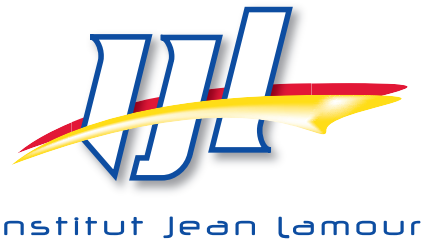
Structure de la surface (010) de $Al_{13}Fe_4$

Émilie Gaudry

Institut Jean Lamour / École des Mines de Nancy

UMR 7198 CNRS - Université de Lorraine

http://gaudry6.blog.univ-lorraine.fr



Institut Jean Lamour - UMR7198

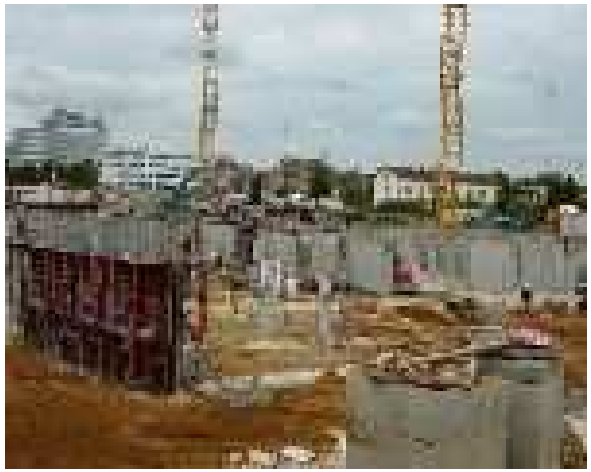
IJL, UMR 7198 CNRS - Université de Lorraine

$\simeq$ 450 personnes

dont $\simeq$ 180 chercheurs / enseignants chercheurs

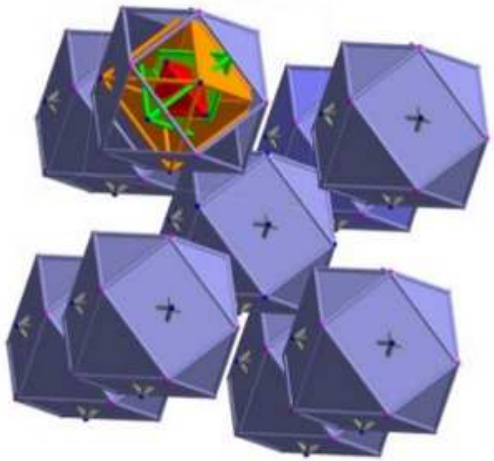
4 départements:

- Physique de la Matière et des Matériaux
- Chimie et Physique des Solides et des Surfaces
- Science et Ingénierie des Matériaux et Métallurgie
- Nanomatériaux, électronique et vivant

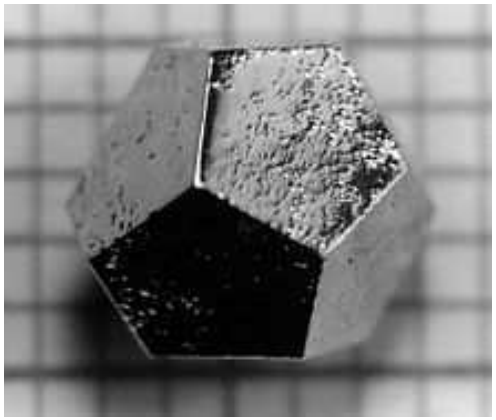


Équipe Métallurgie et Surfaces

- 5 permanents: Jean-Marie Dubois, Vincent Fournée, Julian Ledieu, Marie-Cécile de Weerd, Émilie Gaudry.
- Alliages métalliques complexes: volume, interfaces, surfaces, films minces
- Moyens: Cluster de calcul de l'IJL / IDRIS + plateformes expérimentales



Al_4Cu_9



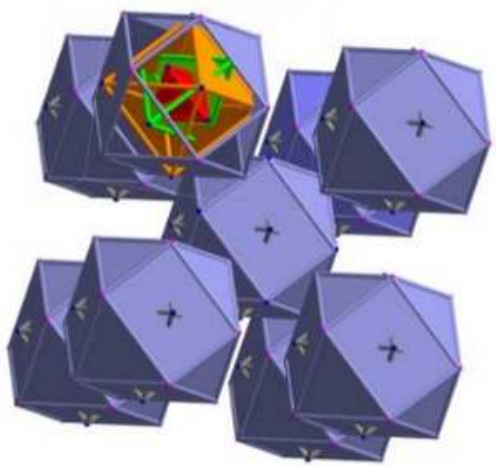
Quasicrystal HoMgZn

Introduction

Structure de la surface (010) de $Al_{13}Fe_4$,

approximant des quasicristaux décagonaux (d-QC)

- Réactivité chimique: semi-hydrogénation de l'acétylène
- Interaction de la structure 3D du système massif avec la structure 2D de surface



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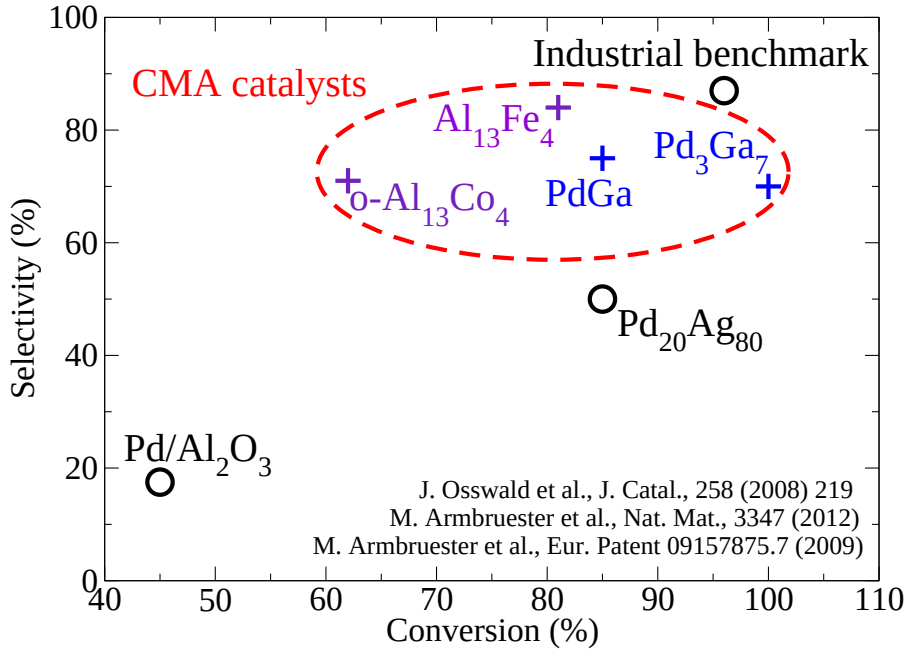

- Une description détaillée de la structure de surface est nécessaire pour la compréhension des propriétés de surface

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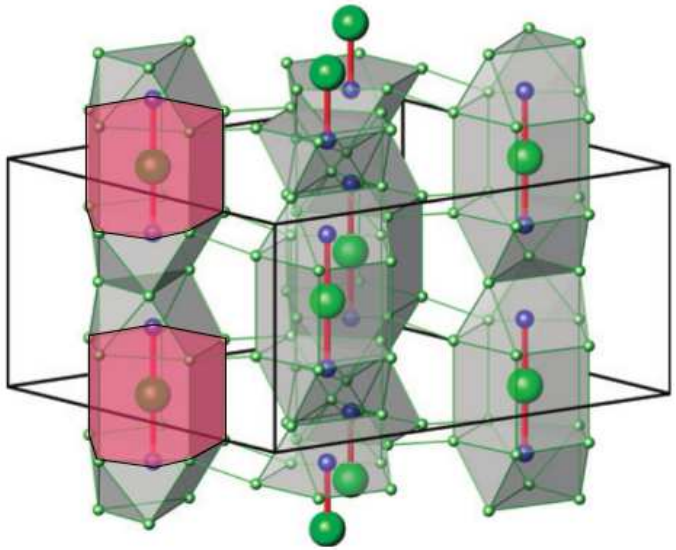
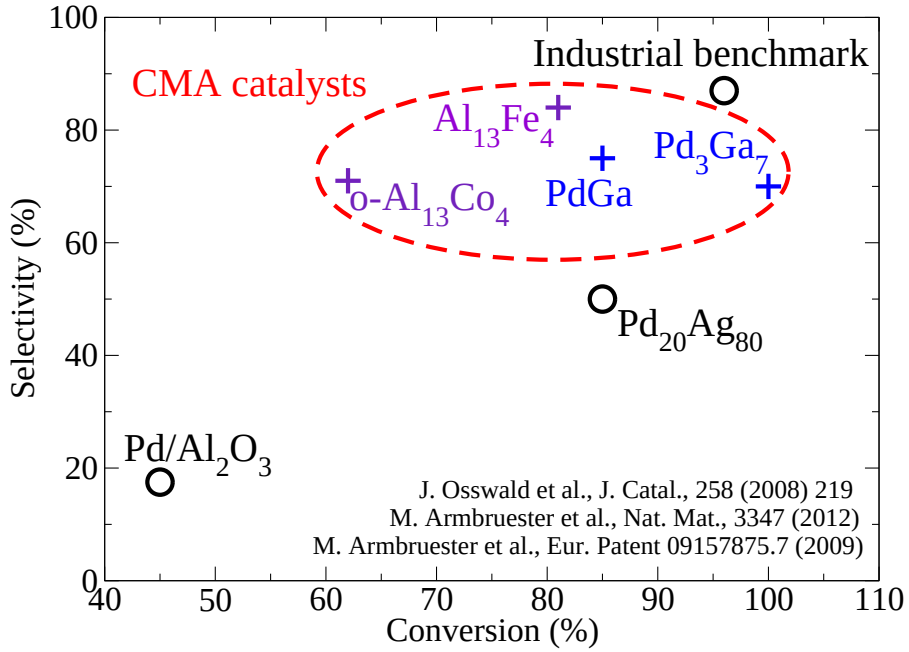
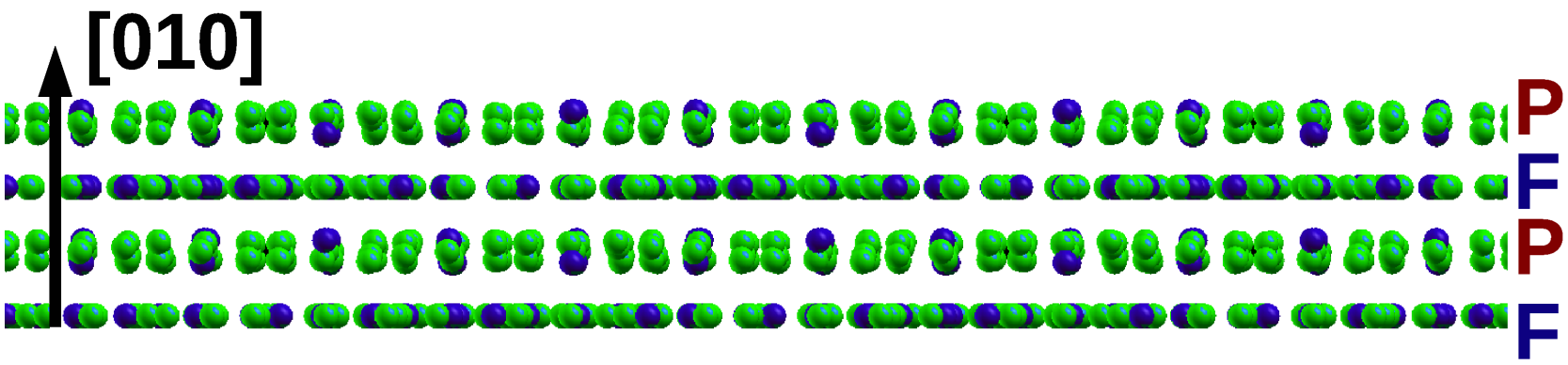


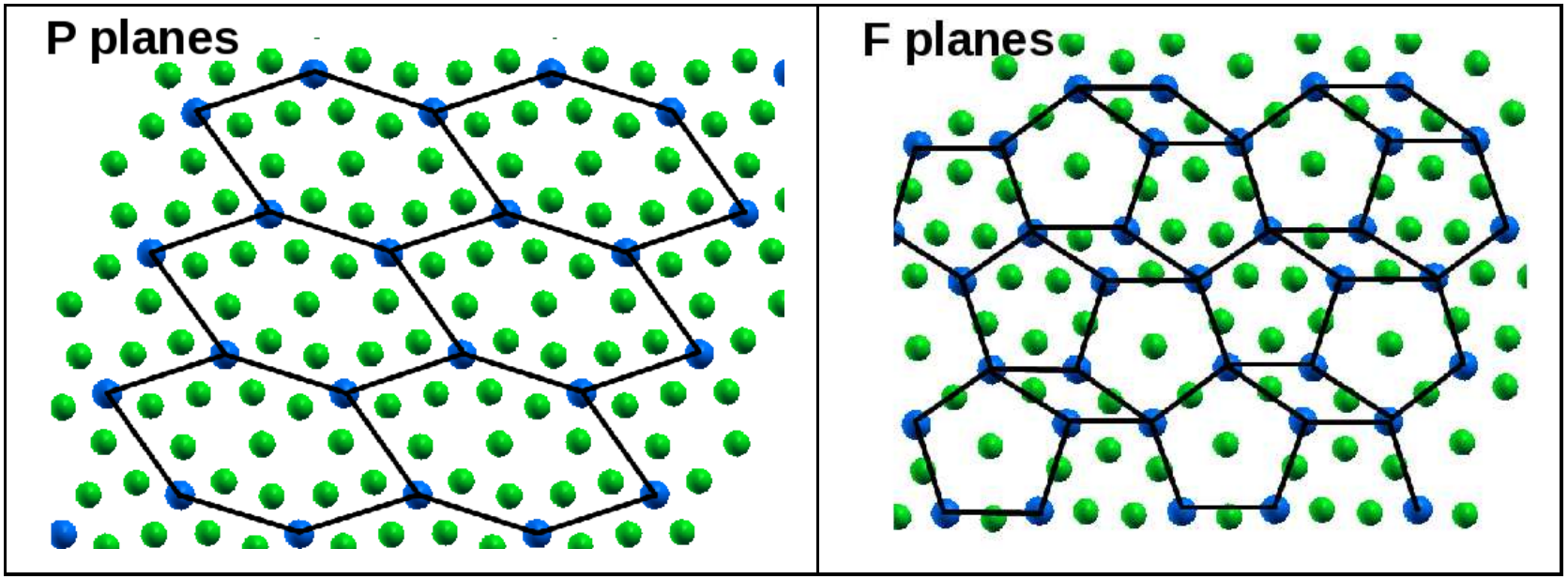


- Une description détaillée de la structure de surface est nécessaire pour la compréhension des propriétés de surface

Structure of the decagonal approximant $Al_{13}Fe_4$

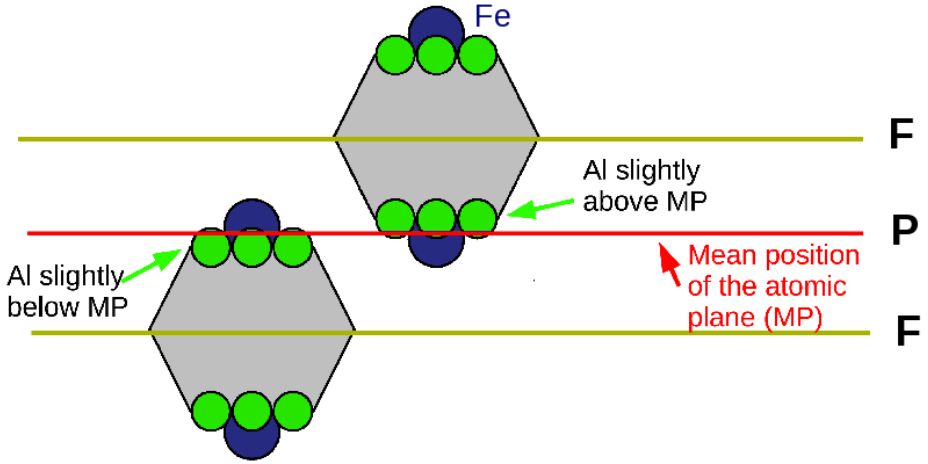
- Crystal structure $C2/m$(mC102): $a = 15.492$ Å, $b = 8.078$ Å, $c = 12.471$ Å, $\beta = 107.69(1)^0$
- Stacking of flat (17 Al + 8 Fe) and puckered (22 Al + 4 Fe) atomic layers along the [010] direction

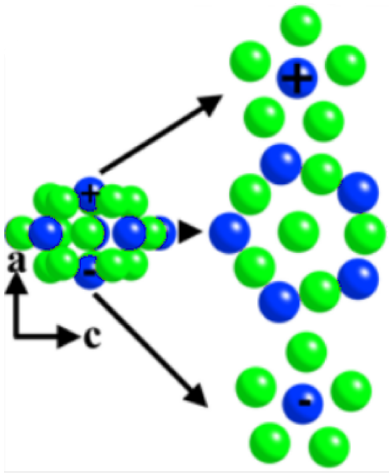


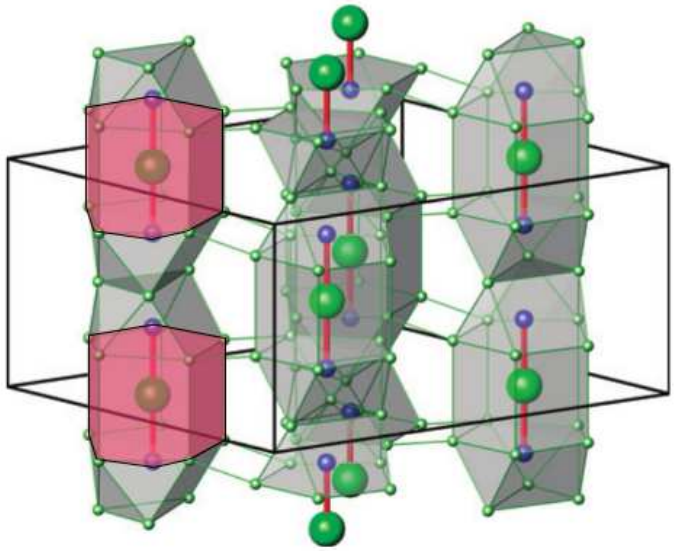


Structure of the decagonal approximant $Al_{13}Fe_4$

- High symmetry atomic clusters (PB) as structural building blocks







PB = 23 atom cluster (16 Al + 7 Co)

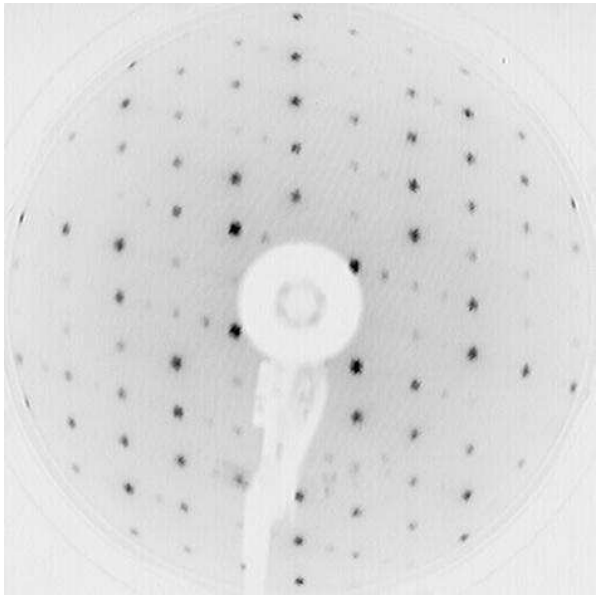
Columns of PB altern. with junction layer

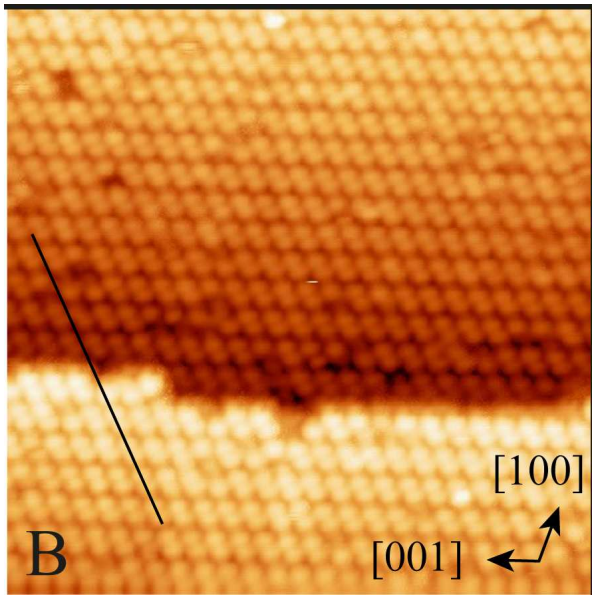
Fe-Al-Fe molecule aligned along [010]

Grin *et al.*, *Z. Kristallogr.*, **209** (1994) 479

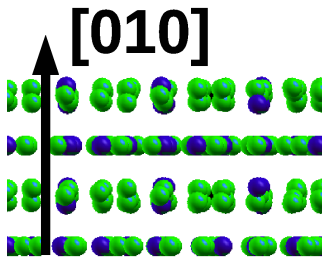
Grin *et al.*, CMA, Wiley (2010).

$Al_{13}Fe_4$: Experimental Results

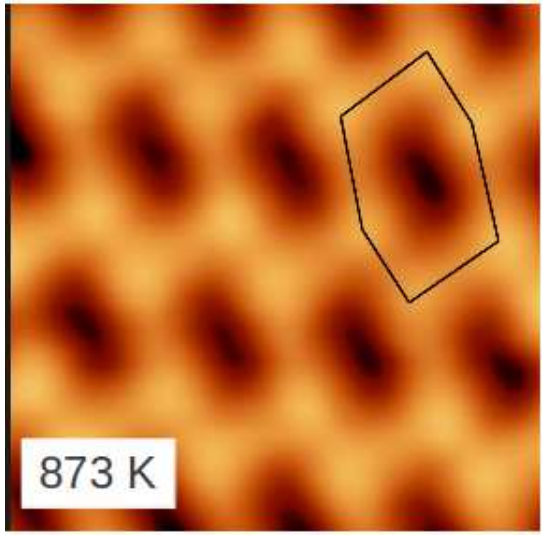




- Single crystal by the Czochralski method (P. Gille et al, Crystal research and technology, **43** (2008) 1161)
- Surface preparation: cycles of Ar^+ bombardment / annealing
- No surface reconstruction (From LEED $\frac{a}{c} = 1.24$, in agree. with Grin et al., Z. Kristallogr., **209** (1994)
- Angle-dependent XPS (not shown here) demonstrates that surface segregation can be disregarded.
- Step height measurements ($\simeq b/2$) highlight a surface plane selection



$Al_{13}Fe_4$: Surface Plane Selection



Step height measurements ($\simeq b/2$)

highlight a surface plane selection

High corrugation

Surface atomic density

Surface composition

} Selection of the P plane

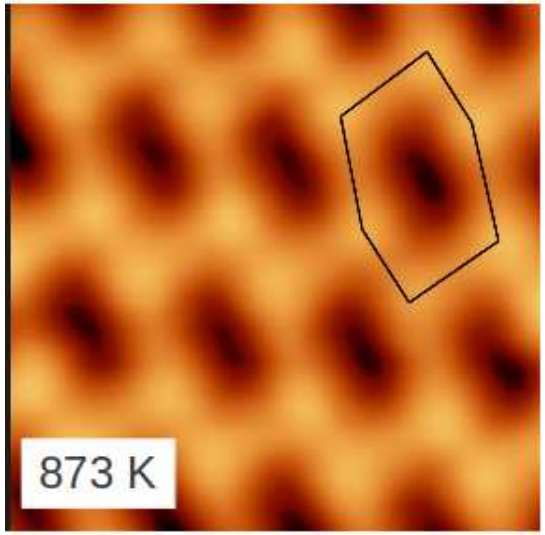
DFT calculations (PAW-PBE)

Calc.	Exp.
a = 15.43 Å	a = 15.49 Å
b = 8.03 Å	b = 8.08 Å
c = 12.43 Å	c=12.47 Å
β = 104^0	β = 107^0

8-layers asymetric slabs

Tersoff-Hamann approximation

$Al_{13}Fe_4$: Surface Plane Selection



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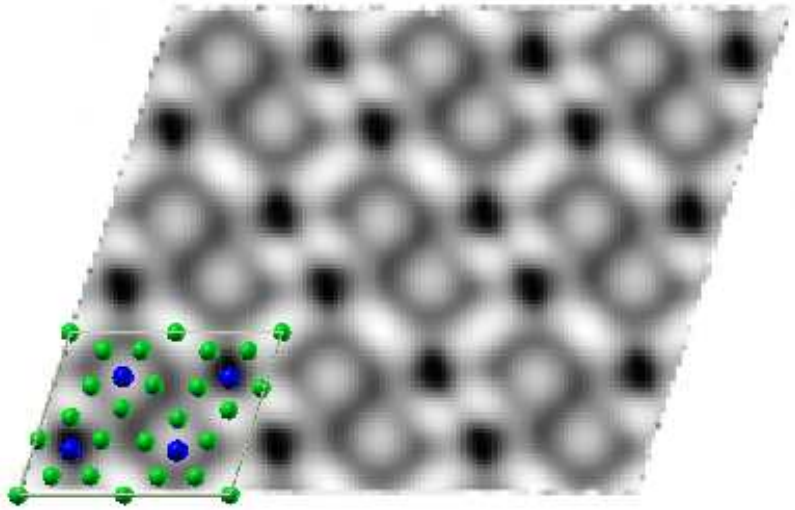
Complete P plane



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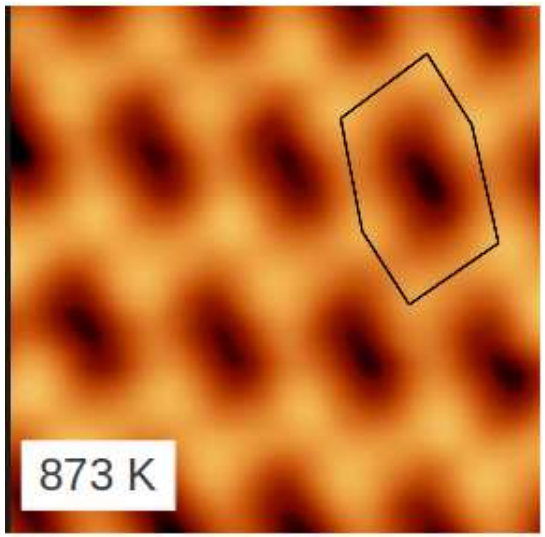
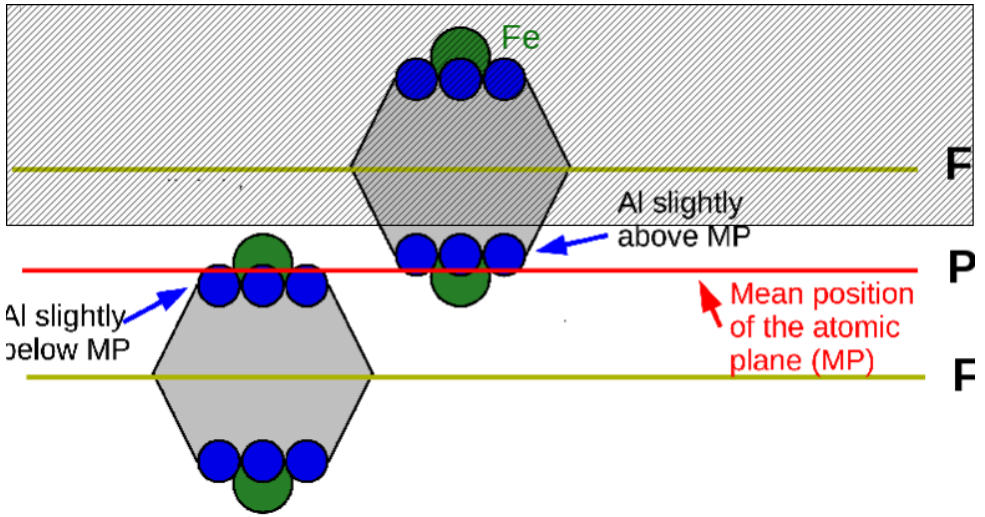
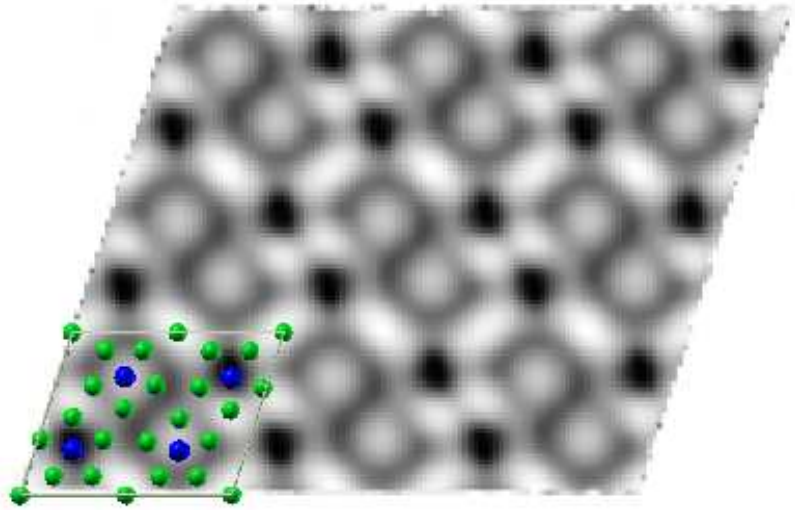
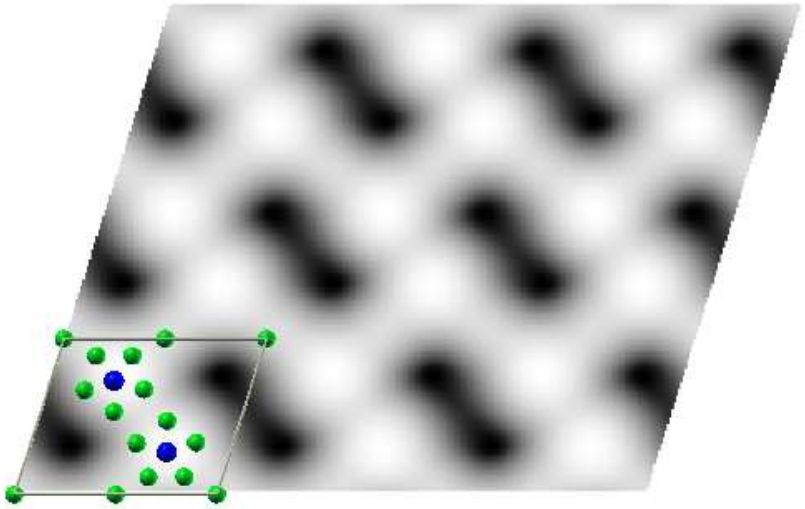
8-layers asymetric slabs ($\simeq$ 200 at.)

Tersoff-Hamann approximation

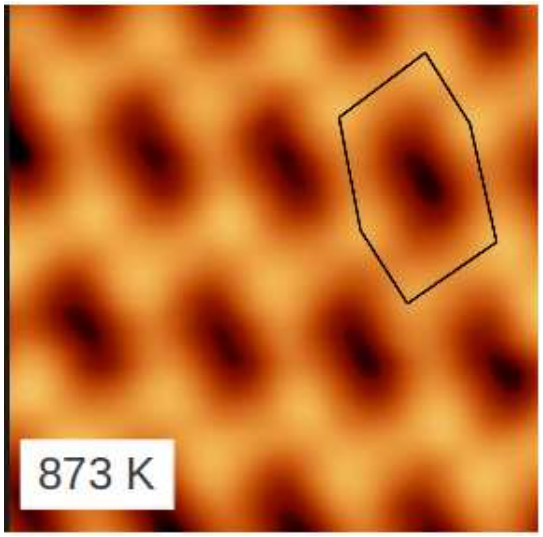
$Al_{13}Fe_4$: Surface Plane Selection

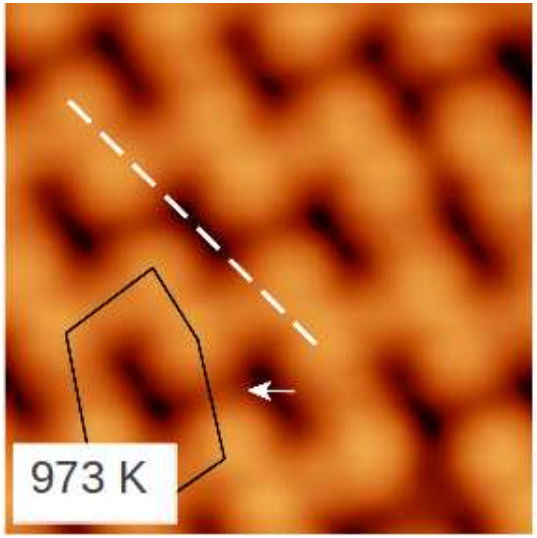




Complete P plane	Incomplete P plane
	

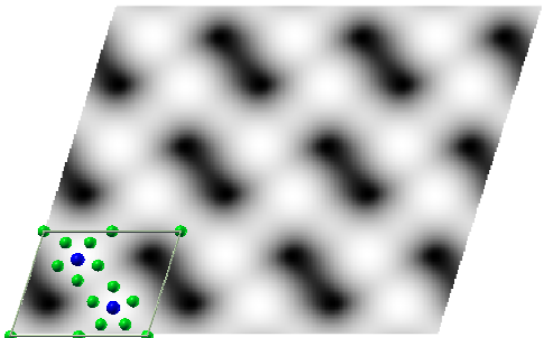
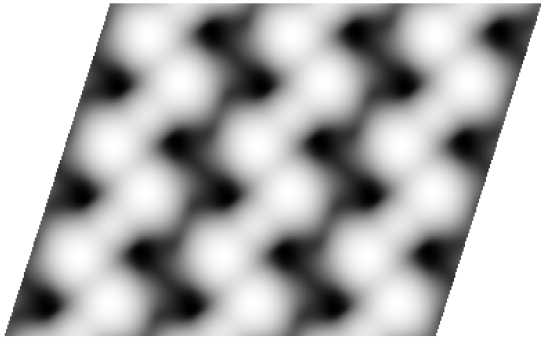
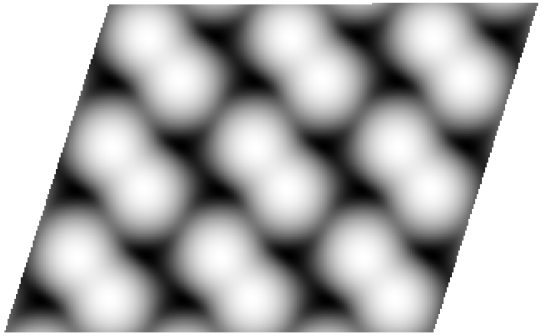
High Resolution STM



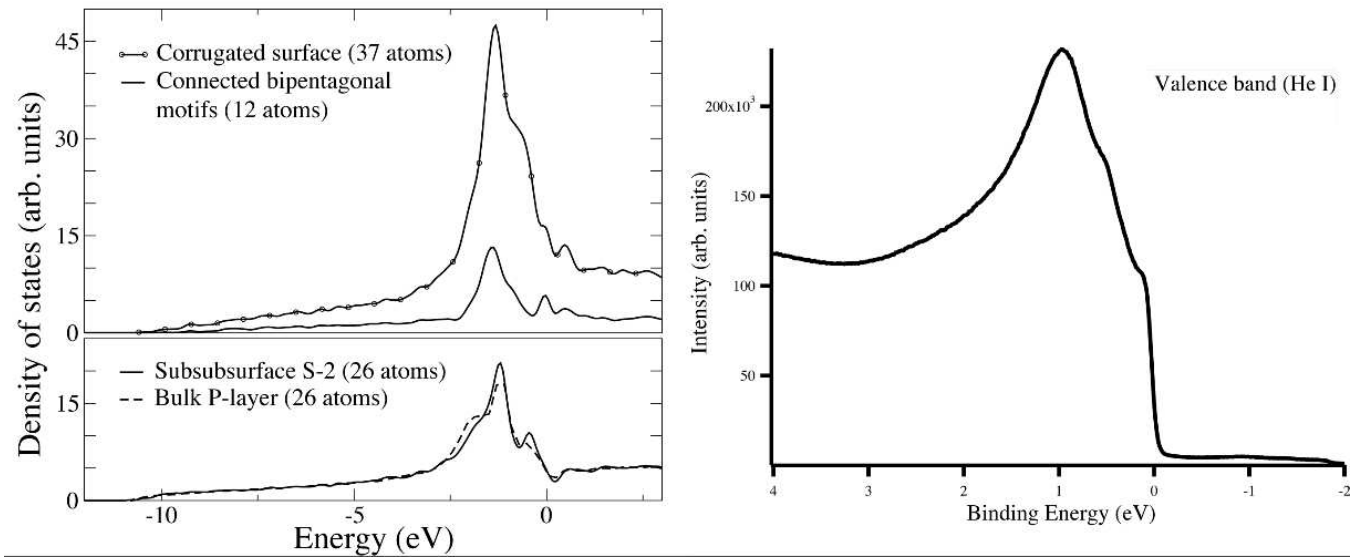


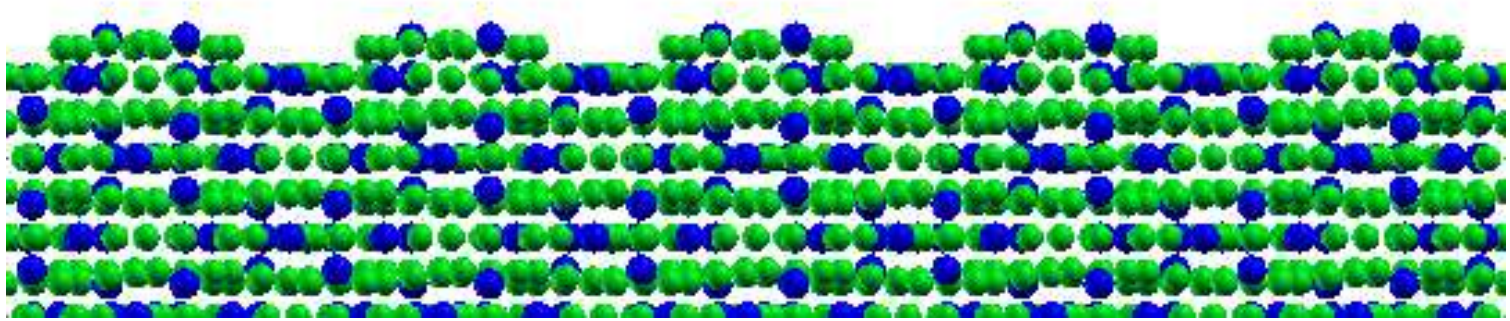
Exp. STM images (5×5 nm)

Calc.: Desorption of surface Al glue atoms $\simeq$ 0.6 eV ($\mu_{Al} = \mu_{Al^{bulk}}$)

		
E_0	$E_1 = E_0 + 4.40 + \mu_{Al}$	$E_1 + 4.33 + \mu_{Al}$

$Al_{13}Fe_4$: Surface Electronic Structure





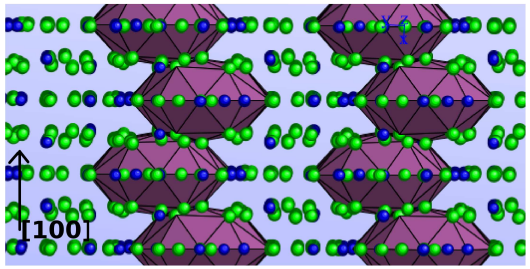
- High corrugated surface (partial exposition of the F subsurface layer)
- DOS dominated by the Fe d-states
- Consistency between the experimental data and the calculated DOS

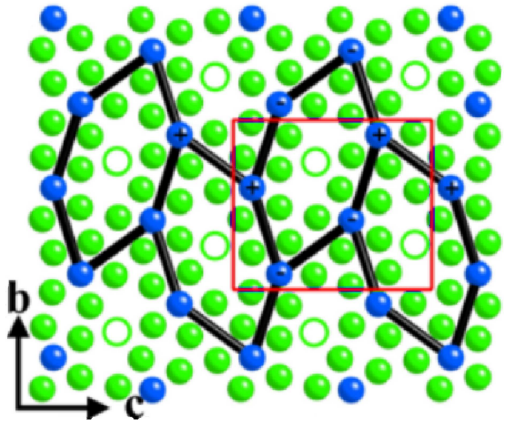
Conclusion

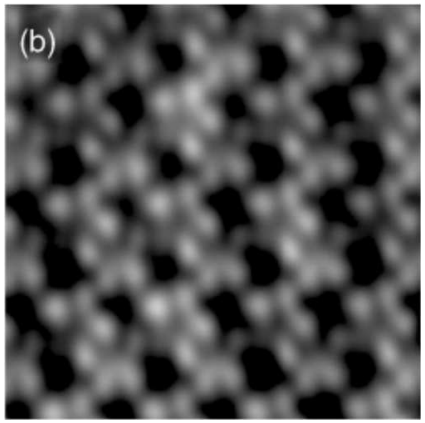
- Surface plane selection: Surfaces form at specific bulk planes charact. by a high atomic density and a high content of the lowest surf. energy element / Consistent with the “plane selection rules” for QCs
- Interplay of the 3D cluster structure with the 2D surface:

Compound	Surface	Pure Bulk trunc.	3D struct. preserv.	Ref.
$Al_{13}Fe_4$	built from the P layer High corrugated surface	no	yes	PRL (2013)
o-$Al_{13}Co_4$ (Czochralski)	Built from the P layer Pure Al plane as surf. term.	almost yes without surf. Co at.	no	PRB 84 (2011) 085411

o-$Al_{13}Co_4$ $Pmn2_1$ (oP102)







- Reactivity: active sites might be the isolated Fe atoms protruding above pentagonal motifs

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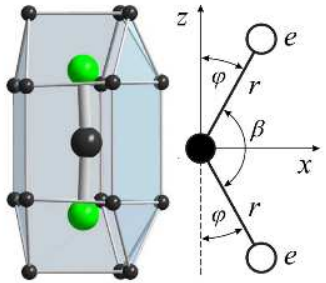
Role of the chemical bonding:

$$E^{AlTM}_{strength} = E^{lac-AlTM}_{f} - (E^{lac-Al}_{f} + E^{lac-TM}_{f})$$

$$E^{AlCo}_{strength} = -0.31eV$$

$$E^{AlFe}_{strength} = -0.66eV$$



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Aknowledgments

S. Alarcón Villaseca, L. Serkovic Loli, R. Addou, J. Ledieu, M.-C. de Weerd, V. Fournée, J.-M. Dubois

Institut Jean Lamour, École des Mines, 54042 Nancy, France

P. Gille and M. Hahne

Ludwig-Maximilians Universität, Theresienstr. 41, München, Germany

Y. Grin

Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, Dresden, Germany

Thank you for your attention!