



NANOALLOYS  
International Research Network

# IMN 2018

International Meeting on Nanoalloys

MAY 22-25

Orléans  
France

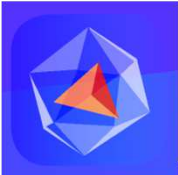


Comprendre le monde,  
construire l'avenir®

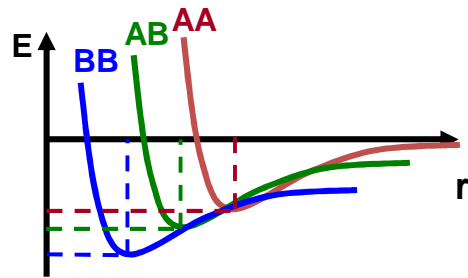
# What is hidden behind phase diagrams and ageing kinetics of nanoalloys

F. Berthier, J. Creuze, B. Legrand

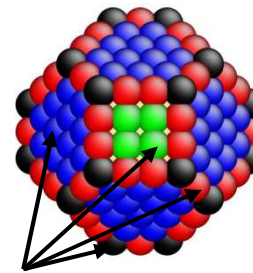
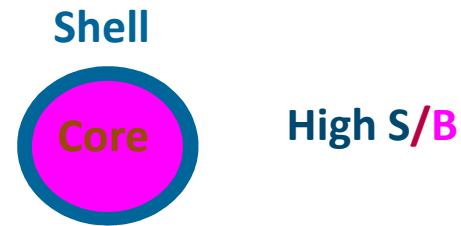
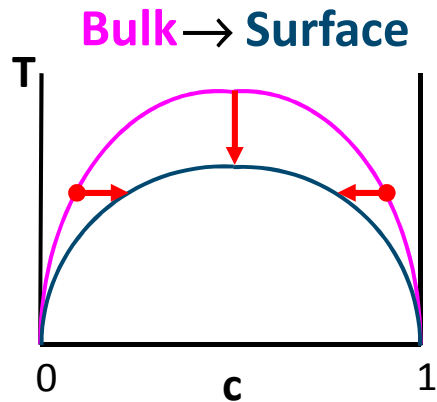
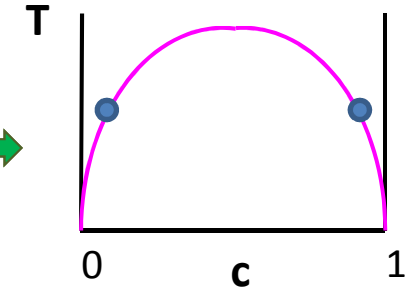
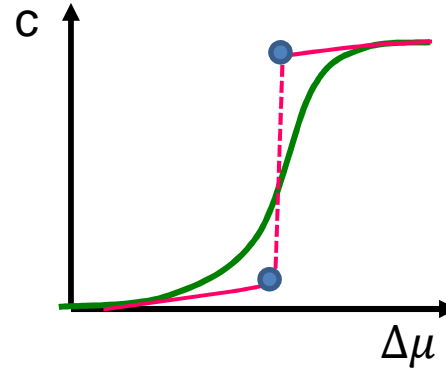




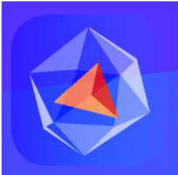
# Bulk $\rightarrow$ surface $\rightarrow$ finite objects



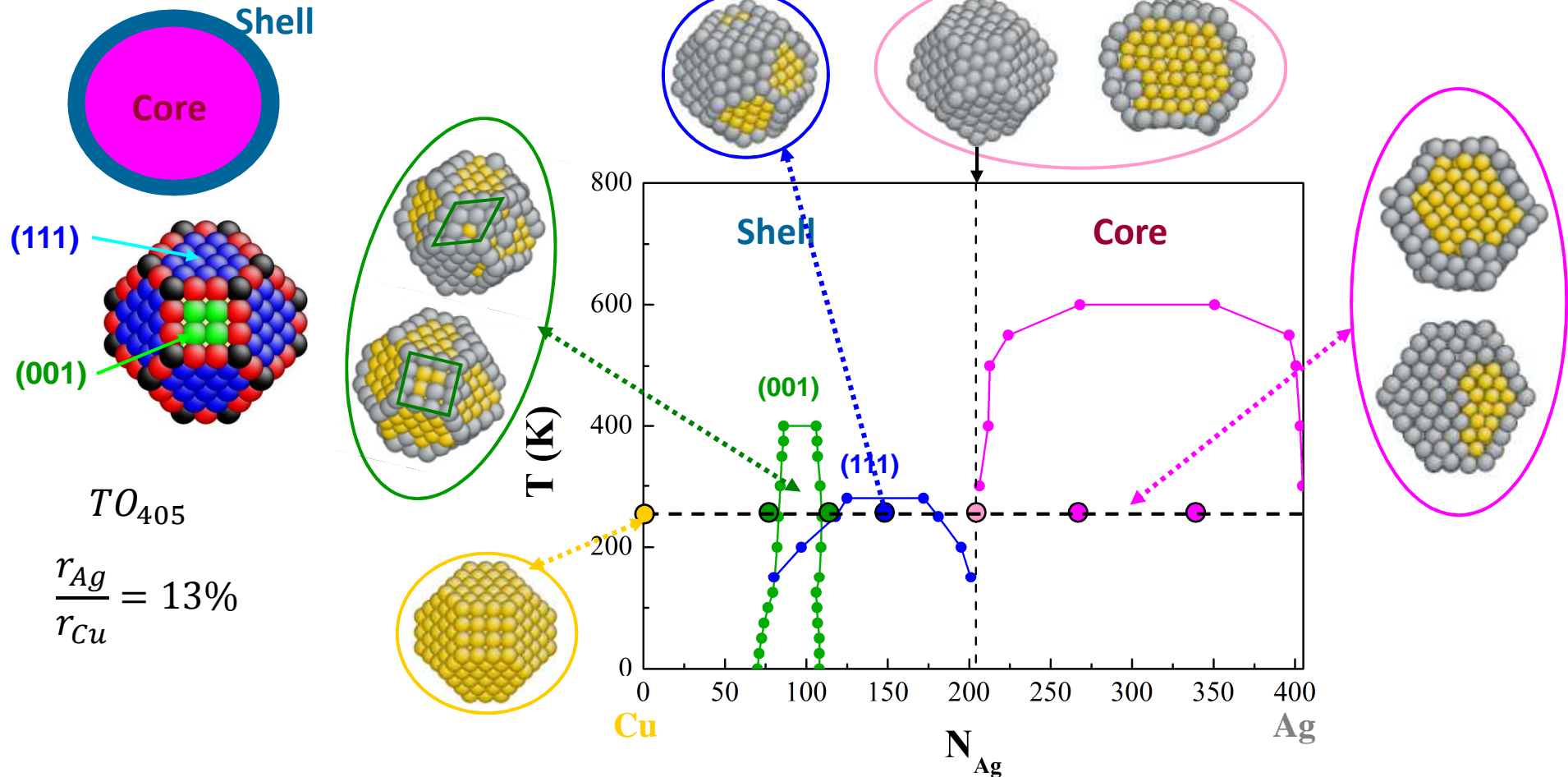
Off Lattice  
Monte Carlo  
simulations



non equivalent sites



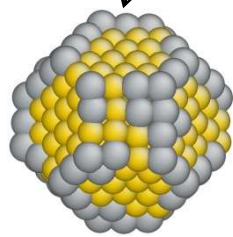
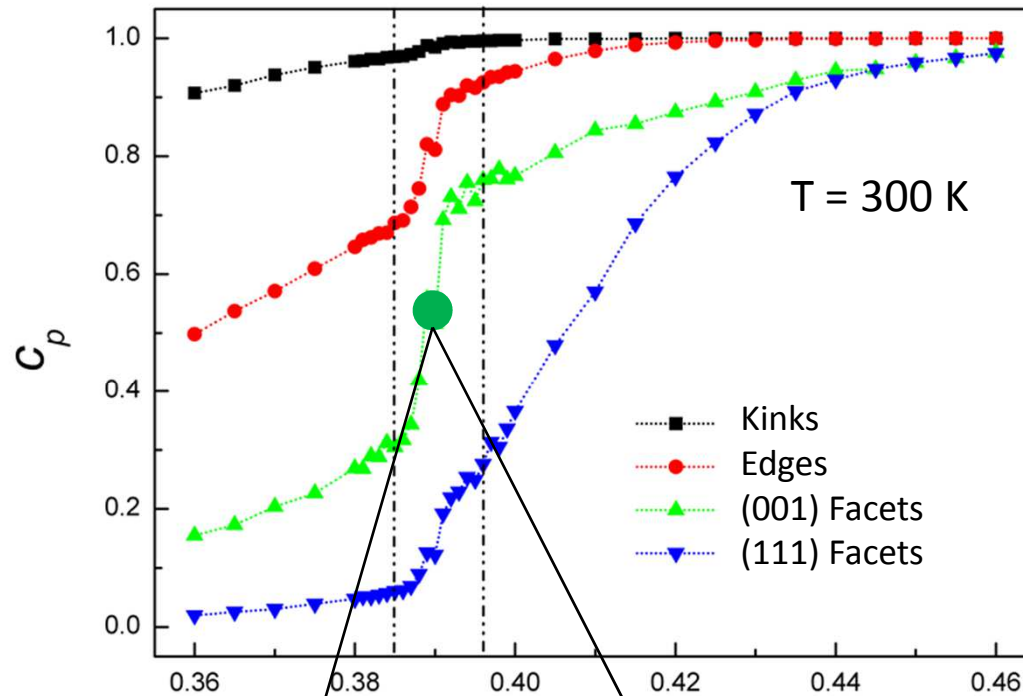
# Multi-objects → Multi Phase Diagrams



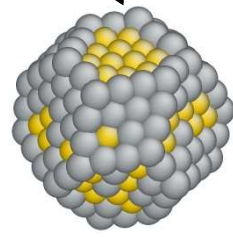
What are the driving forces for each phase separation ?



# Exotic behavior of the (001) facets

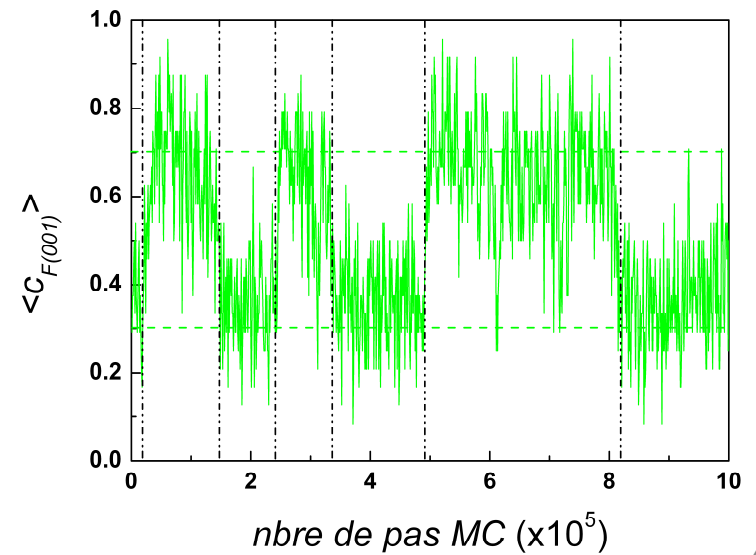


$$c_{(100)} \approx 0,3$$



$$c_{(100)} \approx 0,7$$

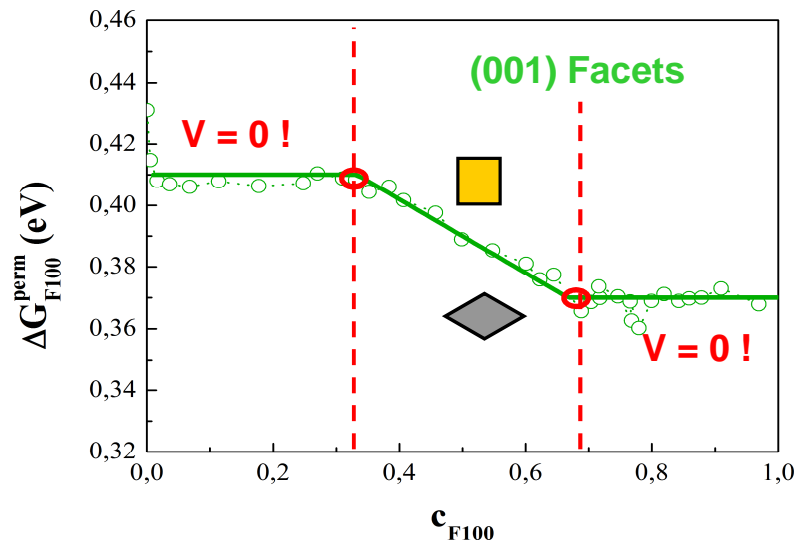
Structural and Chemical Bistability...



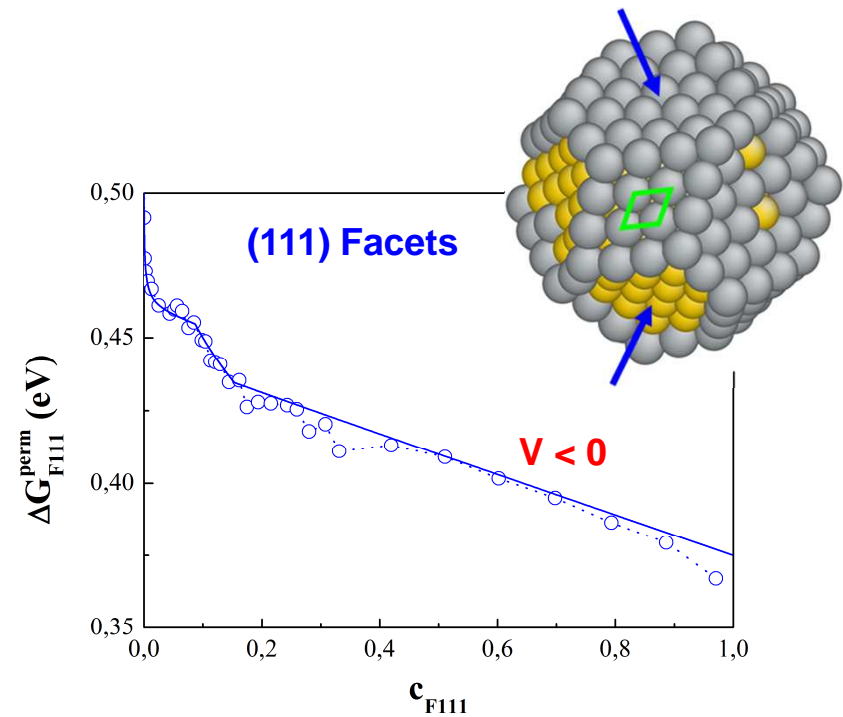


# Mean Field Analysis

$$\frac{c_p}{1 - c_p} = \exp\left(-\frac{\Delta G^{perm} - \Delta\mu}{k_B T}\right)$$



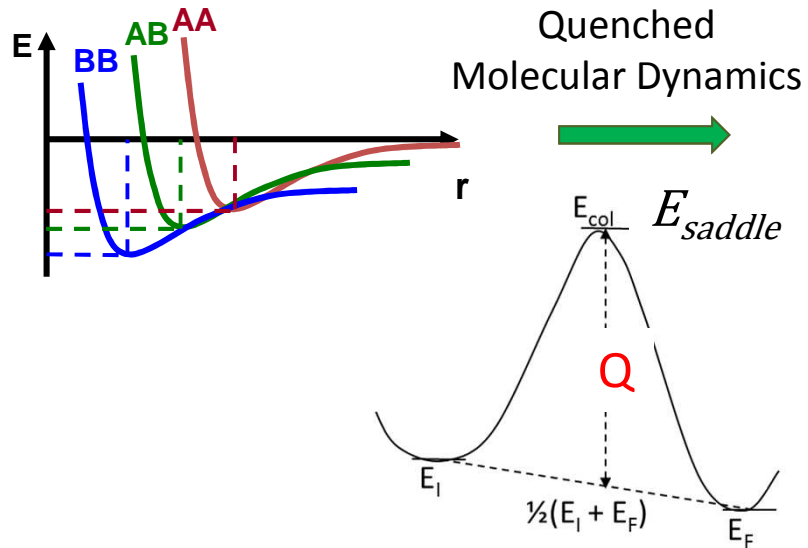
size effect



Chemical effect

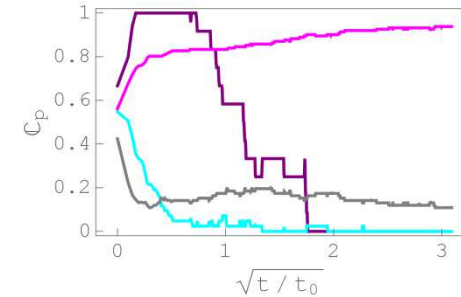


# From equilibrium to kinetics

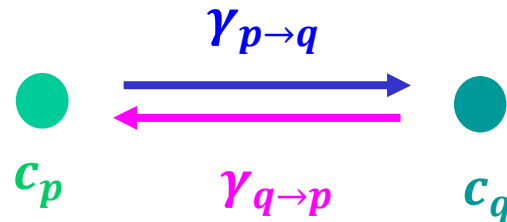


$\tau, V, Q$

Kinetic Monte Carlo simulations



$$P(E_I \rightarrow E_F) = \nu \exp\left(-\frac{E_{saddle} - E_I}{k_B T}\right)$$



Mean Field Approximation  
Site Kinetic

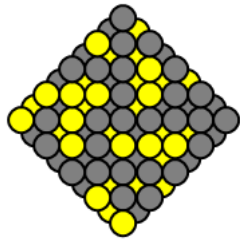
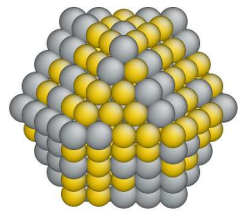
$$\frac{\partial c_p}{\partial (t/t_0)} = \sum_q [(1 - c_p)c_q \gamma_{q \rightarrow p} - c_p(1 - c_q)\gamma_{p \rightarrow q}]$$



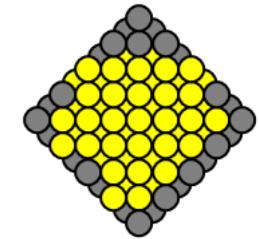
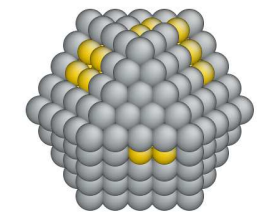
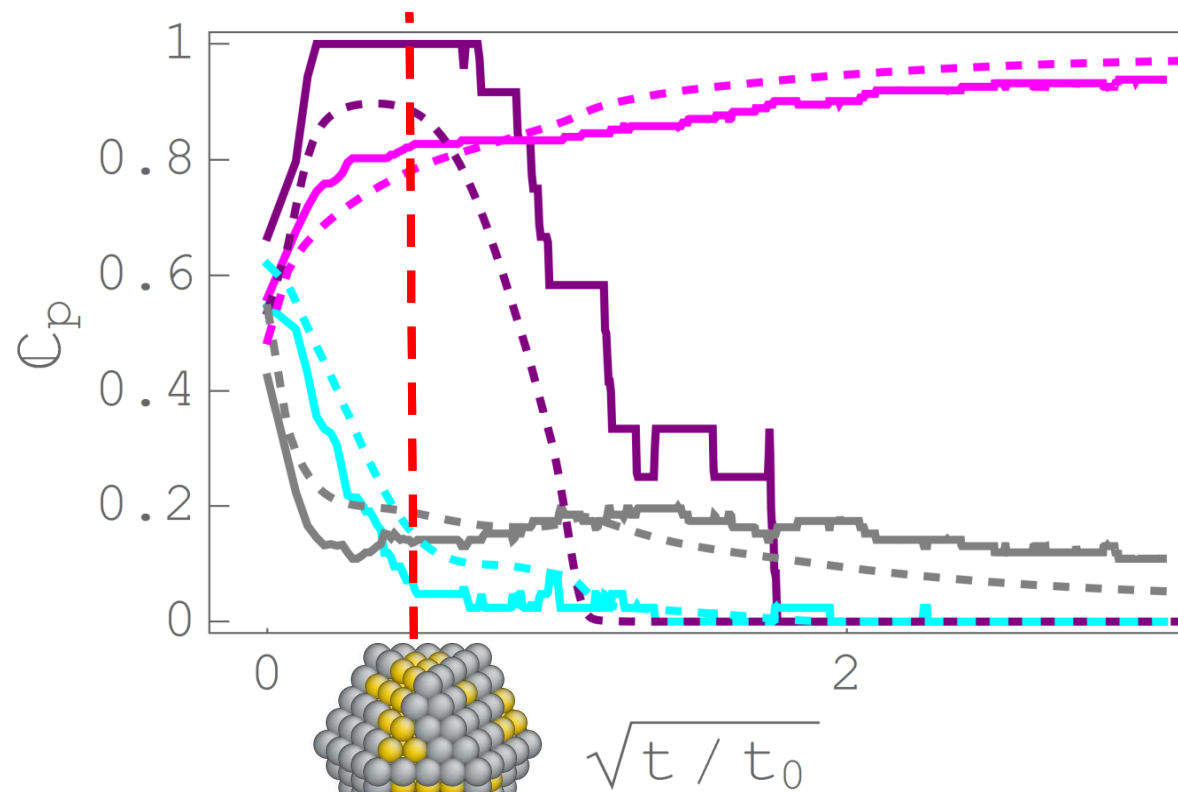
# Ageing kinetics

CuAg

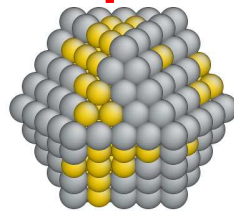
T=250 K



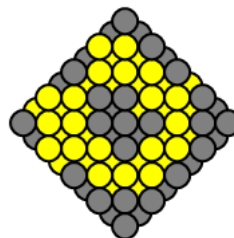
random



Core/Shell



$\sqrt{t/t_0}$



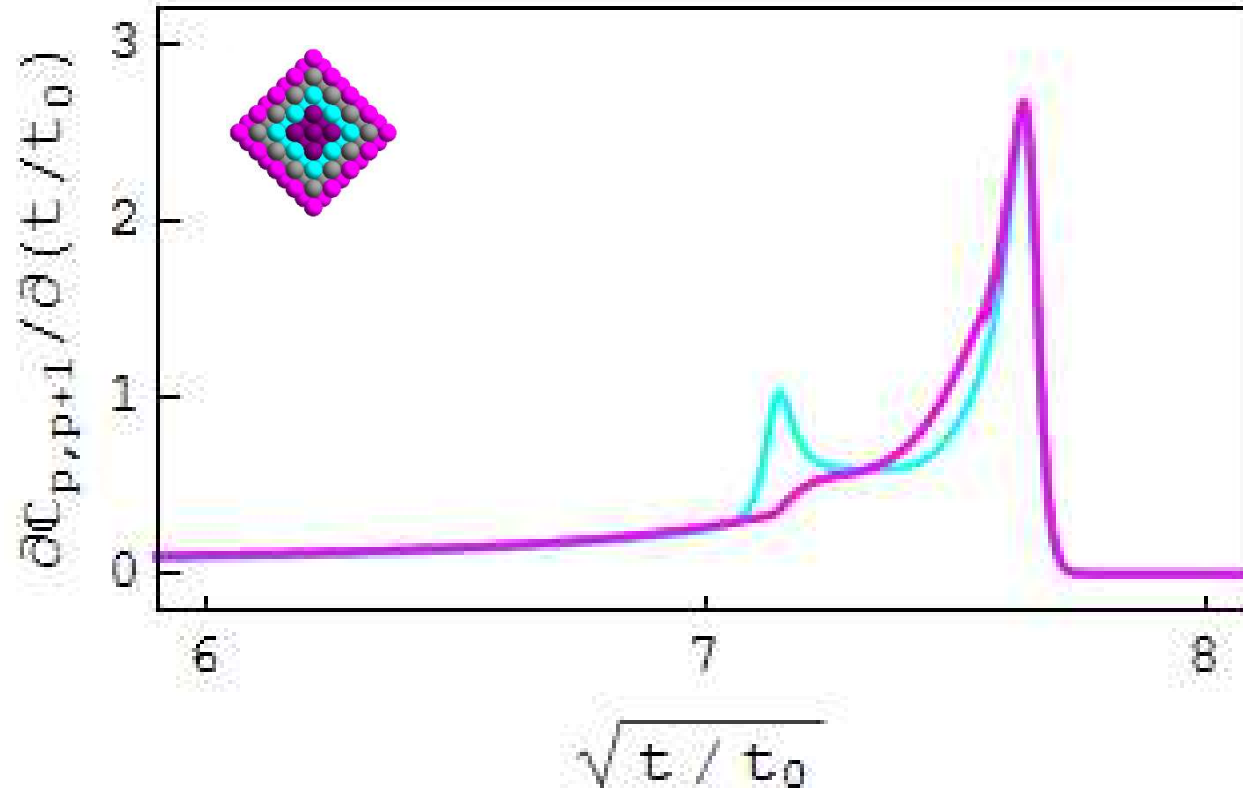
Oignon-like

Kinetic Monte Carlo  
=  
MFA-SK



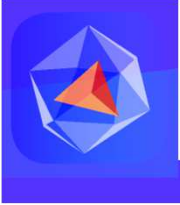
# Mean Field Analysis

Ag : bulk  $\rightarrow$  surface or Cu : surface  $\rightarrow$  bulk ?



Ag : bulk  $\rightarrow$  surface





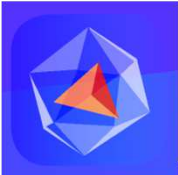
# Conclusions

## The moral of the story :

- atomistic simulations are efficient for the study of bimetallic nanoalloys
- analysis of these simulations by a coherent analytical modelling allows a better understanding

## Ageing kinetics:

- First step.... It's a long way
- it would be interesting to have experimental data to calibrate our simulations.



# Thanks to

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## Internships

## Equilibrium

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## kinetics

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