Electronic Structure:

LDA, LSDA, Tight Binding, DMFT

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A Local Density Approximation (LDA)

B Tight Binding Approximation (TB)

C Local Spin Density Approximation (LSDA)

D Applications and a Hint on Dynamical Mean Field Theory (DMFT)

A few words about DMFT (an ignoramus' view)

- Dynamical mean field theory is very fashionable (gold rush).
- DMFT is not $ab\ initio$.
- DMFT is not parameter free.
- Many people doubt that you (at present) can evaluate ground state geometries and related properties.
- DMFT is a Green's function theory with many different implementations.
- But: DMFT can give a physically motivated access to both high (eV) and low (meV) energy quasi-particle excitations. It can (partly) describe elevated temperature properties, paramagnetism.

- Read A. Georges *et al.*, *Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions*, Rev. Mod. Phys. **68**, 13–125 (1996)!

$LaFe_{12-x}Si_x$:

The ideal material for magnetic cooling?

Facts on magnetic cooling:

- efficiency up to 50% higher than in conventionel (compression) systems
- can potentially save 5% of the world electric energy consumption
- the cooling power is proportional to ΔM and to the operation frequency

$$P \sim \Delta M \nu$$

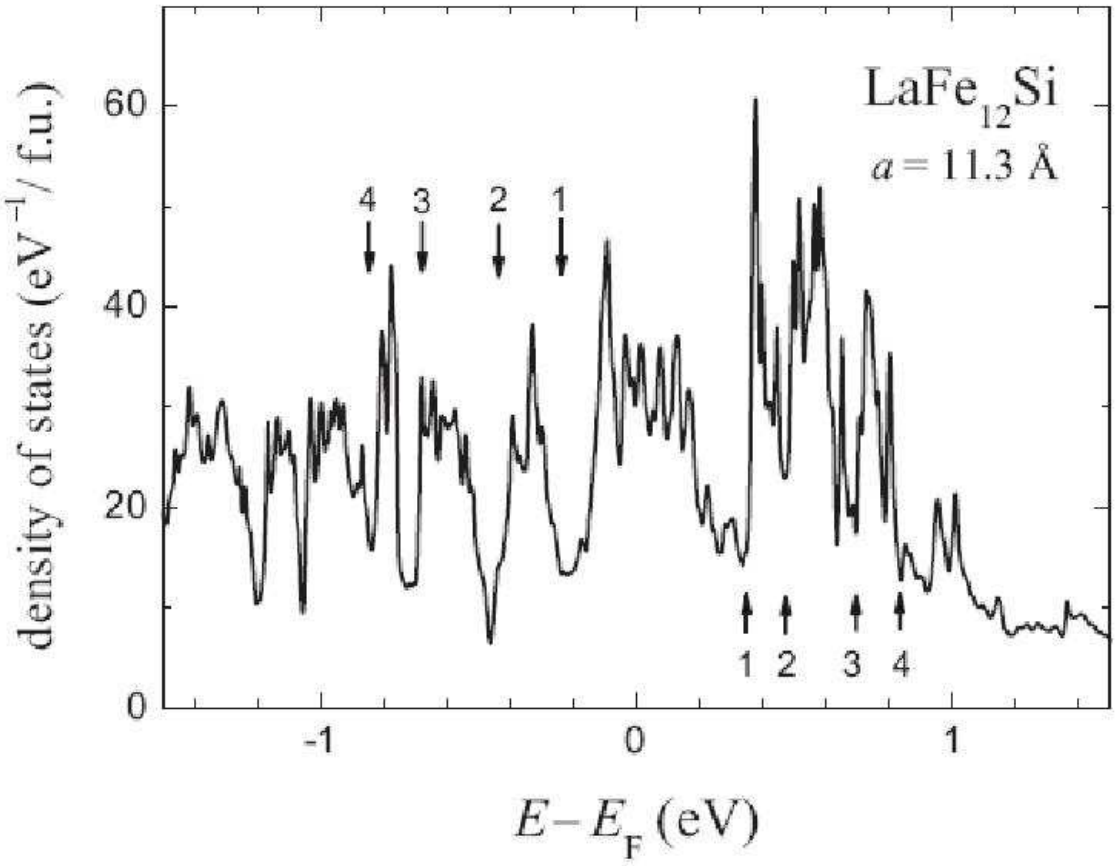
- up to now, all demontrators work with Gd

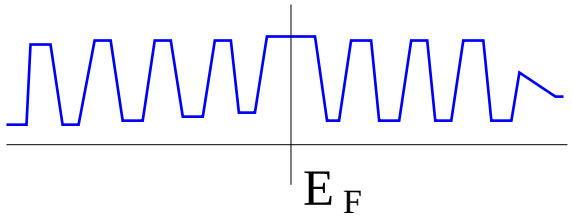
Facts on $LaFe_{12-x}Si_x$:

- "almost pure" iron, $x \approx 1$
- almost no hysteresis, if prepared by melt-spinning
- magnetocaloric effect comparable with or larger than Gd
- operation temperature can be tuned (change x, add Co, add hydrogen)

$LaFe_{12-x}Si_x$:

The reason for its large ΔM and its low hysteresis

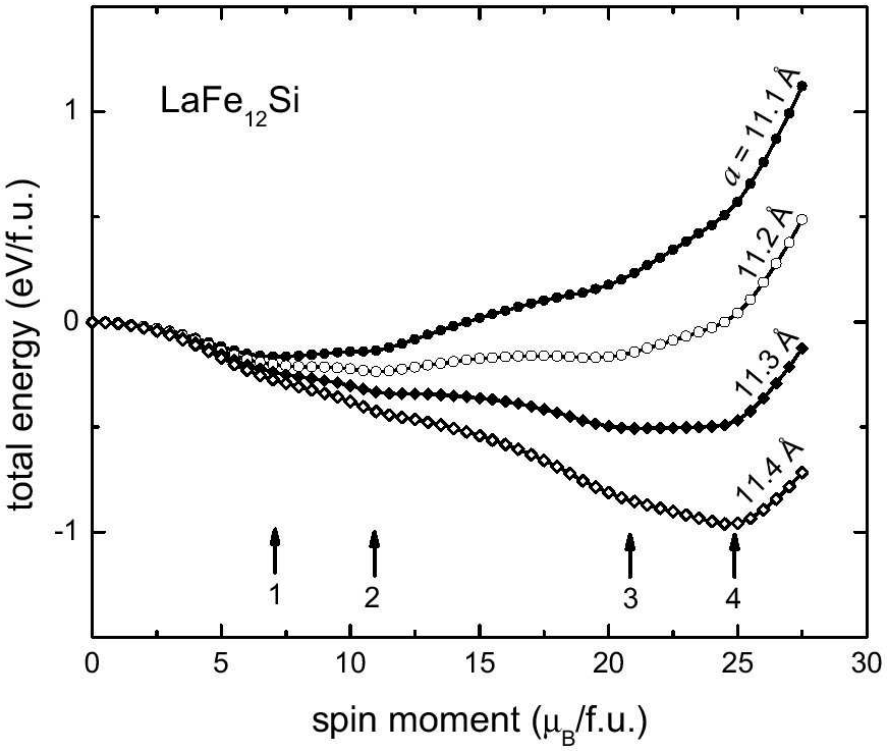


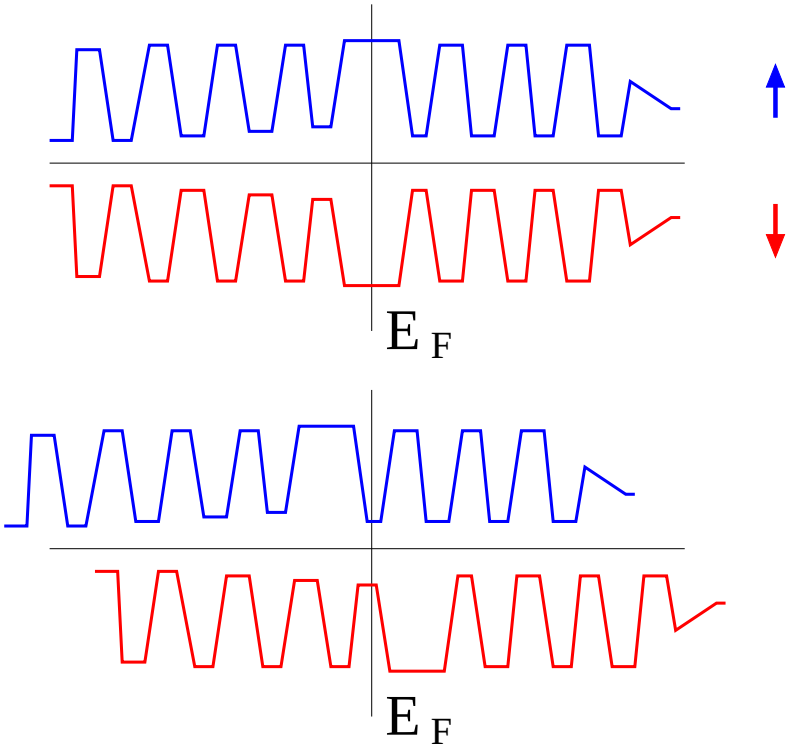


Model for the DOS

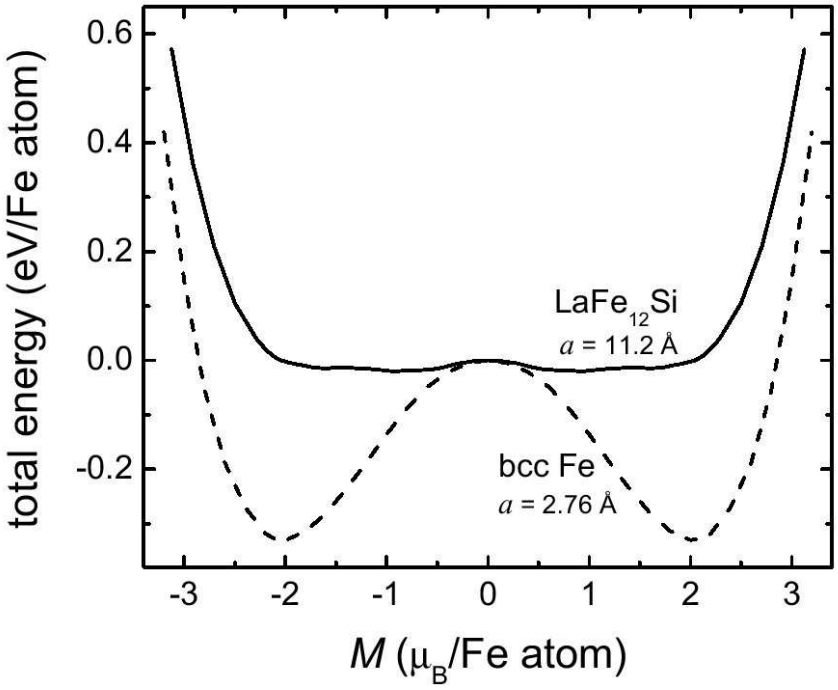
$LaFe_{12-x}Si_x$:

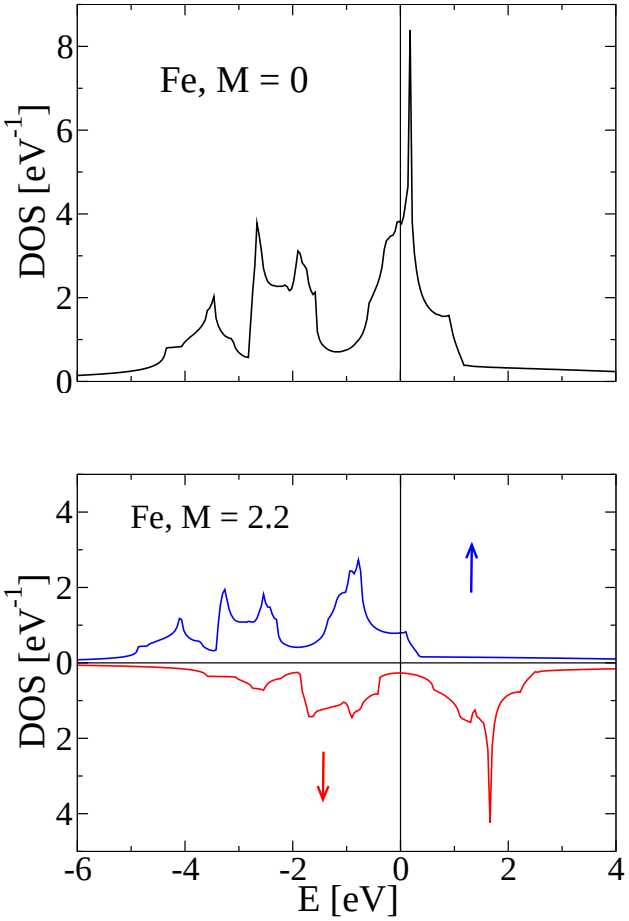
The reason for its large ΔM and its low hysteresis





$LaFe_{12-x}Si_x$: Comparison with bcc iron





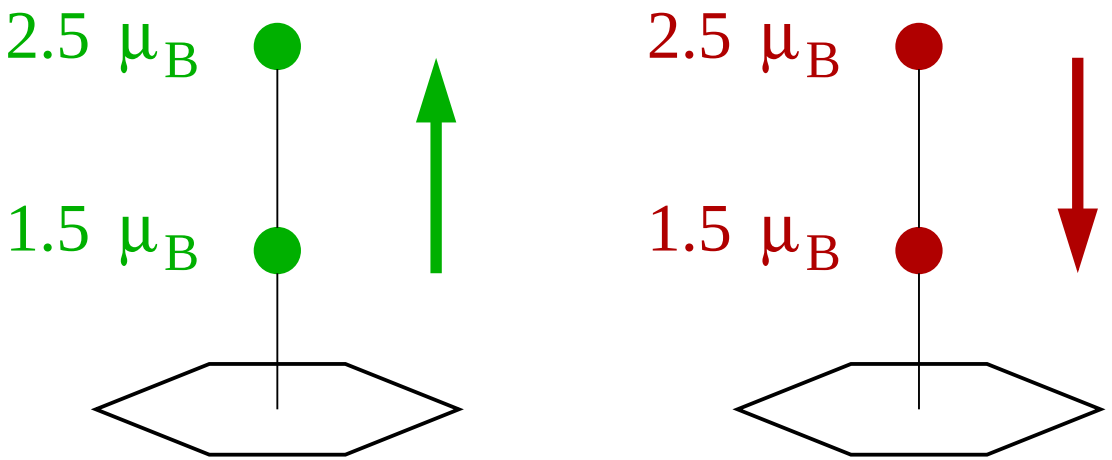
prediction of metamagnetism:

Kuz'min and Richter, PRB 2007;

verification: Lyubina et al. PRL 2008

Subnanometer Magnetic Storage Bits: a Prediction

arXiv.org/abs/0906.4645

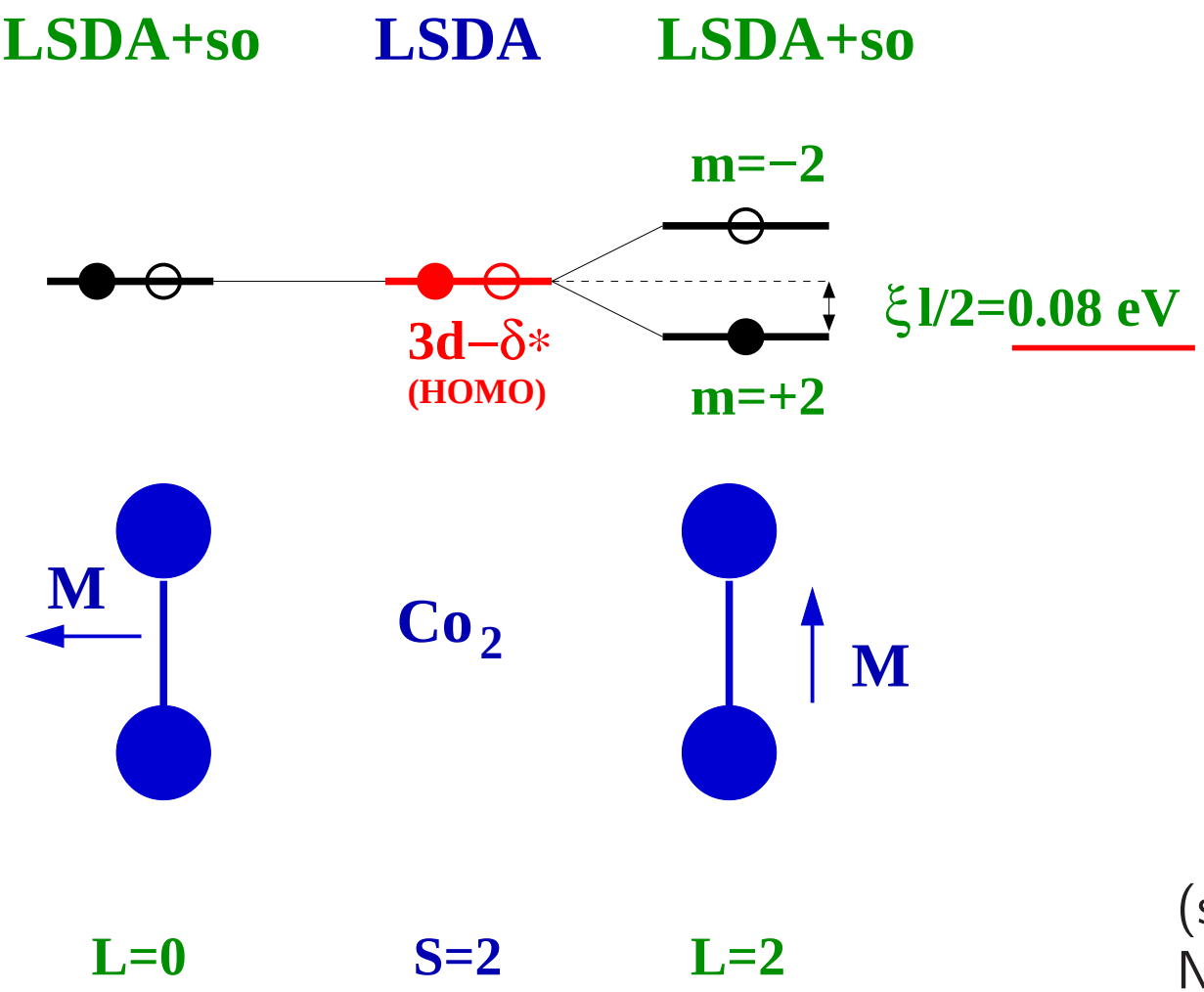


Co-based magnetic storage materials

(MAE: magnetic anisotropy energy, $\geq 40\ kT$ required)

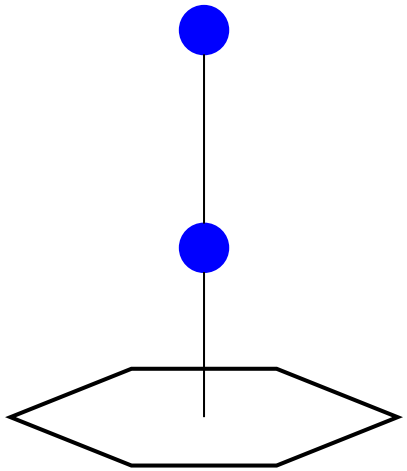
material	MAE per atom	atoms/bit	comments
Co(Cr,Pt)	≈ 0.05 meV	400,000	current bit size about 5,000 nm^3
hcp Co	0.065 meV	15,000	
$L1_0$ CoPt	1 meV	1,000	15 nm^3 per bit seems possible, but such small clusters do not order (Gruner 08)
Co on Pt(111)	9 meV (Gambardella 03)	1 at 3 K?	MAE per atom $\sim 1/$number of Co atoms
predictions for free Co_2	14 meV (Strandberg 07, 08)	2 at 9 K?	(lower estimate) Does bonding reduce the MAE?
	95 meV (Fritsch 08)	2 at 60 K?	(upper estimate)

Huge magnetic anisotropy due to a singly occupied doublet



(see Strandberg *et al.*, Nature Materials 2007)

Idea: a hexagonal symmetry ...



... would not break the degeneracy of (non-relativistic) δ-states!

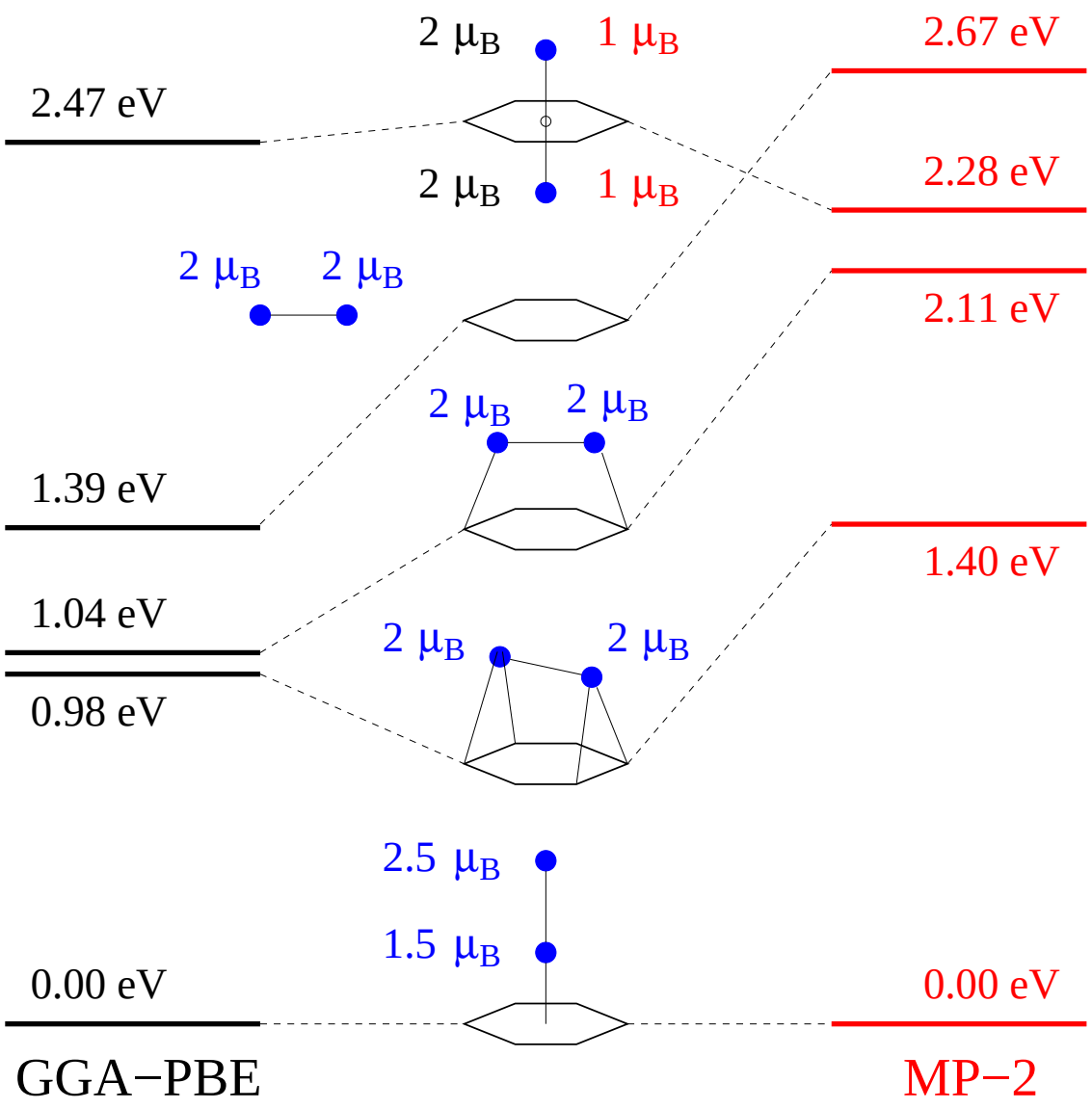
Will the bonding be strong enough?

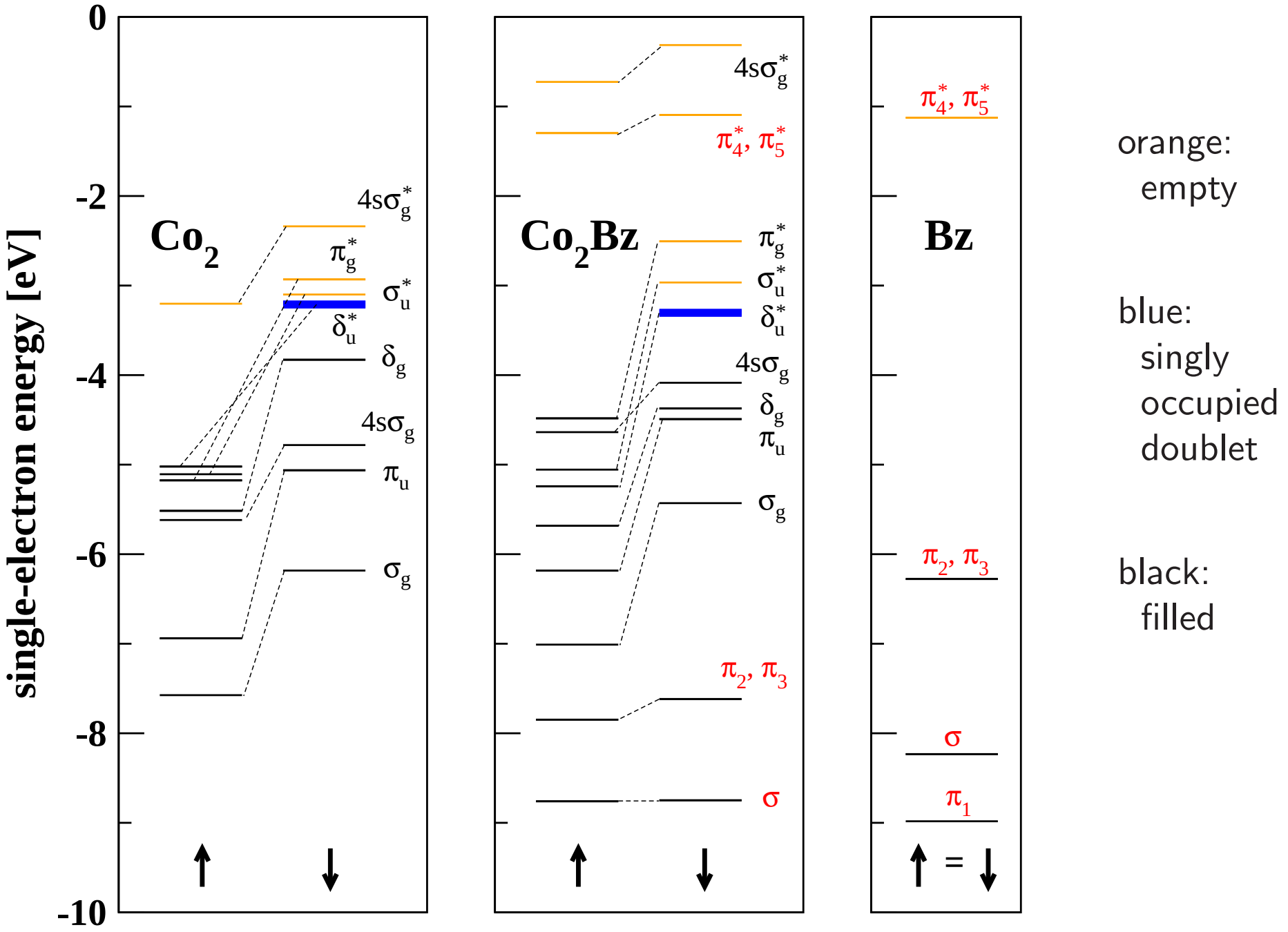
Will magnetism survive?

Check Co_2-benzene as a model for Co_2 on graphene or on graphite!

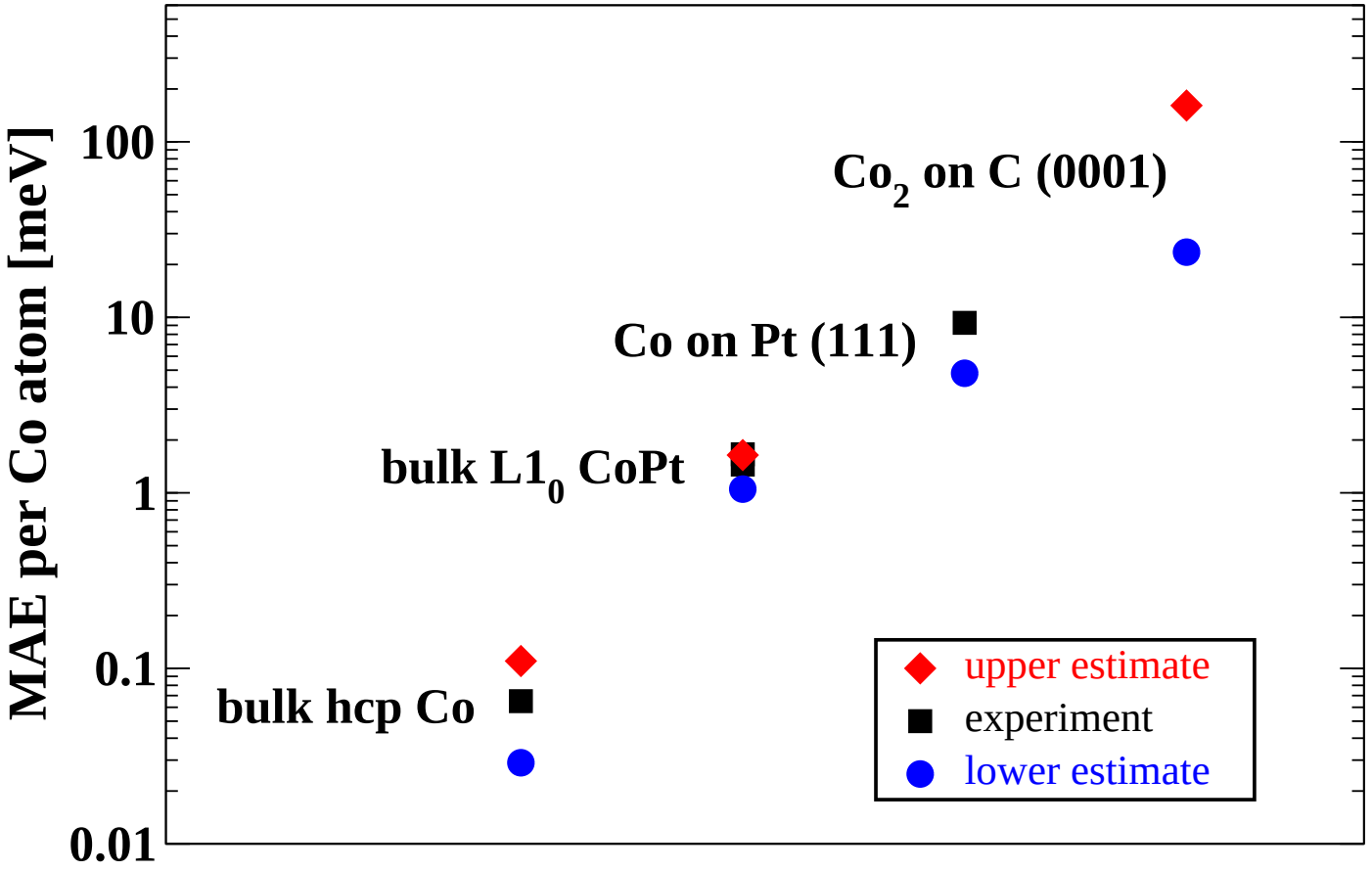
Co_2-benzene: structures and spin states

Perpendicular
Pd_2-benzene
and Pt_2-benzene:
Lüttgens 01




single-electron energy [eV]
0
-2
-4
-6
-8
-10
Co2
4sσg*
πg*
σu*
δu*
δg
4sσg
πu
σg
Co2Bz
4sσg*
π4*, π5*
πg*
σu*
δu*
4sσg
δg
πu
σg
π2, π3
σ
Bz
π4*, π5*
π2, π3
σ
π1
=
orange:
empty
blue:
singly
occupied
doublet
black:
filled

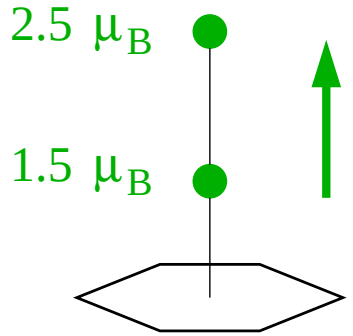
MAE of Co in different systems: heavy metals are not needed



Open problems

- Cheap production of large regular arrays?
- Protection against oxidation without reducing the anisotropy?
- Appropriate read/write technology? arXiv.org/abs/0906.4645
- Cooling . . . ?

Take-home message . . .



You can do predictive theory for magnetic materials!

. . . using advanced electronic structure methods.

method: http://www.fplo.de/