Pt systems

VASP – PAW/GGA spin polarized

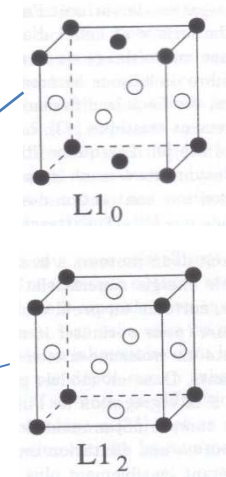
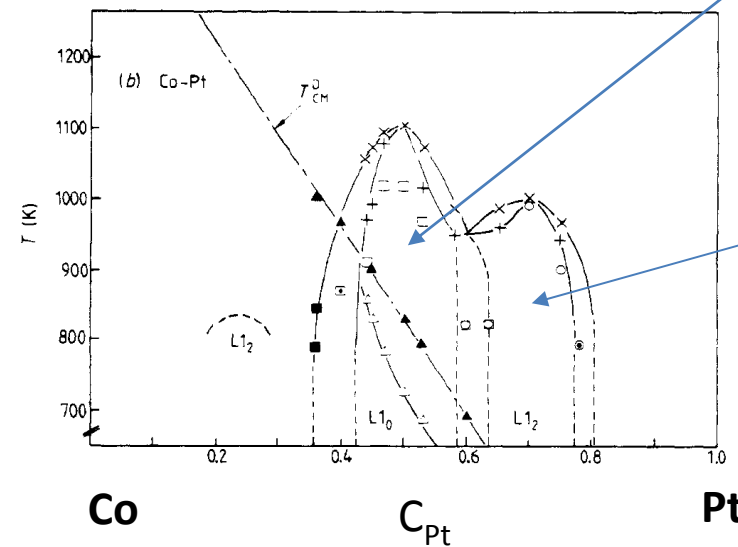
Metal	a (Å)	E _{coh} (eV/at.)	γ ⁽¹¹¹⁾ (eV/at.)	γ ⁽¹⁰⁰⁾ (J/m ²)	γ ⁽¹¹⁰⁾ (eV/at.)
Co	3.52 (3.54)	-5.35 (-4.45)	0.68	2.47 (2.55)	1.31
Pt	3.98 (3.92)	-5.53 (-5.86)	0.64	1.85 (2.48)	1.31

(Exp. values in parenthesis)

DFT Mixing Enthalpies of Co-Pt Bulk Alloys



Experimental Co-Pt Bulk Phase Diagram



TBIM parameters of Co-Pt alloys

- Effective Pair Interactions (EPI): n^{th} neighbors

$$V^n = (V_{\text{CoCo}}^n + V_{\text{PtPt}}^n - 2V_{\text{CoPt}}^n)/2$$

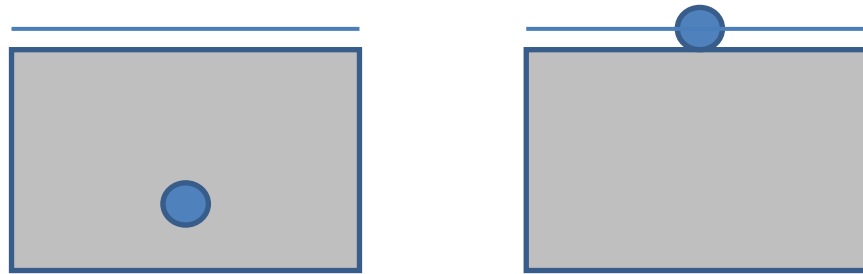
EPI in meV	V^1	V^2	V^3
Co(Pt) SMA	57	33	23
DFT	69	16	?
Pt(Co) SMA	67	16	16
DFT	-8*	-19*	?

*because of magnetic interaction between 2 magnetic impurities

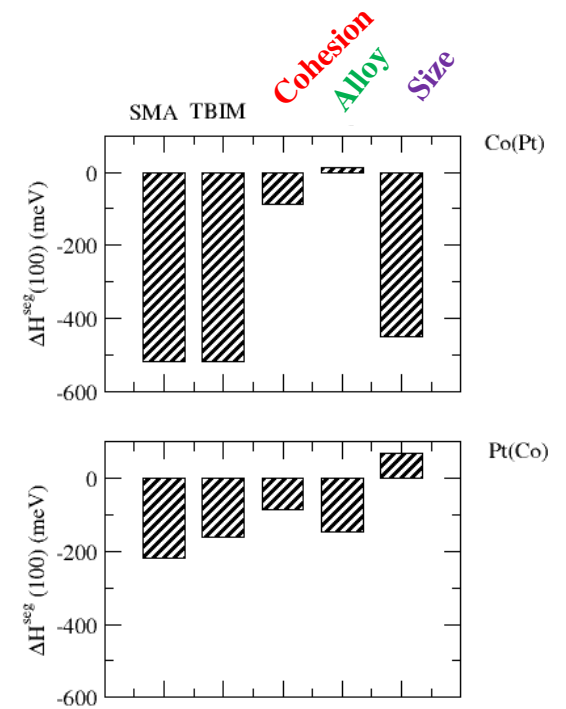
- Two possible EPI models: $(V^1, V^2, V^3) = (67, 16, 16)$ compatible with SMA / DFT
 or
 $(V^1, V^2) = (82, -8)$ fitted to experimental T_c

TBIM / SMA comparison

Segregation enthalpies reconstruction: 3 driving forces in TBIM



(100)	SMA	TBIM	Cohesion	Alloy	Size
Co(Pt)	-0.52	-0.54	-0.10	0.012	-0.449
Pt(Co)	-0.22	-0.18	-0.10	-0.148	0.071



- TBIM Co-Pt systems:
- Bulk
 - Surfaces
 - Clusters

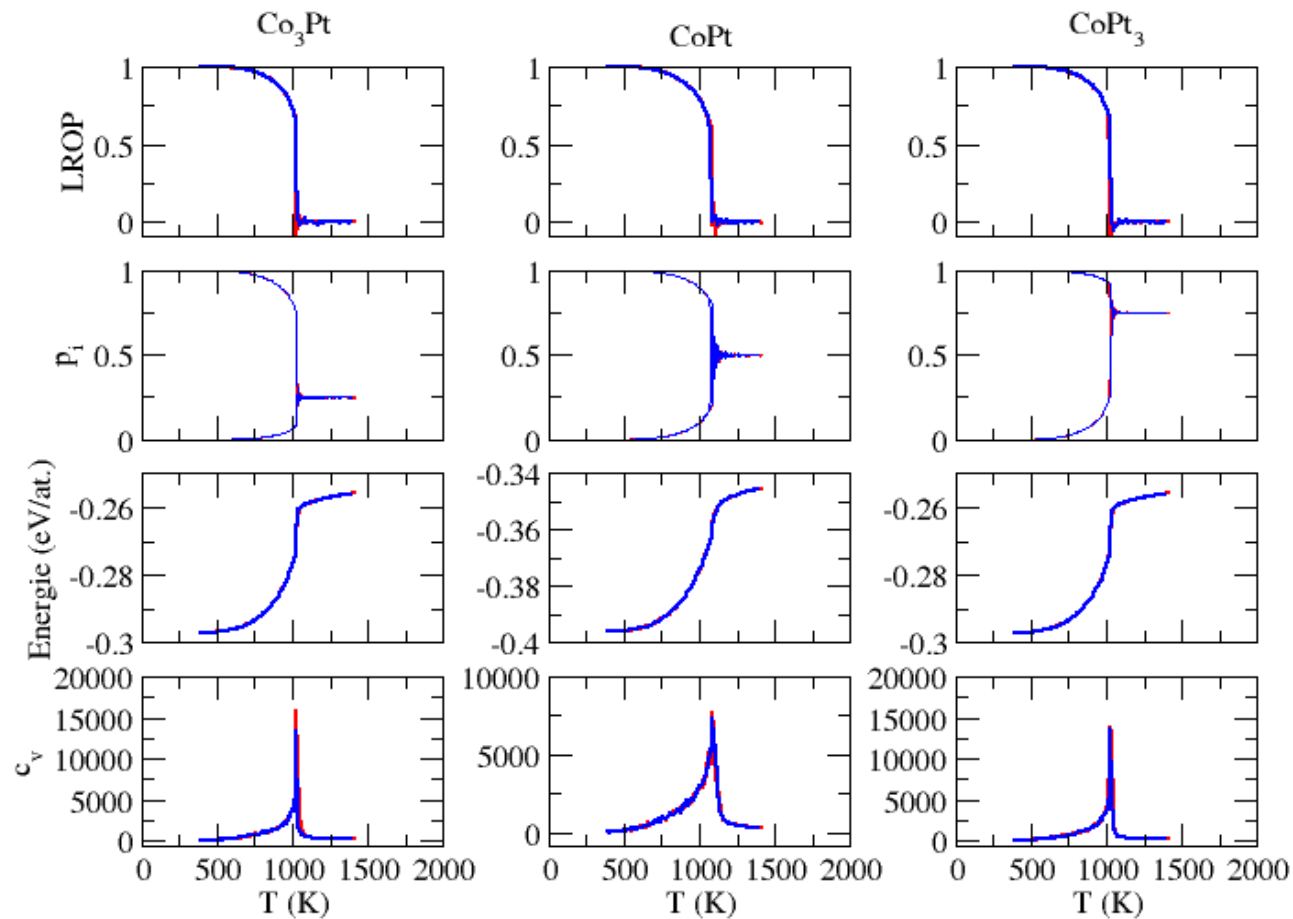
Rigid lattice model

Order/Disorder Transition in TBIM

Bulk $\text{Co}_{1-c}\text{-Pt}_c$ alloys

T_c (K)	v^1	v^2	$v^1 v^2 v^3$
Co_3Pt	1120	1030	
CoPt	1110	1080	
CoPt_3	1120	1030	

TBIM with V^1, V^2, V^3 effective pair interactions



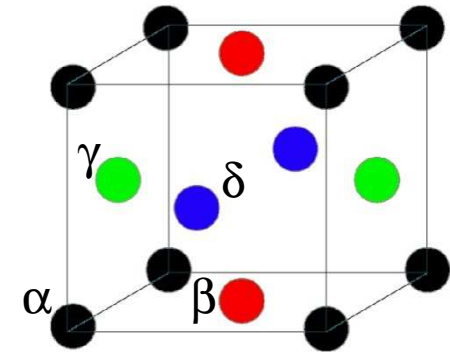
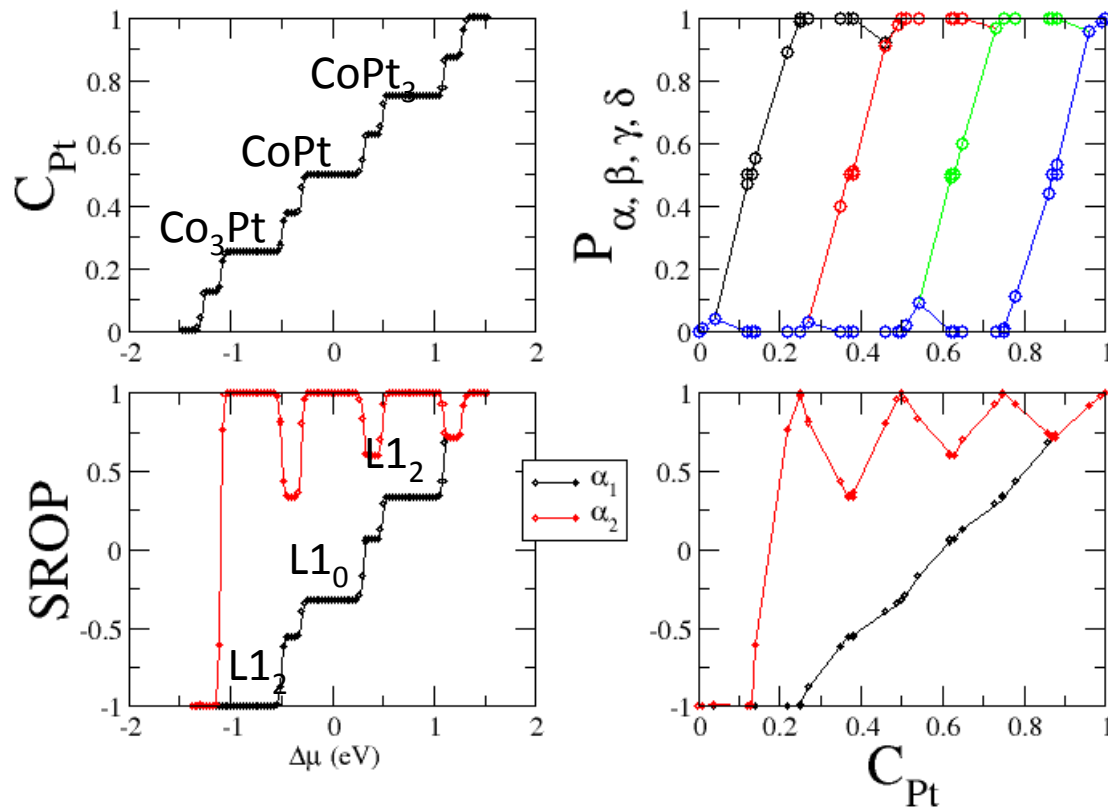
Canonical Monte Carlo Simulations

Bulk $\text{Co}_{1-c}\text{Pt}_c$ Isotherms

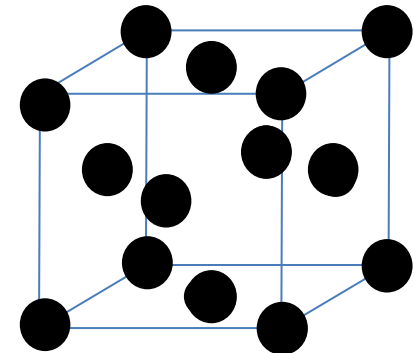
Semi-Grand Canonical Monte Carlo

T = 100 K

TBIM with V^1, V^2, V^3 effective pair interactions

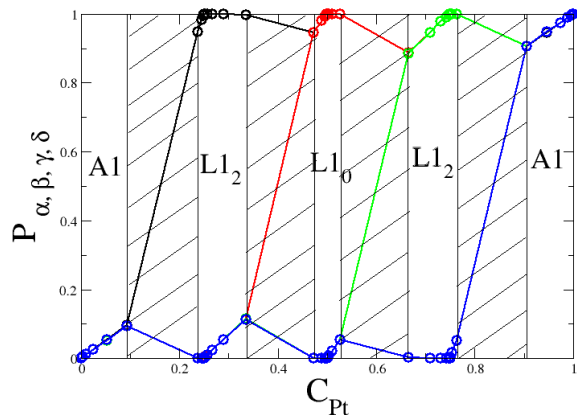


Sublattices in FCC

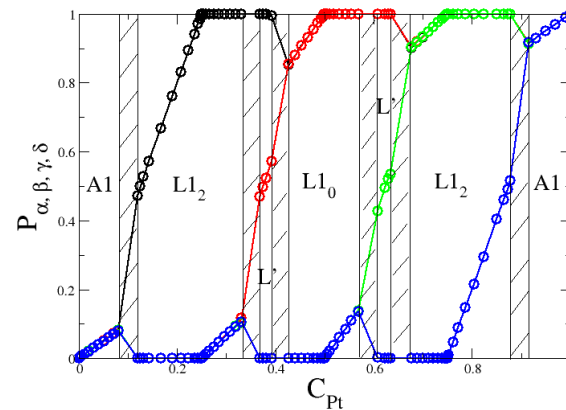


TBIM V^1, V^2

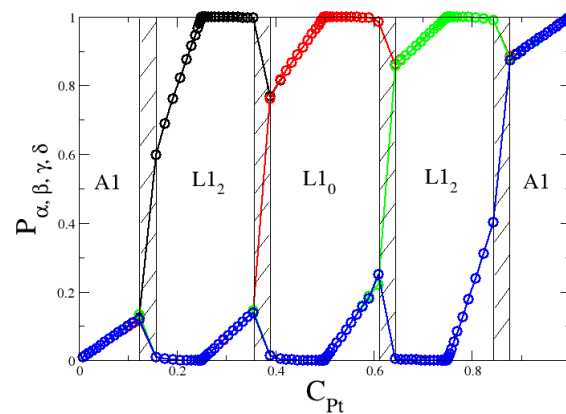
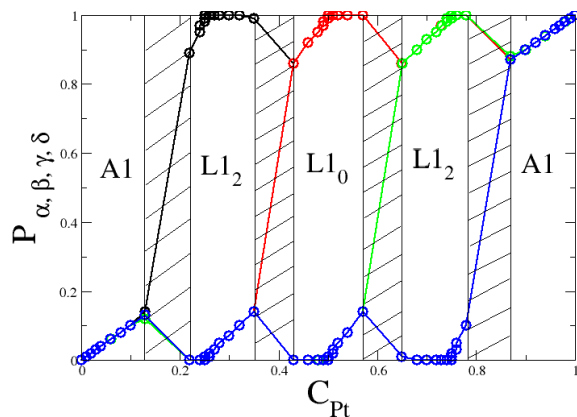
T = 300 K



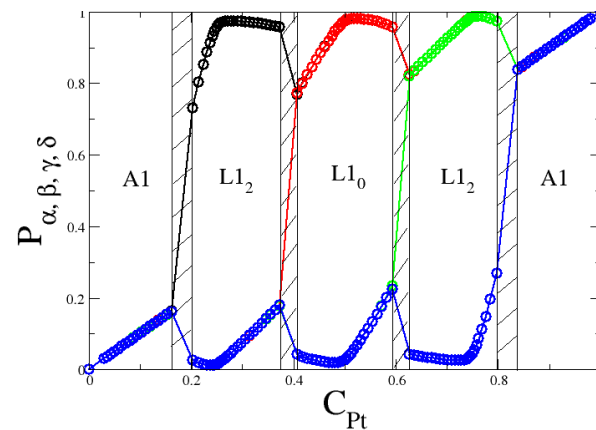
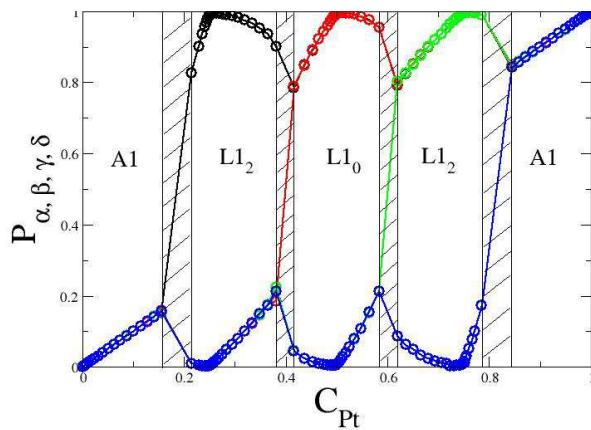
TBIM V^1, V^2, V^3



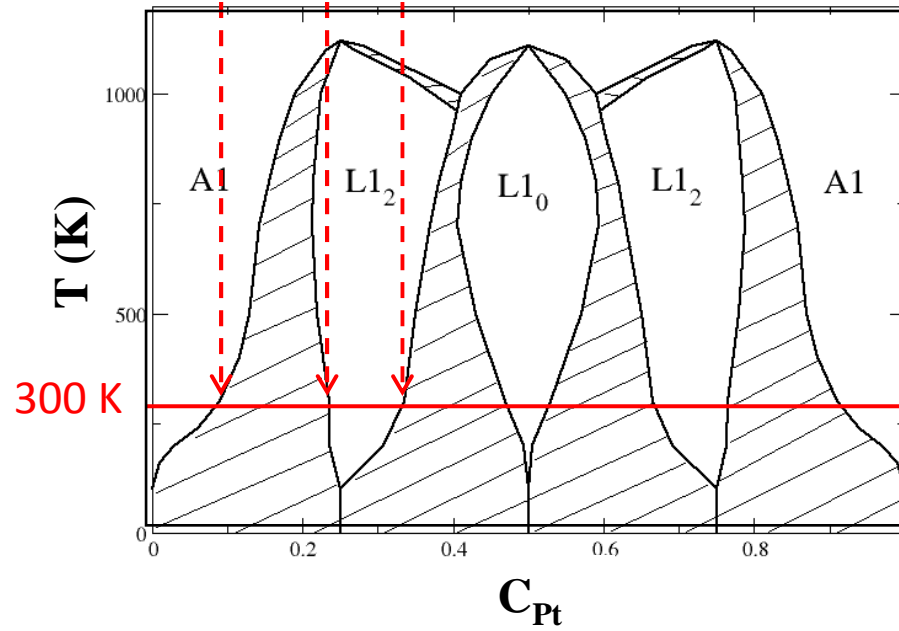
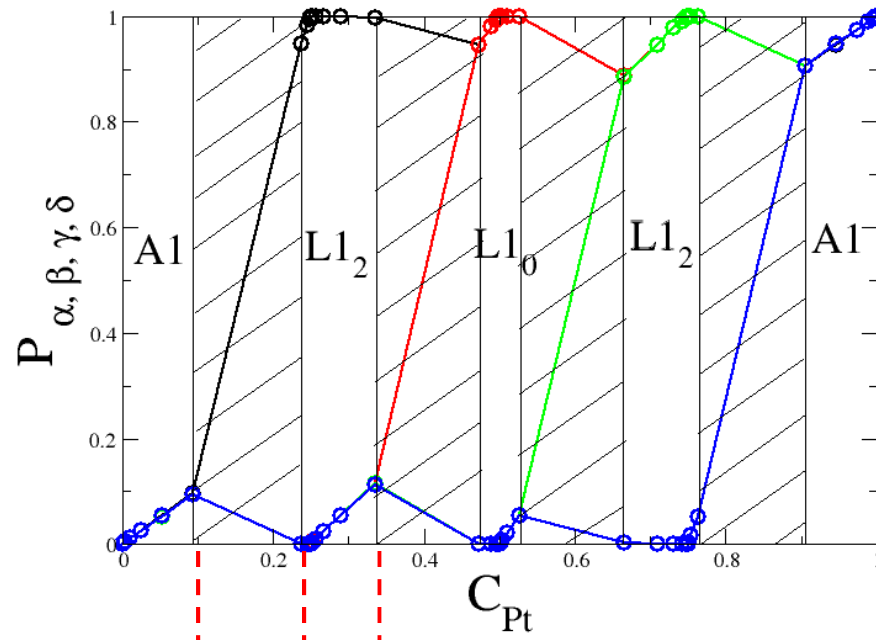
T = 500 K



T = 800 K

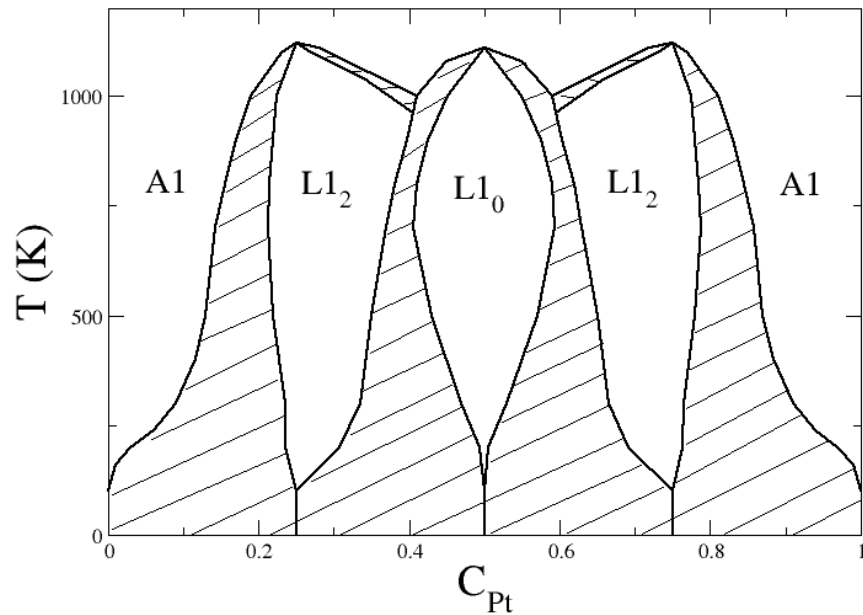


T = 300 K

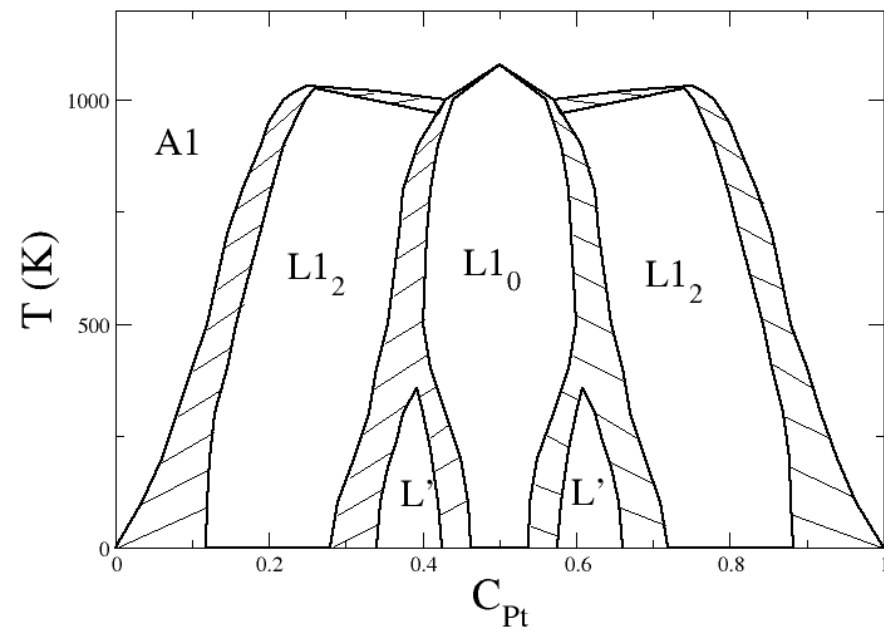


TBIM $\text{Co}_{1-c}\text{-Pt}_c$ Bulk Phase Diagram

V^1, V^2 effective pair interactions



V^1, V^2, V^3 effective pair interactions

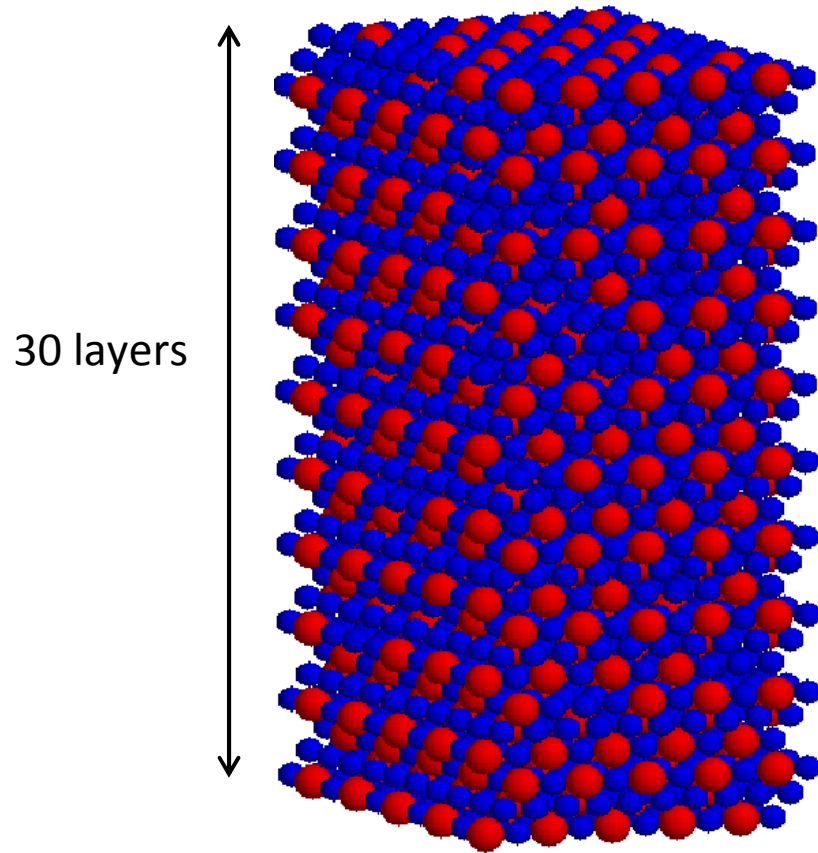


- TBIM Co-Pt systems:
- Bulk
 - Surfaces
 - Clusters

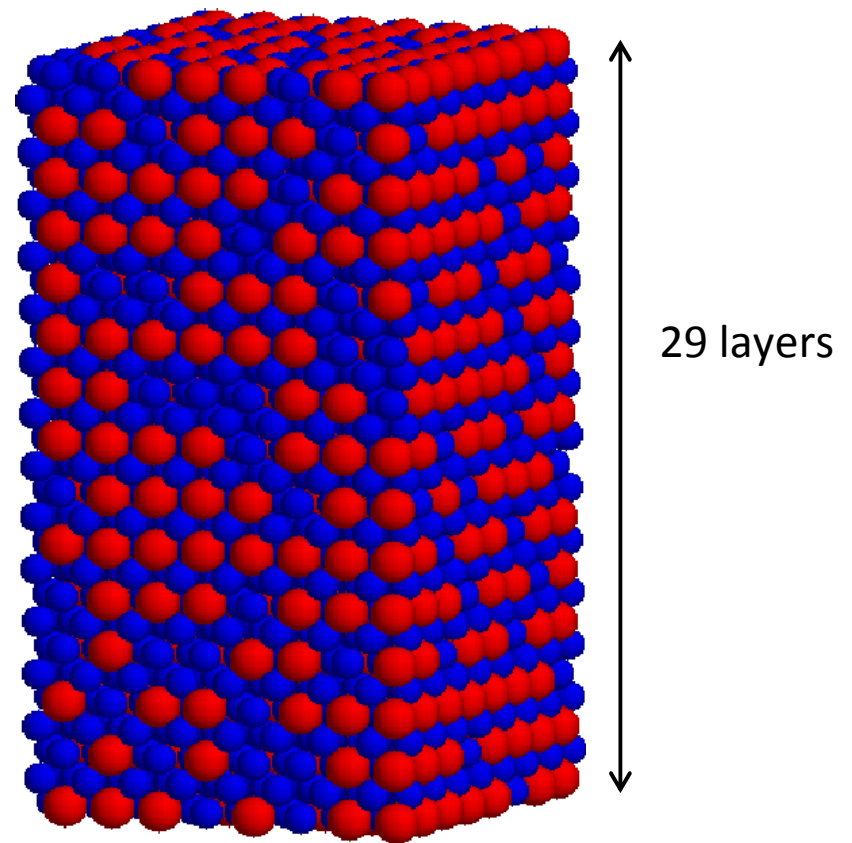
Rigid lattice model

Co_{1-c}-Pt_c (111) and (100) Surfaces

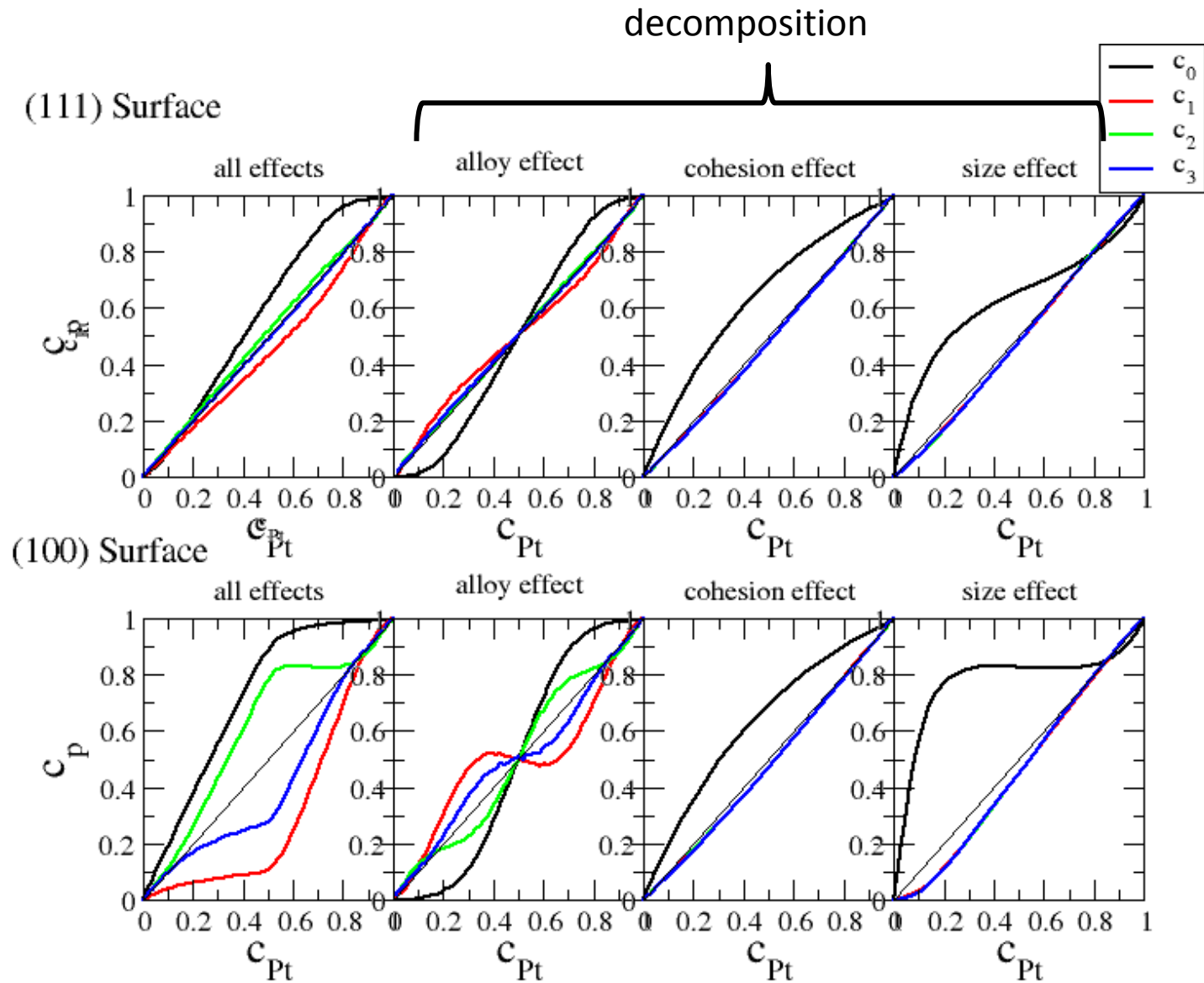
(111)



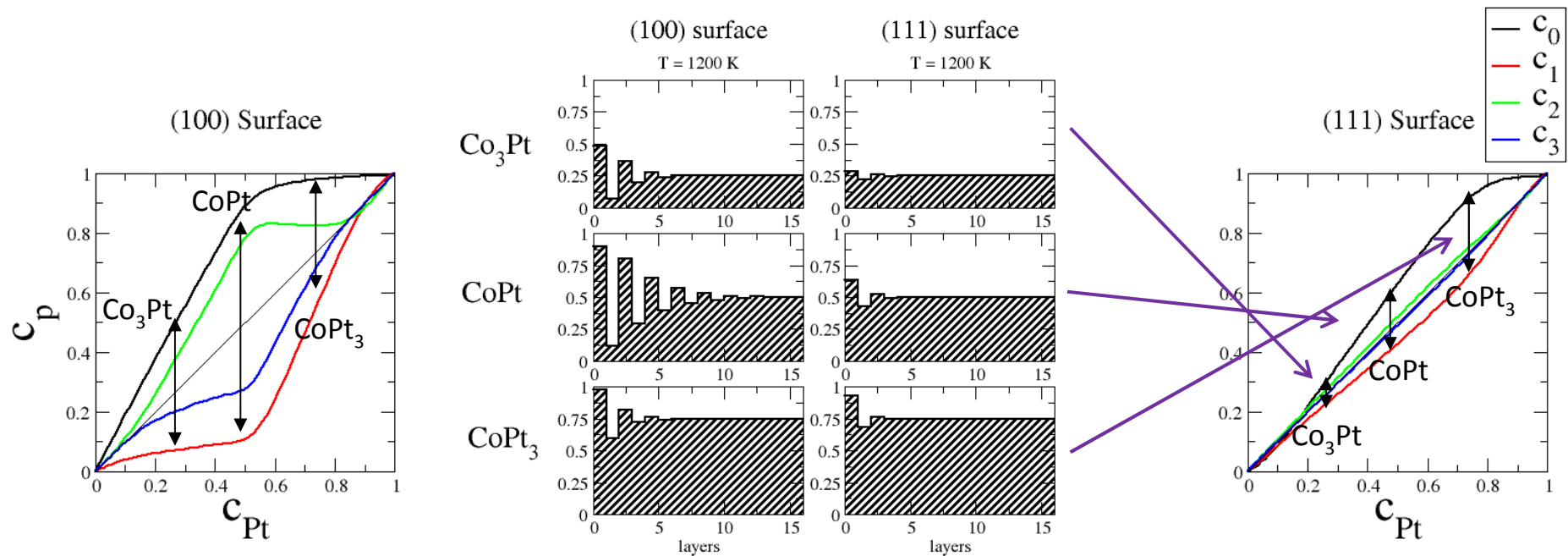
(100)



Surface Segregation Driving Forces @ 1200 K



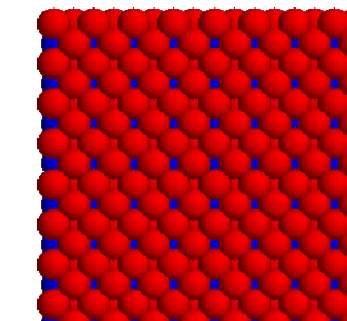
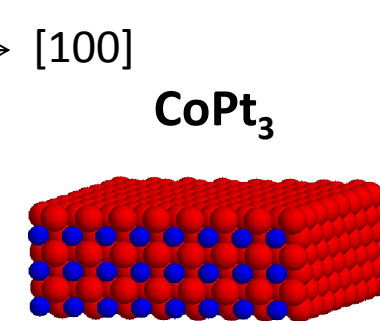
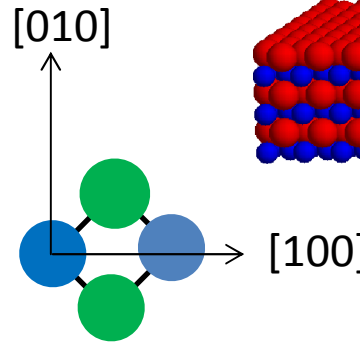
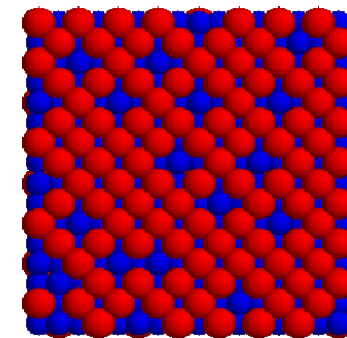
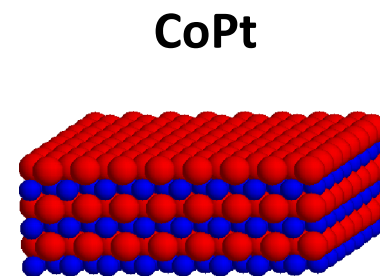
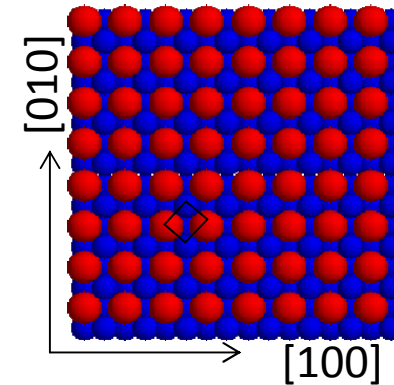
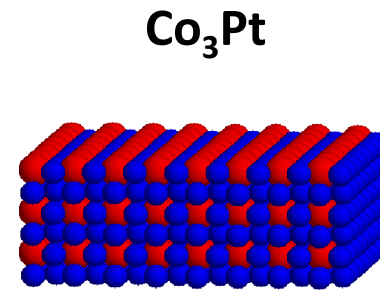
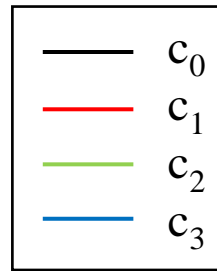
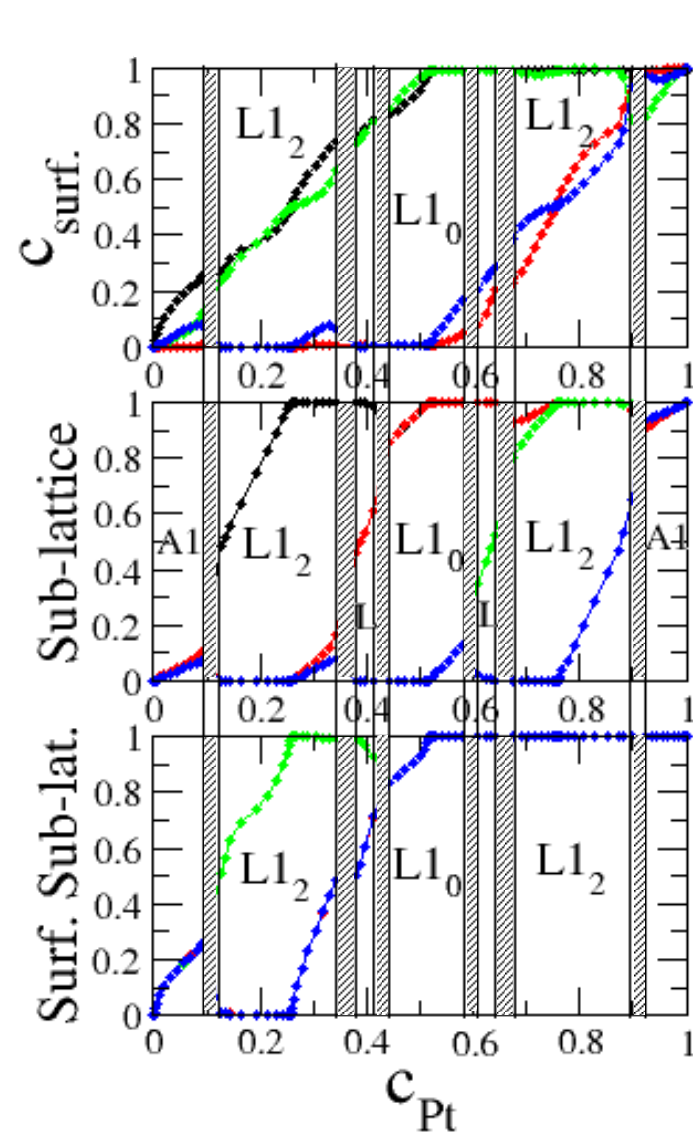
Segregation profiles at $\text{Co}_{1-c}\text{-Pt}_c$ surfaces @ 1200 K



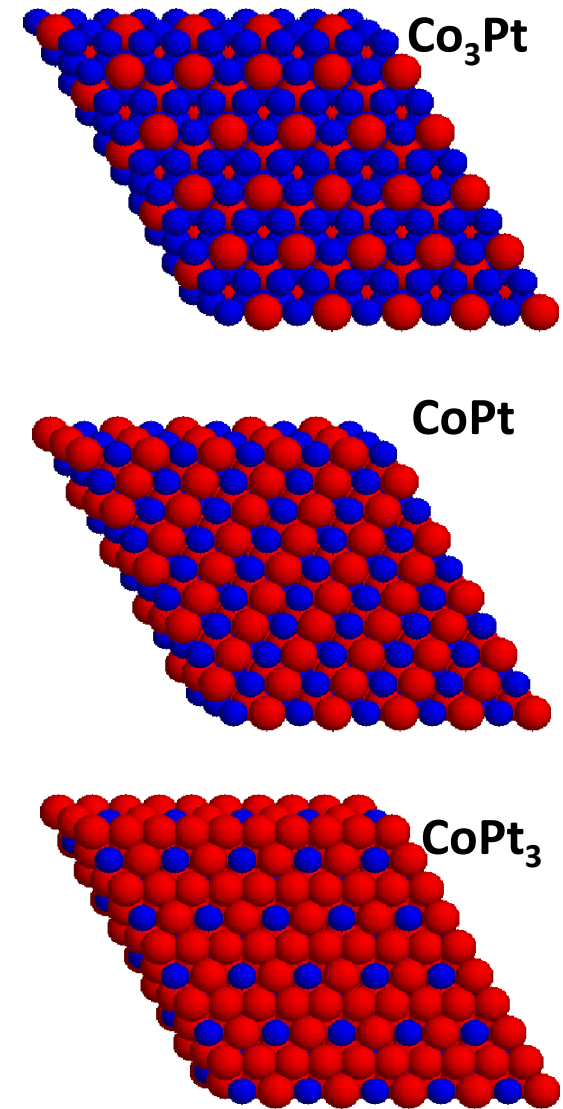
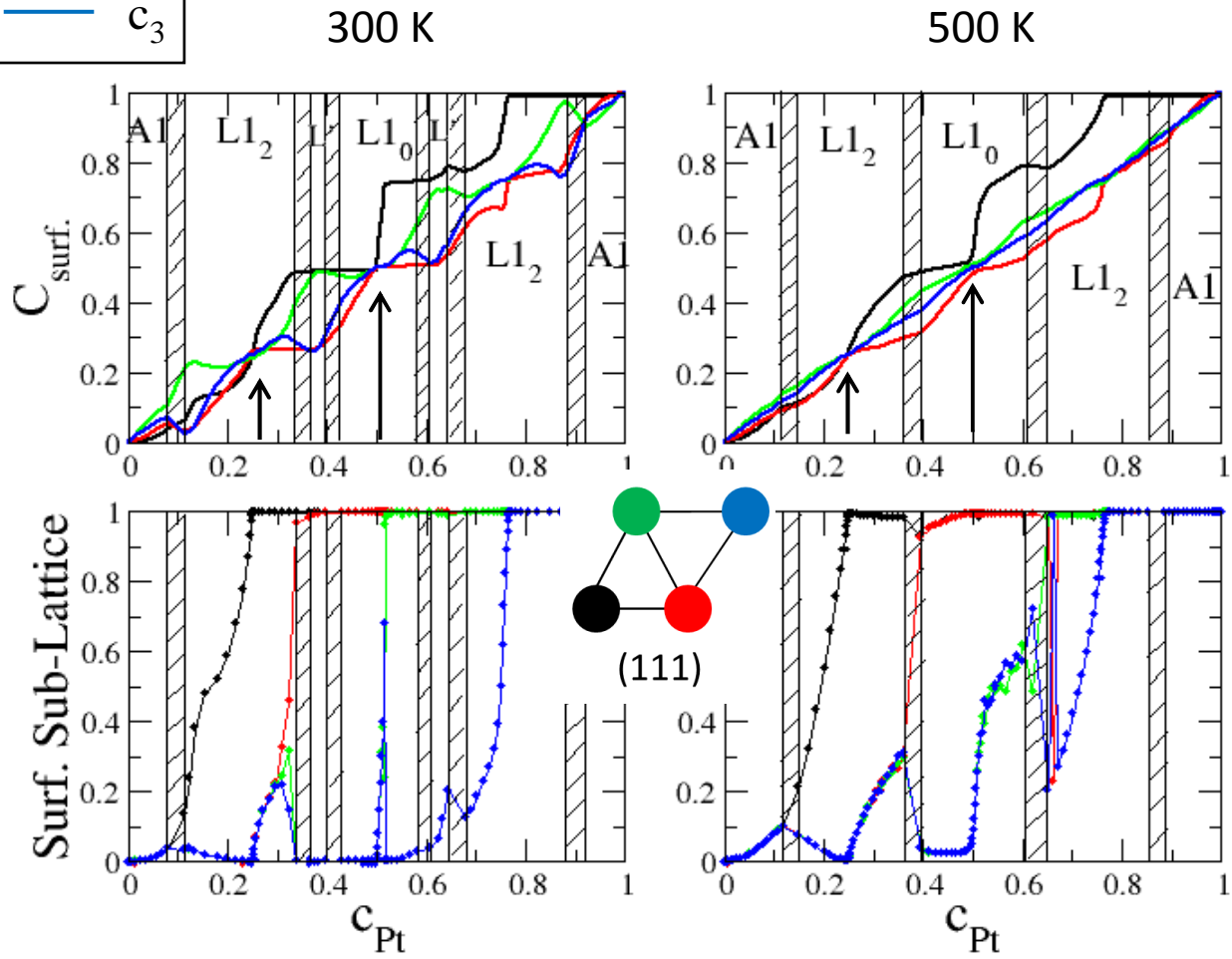
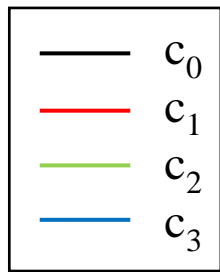
Oscillating profiles with Pt surface segregation, in agreement with experimental results:

- **CoPt_3 (100)** : U. Bardi, A. Atrei, G. Rovida, E. Zanazzi, P. Ross, **Surf. Sci.** **211/212**, 441 (1989).
(111) : Y. Gauthier, R. Baudoing-Savois, J. Bugnard, U. Bardi, A. Atrei, **Surf. Sci.** **276**, 1 (1992).
- **Co_3Pt (100)** : Y. Gauthier, P. Dolle, R. Baudoing-Savois, M. Schmid, P. Varga, **Surf. Sci.** **396**, 137 (1998).
(111) : Y. Gauthier, R. Baudoing-Savois, J. Bugnard, M. Schmid, P. Varga, **Surf. Sci.** **466**, 155 (2000).

(100) Surface Segregation Isotherm @ 300 K



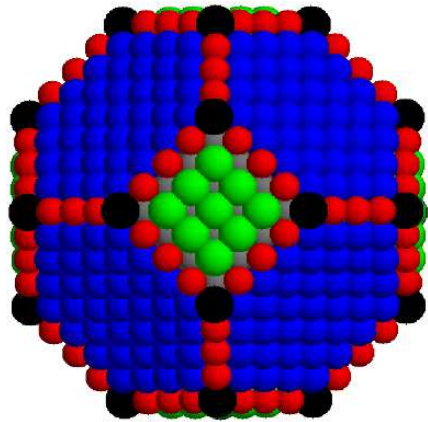
(111) Surface Segregation Isotherm @ 300 K



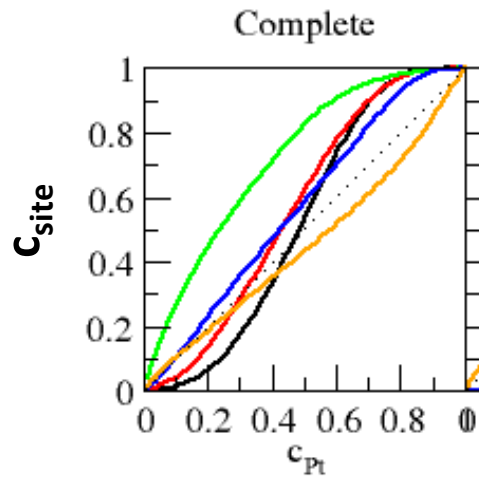
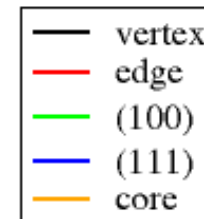
- TBIM Co-Pt systems:
- Bulk
 - Surfaces
 - Clusters

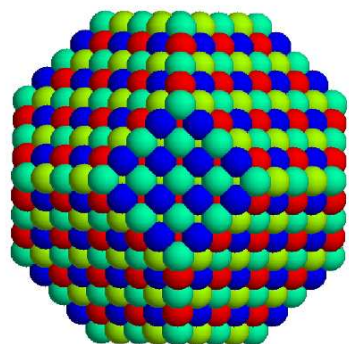
Rigid lattice model

TBIM Cluster Surface Segregation



1289-TOh Cluster @ 1200K

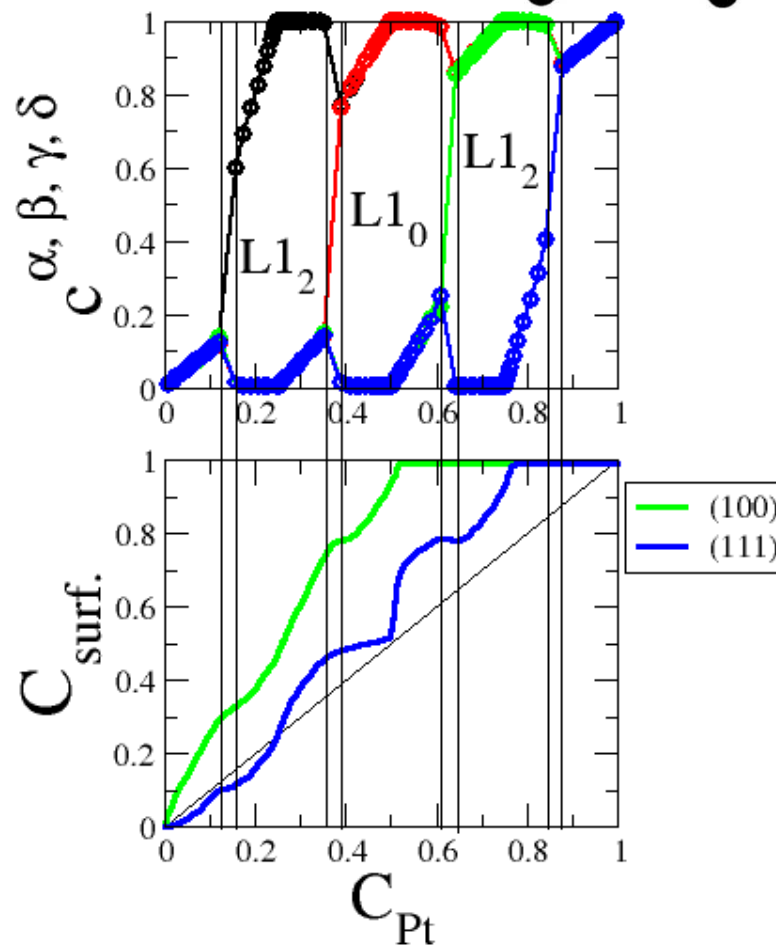
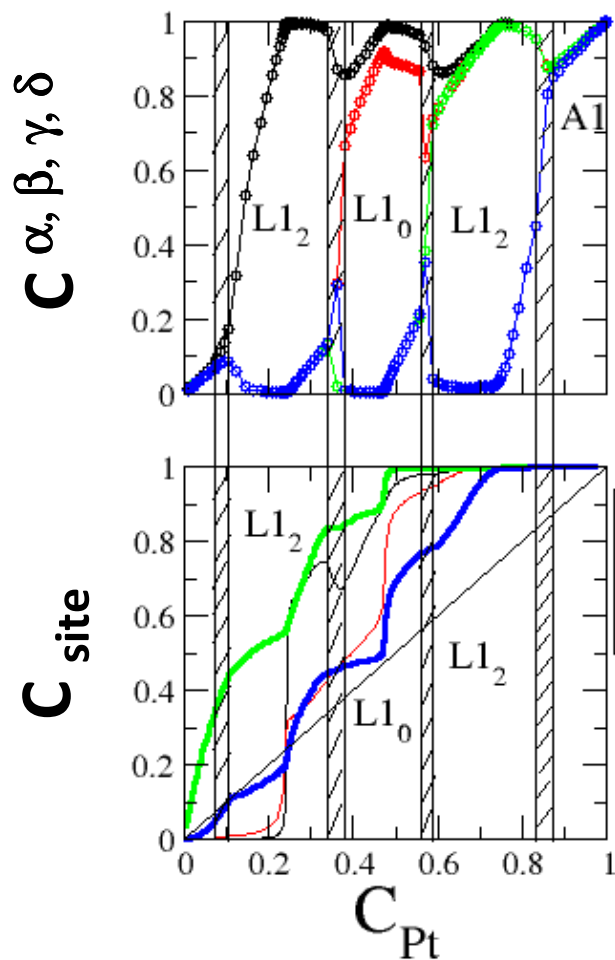
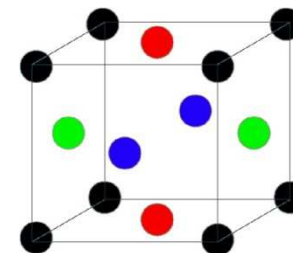




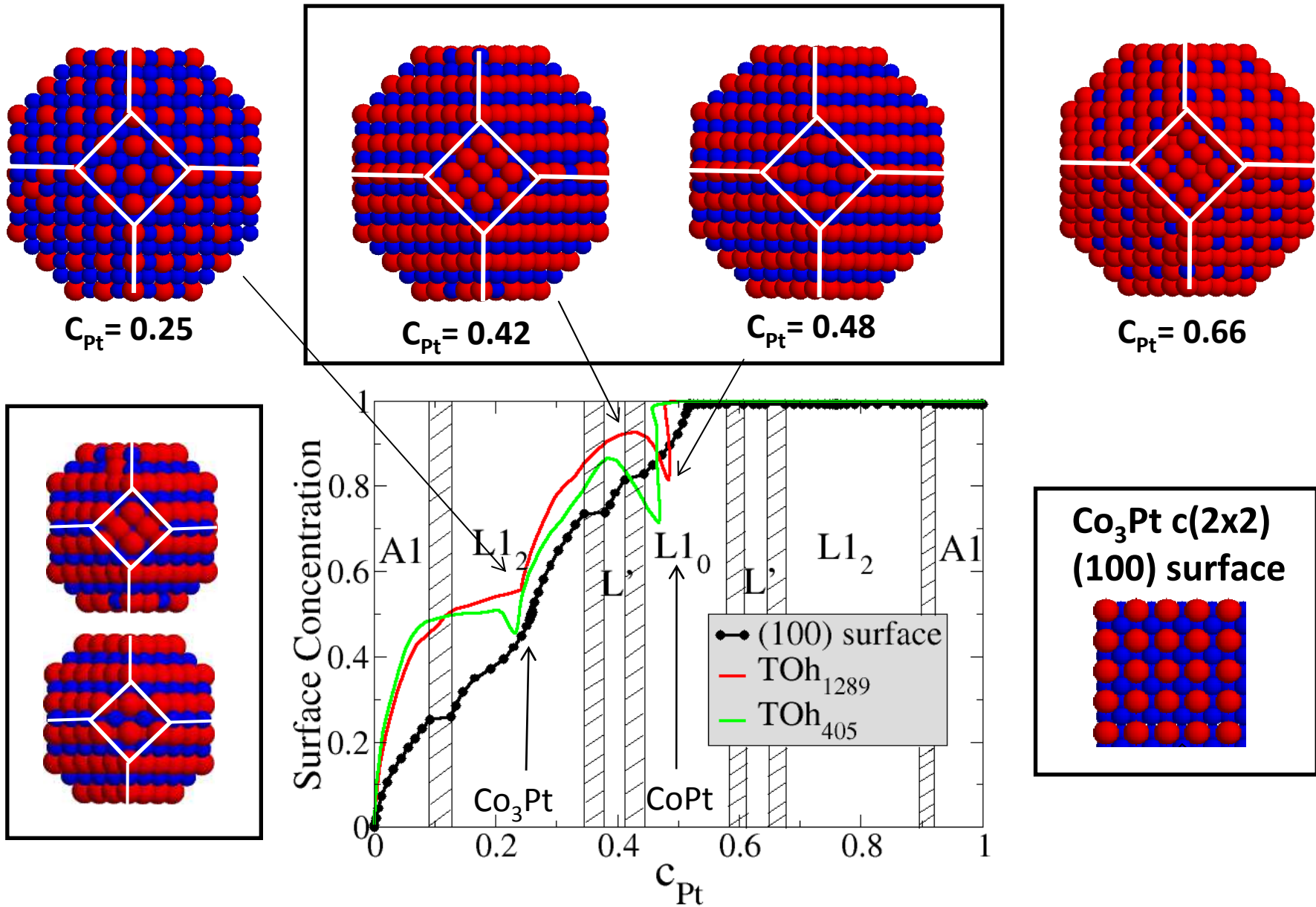
TBIM Cluster Order/Segregation

T = 500 K

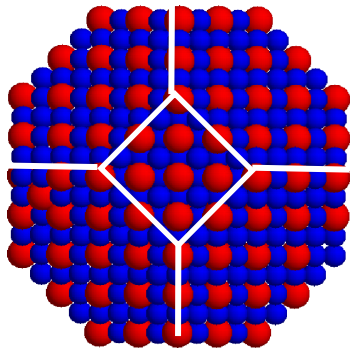
TOh₁₂₈₉



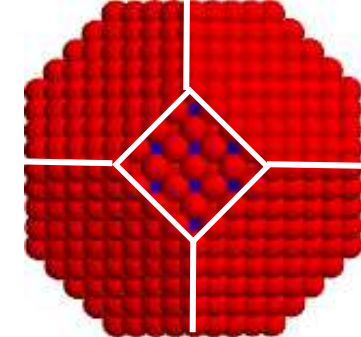
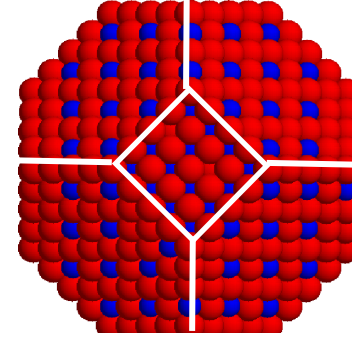
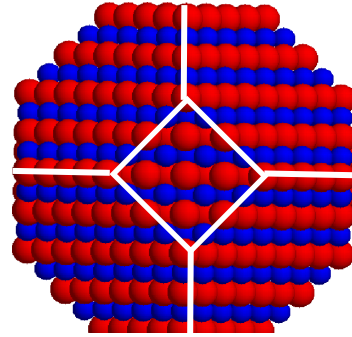
(100) Cluster Facets / (100) surface @ 300 K



(111) Cluster Facets / (111) Surface @ 300 K

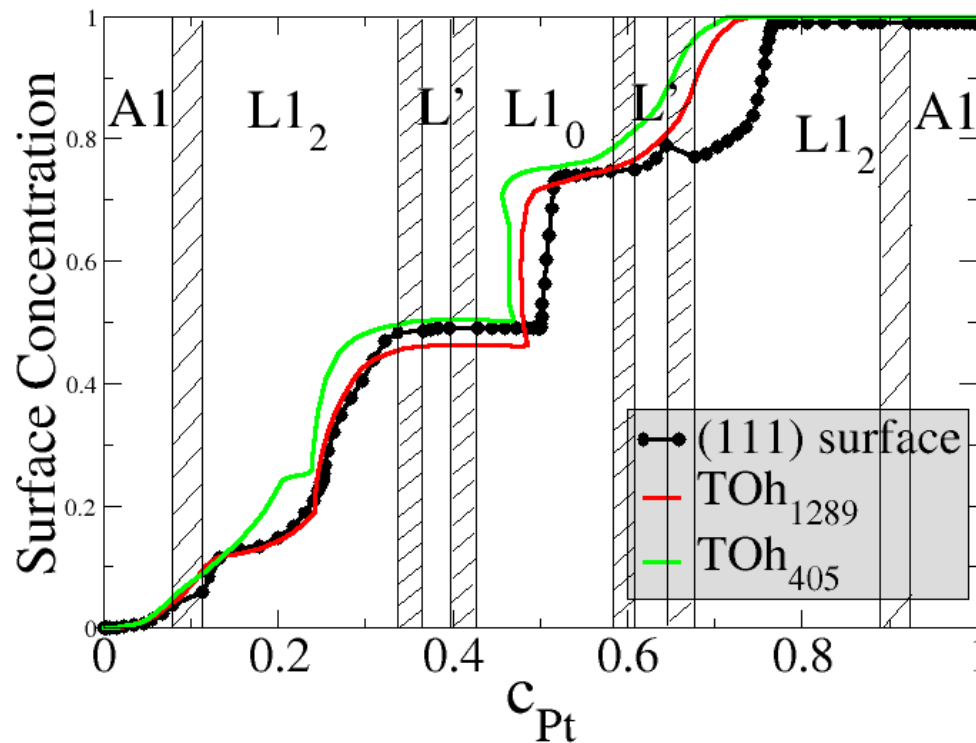
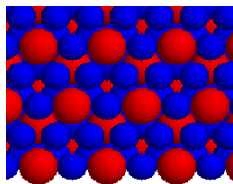


$C_{Pt} = 0.25$

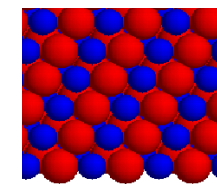


$C_{Pt} = 0.75$

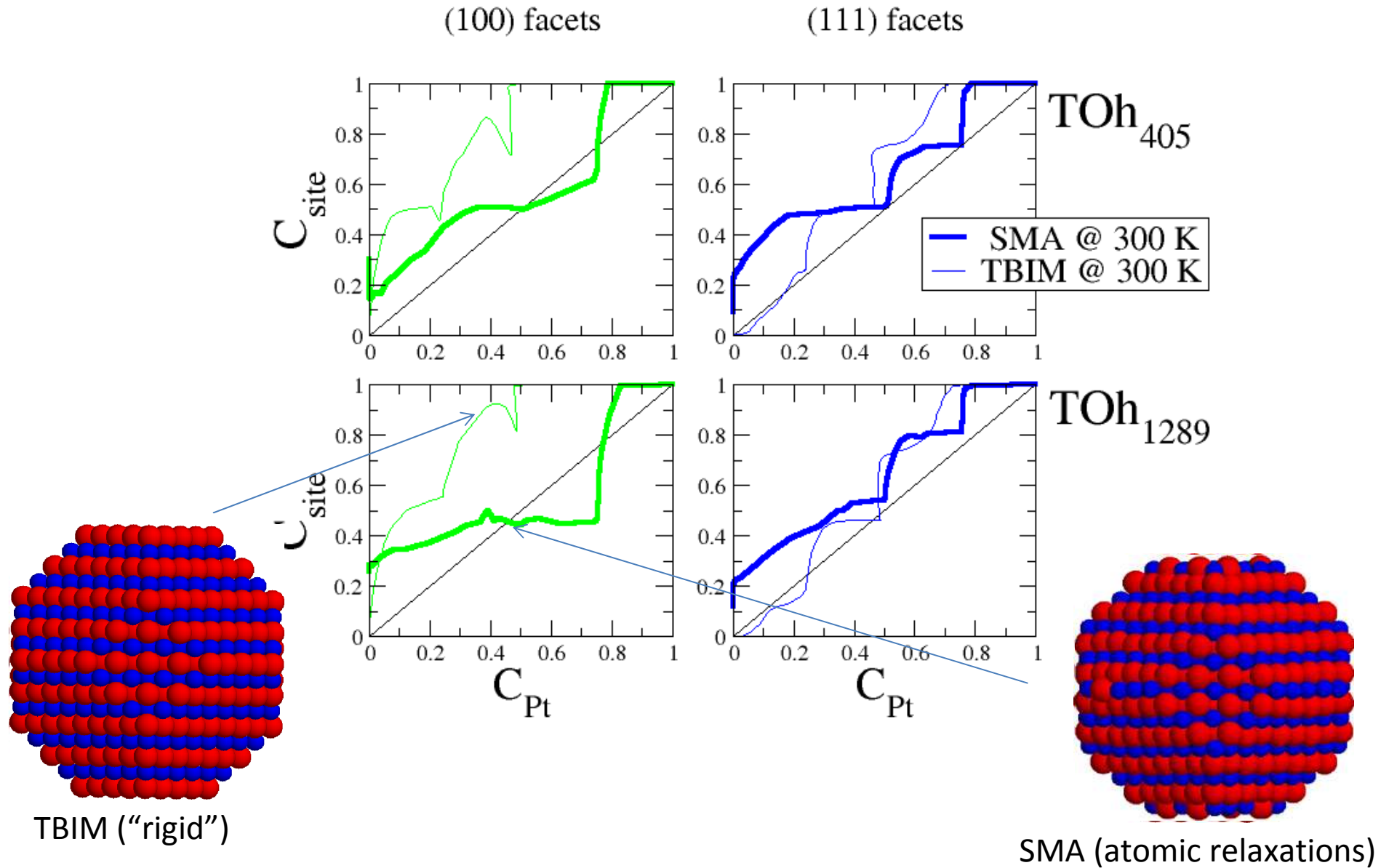
**Co₃Pt c(2x2)
(111)**



**CoPt (2x1)
(111)**



Co_{1-c}-Pt_c nanoalloys isotherms TBIM / SMA



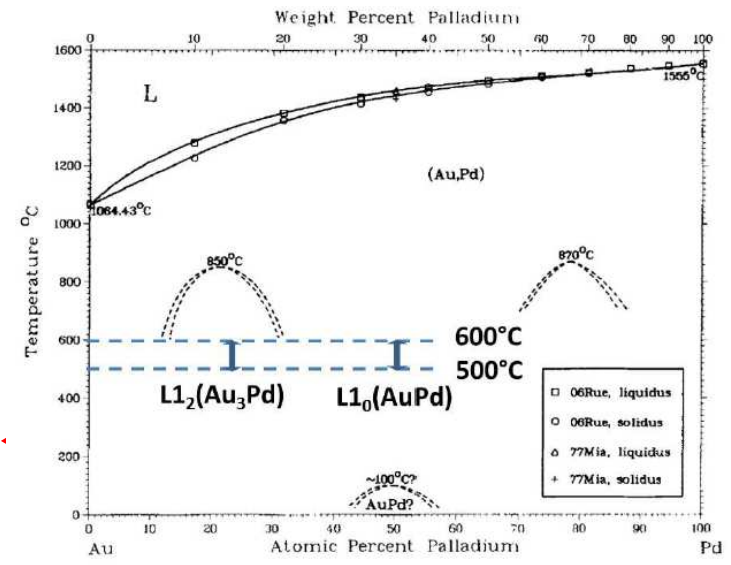
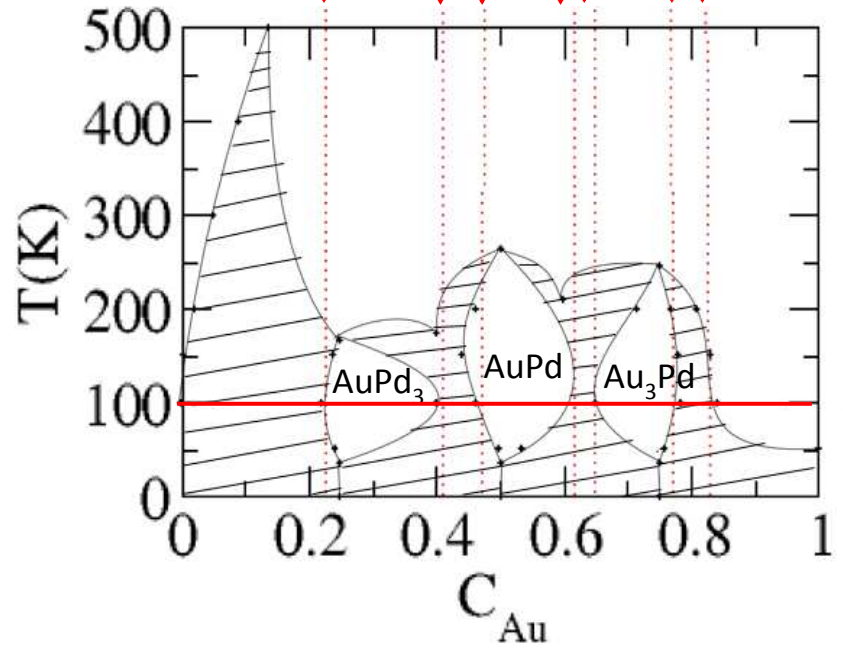
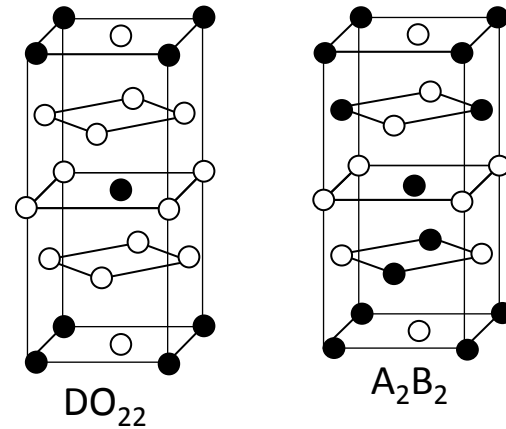
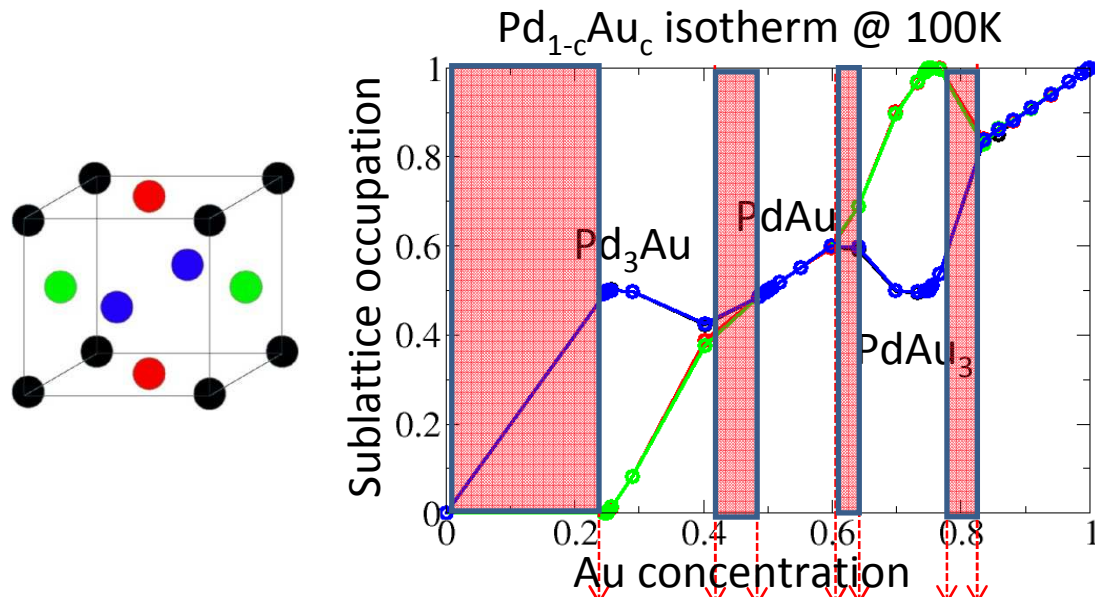
Conclusions sur Nanoalliages Co-Pt :

- $\text{Co}_{1-c}\text{-Pt}_c$ nanoalloys have been studied in the whole range of concentration and temperature in order to describe nanoalloys phase diagrams.
- Pt segregates at high temperature in the disordered state.
- Pt segregation is modified by the core ordering at low temperature:
 - cluster facets reproduce (100) and (111) surface segregation
 - (100) facets segregation compete with the L1_0 ordered phase.
- Atomic relaxations, in particular the tetragonalisation of the L1_0 phase change surface segregation on (100) facets.

Exemple n° 2 : Pd-Au

- ✓ Pd-Au bulk phase diagram
- ✓ Which motif Ih/Dh/TOh at OK ?
- ✓ Chemical ordering/surface segregation

Pd-Au bulk phase diagram: from Monte Carlo isotherms

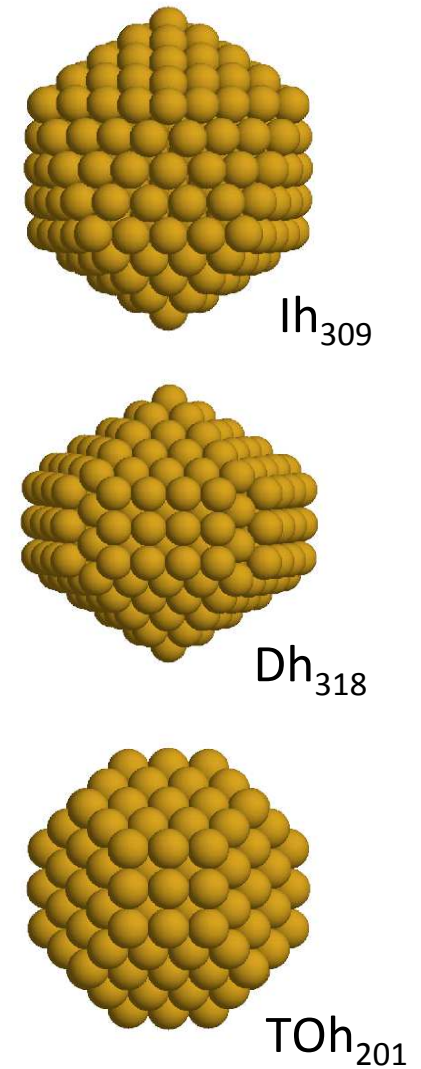
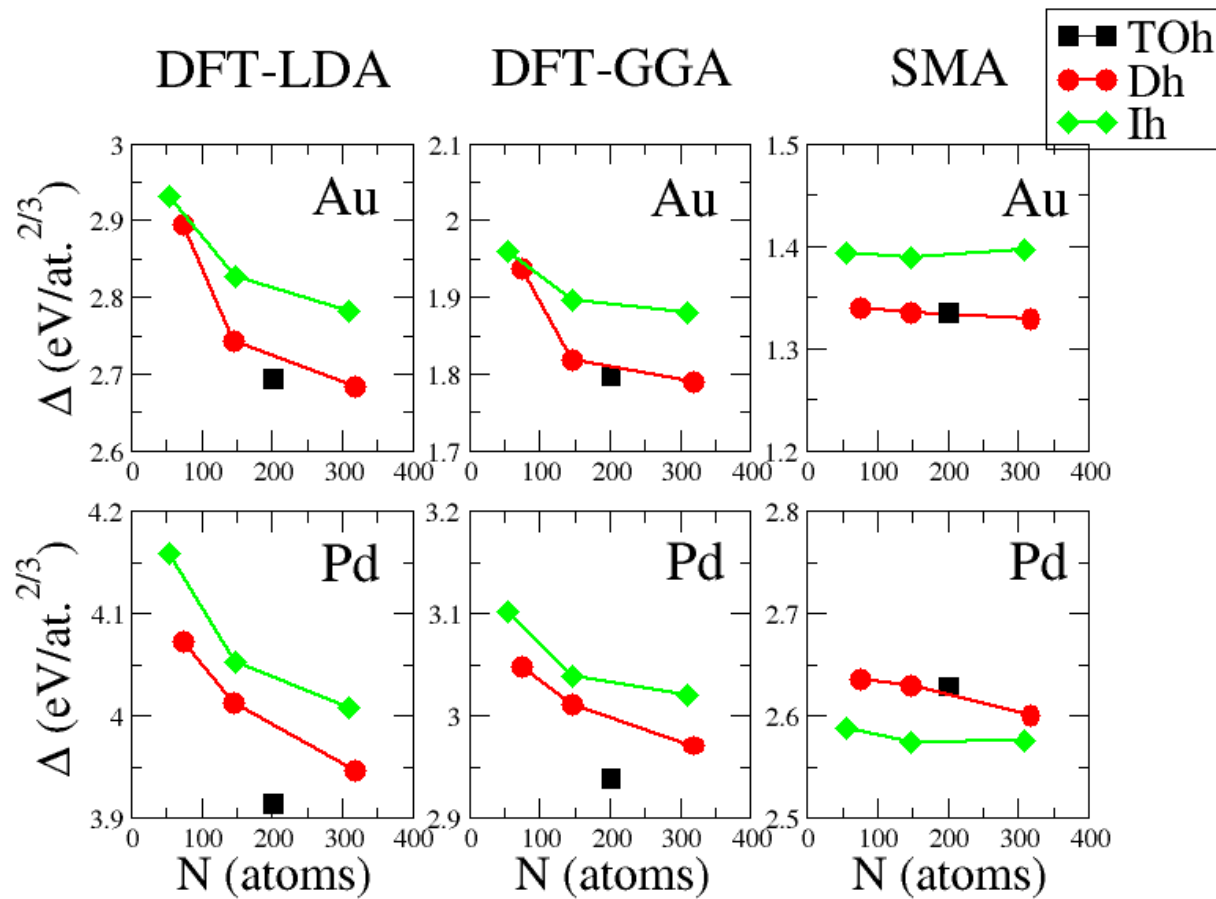


Okamoto et al. (1965)
N.T. Nguyen, PhD (2015)

- ✓ Pd-Au bulk phase diagram
- ✓ Which motif Ih/Dh/TOh at OK ?
- ✓ Chemical ordering/surface segregation

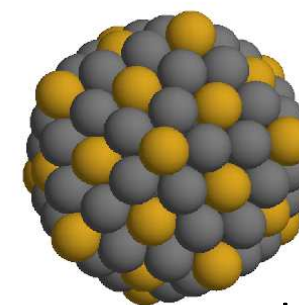
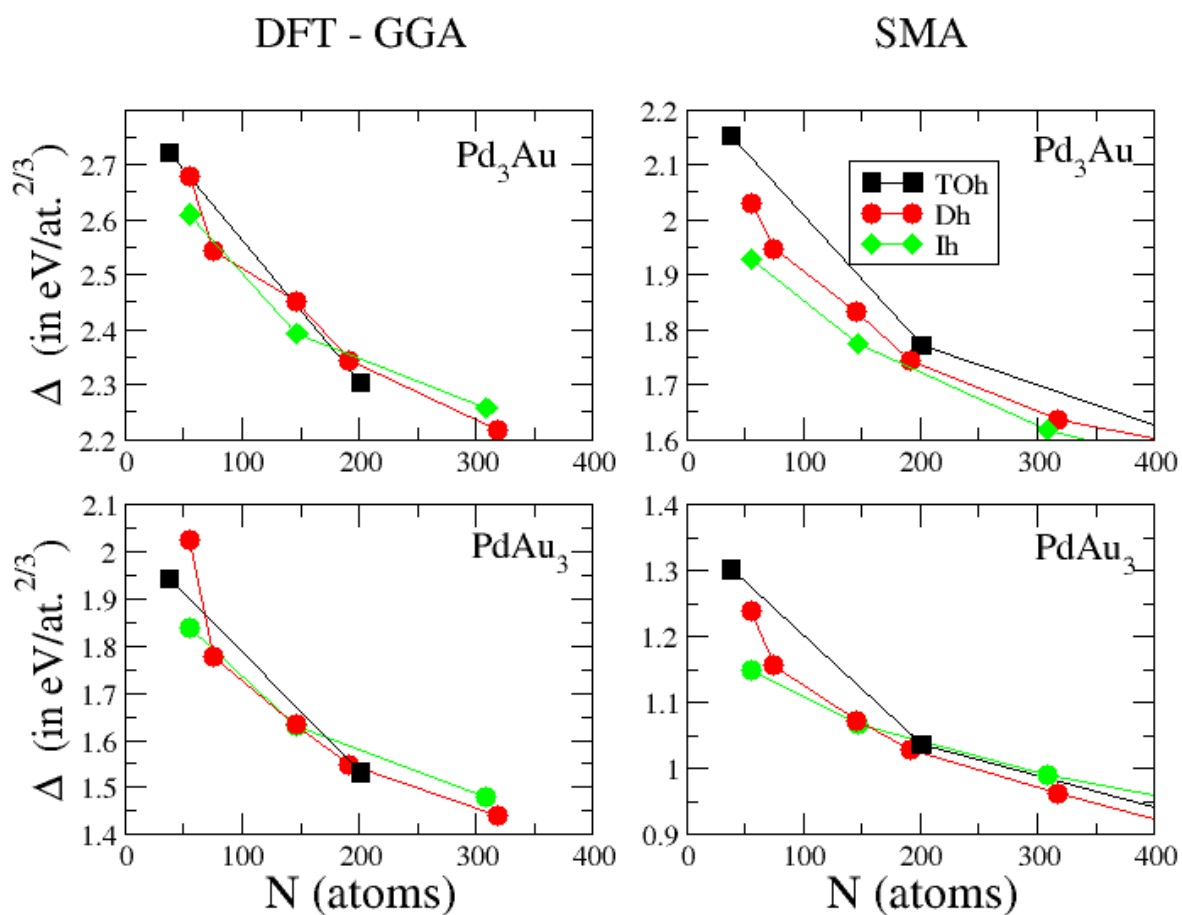
Au and Pd clusters of less than 300 atoms: comparison between DFT and SMA calculations

$$\Delta = (E_N - N E^{coh})/N^{2/3}$$

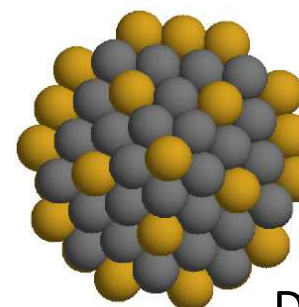


Pd-Au nanoalloys of less than 300 atoms: comparison between DFT and SMA calculations

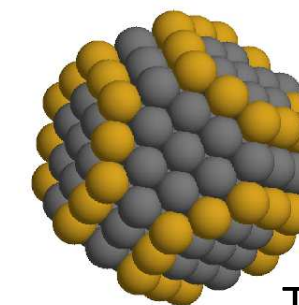
$$\Delta = (E_N - N_{Au} E^{Au} - N_{Pd} E^{Pd})^{2/3}$$



Ih₁₄₇

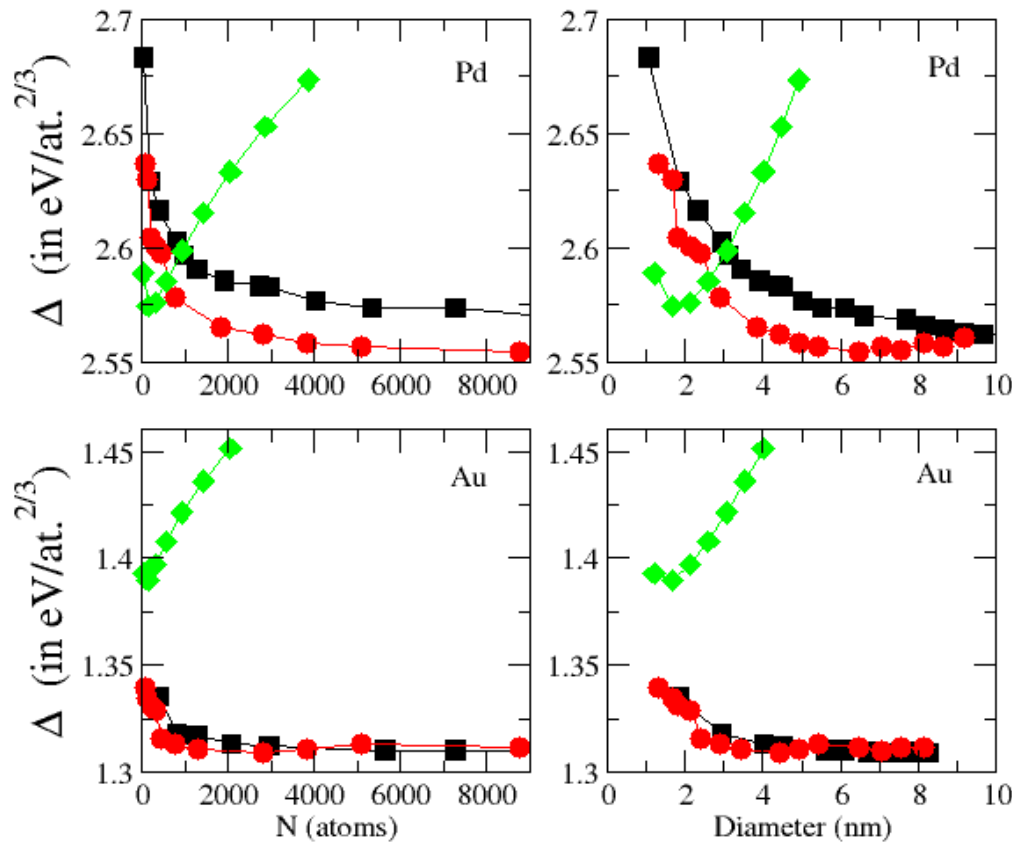


Dh₁₉₂



TOh₂₀₁

Crossover among structural motifs of Pd-Au nanoalloys within the SMA potential



Palladium clusters

- Ih stable < 3nm
- Dh stable < 9 nm
- TOh > 9 nm

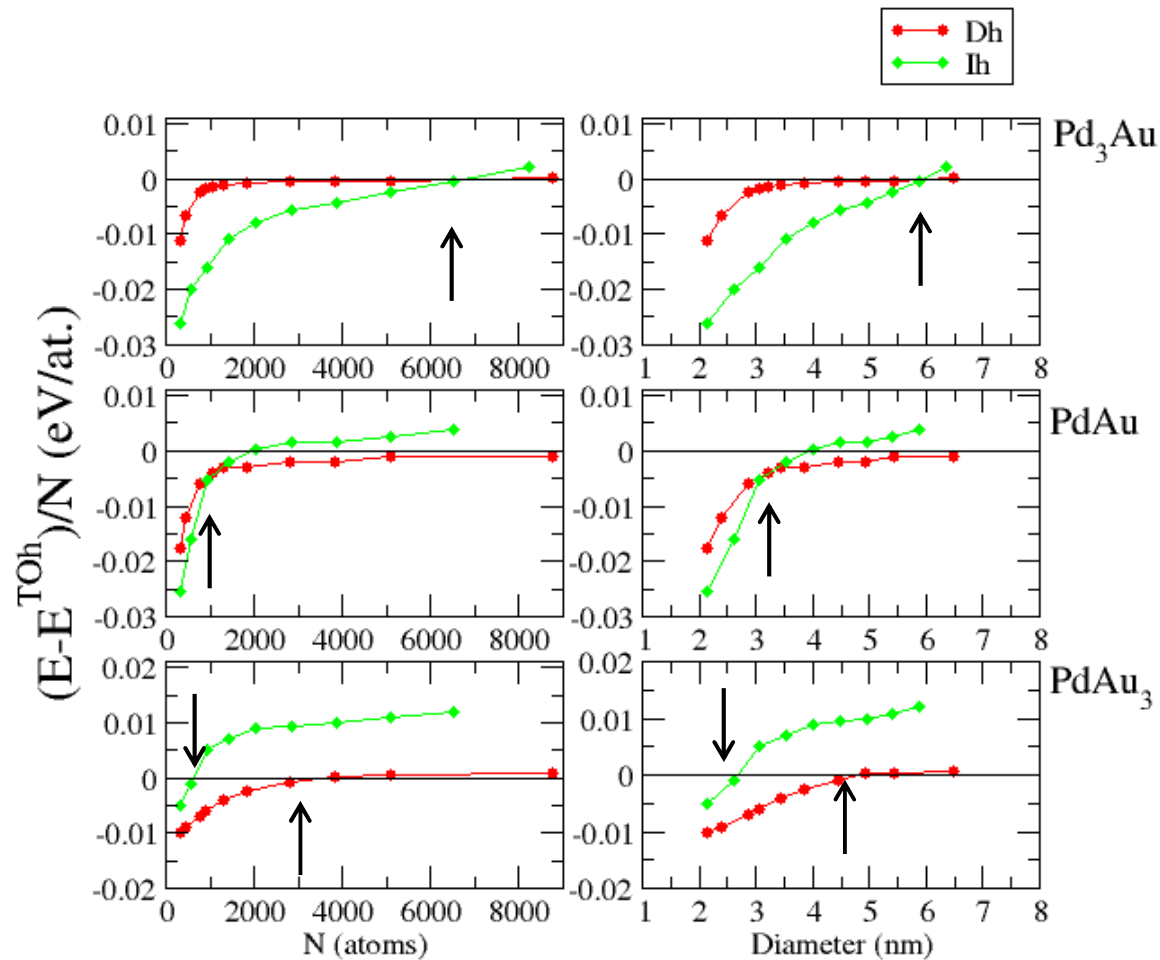
Gold clusters

- Ih unstable
- Dh / TOh stable up to 9 nm

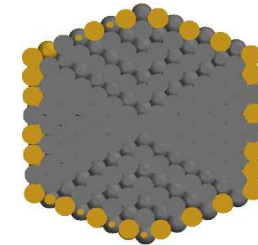
$$N \sim V = \frac{4\pi}{3} R^3 \quad R \sim \left(\frac{N}{4}\right)^{1/3} \quad D = 2R \quad D = \frac{1}{2} \left(\frac{N}{4}\right)^{1/3} \text{ in nm}$$

& 0.25 nm between 2 atoms

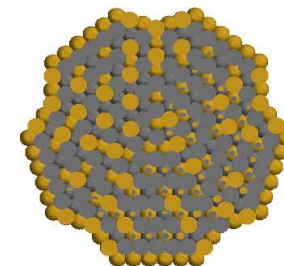
Crossover among structural motifs of Pd-Au nanoalloys within the SMA potential



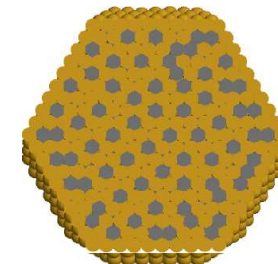
Ih₁₄₁₅ (25% Au)



Dh₂₈₀₂ (50% Au)

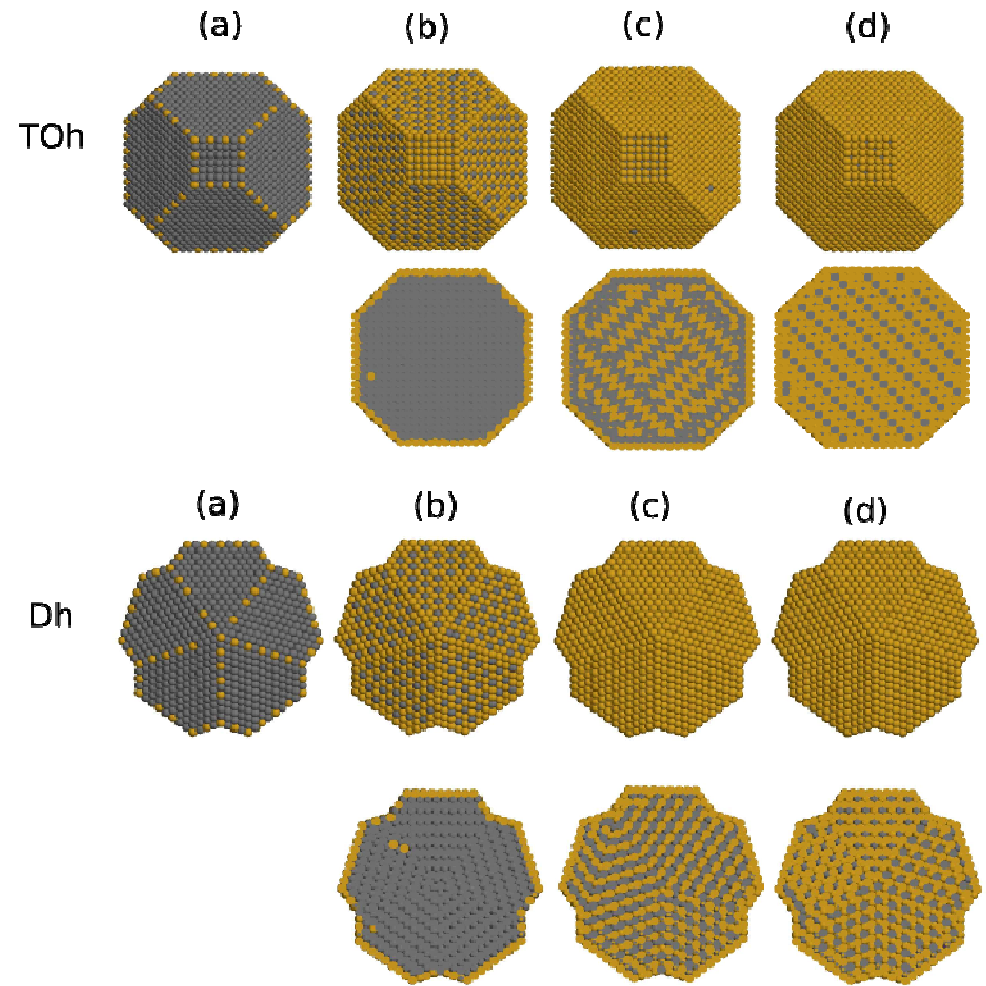
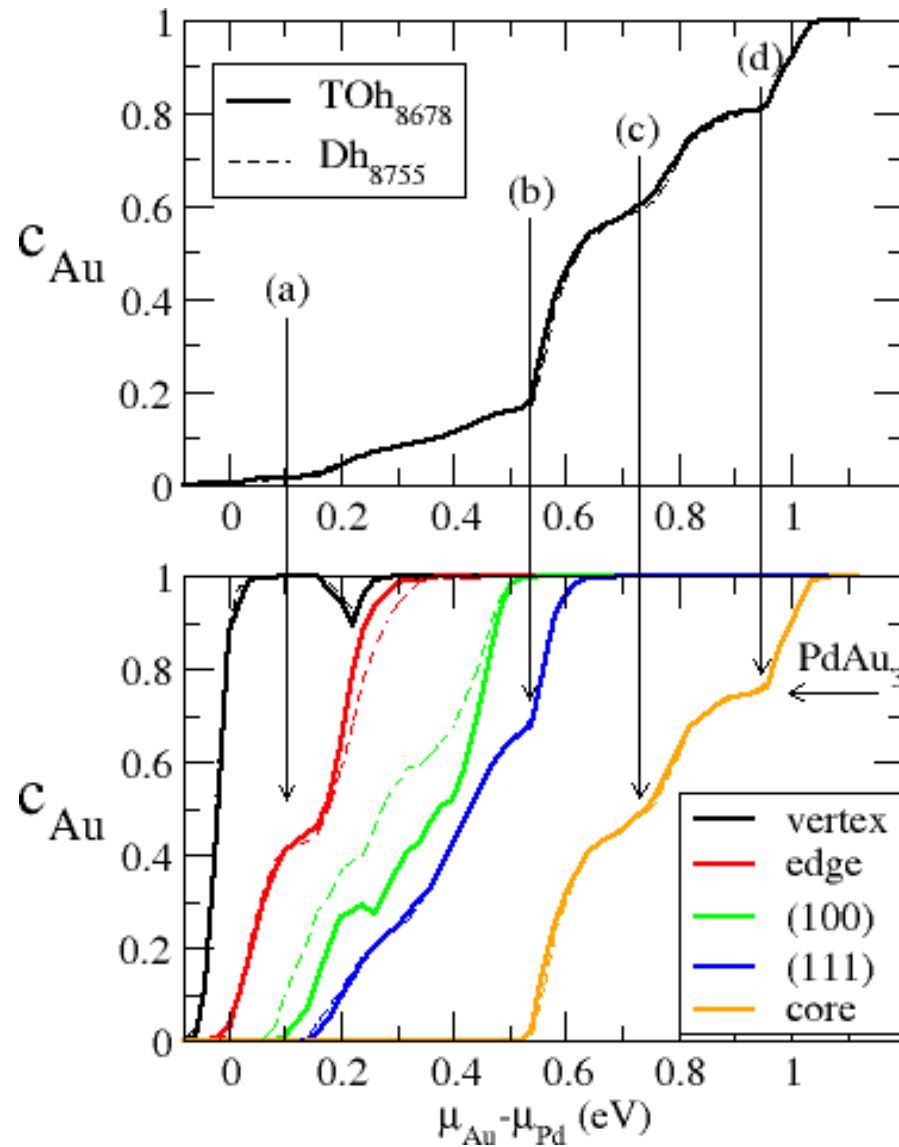


TOh₄₀₃₃ (75% Au)



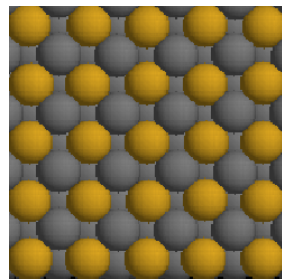
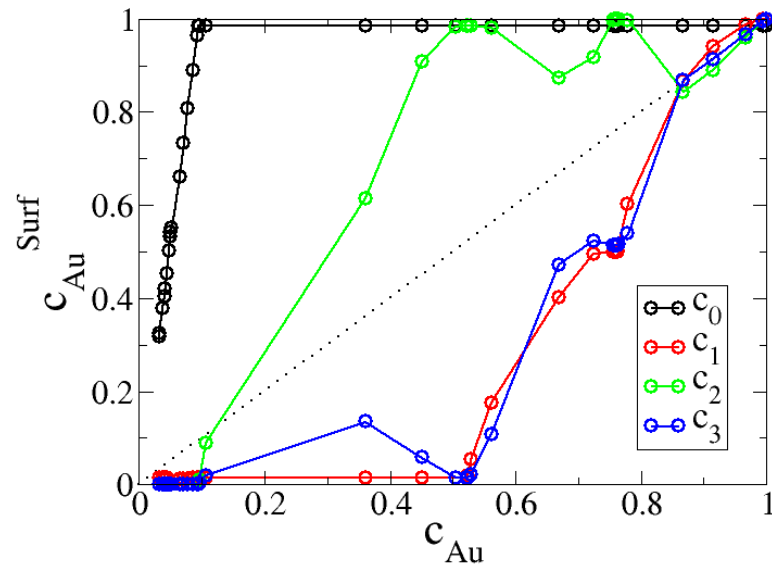
- ✓ Pd-Au bulk phase diagram
- ✓ Which motif $I_h/D_h/T O_h$ at OK ?
- ✓ **Chemical ordering/surface segregation**

Segregation Isotherms for TOh and Dh



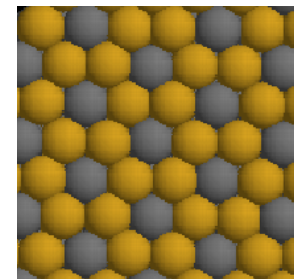
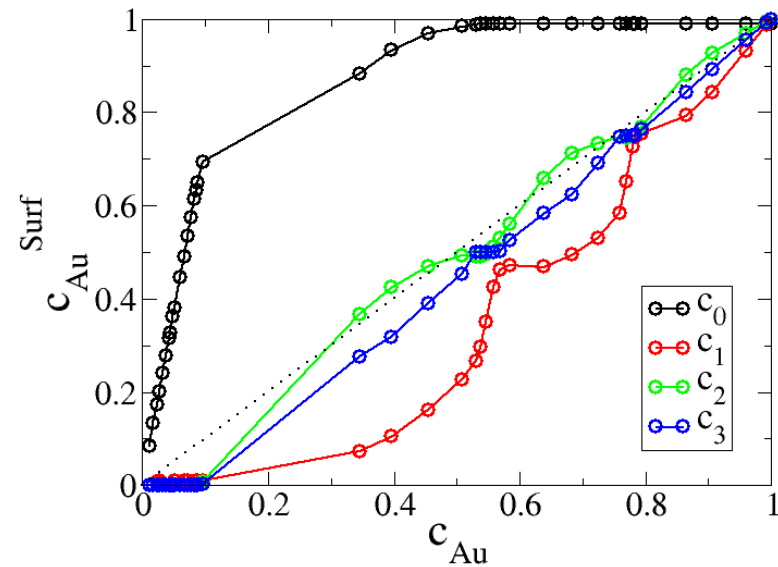
Surfaces reconstruction on (100) and (111) orientations

(100) Pd_{1-c}Au_c Surface



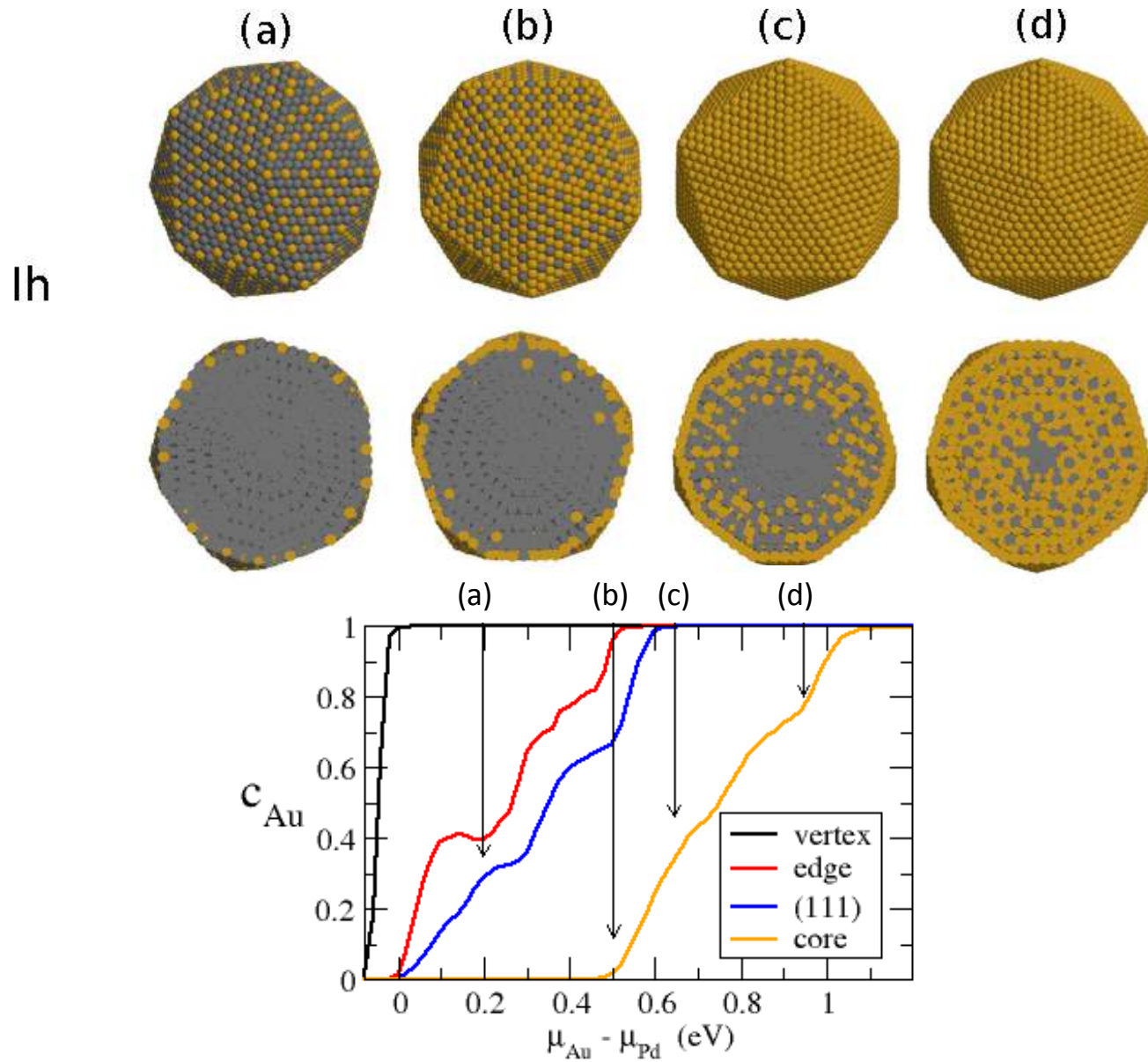
C(2x2) (100)

(111) Pd_{1-c}Au_c Surface

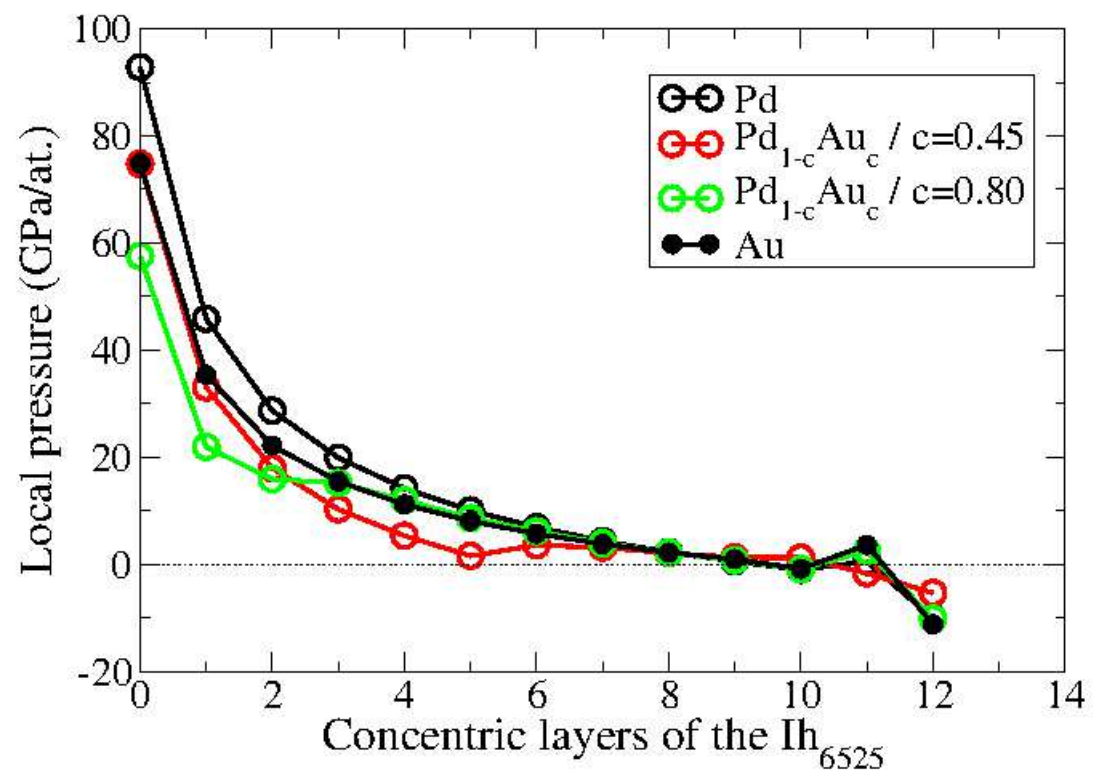
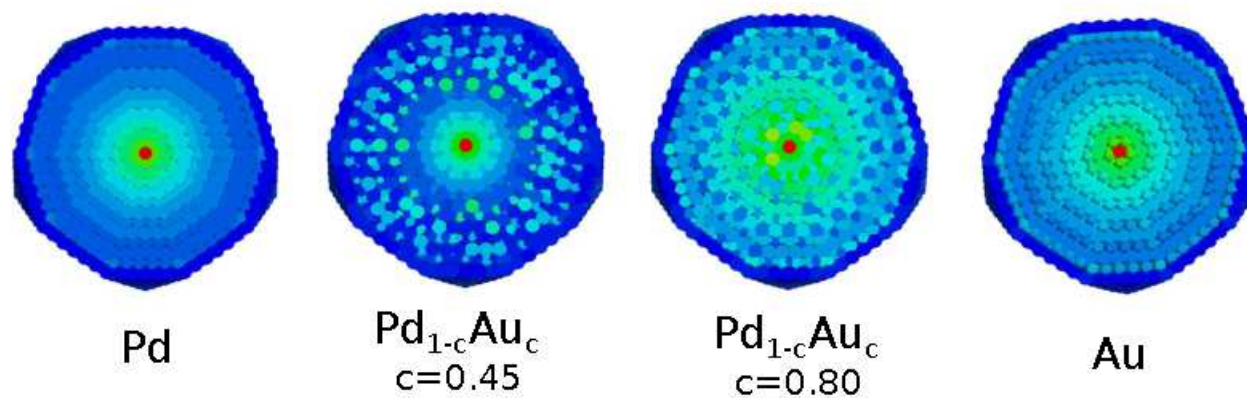


$(\sqrt{3} \times \sqrt{3})R30(111)$

Segregation Isotherms for Ih



Internal Stress inside Ih



Conclusions sur les Nanoalliages Pd-Au:

- Although the **Ih structure is never stabilized in pure Au clusters** and only below 2nm for Pd clusters, **Ih Pd₃Au and PdAu are stable in a large range of size** :
up to 6nm for Pd₃Au and 3nm pour PdAu
- This can be explained by the **stress release induced by the misfit inside the Ih.**
- This is the **first attempt to characterize the structure and morphology of Pd-Au nanoalloys on a large range of size (2 to 7 nm)**
- **Chemical ordering** at the surface: **edges, facets** and in the **core of the nanoalloys**
- The real life is more complex: **gas adsorption** and/or **kinetics effect** in order to be compared to real catalysts.

2. Effet d'environnement sur la structure et la morphologie de nanoparticules supportées

➤ Nanoparticules libres :

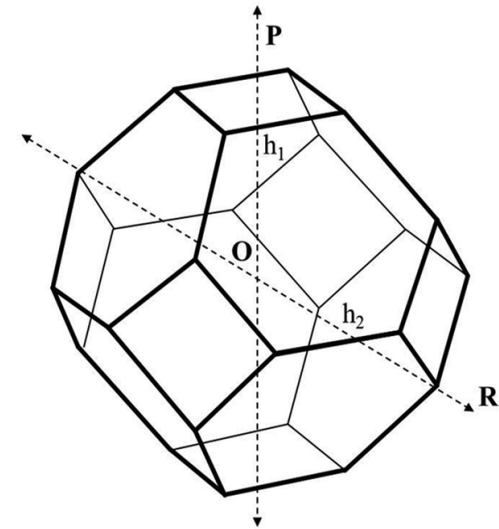
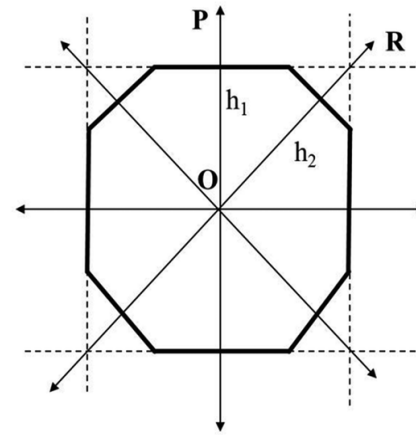
- Potentiel métal-métal + simulation numérique (DM)
- Théorème de Wulff

➤ Nanoparticules supportées:

- Surface d'énergie potentielle métal/support d'oxyde
- Théorème de Wulff-Kaishew

Théorème de Wulff :

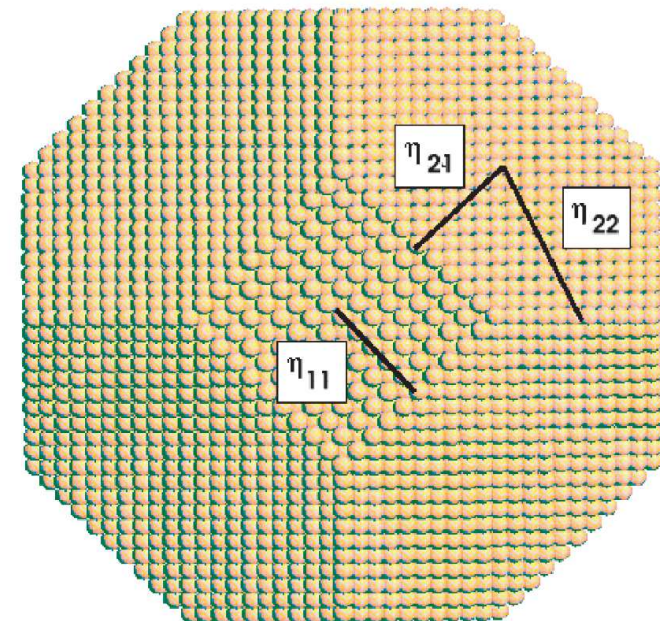
$$\frac{\gamma_i}{h_i} = \text{Constante}$$



Théorème de Wulff « étendu » :

$$\frac{\gamma_i}{h_i} + \frac{1}{2h_i} \frac{\rho_{ij}}{\eta_{ij}} \left(- \frac{3s^2}{2Kh^2} \right) = \text{Cste}$$

Surface stress

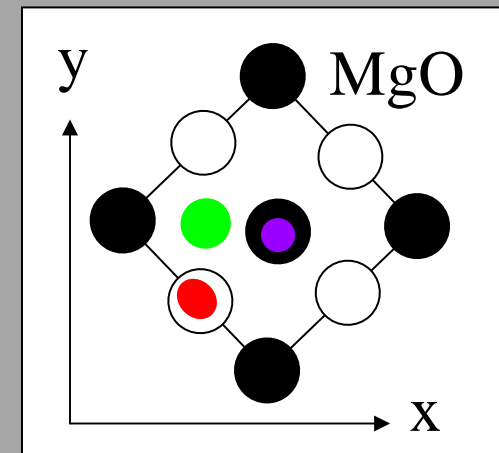
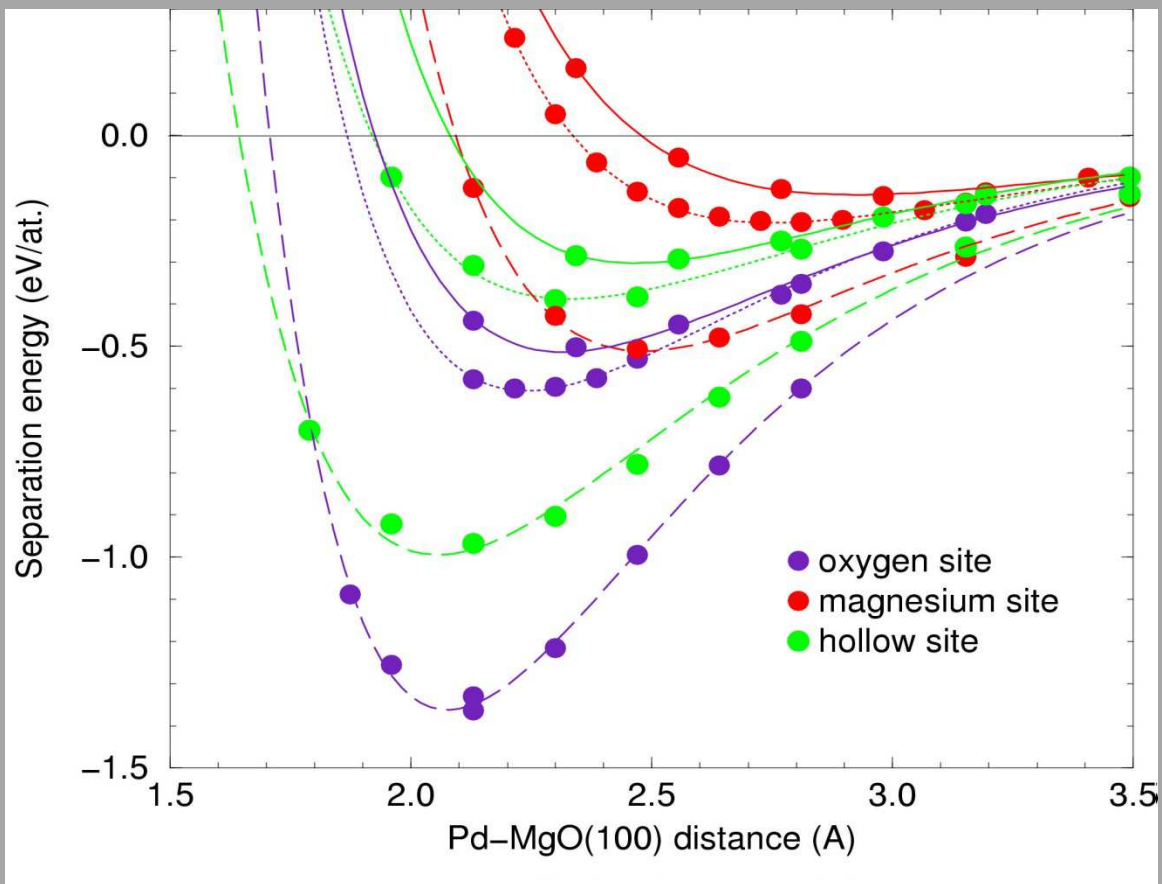


Interactions Métal-MgO(100) ajustées sur des calculs DFT: Surface d'énergie potentielle.

$$E_i(x,y,z,Z) = a_1[\exp(-2a_2(z-a_3)) - 2\exp(-a_2(z-a_3))]$$

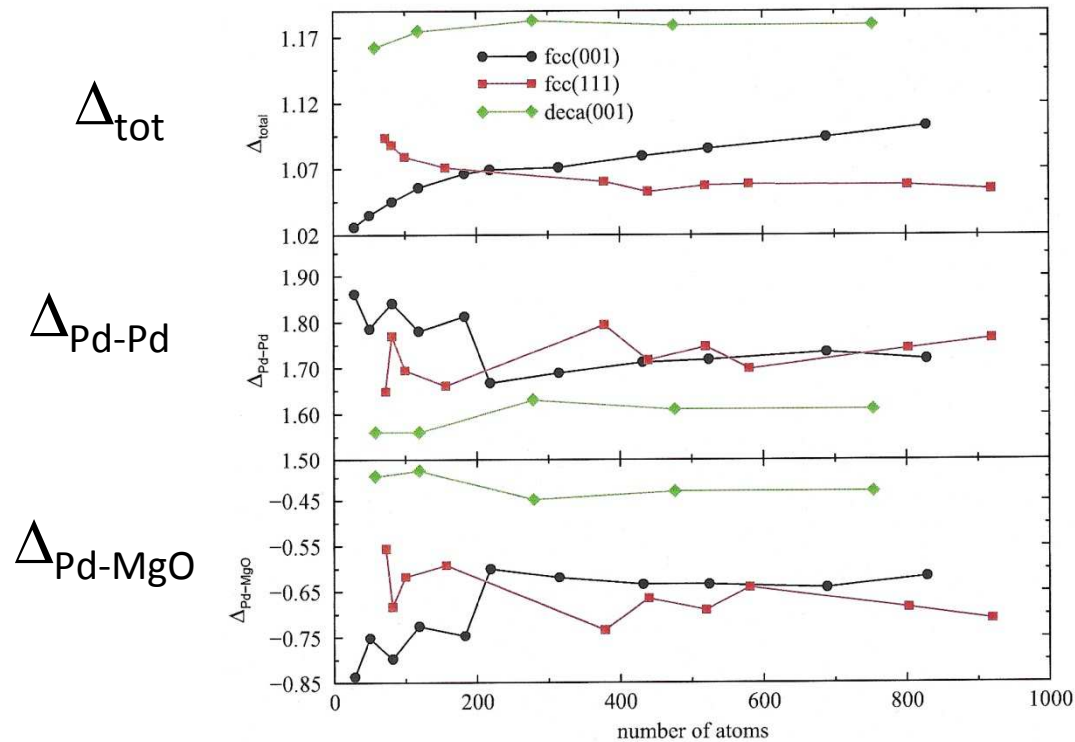
$$a_i(x,y,Z) = b_{i1} + b_{i2}\exp(-Z/b_{i3})$$

$$b_{ij}(x,y) = c_{ij1} + c_{ij2}(\cos x + \cos y) + c_{ij3}[\cos(x+y) + \cos(x-y)]$$



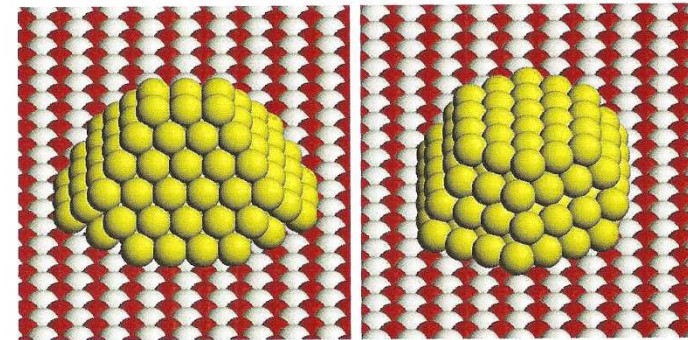
Nanoparticules supportées : quelle épitaxie ?

$$\Delta = \frac{E_{tot} - N\epsilon_{coh}}{N^{2/3}}$$



Pd/MgO(100)

Epitaxie (100) Epitaxie (111)



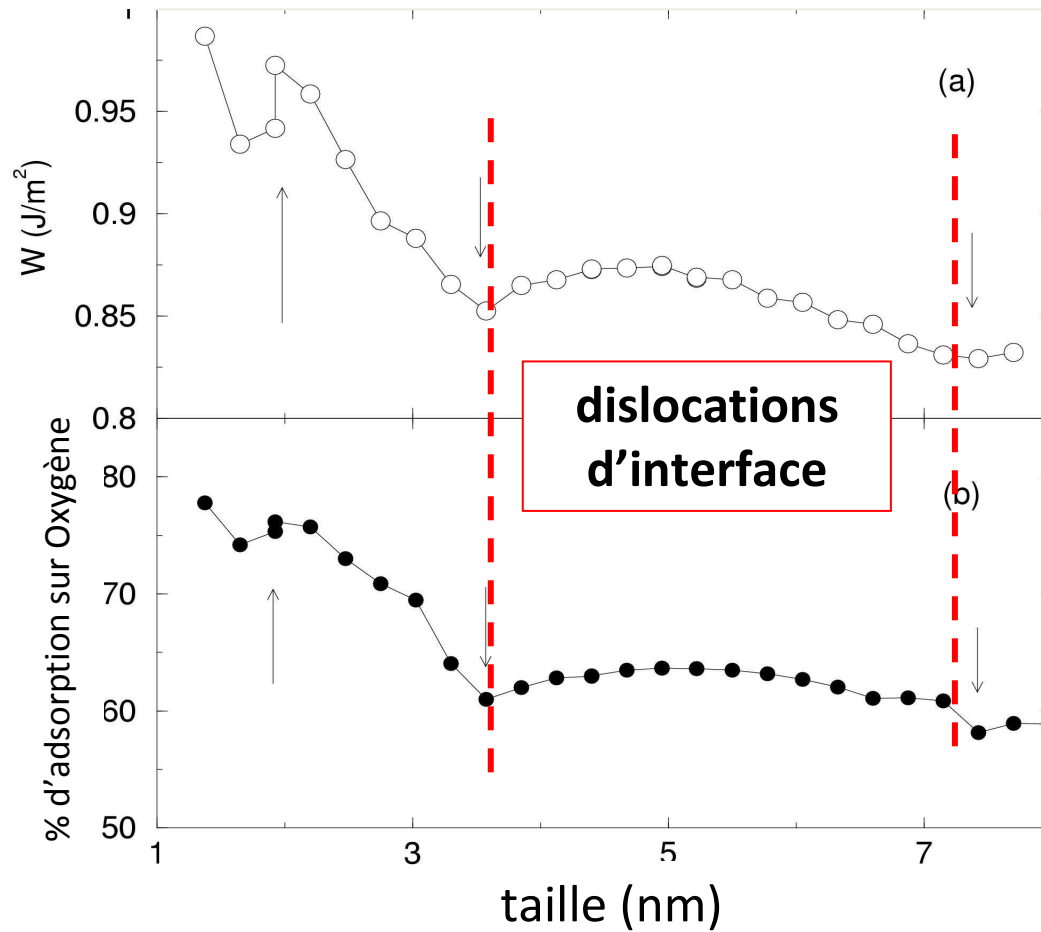
(a) 0.00 eV

(b) 0.20 eV

Goniakowski, Jelea, Mottet, Barcaro, Fortunelli, Kuntova, Nita, Levi, Rossi, Ferrando,

J. Chem. Phys. **130** (2009)

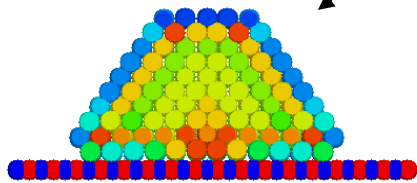
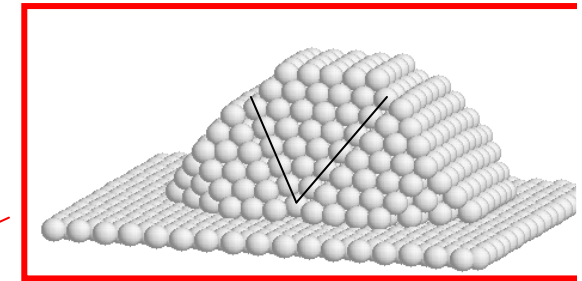
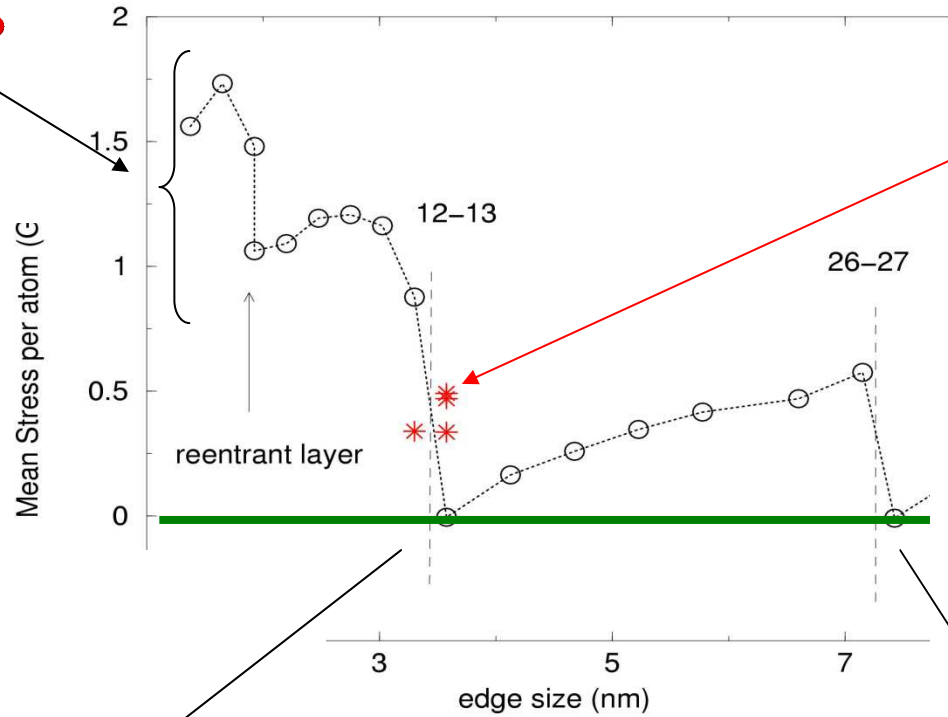
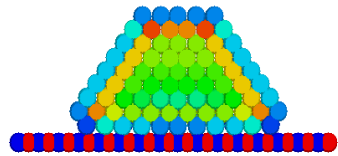
Evolution de l'énergie d'adhésion avec la taille.



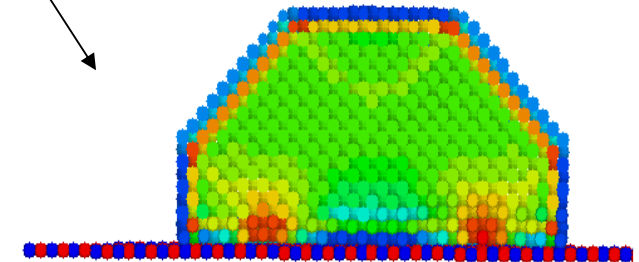
Energie d'adhésion

% d'adsorption sur les sites Oxygène

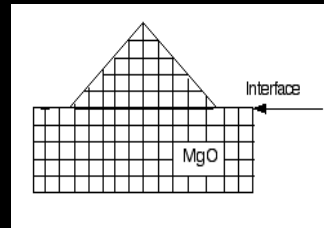
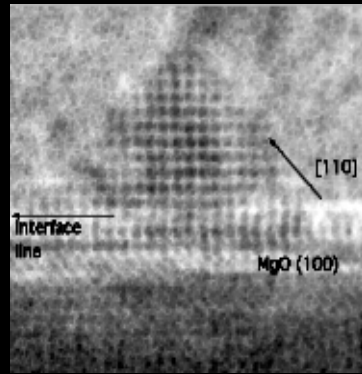
Contrainte induite par le substrat dans les nanoparticules



Dislocations d'interface

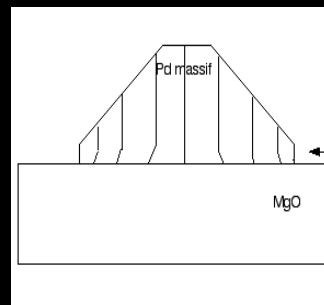
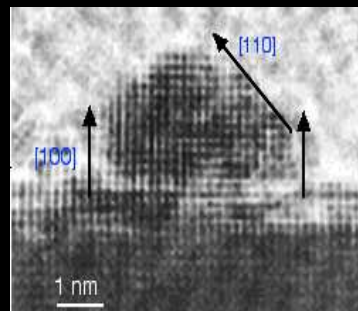


Pd/MgO(100), observation en HRTEM.



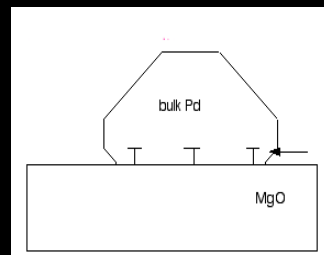
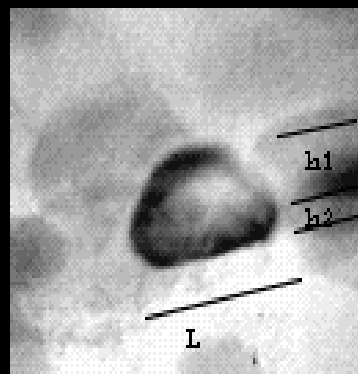
< 3 nm

Accommodation parfaite des agrégats de Pd (dilatation)



5 – 6 nm

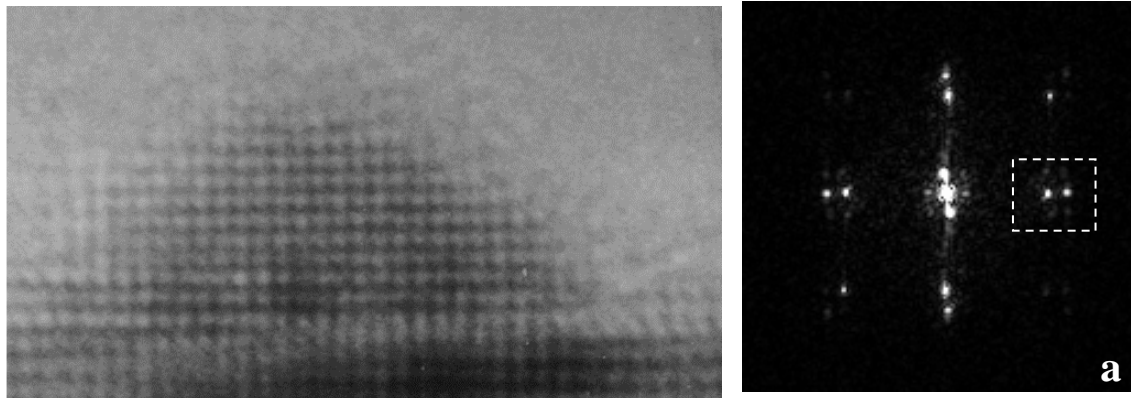
Dilatation uniquement à l'interface



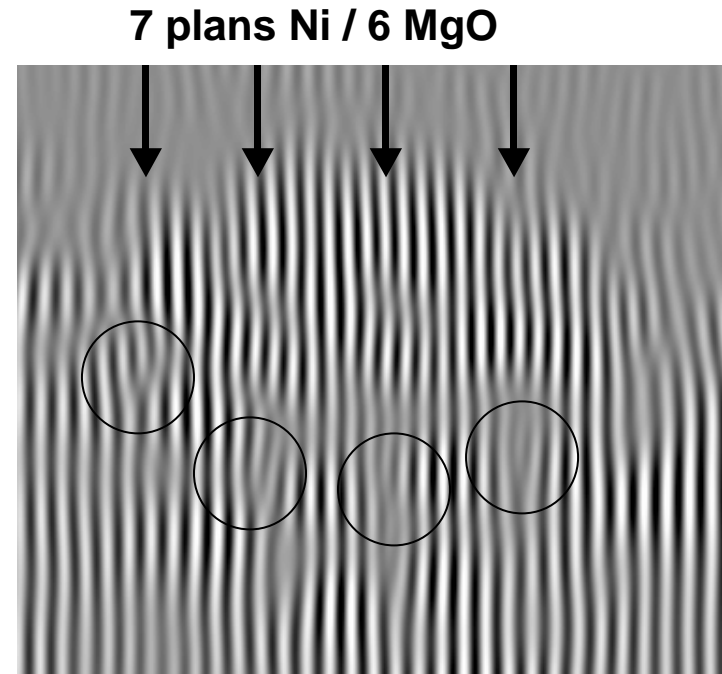
> 10 nm

**Dislocations
Agrégats relaxés**

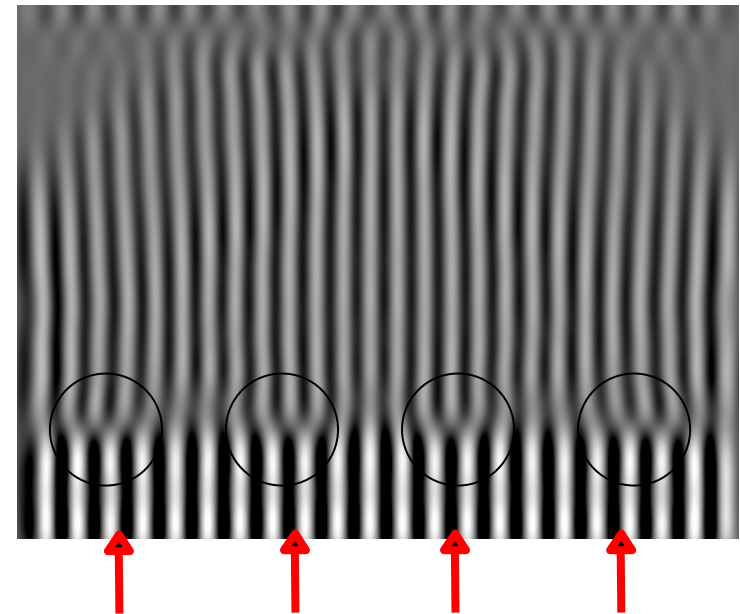
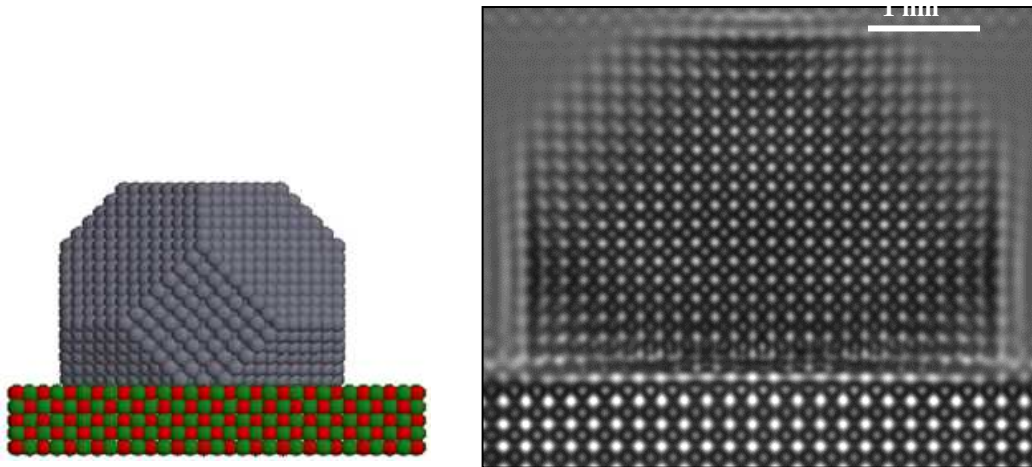
images HRTEM: Ni/MgO(100)



S. Sao-Joao, PhD thesis, Marseille, 2005.



Images simulées : Ni/MgO(100)

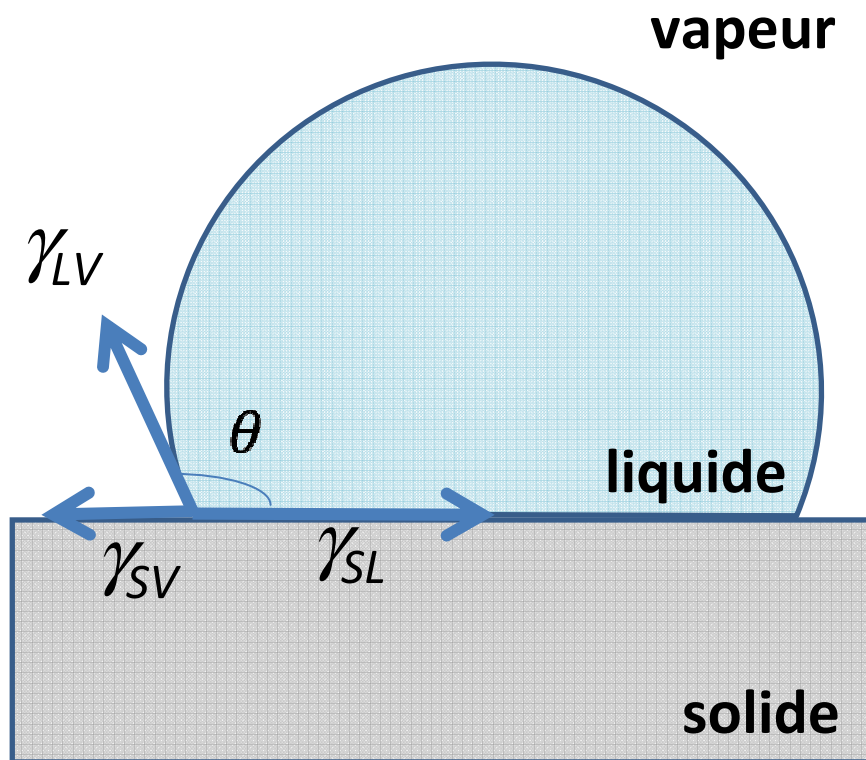


6 plans Ni / 5 MgO

Sao-Joao, Giorgio, Mottet, Goniakowski, Henry, *Surf. Sci.* 600, L86 (2006).

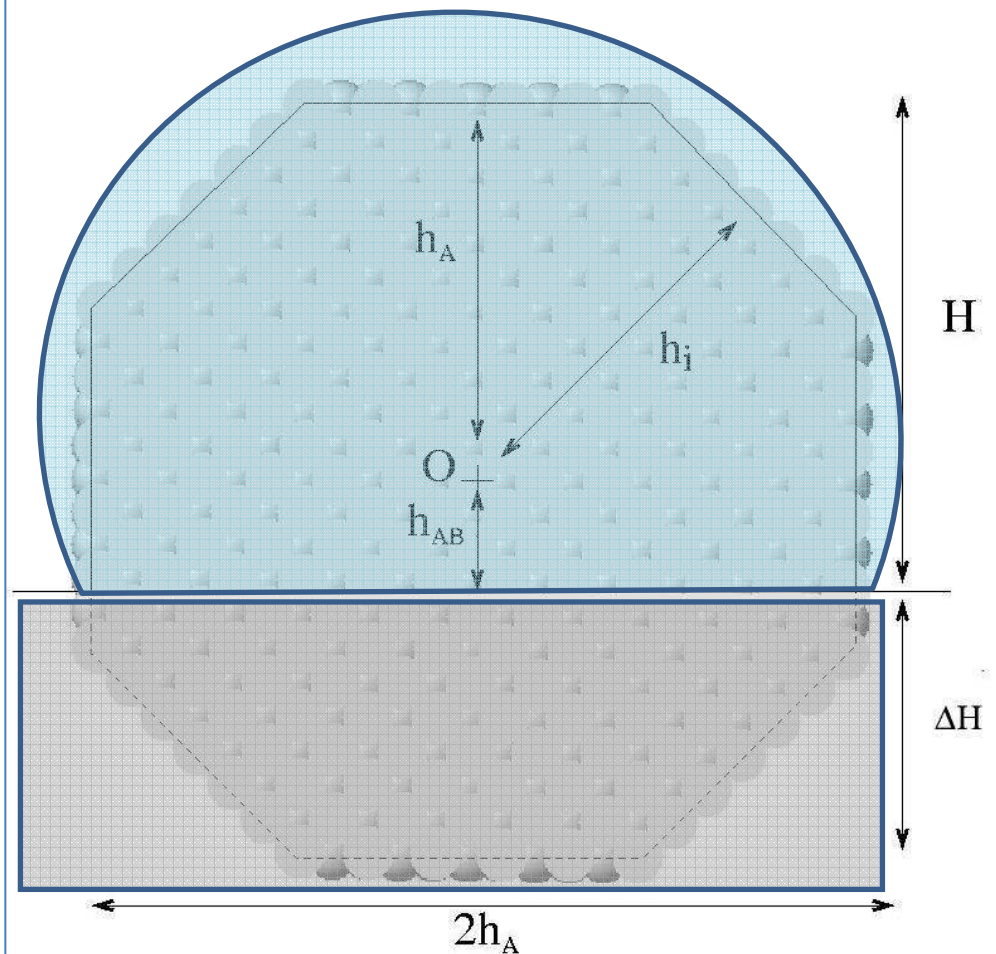
Théorème de Young-Dupré

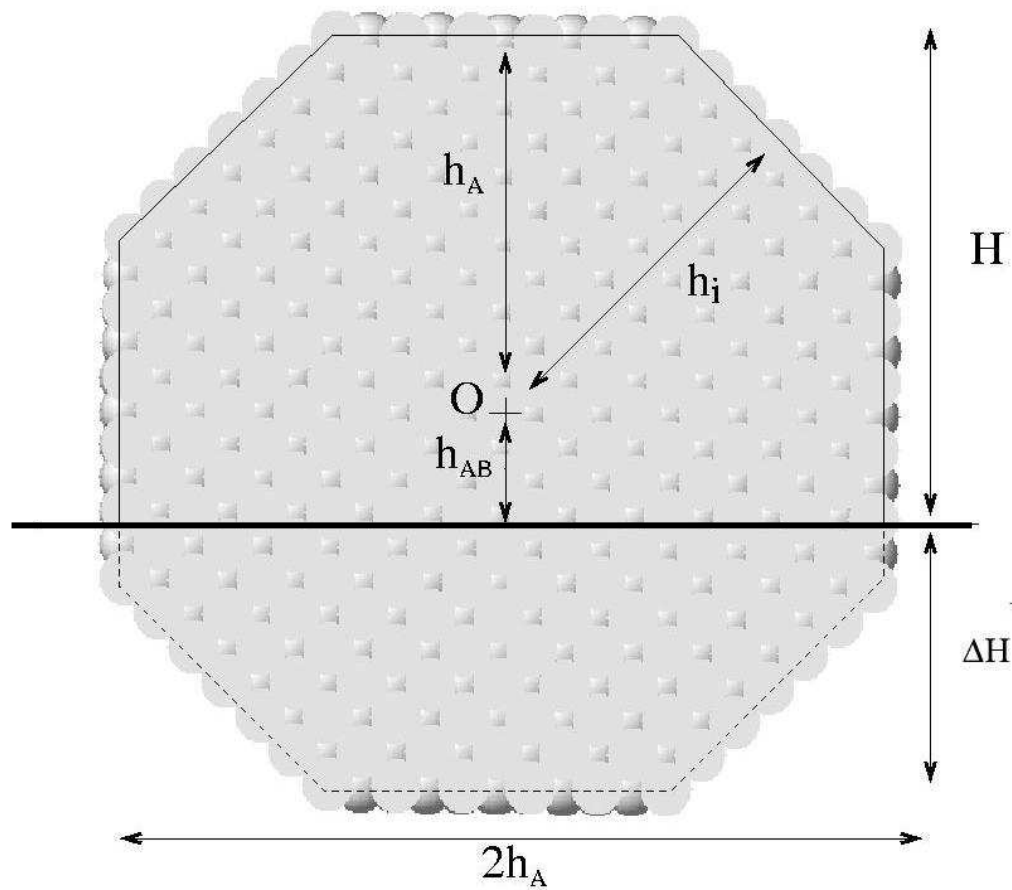
$$\gamma_{LV} \cos \theta = \gamma_{SL} - \gamma_{SV}$$



Théorème de Wulff-Kaishew

$$\frac{\gamma_i}{h_i} = \frac{\gamma_A - \beta}{h_{AB}}$$








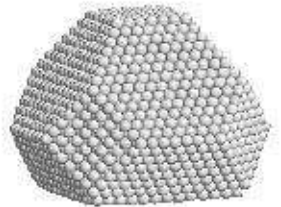


Rapport d'aspect R:

$$R = 1 - \beta / 2\gamma_A$$

	$\gamma_{(100)}$ (J/m ²)	β (J/m ²)	R_{wk}
Pd	0.82	0.91	0.45
Pt	1.15	0.68	0.70

Rapport d'aspect atomistique : Pd, Pt / MgO(100)

métal \ taille	2 nm	3 nm	5-6 nm
Pd	 R=0.5	 R=0.4	 R=0.43
Pt	 R=0.6	 R=0.7	 R=0.8

Wulff-Kaishew

↓

$R_{WK} = 0.45$

$R_{WK} = 0.70$

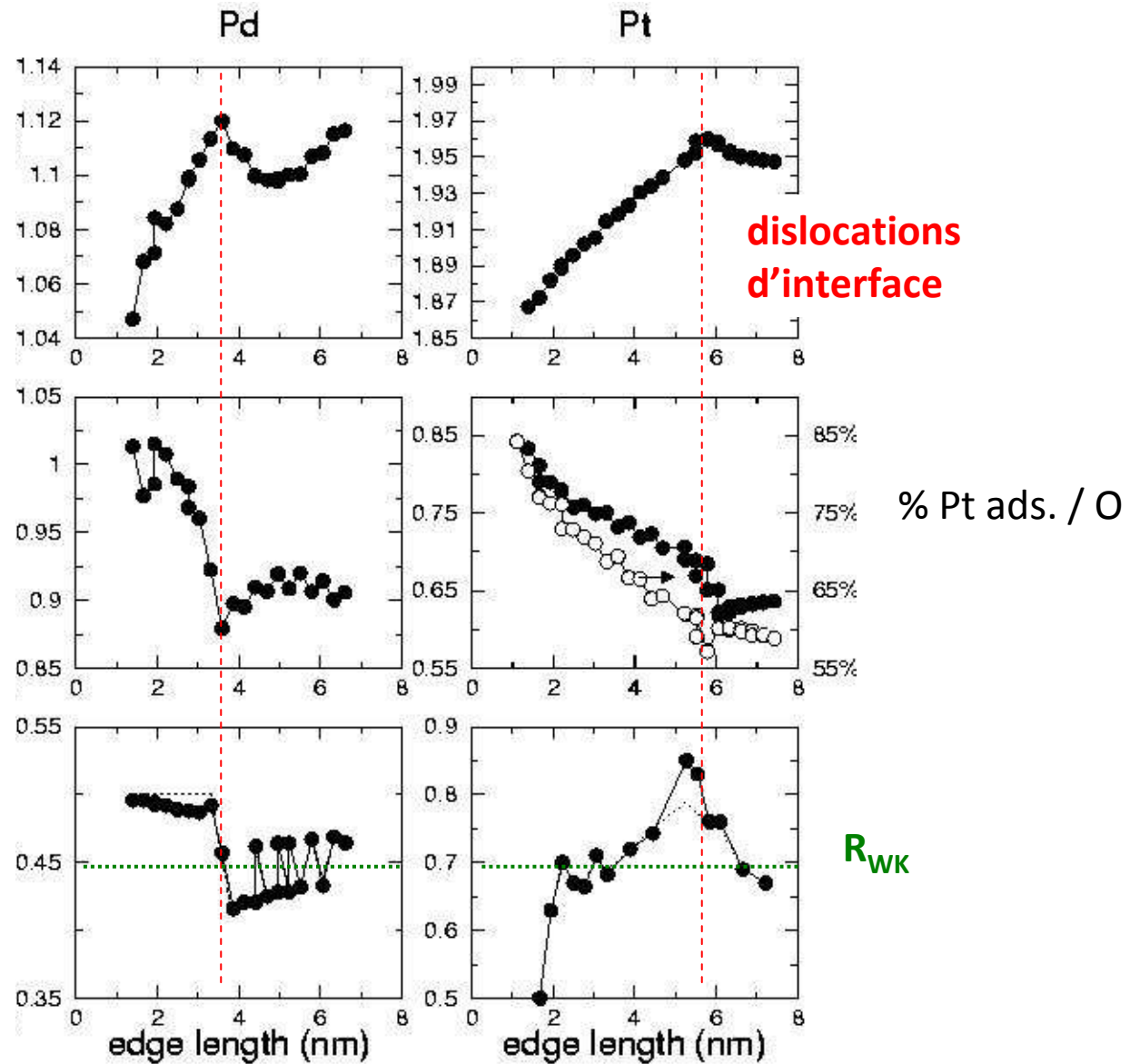
Validité du théorème de Wulff-Kaishew / modèle atomistique

énergie de surface moyenne

énergie d'adhésion

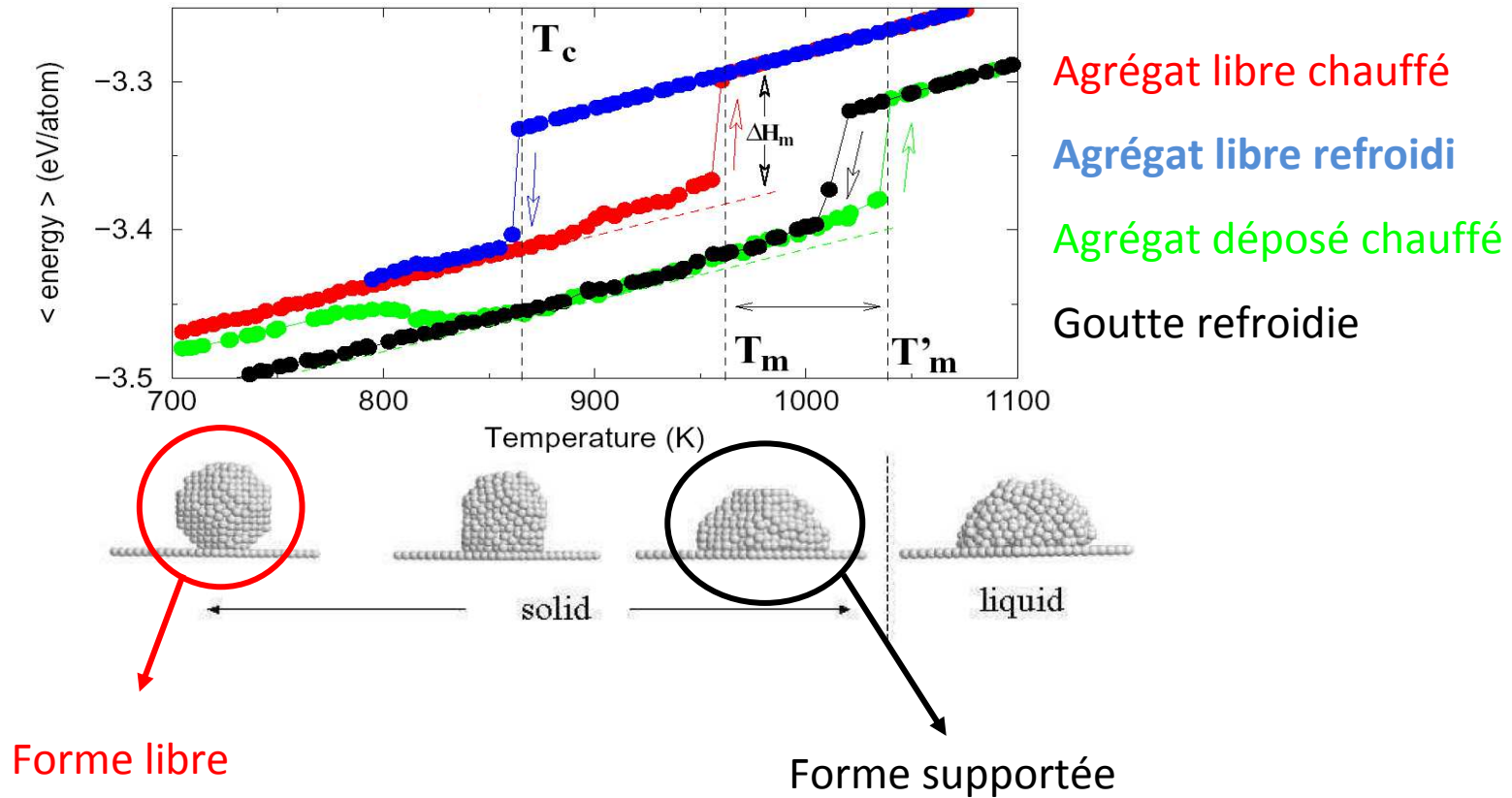
rapport d'aspect

$$R = 1 - \beta / 2\gamma_A$$



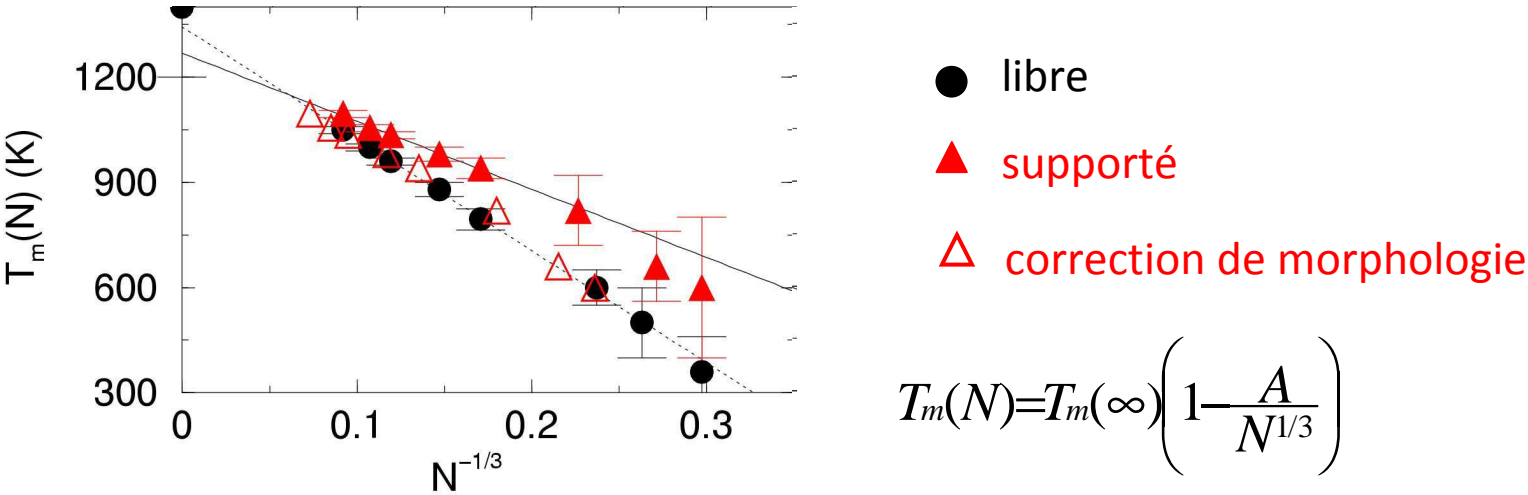
“Théorème de Wulff-Kaishew généralisé” P. Müller, R. Kern, *Surf. Sci.* **457** (2000) 229.

Fusion / Recristallisation

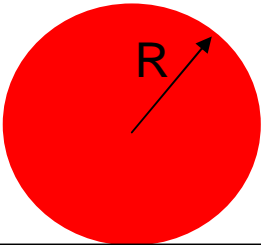


Hypthèse d'ergodicité: la forme recristallisée représente la forme d'équilibre

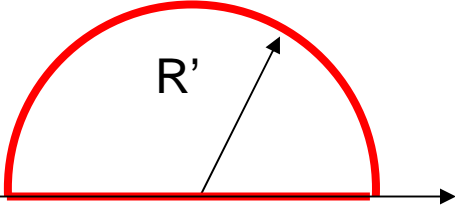
Effet de la morphologie sur la fusion : libre / supporté



Forme libre



Forme supportée



Conservation du volume (nbre d'atomes N)

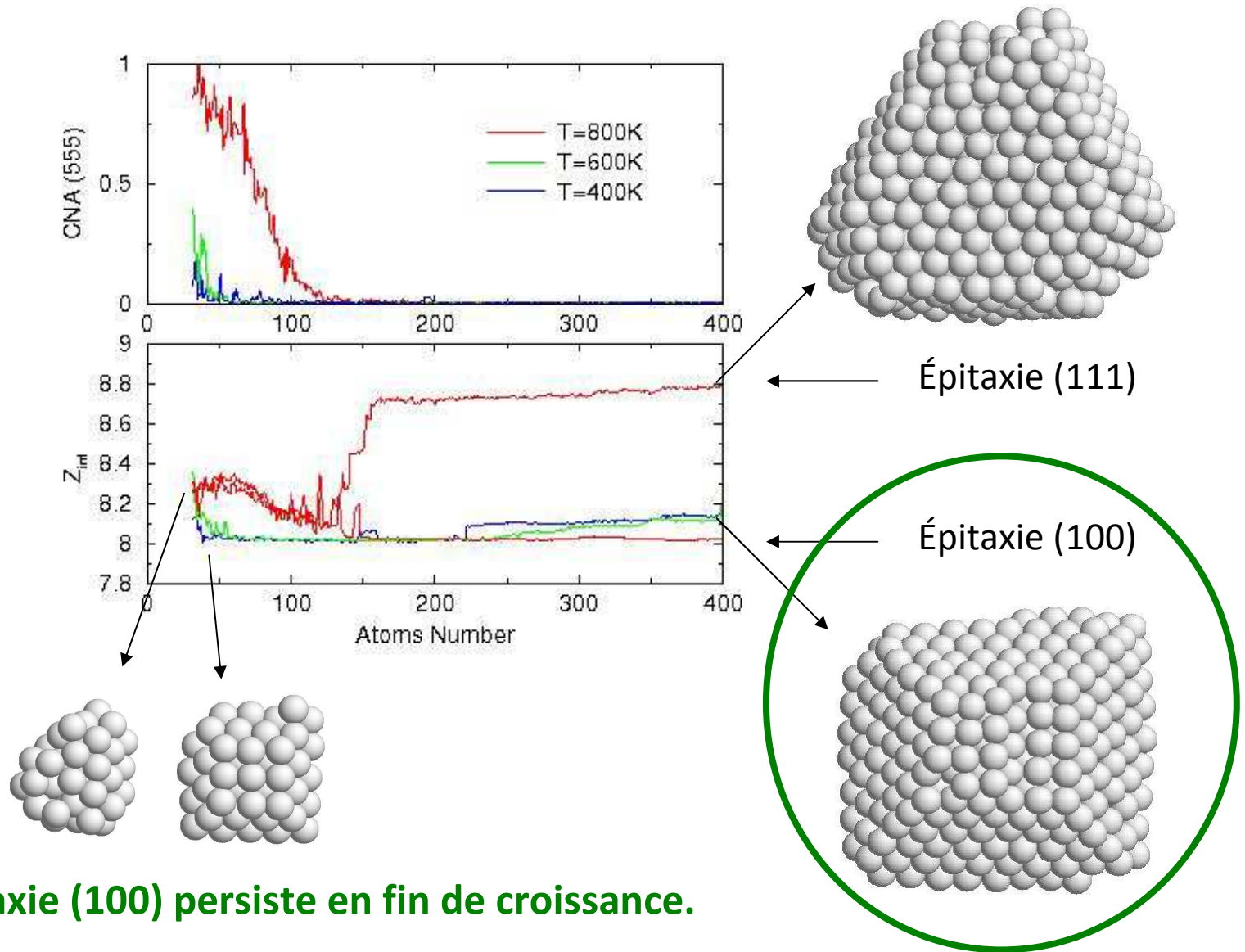
$$V = \frac{4}{3}\pi R^3 = \frac{(4/3)\pi R'^3}{2} \Rightarrow R' = 2^{1/3} \text{ soit } N' \rightarrow 2N$$

Croissance d'agrégats de Pd / MgO(100)

Common Neighbors
Analysis

Signature (555)

Nombre de voisins
métalliques à
l'interface



à $T < 800K$, l'épitaxie (100) persiste en fin de croissance.