DE LA RECHERCHE À L'INDUSTRIE

(Paris, France)

Saclay

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Magneto-Crystalline anisotropy of Fe, Co and Ni slabs : A benchmark from DFT and Tight-Binding models

Ludovic Le Laurent[1], Cyrille Barreteau[1], Troels Markussen[2]

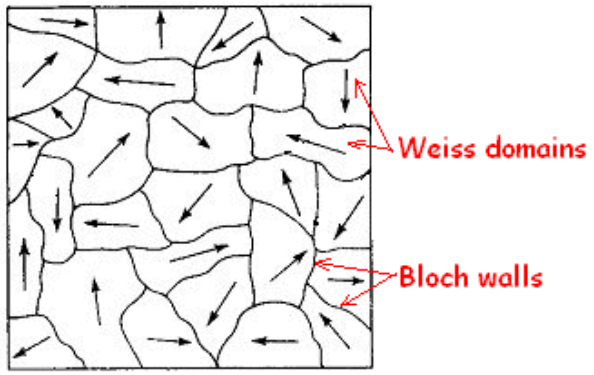
(ludovic.le-laurent@cea.fr)

[1]CEA Saclay, [2]Synopsys

MAGNETIC ANISOTROPY

In magnetic materials :

- Easy-axis magnetization : $E_{syst} = f(\vec{m})$
- Switchable domains → Data storage.

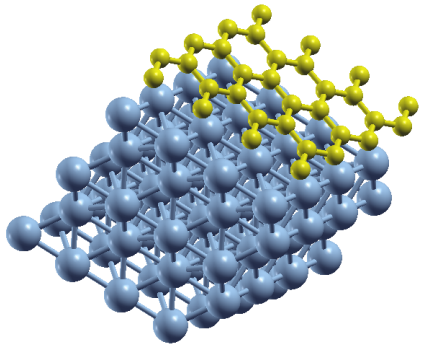


Until which size can we reduce domains ?

→ **Nanoscale systems.**

→ **Smaller ? Thermal fluctuations…**

→ Find system with large Anisotropy.



Why an easy-axis instead of another ? →

Origin is twofold :

- Shape anisotropy.
- Magneto-crystalline anisotropy (MCA).

→ We study the difference of total energy under two different magnetizations :

$$MAE = E_{tot}(m_1) - E_{tot}(m_2)$$

TWO ANISOTROPIES

• Shape anisotropy

- Two magnetizations $\vec{m}_i, \vec{m}_j$, as a magnetic dipole.

$$E_{dip} = \frac{\mu_0}{8\pi} \sum_{i \neq j} \frac{1}{r_{ij}^3} [\vec{m}_i \cdot \vec{m}_j - 3 \frac{(\vec{r}_{ij} \cdot \vec{m}_i)(\vec{r}_{ij} \cdot \vec{m}_j)}{r_{ij}^2}]$$

- Dipole-dipole interaction.

$$E_{dip} = \frac{\mu_0}{8\pi} \sum_{i \neq j} \frac{m_i m_j}{r_{ij}^3} (1 - 3\cos^2(\theta_{ij}))$$

→ **in-plane** magnetization.

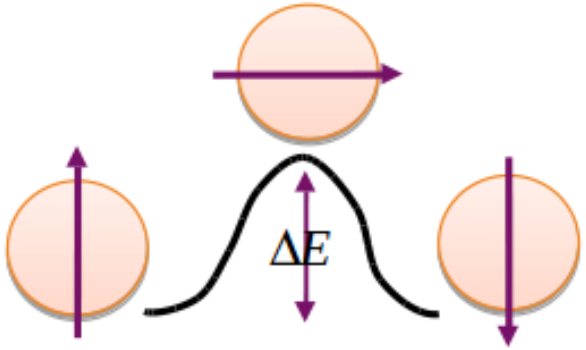
- Independent of crystalline structure.
- Depends only on quantity of matter and shape.
- At big scales, wins always !

• MCA

- H = Schrödinger + Zeeman + Mass velocity + Spin-orbit → relativistic corrections.

- Quantum effects :

$$H^{SOC} = \sum_i \xi_{i,d} \vec{L}_i \cdot \vec{S}_i$$



- SOC breaks spherical invariance.
- MCA depends on symmetry, nature of atoms.
- Dominating at surfaces and interfaces.

TWO ANISOTROPIES

Shape anisotropy

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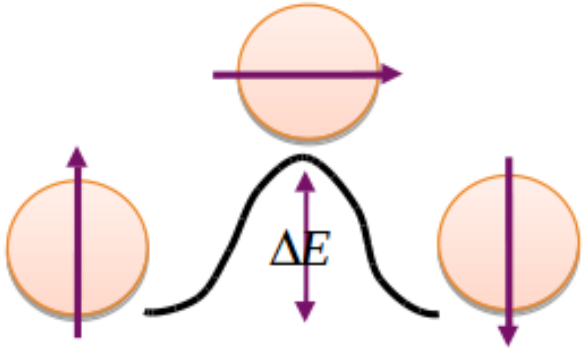

- SOC breaks spherical invariance.
- MCA depends on symmetry, nature of atoms.
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HOW TO CALCULATE MCA (1/2)

- Brute force method (self-consistent) : $MCA = E_{inplane} - E_{outofplane}$ where the two energies are obtained from SCF calculation including SOC.

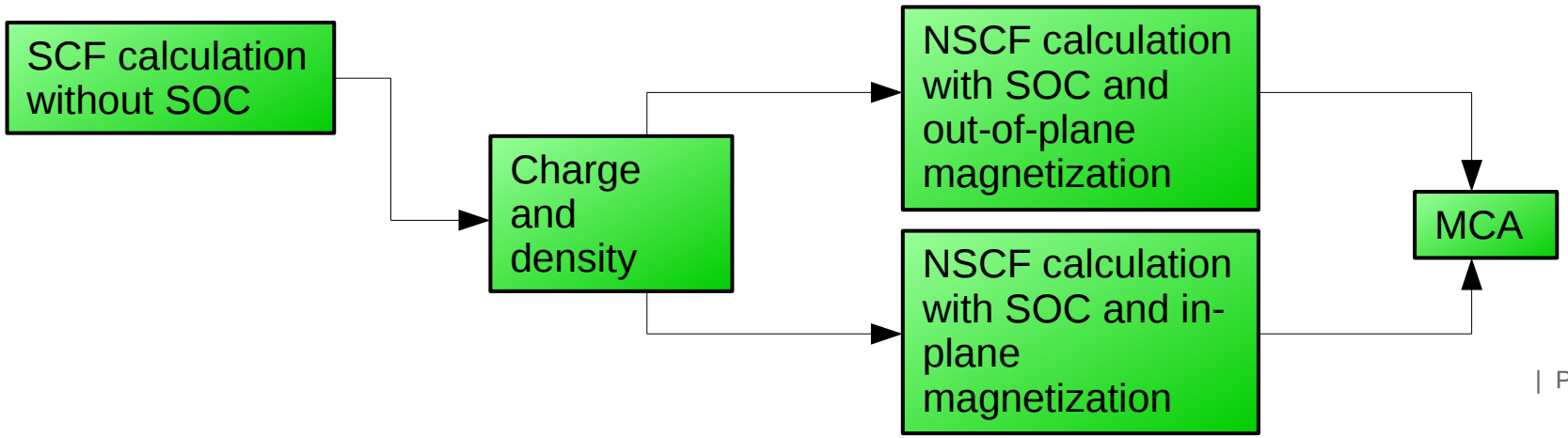
  In principle « exact » but very time consuming and hard to converge
  One should use penalization techniques to obtain energy for any direction.

- Force Theorem method : The variation of energy between a SCF calculation without SOC and with SOC is just the band energy variation. $\Delta E_{tot} = \Delta E_{band}$

$$MCA^{FT} = \int^{E_F^1} E\rho_1(E)dE - \int^{E_F^2} E\rho_2(E)dE$$

$$MCA^{FTgc} = \int^{E_F} (E - E_F)\Delta\rho(E)dE$$, at fixed chemical potential.

Very « fast » and numerically stable but cannot be applied to systems with too large SOC.



HOW TO CALCULATE MCA (2/2)

- Three computational tools : home-made Tight-Binding (TB), Quantum Espresso (DFT QE) and Quantum ATK (DFT QATK).

  → experimentally, MCA really weak, numerically too ! We have to compare different approaches.

TB

Semi-empirical Tight-Binding fitted on Density Functionnal Theory data :

- On-site
- Hopping
- Overlap
- Stoner parameter
- SOC

→ Really fast computational time.

DFT

Quantum Espresso : *Ab initio* expanded on plane waves.

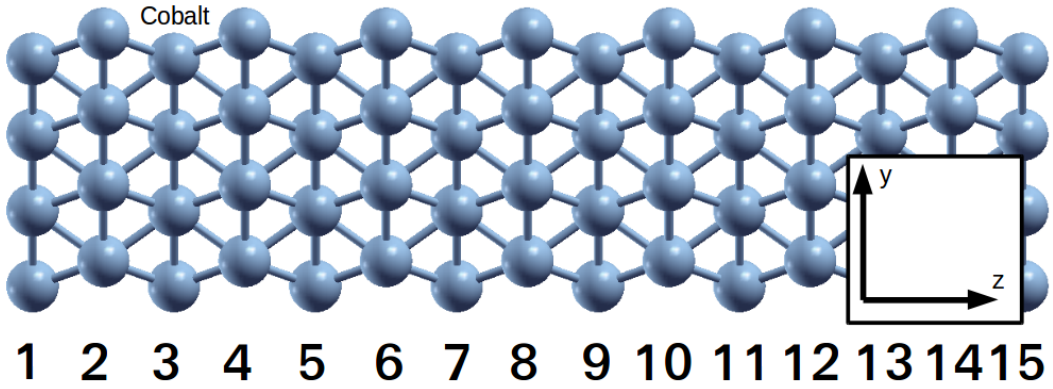
→ complete basis describing the whole system plus void, but huge computational cost.

Quantum ATK : *Ab initio* expanded on Local Atomic Orbitals.

→ localized basis with a really good description of partial system, fast computational time.

TOTAL MCA FOR SLABS : IRON, COBALT AND NICKEL (1/2)

	Fe bcc (001,110,111)	Co fcc (001,110,111)	Co hcp (0001)	Ni fcc (001,110,111)
Lattice parameter (Angström)	a=2,8665	a=3,5447	a=2,5071 c=4,0686	a=3,5249

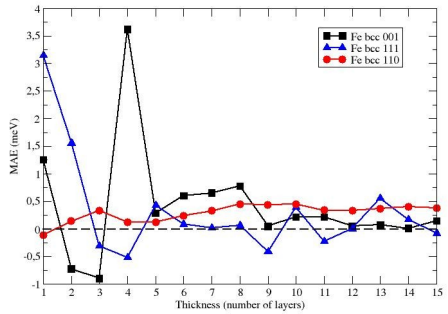


Mesh SCF : 25*25 k-points / Mesh NSCF : 50*50 k-points

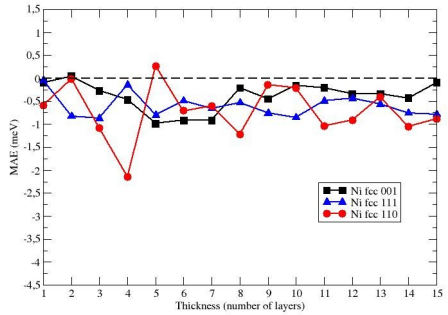
TOTAL MCA FOR SLABS : IRON, NICKEL AND COBALT (2/2)

TB

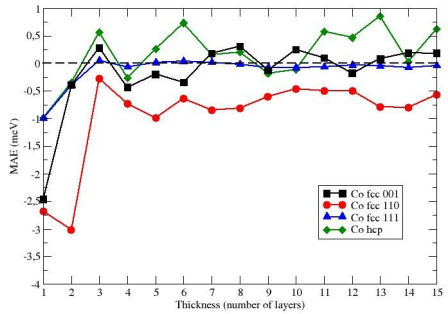
Fe bcc vs thickness (TB)



Ni fcc vs thickness (TB)

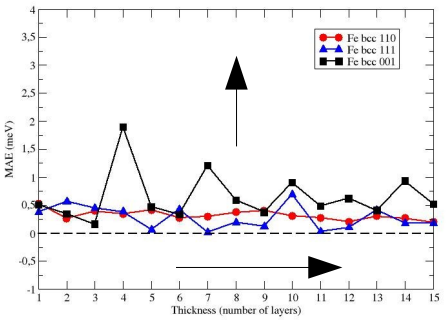


Co fcc and hcp vs thickness (TB)

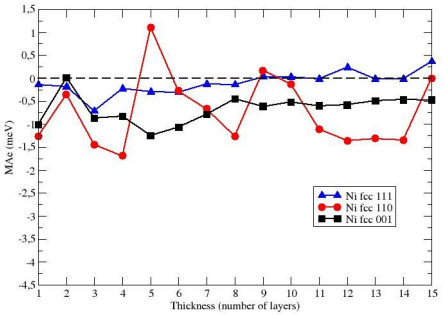


DFT

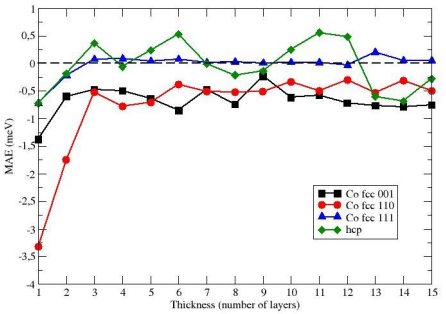
Fe bcc vs thickness (QE)



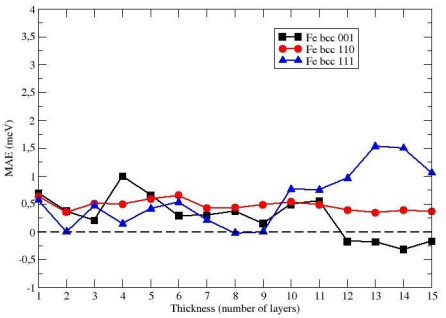
Ni fcc vs thickness (QE)



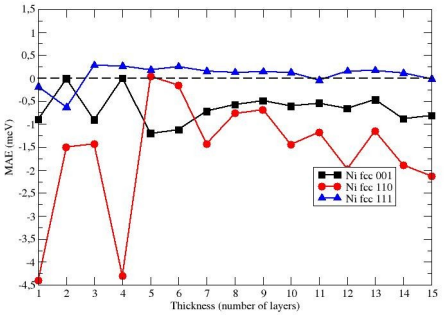
Co fcc and hcp vs thickness (QE)



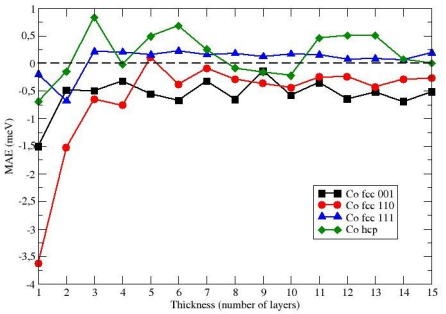
Fe bcc vs thickness (QATK)



Ni fcc vs thickness (QATK)



Co fcc and hcp vs thickness (QATK)

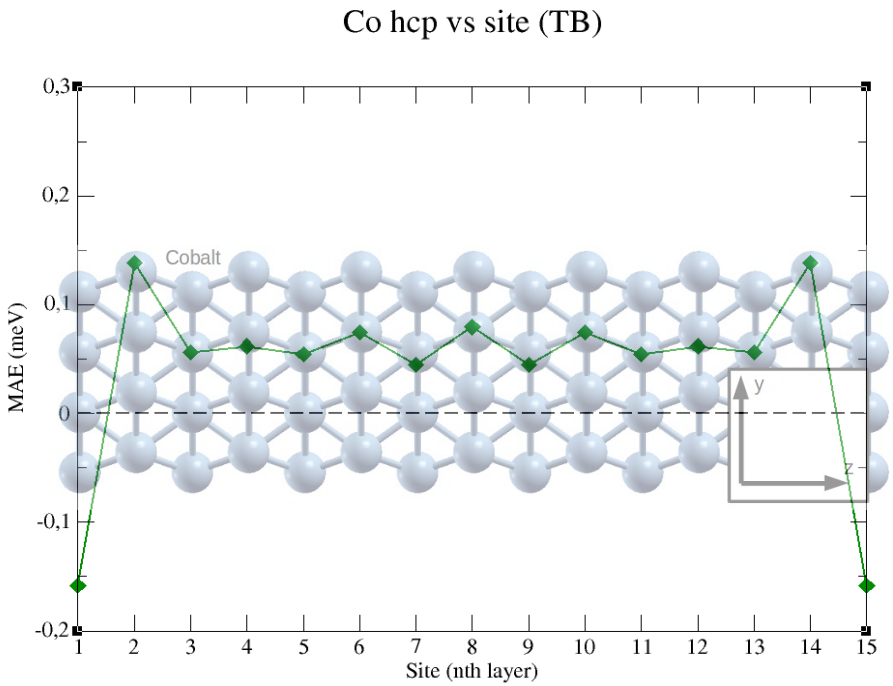


MCA BY LAYERS FOR SLABS : IRON, NICKEL AND COBALT(1/2)

- How to explain oscillations ? It can be interesting to decompose MCA, since we can write :

$$MCA^{FTgc} = \int^{E_F} (E - E_F)\,\Delta\rho(E)\,dE = \sum_{i,\lambda,k} \int^{E_F} (E - E_F)\,\Delta\rho_{i,\lambda,k}(E)\,dE$$

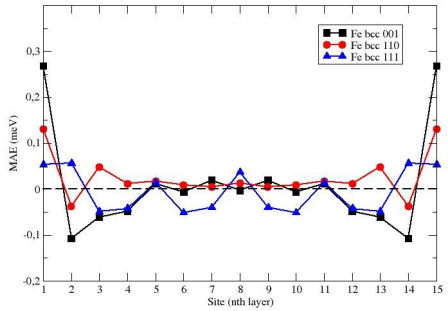
→ decomposition by layers of MCA, index i
→ decomposition by orbitals, index λ
→ large thickness behavior
→ MCA in Brillouin zone, index k
→ band structure



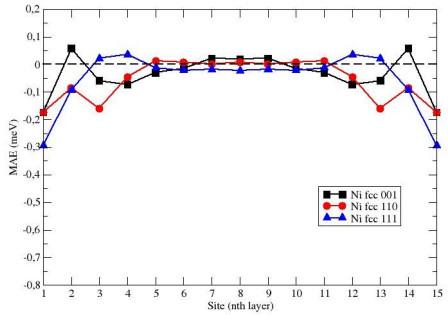
MCA BY LAYERS FOR SLABS : IRON, NICKEL AND COBALT(2/2)

TB

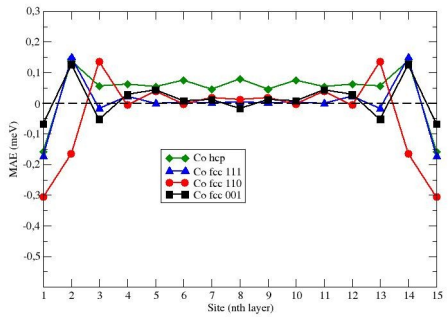
Fe bcc d orbital vs site (TB)



Ni fcc d orbital vs site (TB)

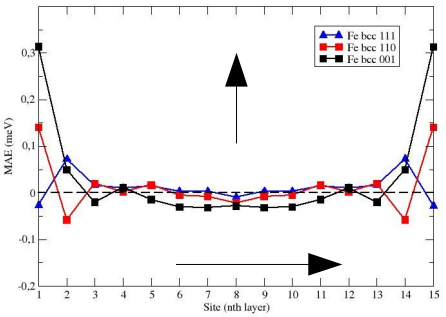


Co fcc and hcp d orbital vs site (TB)

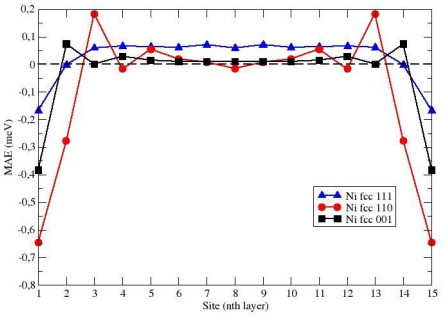


DFT

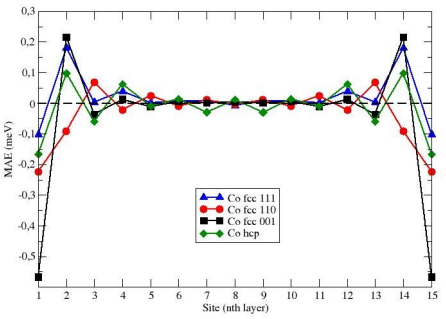
Fe bcc d orbital vs site (QE)



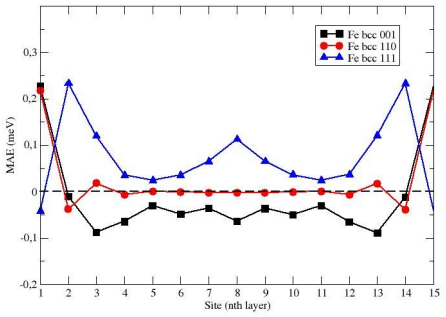
Ni fcc d orbital vs site (QE)



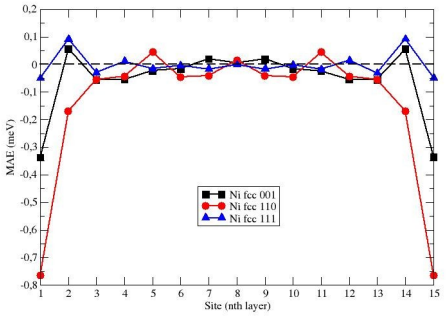
Co fcc and hcp d orbital vs site (QE)



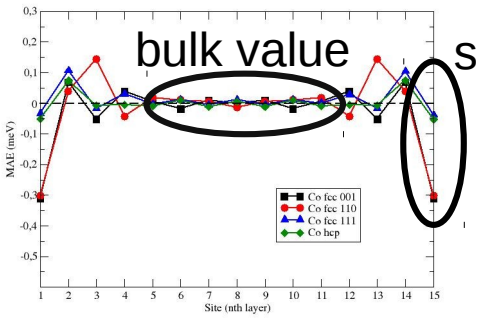
Fe bcc d orbital vs site (QATK)



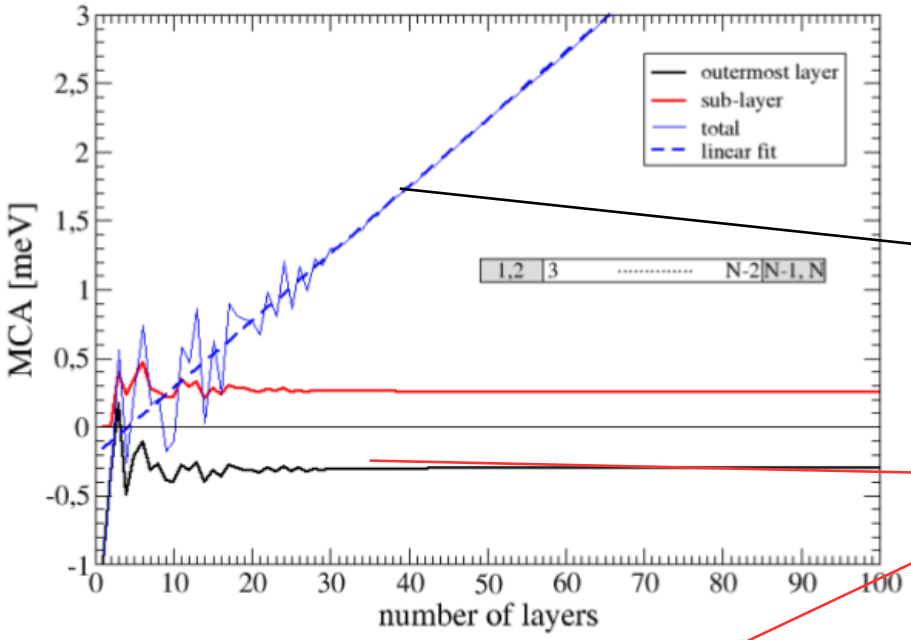
Ni fcc d orbital vs site (QATK)

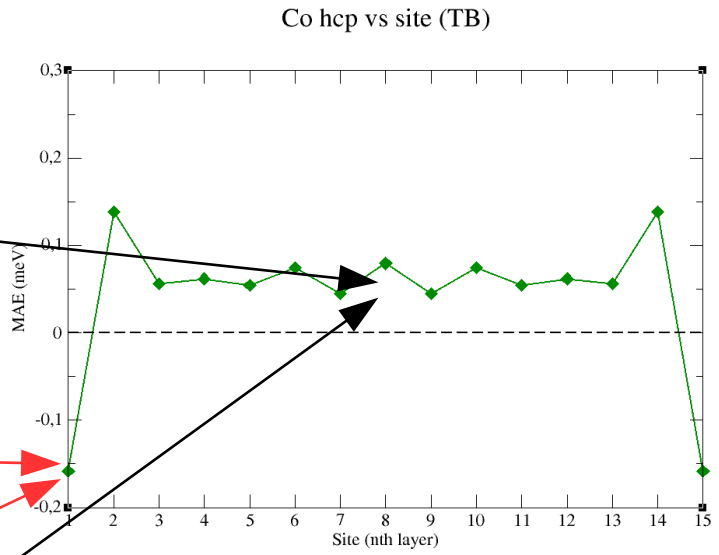


Co fcc and hcp d orbital vs site (QATK)



MCA ANALYSIS IN TIGHT-BINDING : LARGE THICKNESS BEHAVIOR FOR COBALT



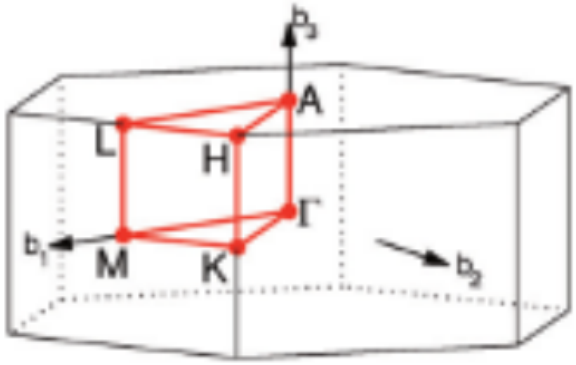


Linear fit :

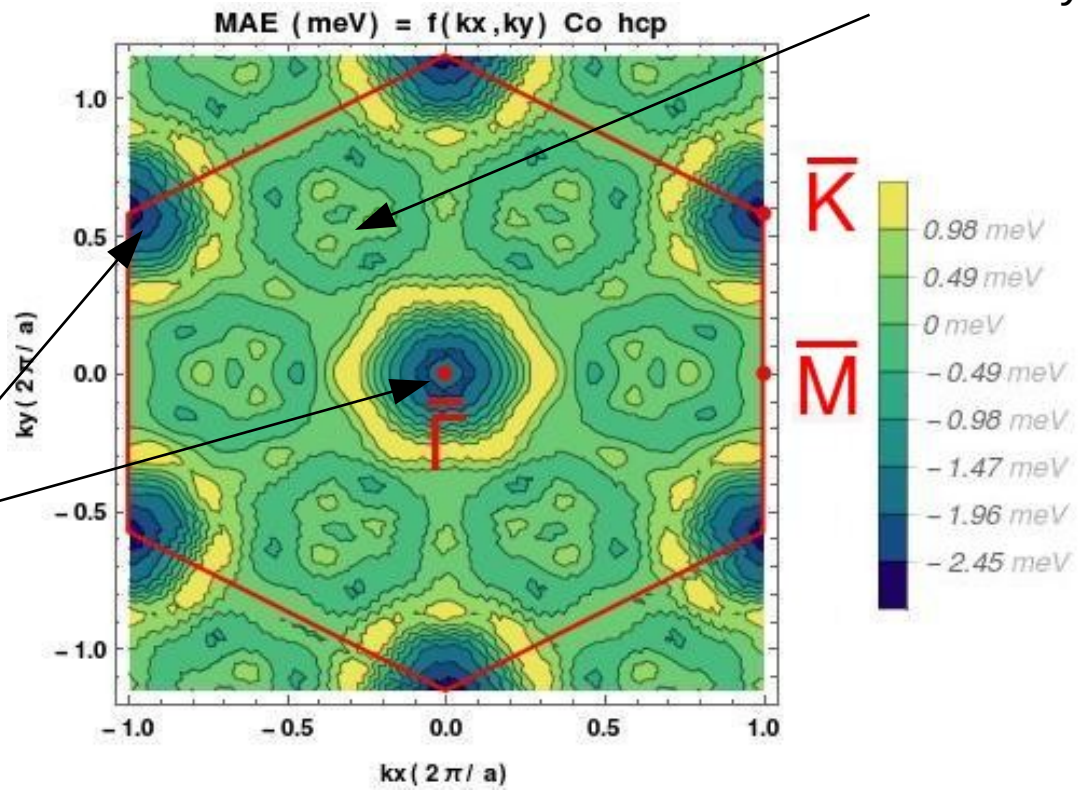
$$MCA = 2MCA_{surf} + NMCA_{bulk}$$

MCA_{bulk} =0.05 meV

MCA ANALYSIS IN TIGHT-BINDING : K-SPACE FOR BULK COBALT

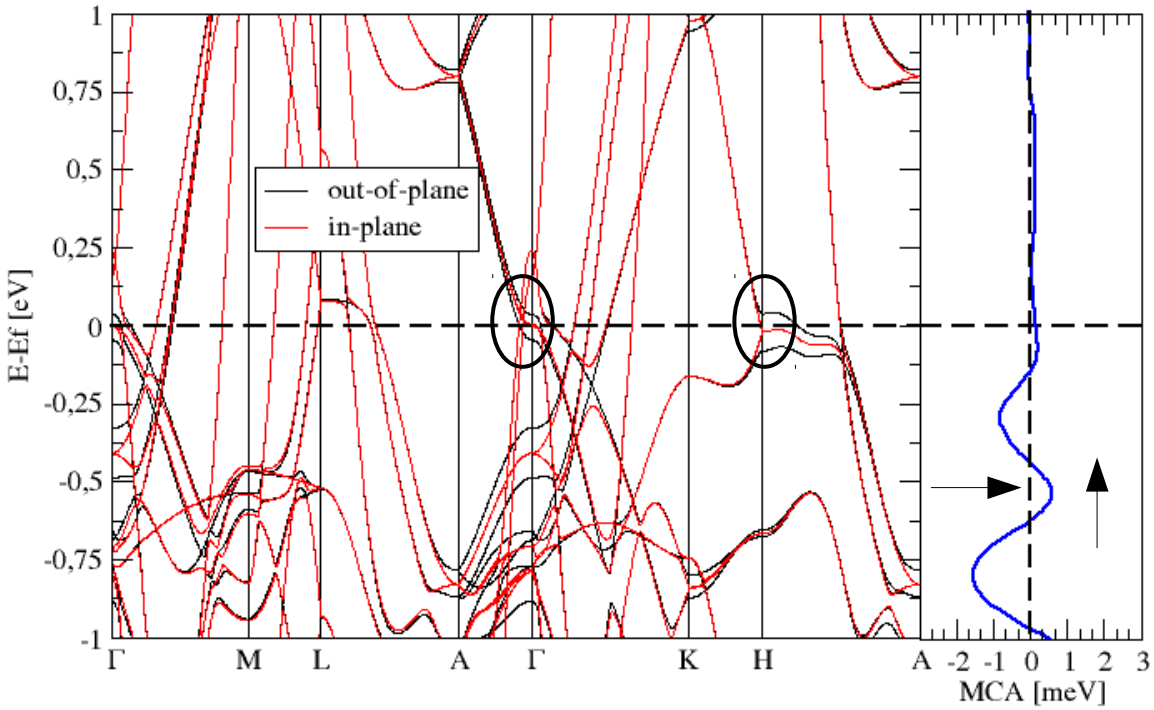


Almost zero everywhere.



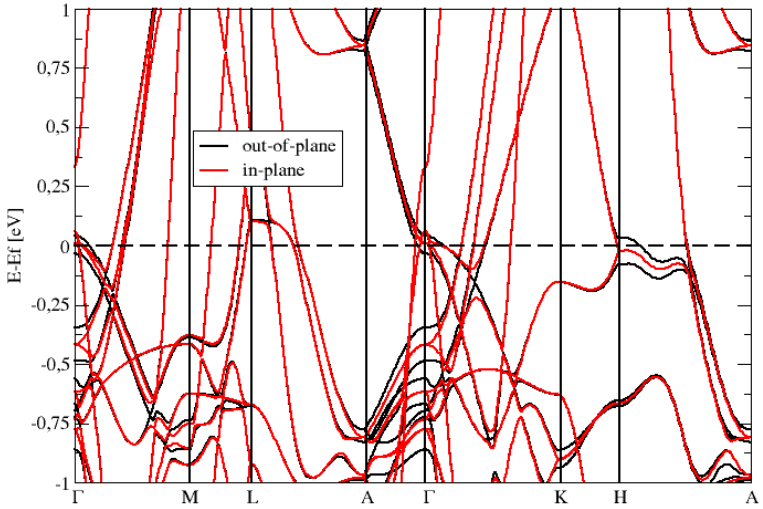
Major contribution to MCA.

MCA ANALYSIS IN TIGHT-BINDING : BAND STRUCTURE FOR BULK COBALT

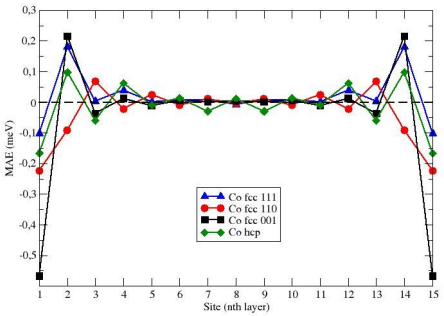


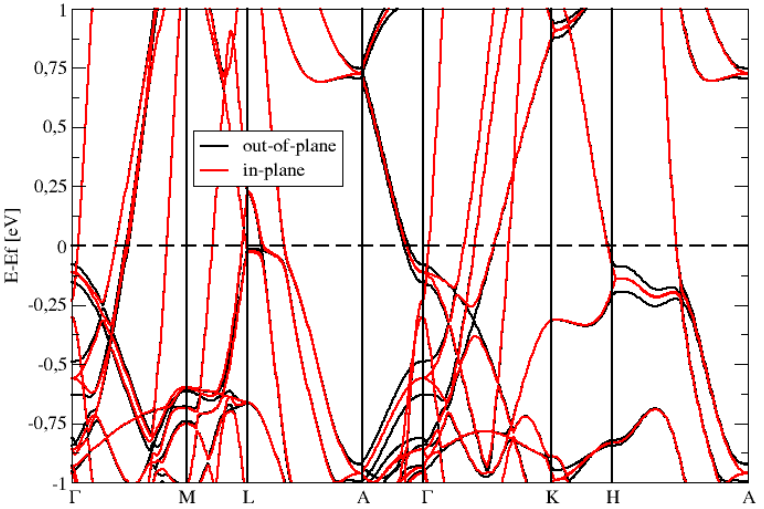
- Most important contributions : high symmetry points H and Γ !
  → tangential bands at Fermi level in one orientation but not in the other one.
- According to the level, MCA varies rapidly !

BAND STRUCTURE IN DFT FOR BULK COBALT

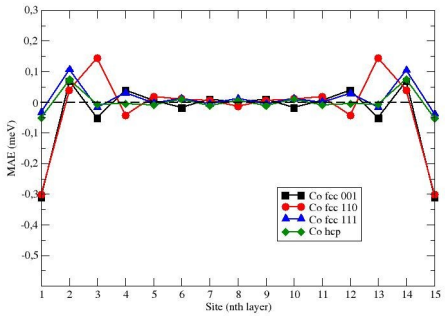


Co fcc and hcp d orbital vs site (QE)





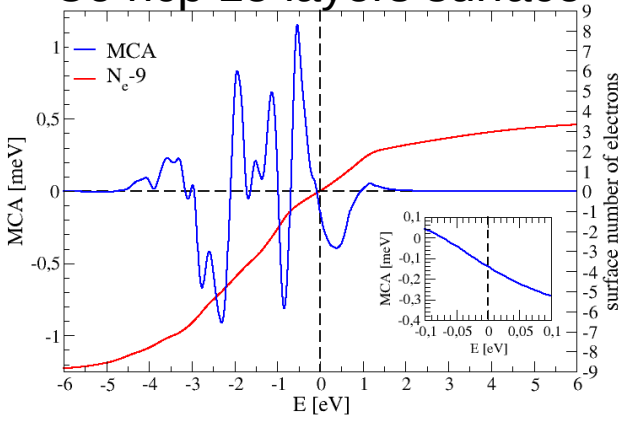
Co fcc and hcp d orbital vs site (QATK)



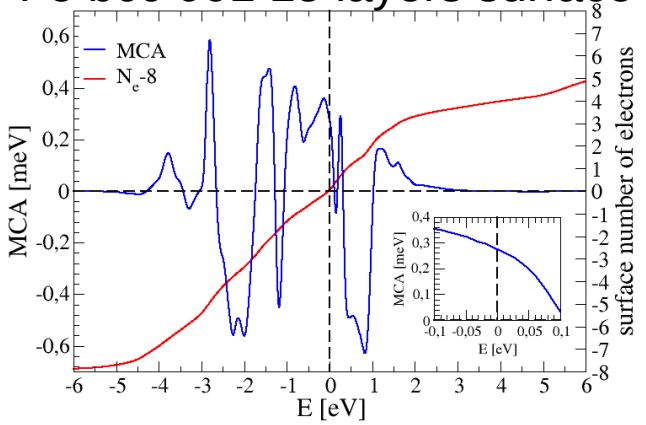
Differences observed in MCA between codes = Slightly differences in band structures according to Fermi level !

FEW IDEAS ABOUT TUNING MCA

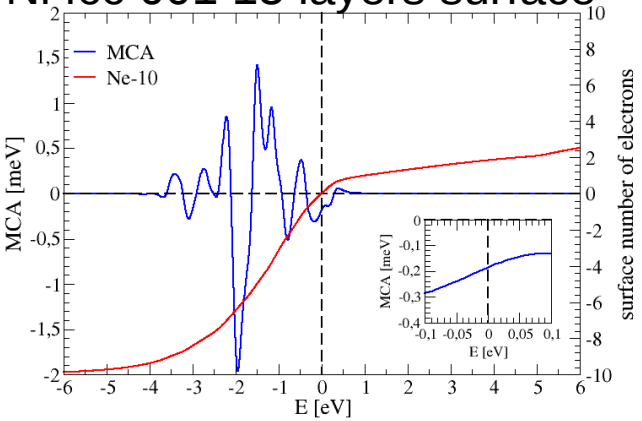
Co hcp 15 layers surface



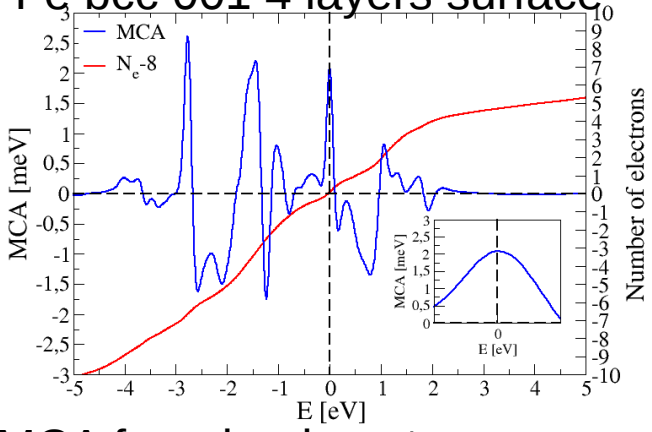
Fe bcc 001 15 layers surface



Ni fcc 001 15 layers surface



Fe bcc 001 4 layers surface



Modifying the filling is a way to pilot MCA from in-plane to out-of-plane orientation :

- Electric field → 1.10^10 V/m for only 0,05 electrons…
- Molecules and charge transfer.

AKNOWLEDGEMENTS

FET open Grant No. 766726

COncepts and tool**S** in **M**olecular spintron**ICS**

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THANK YOU FOR YOUR ATTENTION

QUESTIONS?

COMMENTS?