ICGM

Institut Charles Gerhardt Montpellier

**CHEMISTRY: MOLECULES TO MATERIALS**

# Toward an Accurate Theoretical Description of Gold-based Nanocatalysts Under Reactive Media

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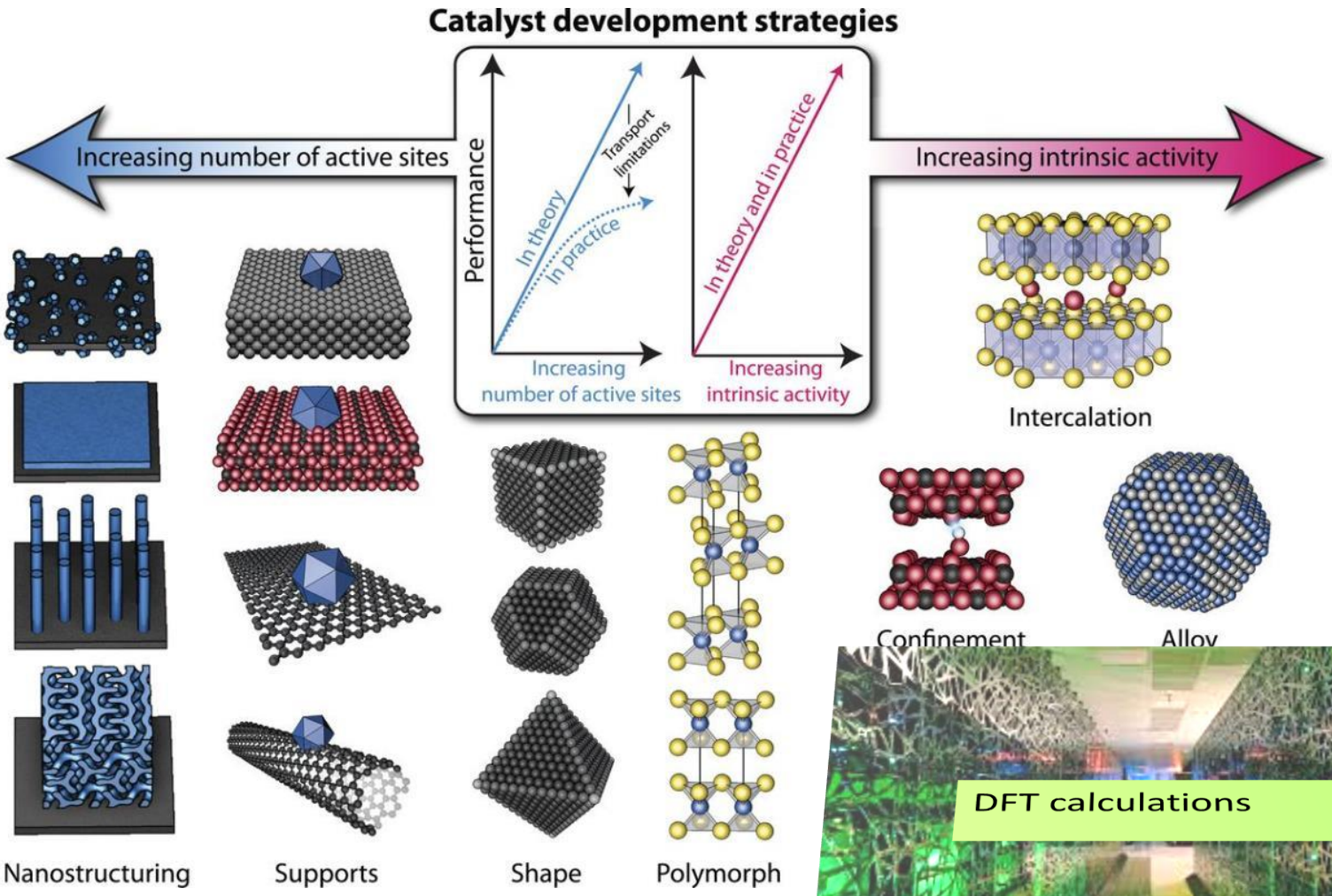
# The context: Theoretical description of nanocatalysts



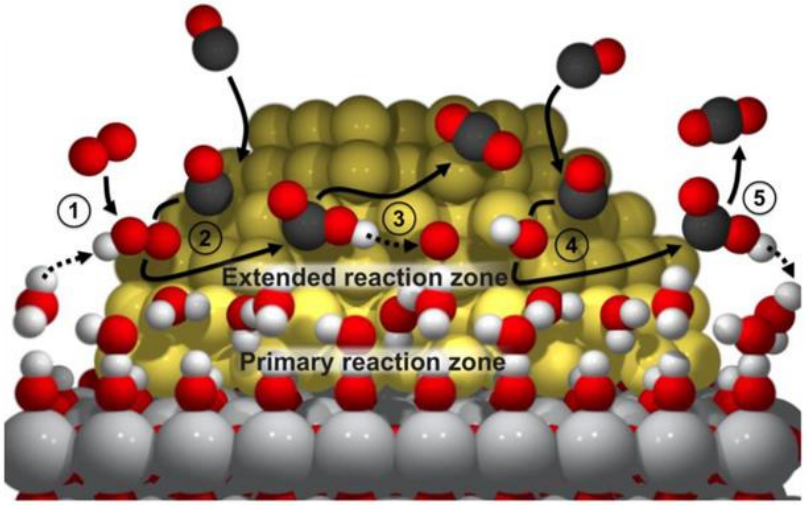




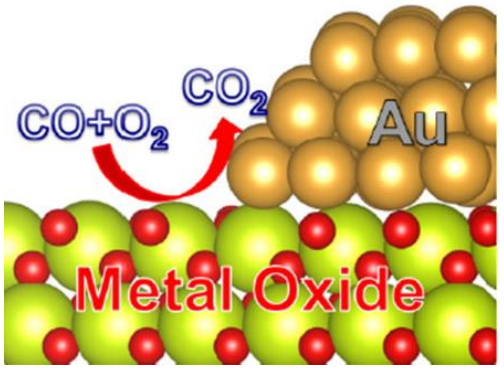
Seh, Z. W. *et al. Science* 355, eaad4998 (2017).

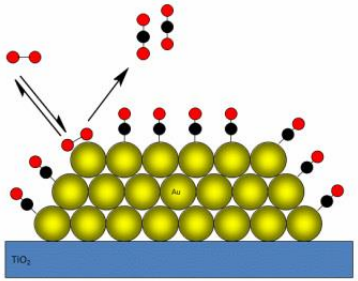
# Subject: Gold based nanocatalysts under reactive media

**Problematic**: Gold shows remarkable catalytic activity for CO oxidation even at room temperature. Despite extensive studies, the mechanism of catalysis by gold nanoparticles is still unclear, in particular in relation to CO oxidation at room temperature.



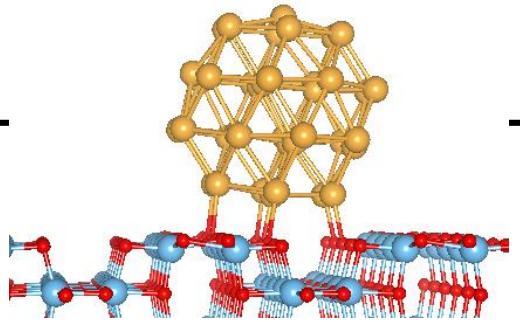

Chandler B.D. et al. Science, 2014, 345, p. 1599.



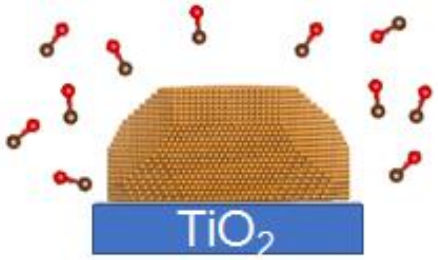



# Goal: Structure and morphology changes under working conditions

- Modeling supported Au-Cu nanoparticles



- Identification of the shape evolution of GNP under $O_2$ gas: MSR model



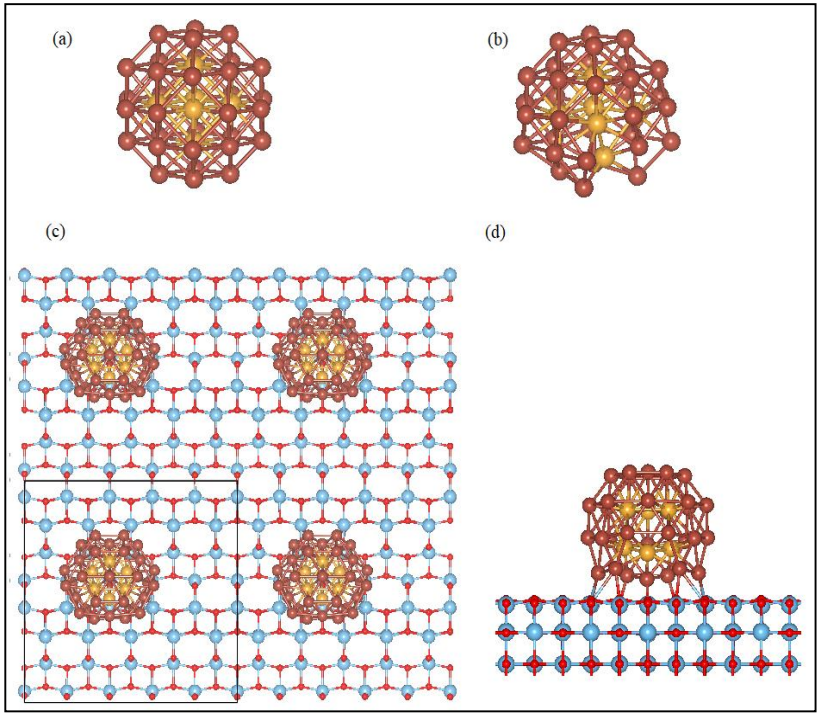
# Modeling supported Au-Cu Nanoparticles

Context: Optimization of Au-Cu catalysts

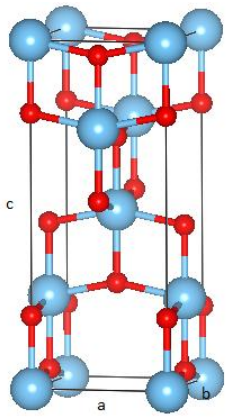
Goal: to model “realistic” systems: supported catalysts

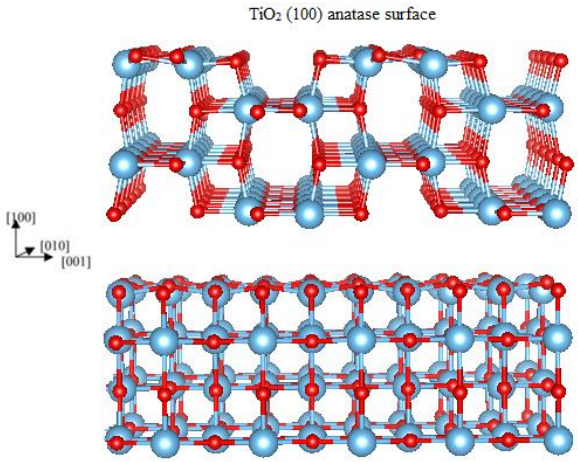
Main questions:

✓The effect of the support
(small nb of atoms/Nbands ; large nb ok Kpoints)
✓ The effect of the gas
(Large nb of atoms/Nbands ; small nb of Kpoints)
✓ The minimum energy structures of AuCu nanoalloys : Hybrid functionals
(non easy convergence)



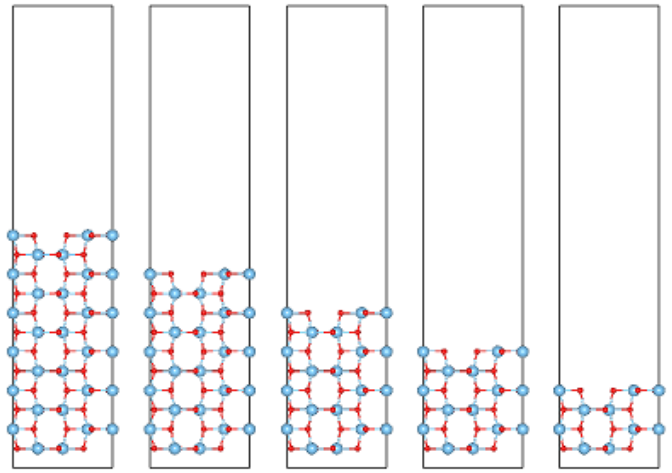
# Modeling Au-Cu : The effect of the support




From the bulk to the surface

Surface energy calculations following the Fiorentini and Methfessel method: f(x)=ax+b
b= (Eslab-Ebulk)/2xA



## The Hubbard correction is used for the description of strongly correlated materials:

In titanium oxide, the 3d orbitals do not overlap with the oxy
on the titanium atoms. Thus an probative semi-empirical ap
Hubbard model leads to an effective Hamiltonian to treat th

| KPOINTS | NKPTS | E(eV) | a(Å) | c(Å) | d((Å) | Band gap (eV) |
|---|---|---|---|---|---|---|
| 29x29x11 | 720 | -107,947 | 3,788 | 9,487 | 1,987 | 2,1985 |
| **33x33x13** | **1071** | **-107,952** | **3,789** | **9,489** | **1,988** | **2,1985** |
| 39x39x15 | 1680 | -107,951 | 3,789 | 9,489 | 1,988 | 2,1985 |
| 43x43x17 | 2277 | -107,952 | 3,789 | 9,489 | 1,988 | 2,1985 |

rials. In the Hubbard model, the electron-electron repuls
parameter $U$. The DFT+$U$ total energy is given as the
correction term that depends on the orbital occupation r

$$E^{DFT+U}[\rho, n_s] = E^{DFT}[\rho] + E$$

In the $U$ total electronic energy, the contributions of c
tionals are counted. This is the reason why one has to ir
as follows:

$$E^{U}[n_s] = E_0^{U}[n_s] - E^{dc}[n_s] \quad (2.7)$$

where $E_0^U[n_s]$ is a term derived accordingly to the HF treatment of electron-electron interaction of electrons within the shell $s$ and $E^{dc}[n_s]$ is a double counting term which represents the electron-electron interaction contribution of the shell $s$ that is already present

2x1 surface slab = KPOINT (33x13x1)

# Methodology

Optimisation of $TiO_2$(100) surface
+
Correction de Hubbard
*********
119 irreducible k-points
Nodes=6 :NPAR=4/KPAR=6

4 layers: 48 (16 Ti + 32 O) atoms : NBANDS= 232
5 layers: 60 (20 Ti + 40 O) atoms : NBANDS= 288
6 layers: 72 (24 Ti + 48 O) atoms : NBANDS= 352
7 layers: 84 (28 Ti + 56 O) atoms : NBANDS= 408
8 layers: 96 (32 Ti + 64 O) atoms : NBANDS= 472

```
executed on          Linux_Intel date 2017.08.24  14:54:14
running on  168 total cores
distrk:  each k-point on   28 cores,    6 groups
distr:  one band on NCORES_PER_BAND=   7 cores,    4 groups
```

Votre job ( 3433111 ) a déclenché un débordement mémoire. Il a tourné sur des nœuds qui disposent de 64 Go de mémoire. La machine Occigen dispose de nœuds avec 128 Go que vous pouvez adresser en rajoutant une option à la soumission de votre job ( https://www.cines.fr/calcul/faq-calcul-intensif/#tabs-2 ). Attention, cette solution est réservée aux

travaux justifiant ce besoin mémoire.

The problem was solved by concidering Nnodes=KPOINTS

```
executed on          Linux_Intel date 2017.09.11  12:47:15
running on 2856 total cores
distrk:  each k-point on   24 cores,  119 groups
distr:  one band on NCORES_PER_BAND=   3 cores,    8 groups
```

Cost: 27 100 core.h !!!

# Modeling Au-Cu : The effect of the reactive gas

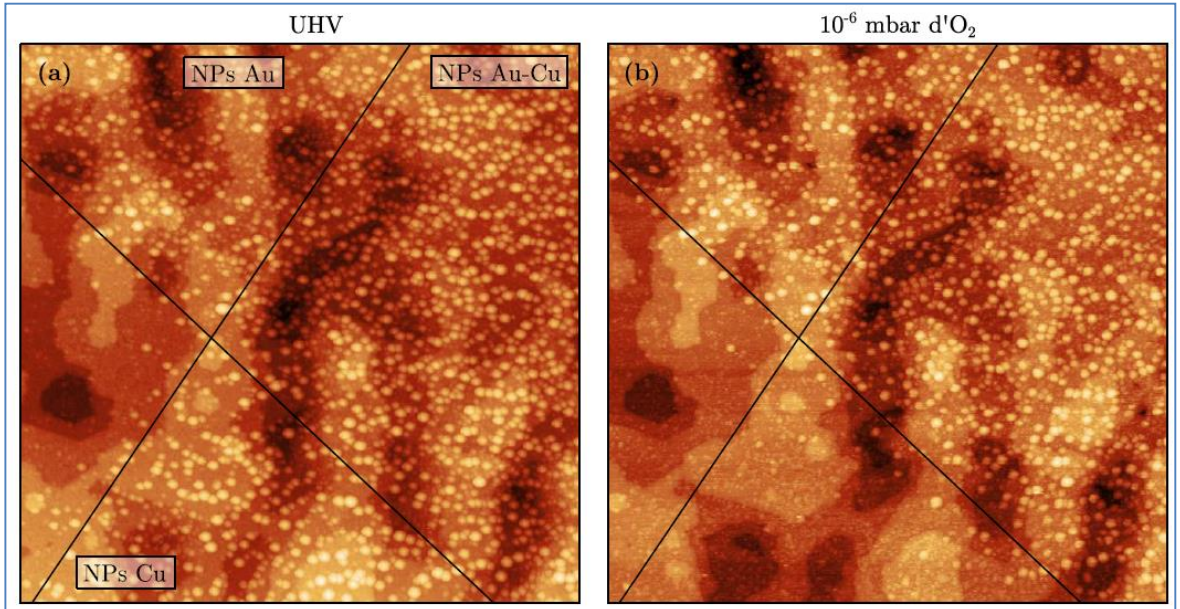
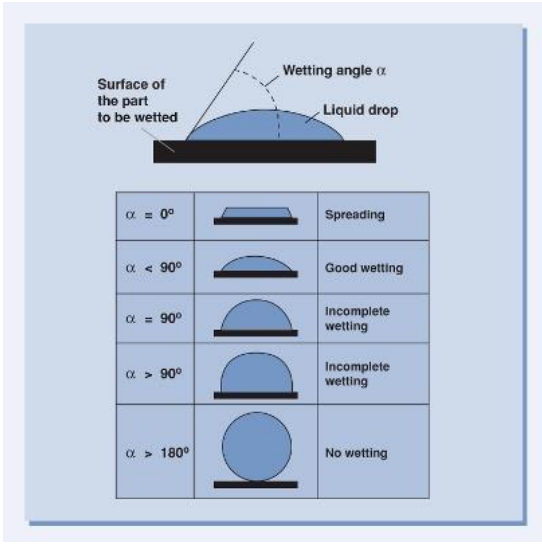


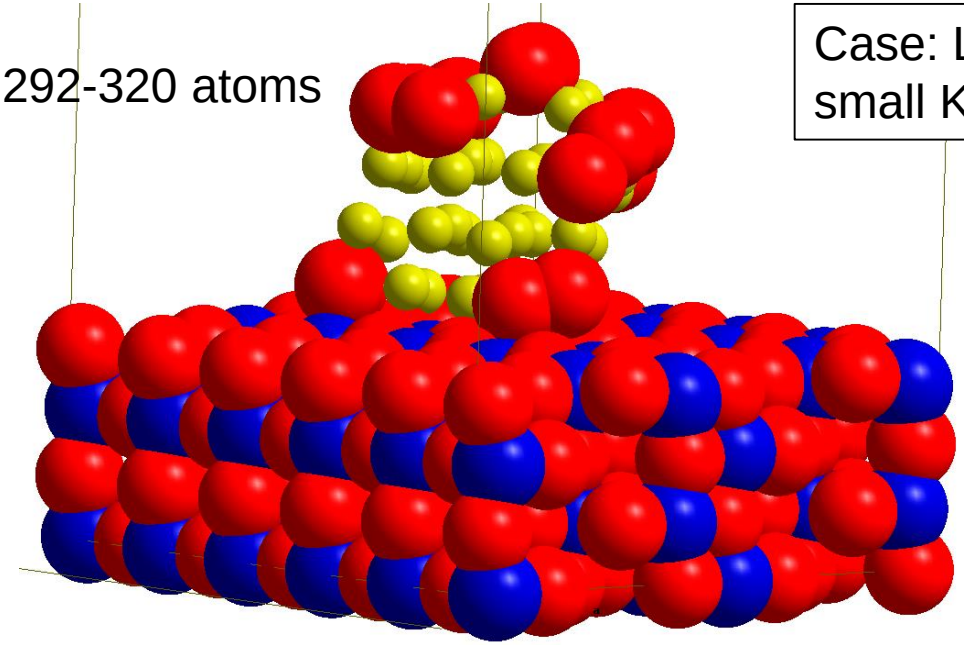

**Figure 16** – *Image STM* $300 \times 300\ nm^2$ *obtenues après une séquence d'évaporation Au puis Cu (a) et réalisée avec la méthode d'ombrage qui permet de synthétiser sur la même surface des NPs d'Au, de Cu et d'Au-Cu. Des changements se produisent pour les NPs de Cu après introduction de* $10^{-6}$ *mbar d'*$O_2$ *(b).*




The supported Cu nanoparticles disappear under $O_2$ pressure: Wetting phenomena

# Modeling Au-Cu : The effect of the reactive gas

292-320 atoms



Case: Large NBANDS/ small KPOINTS

```
POSCAR
   1.00000000000000
     19.1050000000000004    0.0000000000000000    0.0000000000000000
      0.0000000000000000   19.0590000000000011    0.0000000000000000
      0.0000000000000000    0.0000000000000000   29.1945000000000014
   Ti   O    Cu   O
    80   160    38    14
Selective dynamics
Direct
  0.0000000000000000  0.0512922599999968  0.0000000000000000   F   F   F
  0.0999996500000009  0.3012928400000021  0.0654401800000031   F   F   F
  0.0999996500000009  0.1762925499999994  0.0000000000000000   F   F   F
  0.0000000000000000  0.4262931299999977  0.0654401800000031   F   F   F
  0.0000000000000000  0.5512933099999984  0.0000000000000000   F   F   F
  0.0999996500000009  0.8012938899999966  0.0654401800000031   F   F   F
  0.0999996500000009  0.6762936000000010  0.0000000000000000   F   F   F
  0.0000000000000000  0.9262941799999993  0.0654401800000031   F   F   F
  0.1999994800000024  0.0512922599999968  0.0000000000000000   F   F   F
  0.2999991300000033  0.3012928400000021  0.0654401800000031   F   F   F
  0.2999991300000033  0.1762925499999994  0.0000000000000000   F   F   F
```

```
 Dimension of arrays:
   k-points           NKPTS =      5   k-points in BZ     NKDIM =      5   number of bands    NBANDS=   1458
   number of dos      NEDOS =    301   number of ions     NIONS =    292
   non local maximal  LDIM  =      6   non local SUM 21+1 LMDIM =     18
   total plane-waves  NPLWV = ******
   max r-space proj   IRMAX =   1731   max aug-charges    IRDMAX=   5046
   dimension x,y,z NGX =    96 NGY =   96 NGZ =  144
```

# Computational cost

Pour nos systèmes comprenant plus de 300 atomes, les tests de calculs (load balancing et communication bandwidth) ont montré un débordement de mémoire pour les calculs avec moins de 480 cœurs. Une fois nous avons déterminé le nombre de nœuds qu'il nous fallait pour des questions de mémoires, nous avons effectué des tests pour l'efficacité (malheureusement pas beaucoup de tests de peur de gaspiller nos heures) et voici un exemple des résultats :

Nanoparticule de Au-Cu couverte de $O_2$ et déposée sur un support TiO2 : 314 atomes, 1494 NBANDS

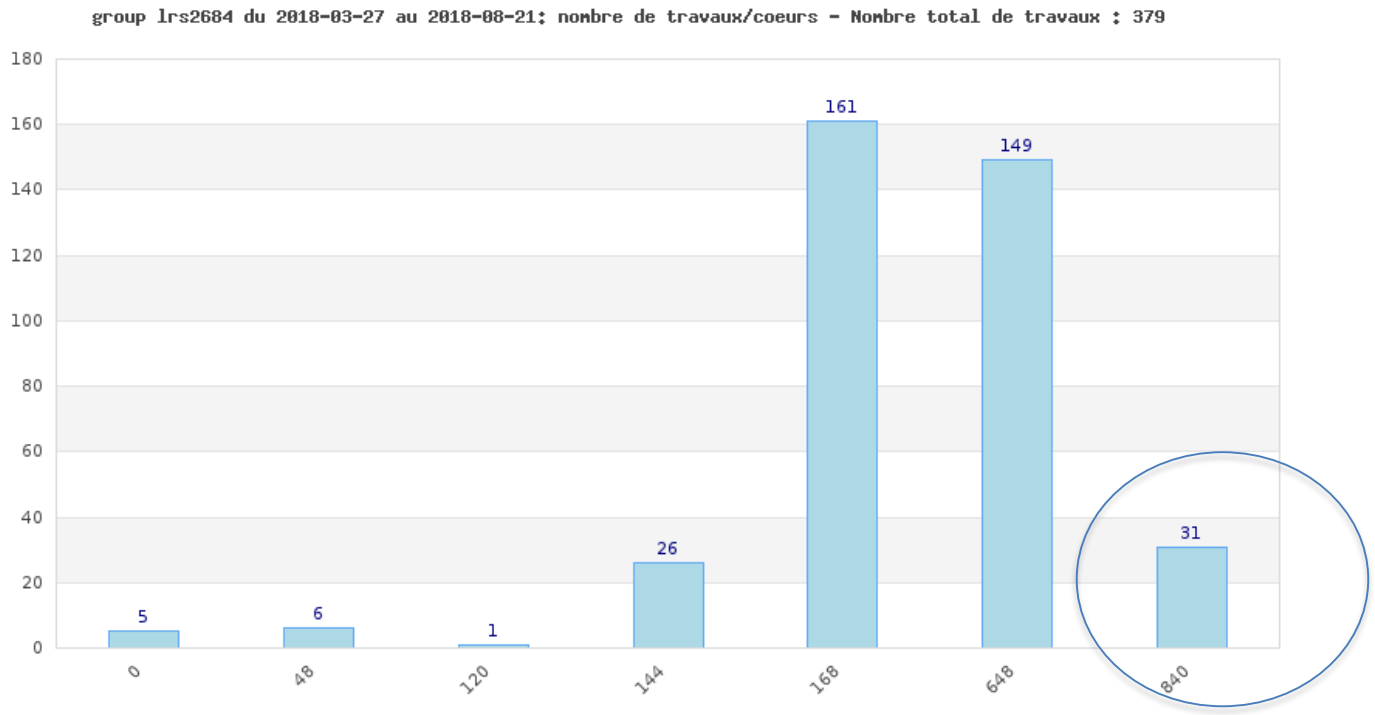
Sur 20 nœuds de 24 cœurs (480 cœurs) : un LOOP+ coute : 480*3891/3600 soit 518 cores.hours ...
LOOP+:  cpu time 3897.27: real time 3898.03
Sur 25 noeuds de 24 coeurs (600 coeurs) : un LOOP+ coute : 600*3562/3600 soit 593 cores.hours
LOOP+:  cpu time 3562.86: real time 3562.20
Sur 35 noeuds de 24 coeurs (840 coeurs): un LOOP+ coute : 840*996s/3600 soit 232 cores.hours
LOOP+:  cpu time  996.67: real time 1000.01

Un calcule qui converge c'est 147 LOOP+, ce qui fait 34 104 cores.hours

**Cela veut dire qu'un calcul sur 840 cœurs coute deux fois moins de ressources que le même calcul sur 480 cœurs.**

Pour plus de documentation sur le sujet voir le témoignage de Peter Larsson sur ce sujet.
https://www.nsc.liu.se/~pla/blog/2014/01/30/vasp9k/

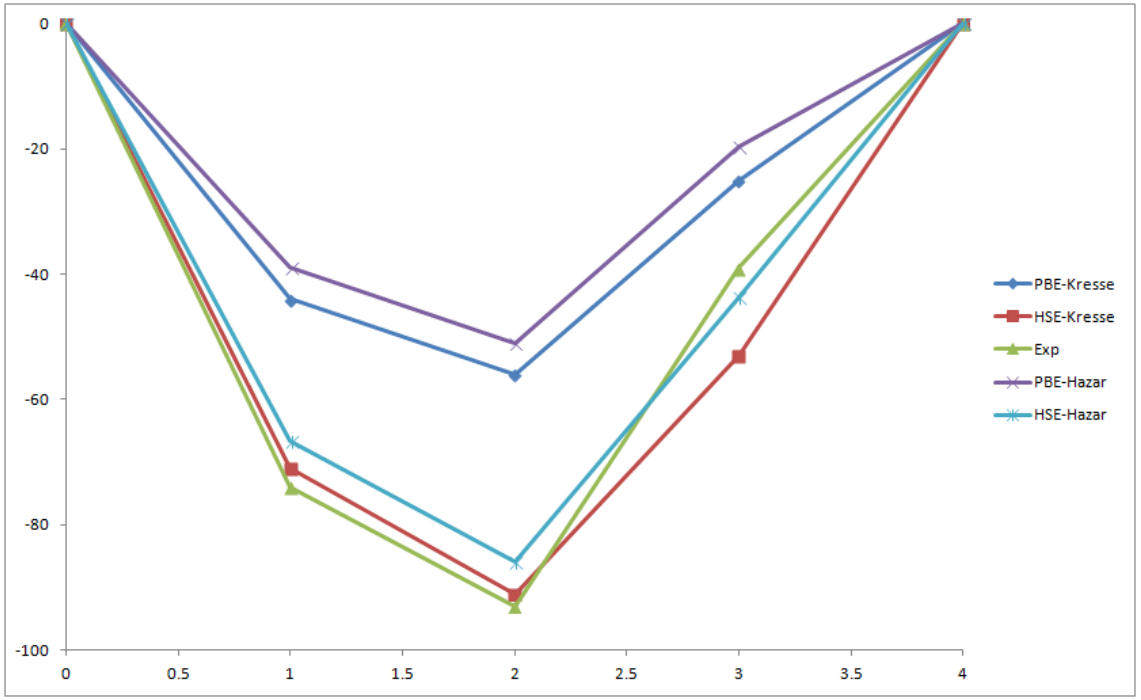
| configuration | Date de soumission | Classe | Partition | Code retour | walltime en (seconde) | Nbr Coeurs demandés | Nbr Coeurs comptabilisés | Mémoire reservée en Mo | secondes correpondantes | Heures correpondantes | Total /jour-semaine |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CSAu6Cu32_HFstep | 01/08/2017 14:00 | gros | all | COMPLETED | 42 883 | 840 | 840 | 102 400 | 36 021 720 | 10 006 | |
| CSAu6Cu32_HFterr | 01/08/2017 14:04 | gros | all | COMPLETED | 42 524 | 840 | 840 | 102 400 | 35 720 160 | 9 922 | |
| CSAu6Cu32_SFterr | 01/08/2017 14:10 | gros | all | COMPLETED | 82 400 | 840 | 840 | 102 400 | 69 216 000 | 19 227 | |
| RAAu8Cu30_HFstep | 01/08/2017 14:14 | gros | all | COMPLETED | 44 913 | 840 | 840 | 102 400 | 37 726 920 | 10 480 | |
| RAAu8Cu30_HFterr | 01/08/2017 16:26 | gros | all | COMPLETED | 33 719 | 840 | 840 | 102 400 | 28 323 960 | 7 868 | |
| | | | | | | | | | | | 57 503 |
| CSAu6Cu32_HFstep | 02/08/2017 12:31 | gros | all | COMPLETED | 9 880 | 840 | 840 | 102 400 | 8 299 200 | 2 305 | |
| CSAu6Cu32_HFterr | 02/08/2017 12:56 | gros | all | COMPLETED | 33 669 | 840 | 840 | 102 400 | 28 281 960 | 7 856 | |
| CSAu6Cu32_SFterr | 02/08/2017 13:01 | gros | all | COMPLETED | 25 218 | 840 | 840 | 102 400 | 21 183 120 | 5 884 | |
| RAAu8Cu30_HFstep | 02/08/2017 13:17 | gros | all | COMPLETED | 30 311 | 840 | 840 | 102 400 | 25 461 240 | 7 073 | |
| | | | | | | | | | | | 23 118 |
| CSAu6Cu32_HFstep | 03/08/2017 10:25 | gros | all | COMPLETED | 35 111 | 840 | 840 | 102 400 | 29 493 240 | 8 193 | |
| CSAu6Cu32_HFterr | 03/08/2017 10:31 | gros | all | COMPLETED | 6 888 | 840 | 840 | 102 400 | 5 785 920 | 1 607 | |
| CSAu6Cu32_SFterr | 03/08/2017 10:35 | gros | all | COMPLETED | 934 | 840 | 840 | 102 400 | 784 560 | 218 | |
| RAAu8Cu30_HFstep | 03/08/2017 10:38 | gros | all | COMPLETED | 4 342 | 840 | 840 | 102 400 | 3 647 280 | 1 013 | |
| RAAu8Cu30_HFterr | 03/08/2017 12:31 | gros | all | COMPLETED | 2 622 | 840 | 840 | 102 400 | 2 202 480 | 612 | |
| RAAu8Cu30_SFterr | 03/08/2017 12:35 | gros | all | COMPLETED | 995 | 840 | 840 | 102 400 | 835 800 | 232 | |
| | | | | | | | | | | | 11 875 |
| RAAu8Cu30_HFstep | 04/08/2017 12:12 | gros | all | COMPLETED | 801 | 840 | 840 | 102 400 | 672 840 | 187 | |
| RAAu8Cu30_HFterr | 04/08/2017 12:15 | gros | all | COMPLETED | 21 972 | 840 | 840 | 102 400 | 18 456 480 | 5 127 | |
| RAAu8Cu30_SFterr | 04/08/2017 12:25 | gros | all | COMPLETED | 848 | 840 | 840 | 102 400 | 712 320 | 198 | |
| Skin-Heart_AuCu3-Cu_Au8Cu3 | 04/08/2017 12:37 | gros | all | COMPLETED | 13 777 | 840 | 840 | 102 400 | 11 572 680 | 3 215 | |
| | | | | | | | | | | | 8 727 |
| | | | | | | | | | | | |
| | | | | | | | | | | | **101 223** |




31*10 000h = 310 000h (en 4mois et demi)

# Minimum energy structure of Au-Cu NPs: HSE06 vs. PBE

Calculation of the formation energies for the bulk

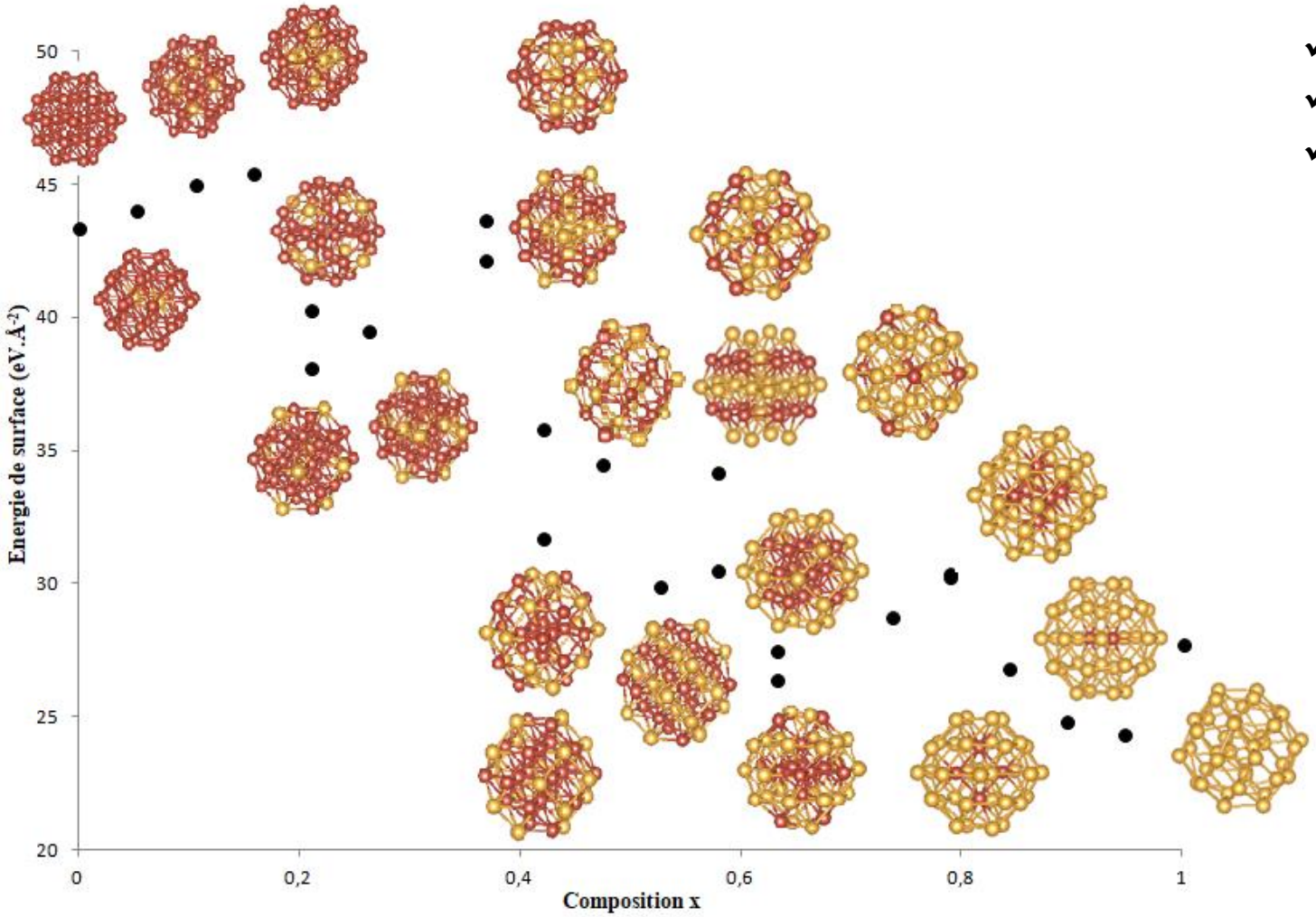



```
# ----------------
# Electronic minimization
# ----------------
  PREC   = NORMAL
#   ALGO   = Damped pour HSE06
 ALGO   = Damped
#  ALGO   = N
 PRECFOCK = Fast
  TIME = 0.4
#   EDIFF  = 1e-6
  EDIFF  = 1e-8
  ENCUT = 600
  LHFCALC = .TRUE.
  HFSCREEN = 0.2
# ----------------
# Ionic relaxation
# ----------------
  NSW    = 301
```

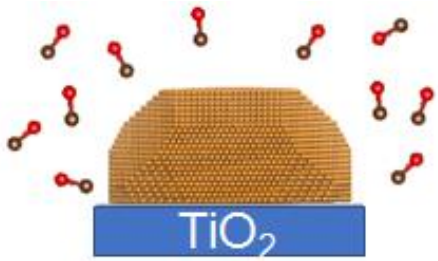
HSE06 gives results in very good concordance with experimental results

Stability of different AuCu alloy types:

- ✓Core_Shell
- ✓Regular_Alloy
- ✓Skin_Heart



➢Identification of the shape evolution of GNP under O2 gas: MSR model



# State of the art : Structure and morphology changes under working conditions

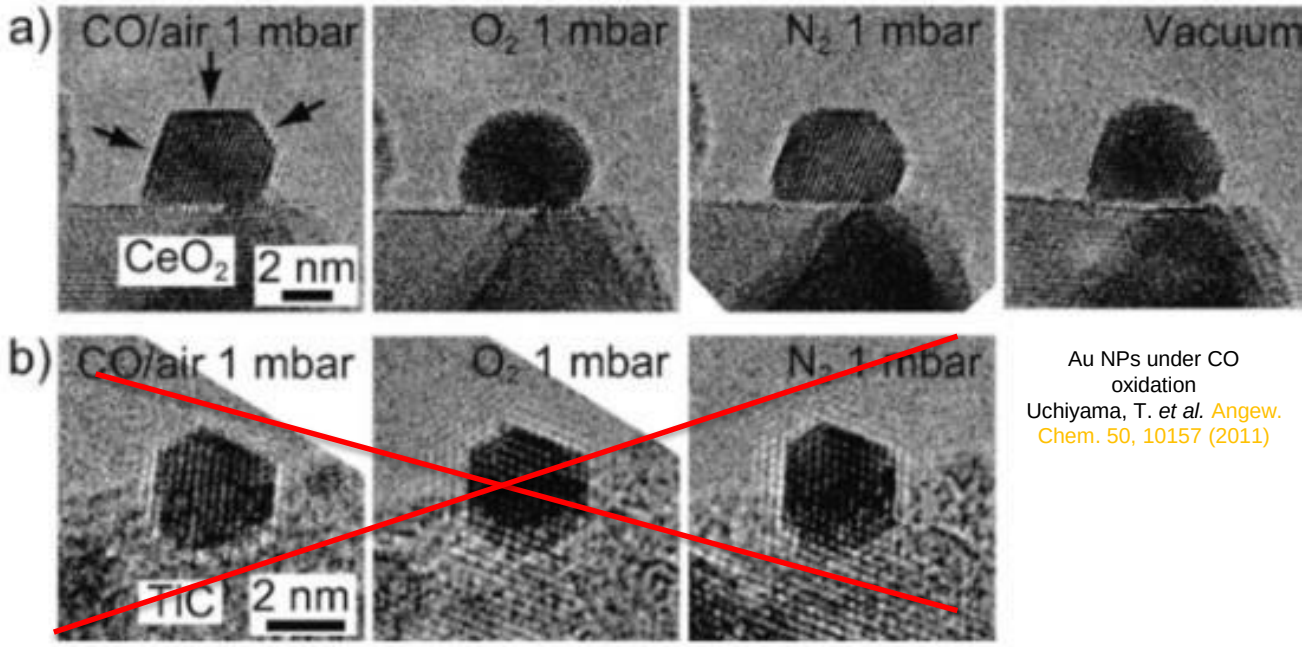
**GNP supported on $CeO_2$ in various environments at room temperature.**

⇒During CO oxidation in CO/air gas mixture, the GNP appeared to be faceted in the form of a stable polyhedron enclosed by the major {111} and {100} facets.

⇒Unexpectedly, the GNP behaved differently, and became rounded in pure $O_2$ gas. The GNP exhibited major facets in both inactive $N_2$ gas at 1 mbar and in vacuum.

⇒ GNPs supported on crystalline TiC remained polyhedral in all of the gas environments including pure $O_2$ gas.

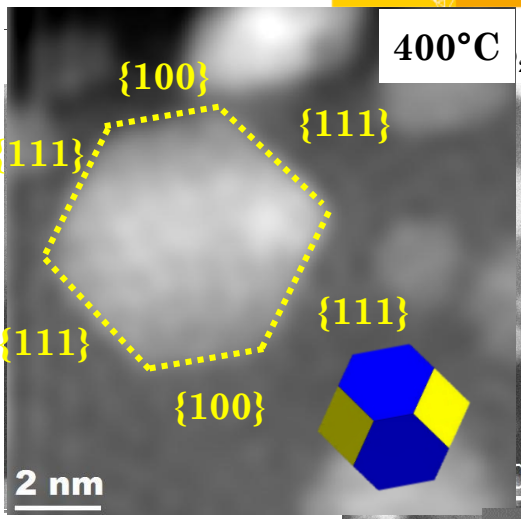
## Gold nanoparticles

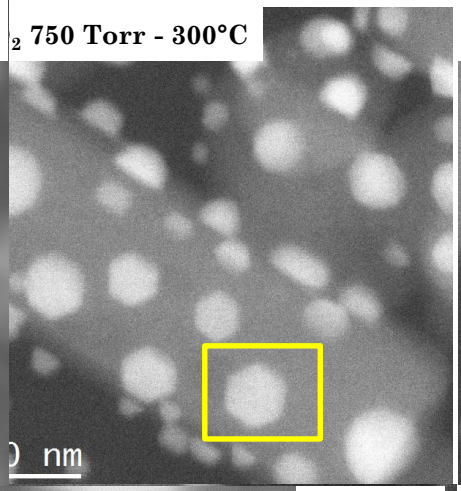


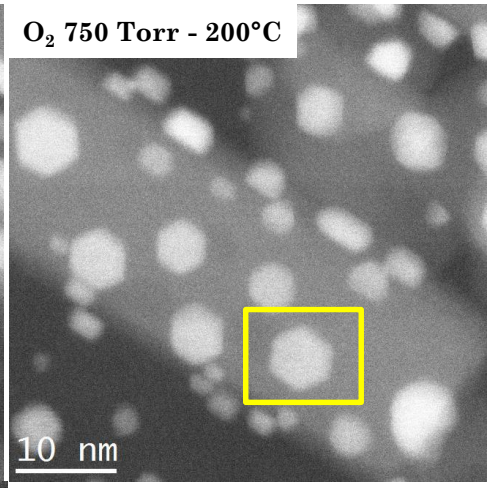

Au NPs under CO oxidation
Uchiyama, T. *et al.* Angew. Chem. 50, 10157 (2011)

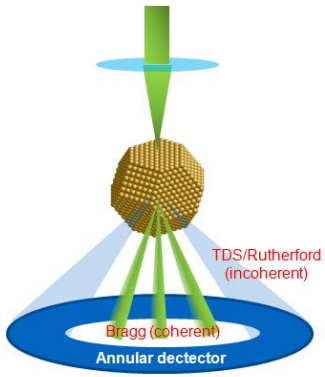
What could be the link between reactivity and morphology changes ?

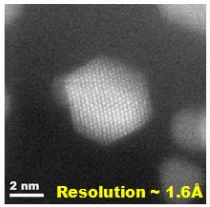
# State of the art : Structure and morphology changes under working conditions

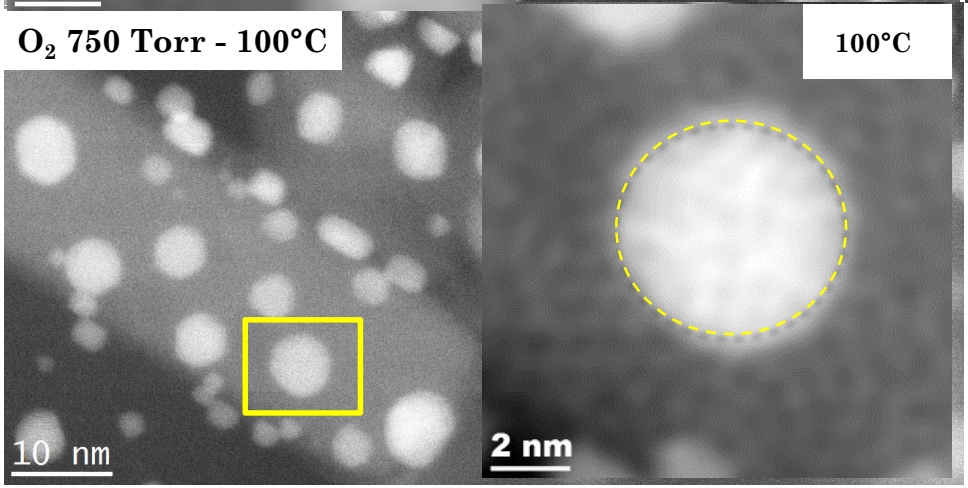



MPQ Jaysen Nelayah and Adrian Chmielewski

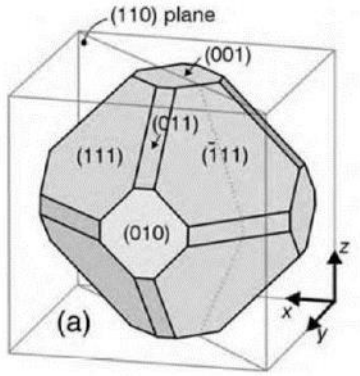
373 K < T < 273 K : Rounding of the NPs

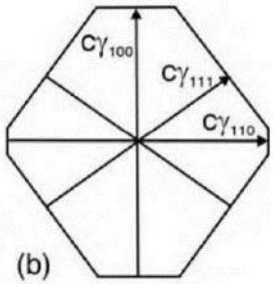
# Identification of the shape evolution of GNP under $O_2$ gas

## Equilibrium crystal shape: the Wulff construction

Under vacuum

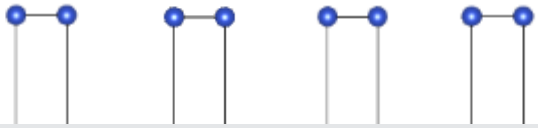
• The distance of a surface plane from the center-of-mass of the crystal is proportional to the surface energy of this plan



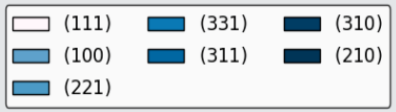



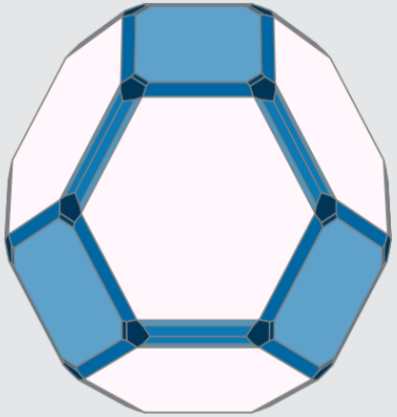

$d_{hkl} = C\,\gamma_{hkl}$ (c is a constant)

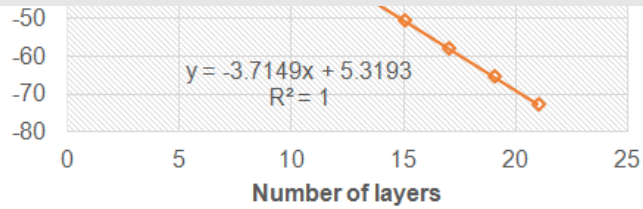
## DFT calculations of $\gamma_{hkl}$



| Miller Indices (hkl) | Surface Energy ($J/m^2$, $eV/Å^2$) | Area Fraction | Slab (CIF) |
|---|---|---|---|
| (111) | 1.31, 0.08 | 0.60 | |
| (332) | 1.43, 0.09 | 0.00 | |
| (322) | 1.45, 0.09 | 0.00 | |
| (100) | 1.47, 0.09 | 0.20 | |
| (221) | 1.48, 0.09 | 0.03 | |
| (331) | 1.52, 0.09 | 0.06 | |
| (311) | 1.54, 0.10 | 0.08 | |
| (110) | 1.56, 0.10 | 0.00 | |
| (321) | 1.58, 0.10 | 0.00 | |
| (310) | 1.59, 0.10 | 0.01 | |
| (210) | 1.60, 0.10 | 0.03 | |
| (320) | 1.62, 0.10 | 0.00 | |
| (211) | 1.63, 0.10 | 0.00 | |



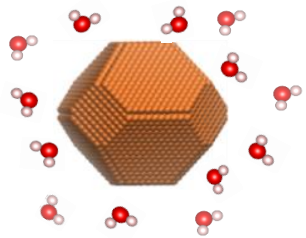






Fiorentini, V.; Methfessel, M. J. Phys.: Condens. Matter 1996, 8,6525

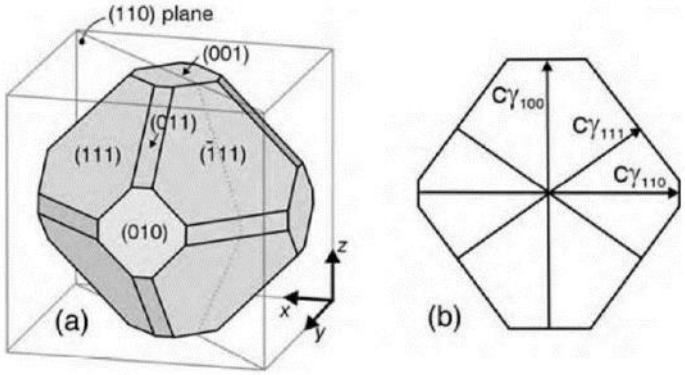
# Identification of the shape evolution of GNP under $O_2$ gas

## Equilibrium crystal shape: the Wulff construction



Under vacuum | Under gaz

- The distance of a surface plane from the center-of-mass of the crystal is proportional to the surface energy of this plan




$d_{hkl} = C\,\gamma_{hkl}$ (c is a constant)

$d^{int}_{hkl} = C\,\gamma^{int}_{hkl}$

$$\gamma^{int}_{hkl} = \gamma_{hkl} + \theta(E^{ads}_{hkl}/A^{at}_{hkl})$$

$\gamma_{hkl}$: surface energy under Vacuum (DFT)

$E^{ads}_{hkl}$: adsorption energy (DFT)

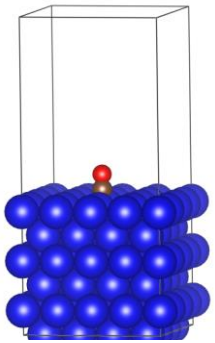
$A^{at}_{hkl}$: surface area per atom (DFT)

$\theta$ is $(T, P, E^{ads}_{hkl})$ dependent, described by Langmuir isotherm

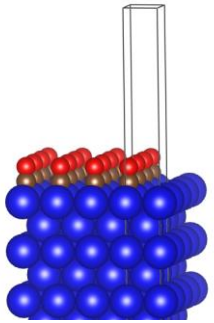
$$\frac{\theta}{1-\theta} = PK = P\,exp\left(-\frac{\Delta G}{k_b T}\right) = Pexp(-\frac{E^{ads}_{hkl} - T(S_{ads} - S_{gas})}{RT})$$

*B. Zhu, et al., Nano Lett. 16,* 2628, (2016)

# Identification of the shape evolution of GNP under $O_2$ gas



C(4x4) slab model



C(1x1) slab model

Including the **lateral interaction** between adsorbates

$\theta$ is described by the **F-G isotherm**:

$$PK = \frac{\theta}{1-\theta} e^{-c\theta},\ c = \frac{zw}{RT}$$

$$K = exp\left(-\frac{\Delta G}{k_b T}\right) = \exp\left(-\frac{E_{ads} - T\left(S_{ads} - S_{gas}\right)}{RT}\right)$$

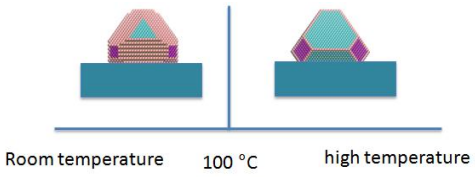
$z$: coordination number of the surface site

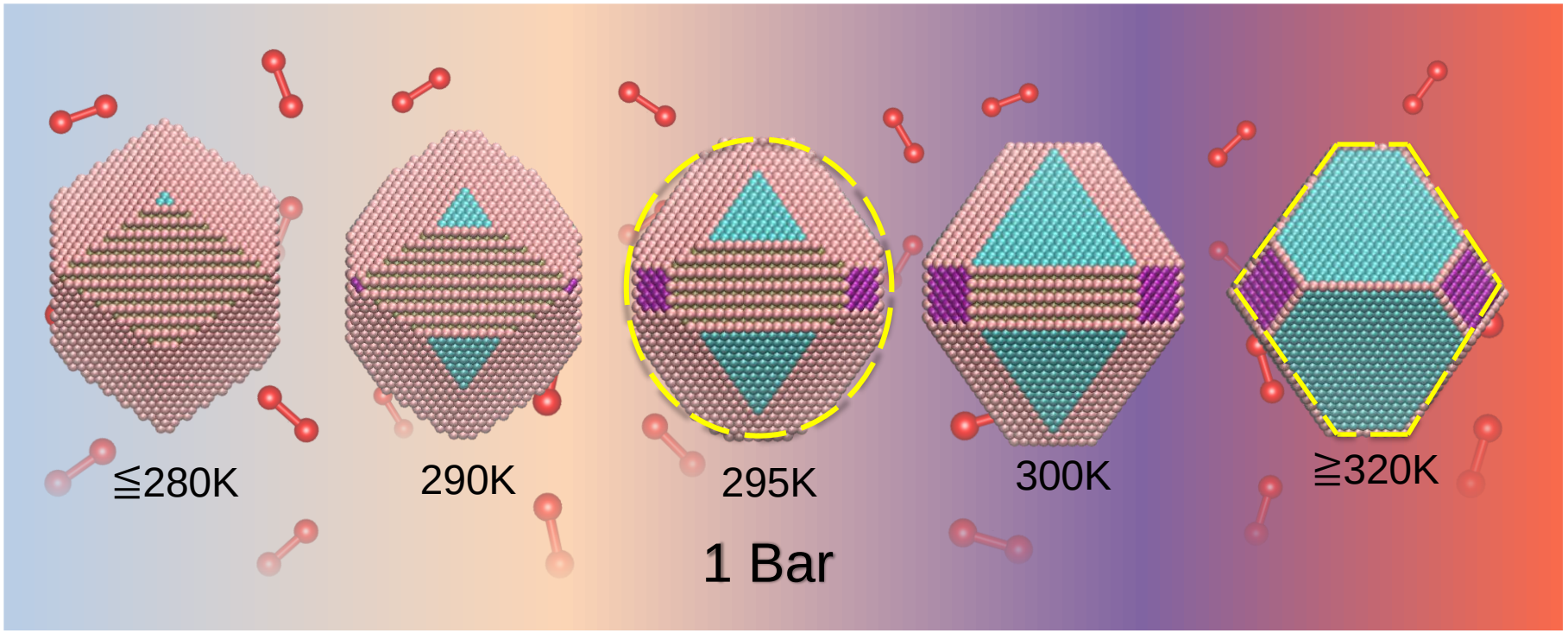
$w$: lateral interaction (DFT)

$$\gamma_{hkl}^{int} = \gamma_{hkl} + \theta\left(\left(E_{hkl}^{ads} - zw\theta\right)/A_{hkl}^{at}\right)$$

# Results: shape evolution of GNP under $O_2$ gas

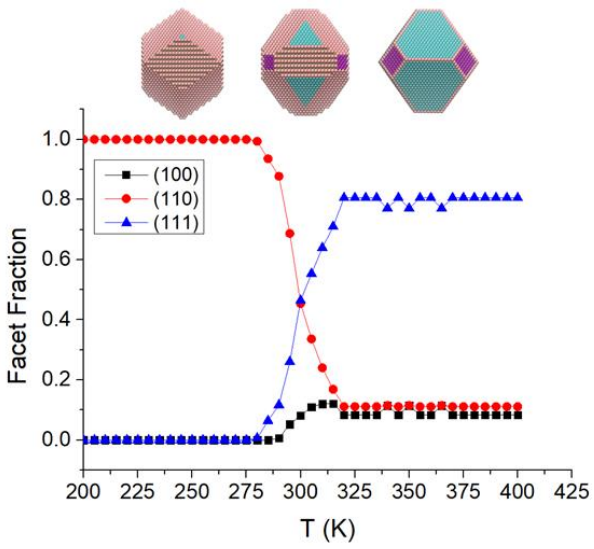
DFT-D3 calculations of Eads $O_2$ molecule ($d_{Au-Au}$=4.07 Å):
Au (111) =  0.00 eV
Au(100) = -0.22 eV
Au(110) = -0.34 eV



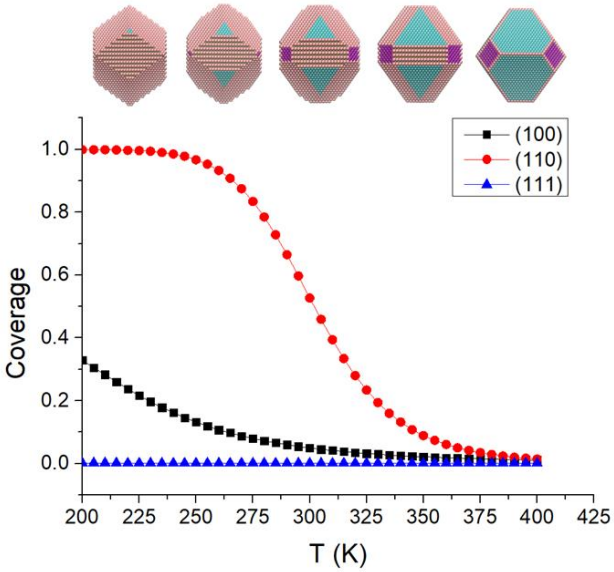



# Results: shape evolution of GNP under $O_2$ gas

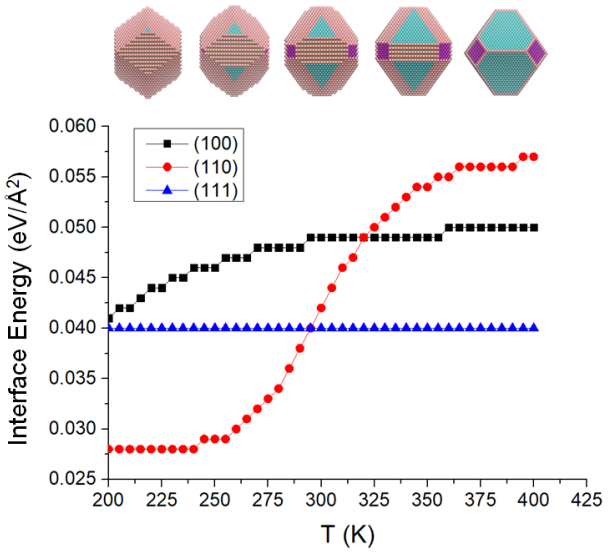
Facet fractions




$O_2$ coverage

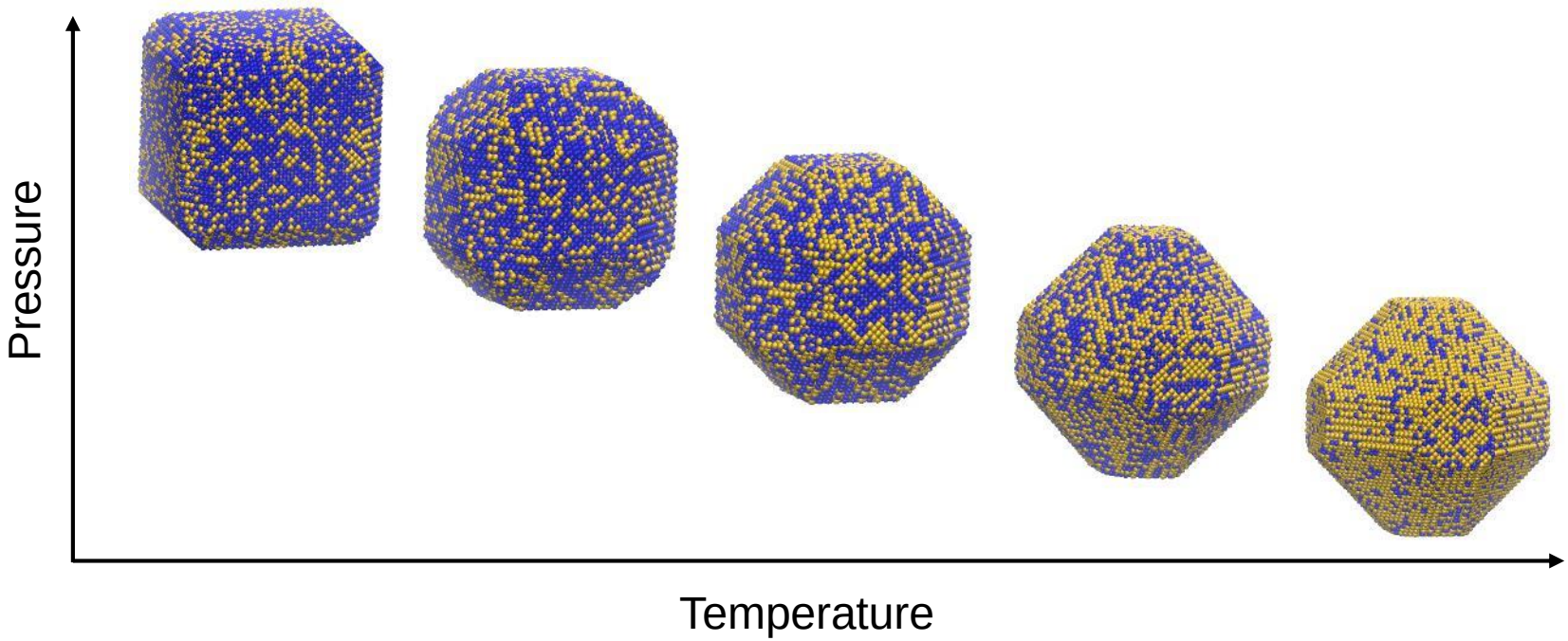



Interface energy



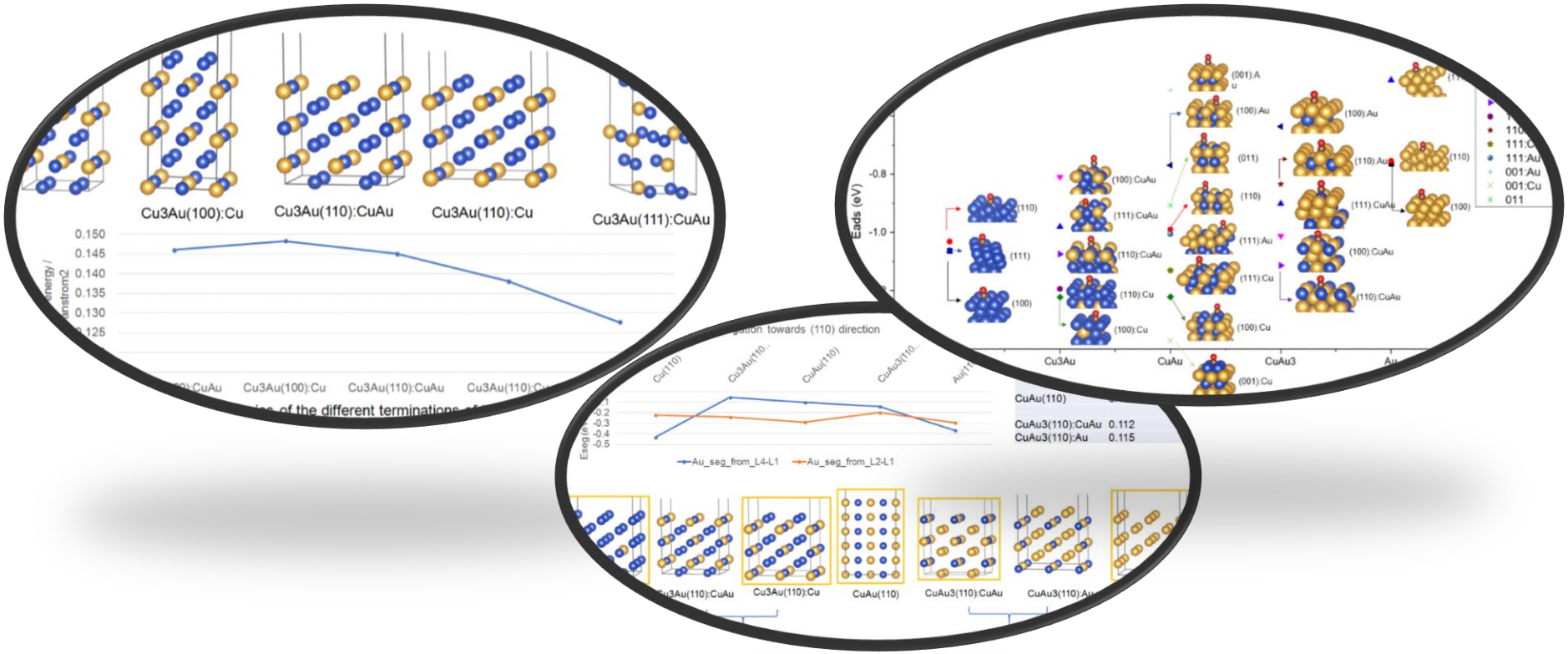

Evolution of active sites as a function of T

# Ongoing calculations: MSR model for nanoalloys




Ongoing work: Modeling Au-Cu NPs under CO gas

# Ongoing: MSR model for nanoalloys




$$\gamma_{alloy}^{int} = \underline{\gamma_{alloy}} + \underline{f(\Delta H_{seg})} + \underline{f(\Delta H_{ads})}$$

$\gamma_{alloy}^{int}$ *is* ***T, P, $E_{seg}$,*** *and* ***$E_{ads}$*** *dependent!*

# Methodology

```
SYSTEM =

ISTART = 0
ICHARG = 2
PREC = Normal
ISPIN = 2
GGA = PE
IVDW = 11

ENCUT = 400
EDIFF = 1E-5
NELM = 200
NELMIN = 8
ISMEAR = 0
SIGMA = 0.1

IBRION = 2
ISIF = 2
EDIFFG = -0.02
NSW = 500
ISYM = 0
POTIM = 0.2

ALGO = F
LDIAG = T
LREAL = Auto

LWAVE = F
LCHARG = F

NPAR = 2
KPAR=2
```

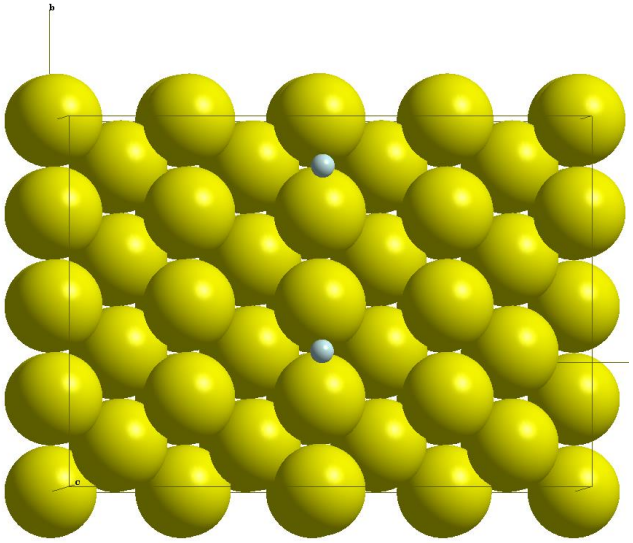
```
#!/bin/sh
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=28
#SBATCH --ntasks=56
#SBATCH --time=24:00:00
#SBATCH --exclusive
#SBATCH --output vasp.5.4.4.%J.out
#SBATCH --constraint=BDW28
##SBATCH --qos=bonus

module load purge

module load intel/18.0 openmpi/intel/2.0.1
module list

ulimit -s unlimited
export OMPI_MCA_coll_tuned_use_dynamic_rules=1
export OMPI_MCA_coll_tuned_alltoall_algorithm=4
export OMPI_MCA_coll_tuned_bcast_algorithm=6

srun --mpi=pmi2 -K1 --resv-ports
/home/alloy/VASP.5.4.4/vasp.5.4.4/bin/vasp_ncl"
```



Au(110): 96 atoms Au +2H

```
vasp.5.3.3 18Dez12 (build Mar 13 2017 10:09:23) complex

executed on          Linux_Intel date 2018.09.10  11:24:02
running on   56 total cores
distrk:  each k-point on   28 cores,    2 groups
distr:  one band on NCORES_PER_BAND=  14 cores,    2 groups
```

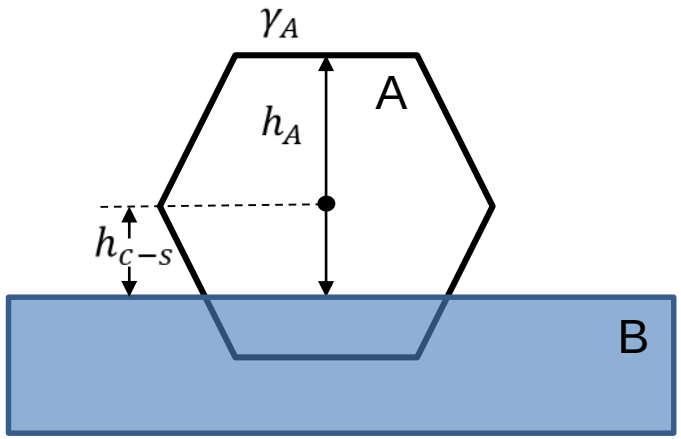
```
Dimension of arrays:
  k-points           NKPTS =      2   k-points in BZ     NKDIM =      2   number of bands    NBANDS=    682
  number of dos      NEDOS =    301   number of ions     NIONS =     96
  non local maximal  LDIM  =      6   non local SUM 21+1 LMDIM =     18
  total plane-waves  NPLWV = 564480
```

# Computational cost

| Job_description | Number of atoms | Nb cores/job | Nb runs (x24h) | Calculation time in cpu |
|---|---|---|---|---|
| Optimizations of surfaces : (111), (100), (110), (221), (331) | 54 et 108 atoms | 168/56 | 2-3 run per surface | 30 720 |
| Adsorption of $O_2$ on (111), (100), (110), (221), (331) | 64 et 118 atoms | 168/56 | 3-6 run per system | 46 080 |

# MSR model for Supported Metal NPs

- **Wulff-Kaischew theorem:** the distance from the center to the contact surface $h_{AB}$ is proportional to the contact surface energy: $\gamma_{c-s}$




$$\frac{\gamma_A}{\gamma_{c-s}} = \frac{h_A}{h_{c-s}} \qquad \gamma_{c-s} = \gamma_{AB} - \gamma_B$$

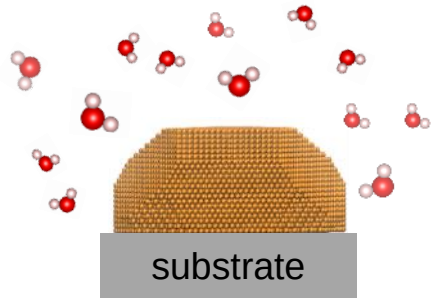
$$\gamma_{AB} = \gamma_A + \gamma_B - E_{adh}$$

$\gamma_{AB}$: interface energy between A and B.

$E_{adh}$: adhesion energy

- **Wulff-Kaischew in the environment:**

$$\gamma^{int}_{A(hkl)} = \gamma_{A(hkl)} + \theta_A \frac{E^{ads}_{A(hkl)}}{A^{at}_{A(hkl)}}$$



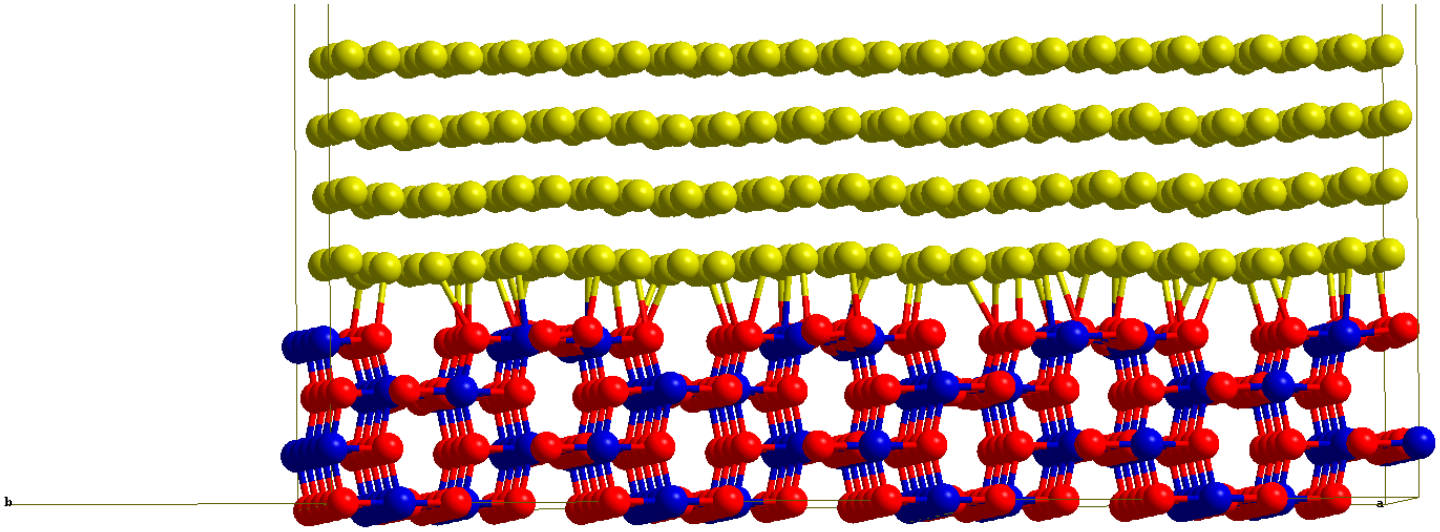

$$\gamma^{E}_{c-s} = \gamma_{AB} - \gamma^{int}_{B(hkl)} = \gamma_{AB} - \gamma_B - \left(\frac{\theta_B E^{ads}_B}{A^{at}_B}\right) = \gamma_A - E_{adh} - \left(\frac{\theta_B E^{ads}_B}{A^{at}_B}\right)$$

$\theta_A$ , $\theta_B$ are described by Langmuir isotherm

# DFT calculations of system with 700 atoms !! YES VASP CAN!

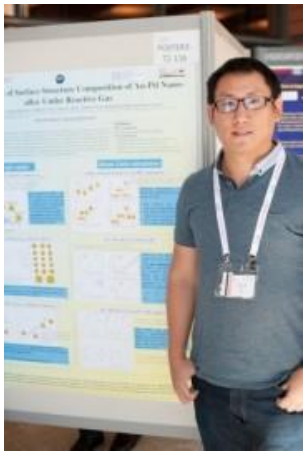
Adhesion energy calculations:
Size mismatch ⟹ (13x3) unit cell for Au(111)
696 atomes
NBANDS=3920
K=gama
35 nodes/840 cores

30 LOOP+ = 4752 core.h



# Acknowledgements

**Jun Meng (2018-2019)** (Institut Charles Gerhardt, Montpellier)



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**Marwa Dhifallah (2015-2018)** (Institut Charles Gerhardt, Montpellier)

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CHEMISTRY: MOLECULES TO MATERIALS