Ab initio investigations of the magnetoelectric properties of materials

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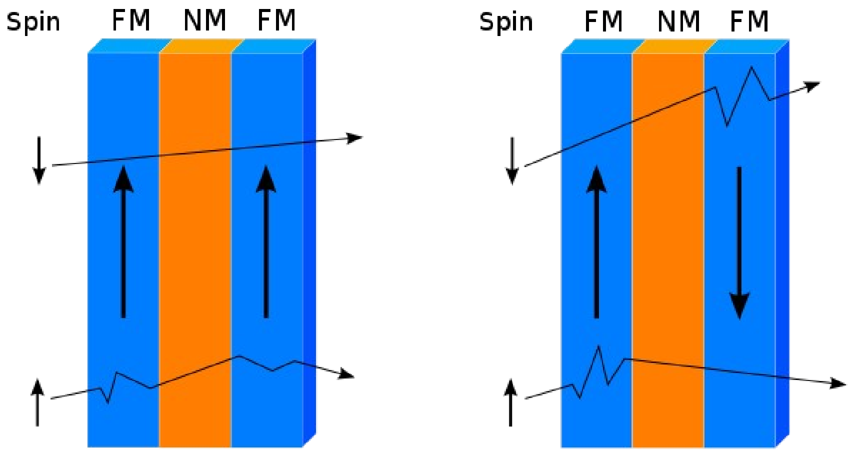
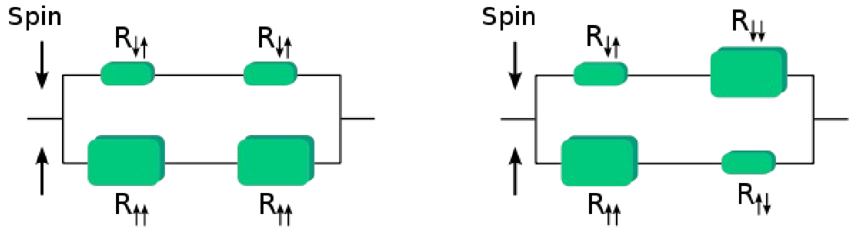
New materials for spintronic devices

Magnetoresistive device





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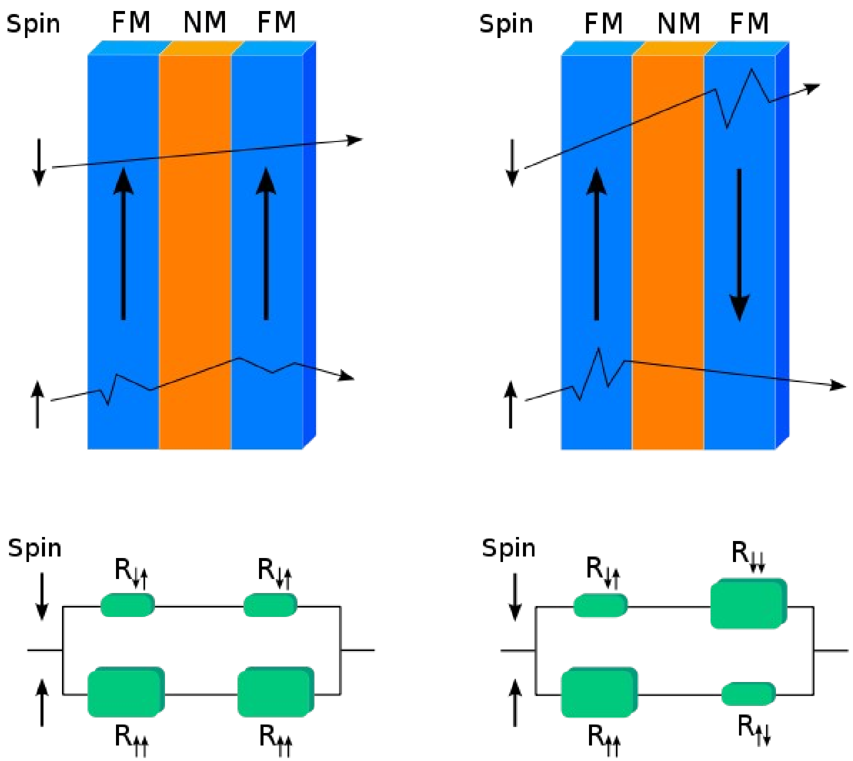

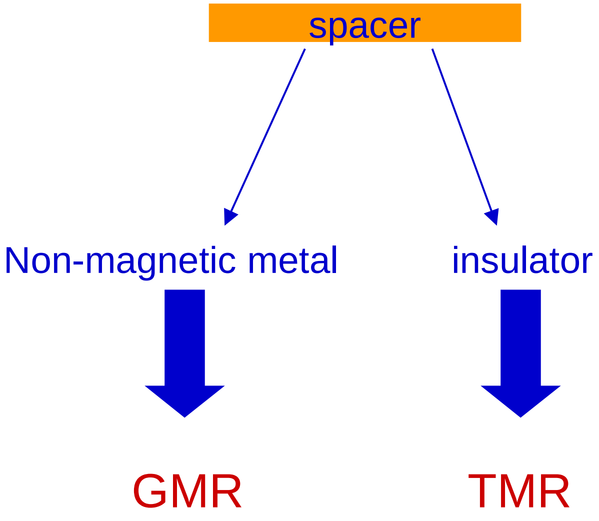

spacer

Non-magnetic metal

insulator

GMR

TMR

The insulator spacer layer can be :

- magnetic : spin dependent tunnel barrier

- ferroelectric : two other conduction states (four state memory)

Motivation

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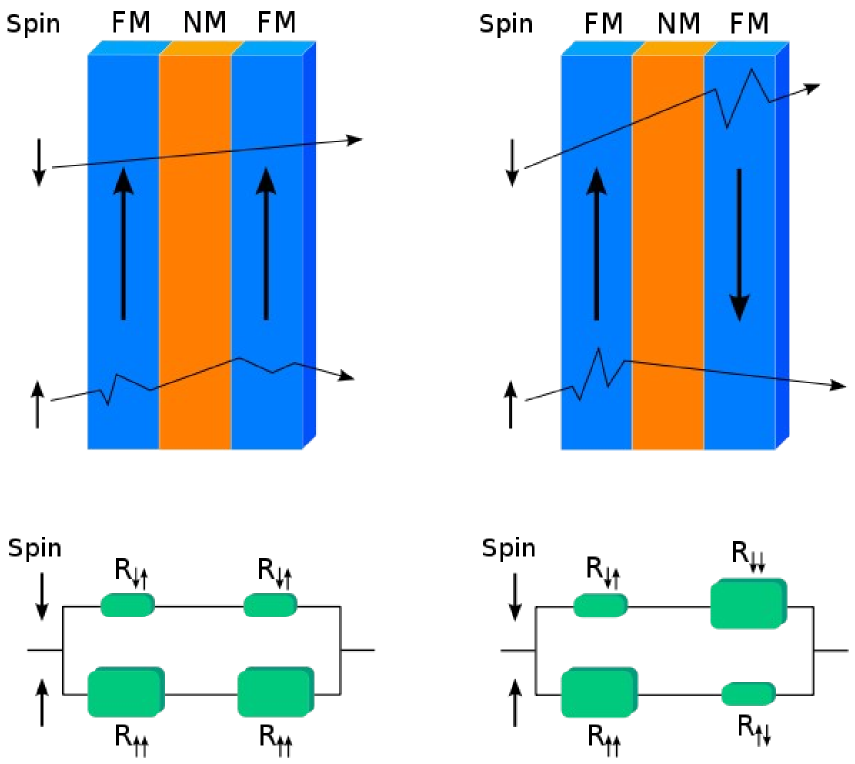

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Functional materials with remarkable properties
→ ***impact on transport***

Motivation

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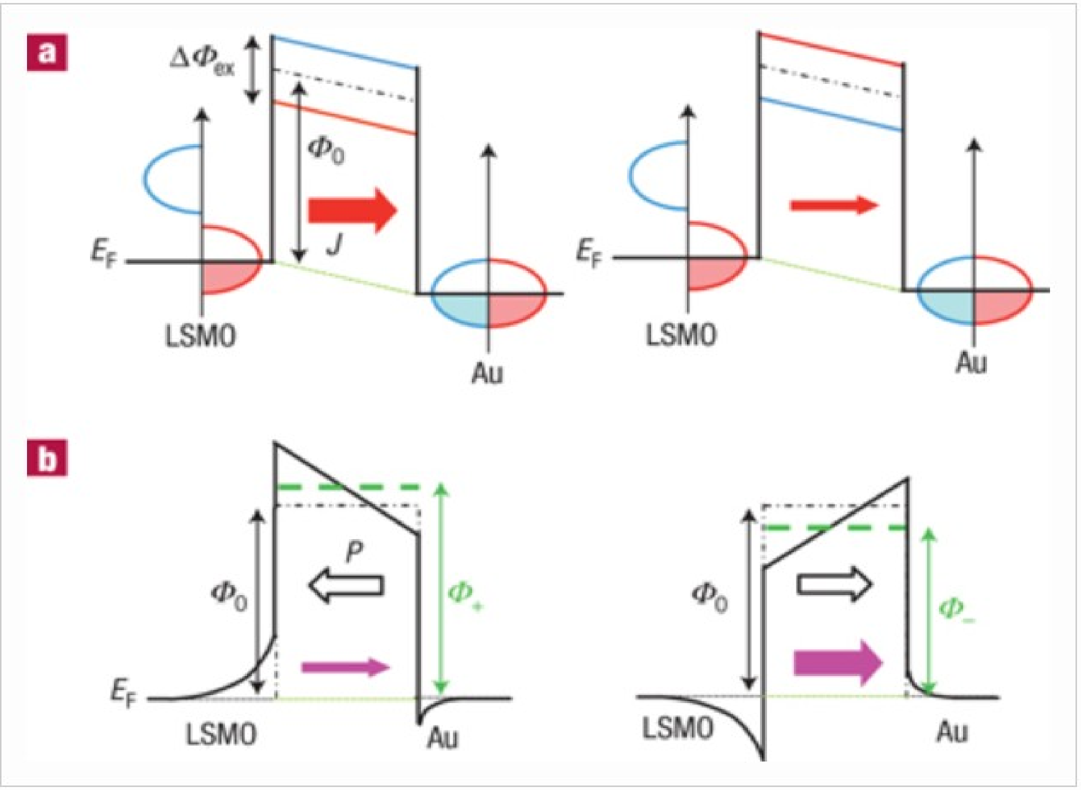
Schematic potential profile seen by the tunnelling electrons



LSMO :
Half metallic electrode (spin up)

Magnetic barrier :
M parallel to **M**(LSMO) : high current
M opposite to **M**(LSMO) : low current

Au : collecting electrode

Martin Gajek, Manuel Bibes, Stéphane Fusil, Karim Bouzehouane, Josep Fontcuberta, Agnès Barthélémy & Albert Fert, Nature Materials 6, 296 - 302 (2007)

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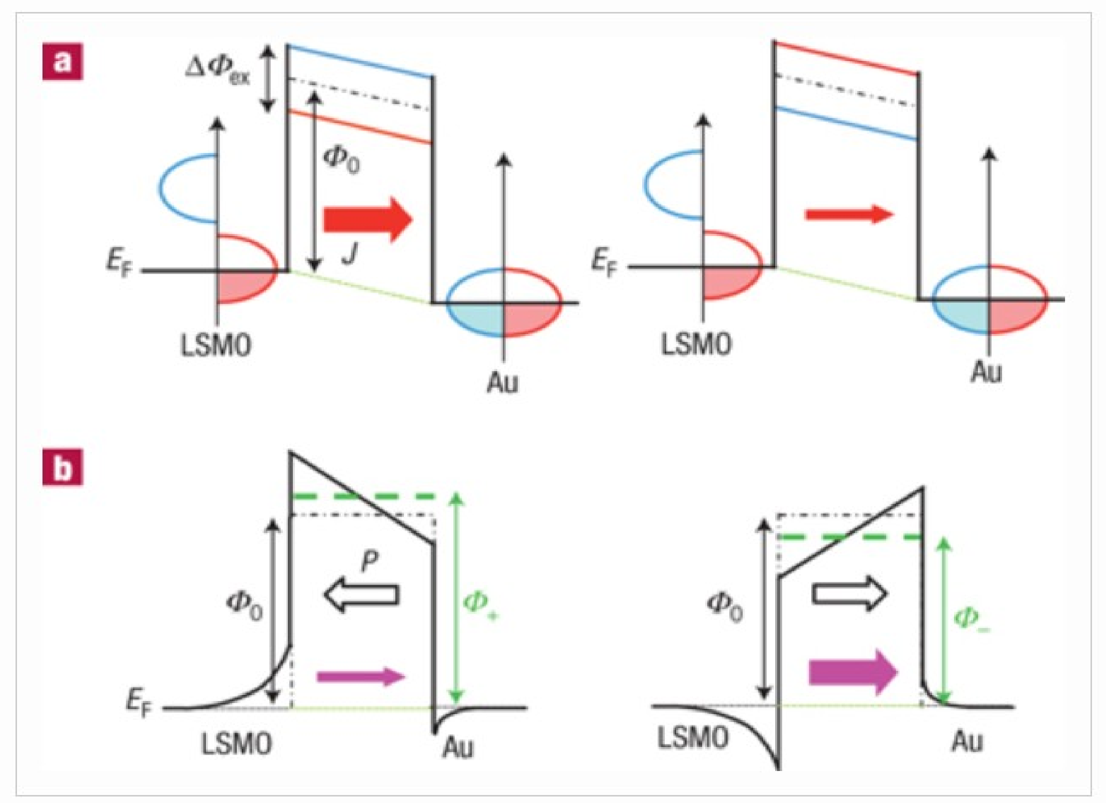

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Non magnetic / ferroelectric barrier : the current depends on the direction of **P**

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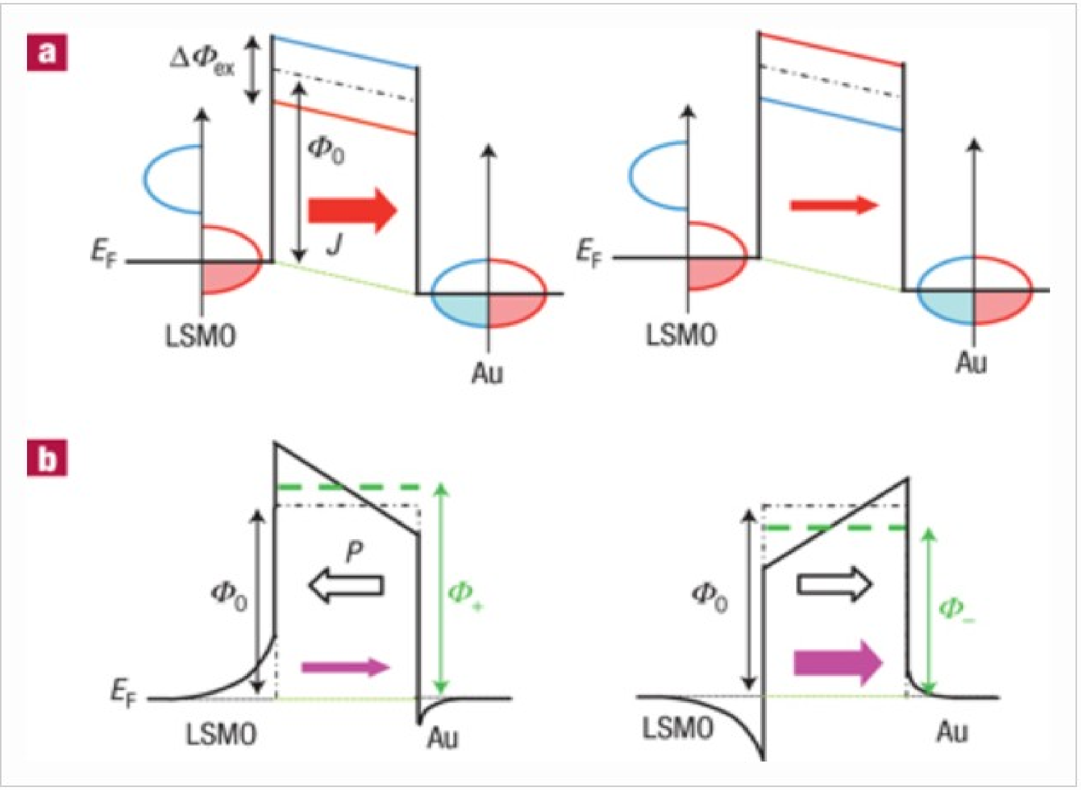

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Combine magnetism and polarization
→ ***more than two (4, 8) state device***

Motivation

Magnetoelectric multiferroics

Magnetic Multiferroics

Ferromagnetism

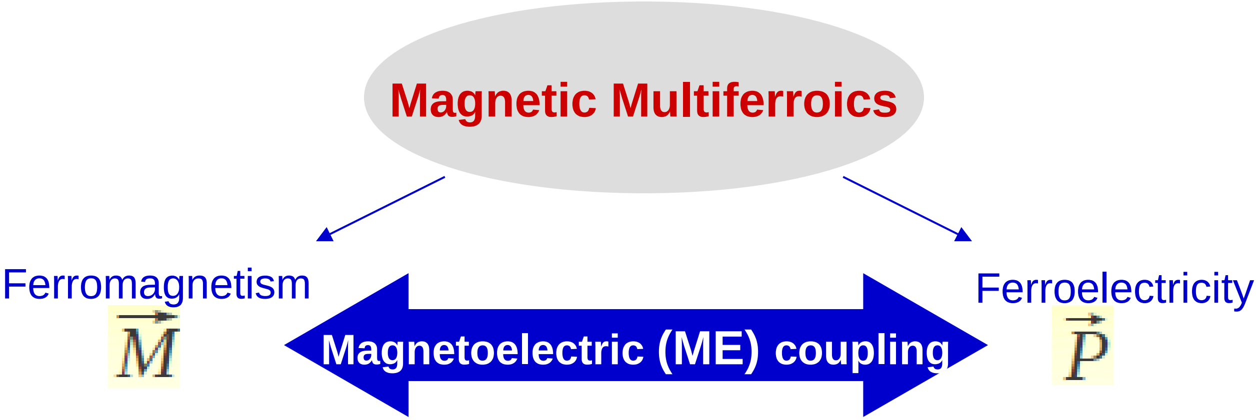
$\vec{M}$

Ferroelectricity

$\vec{P}$

Motivation

Magnetoelectric multiferroics



Magnetic Multiferroics

Ferromagnetism $\vec{M}$

Magnetoelectric (ME) coupling

Ferroelectricity $\vec{P}$

$$F = \ldots \; - \alpha \, \vec{E} \, . \, \vec{H} + \ldots$$

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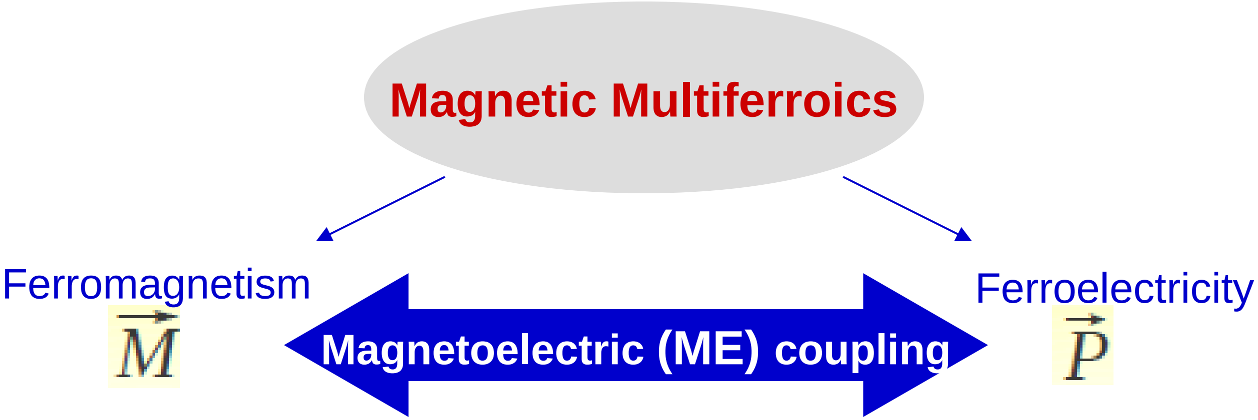
Magnetoelectric multiferroics



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$$F = \dots \ - \alpha \, \vec{E} . \vec{H} + \dots$$

Strong ME coupling

↓

Possible control of :

$\vec{P}$ by $\vec{H}$ $\vec{M}$ by $\vec{E}$

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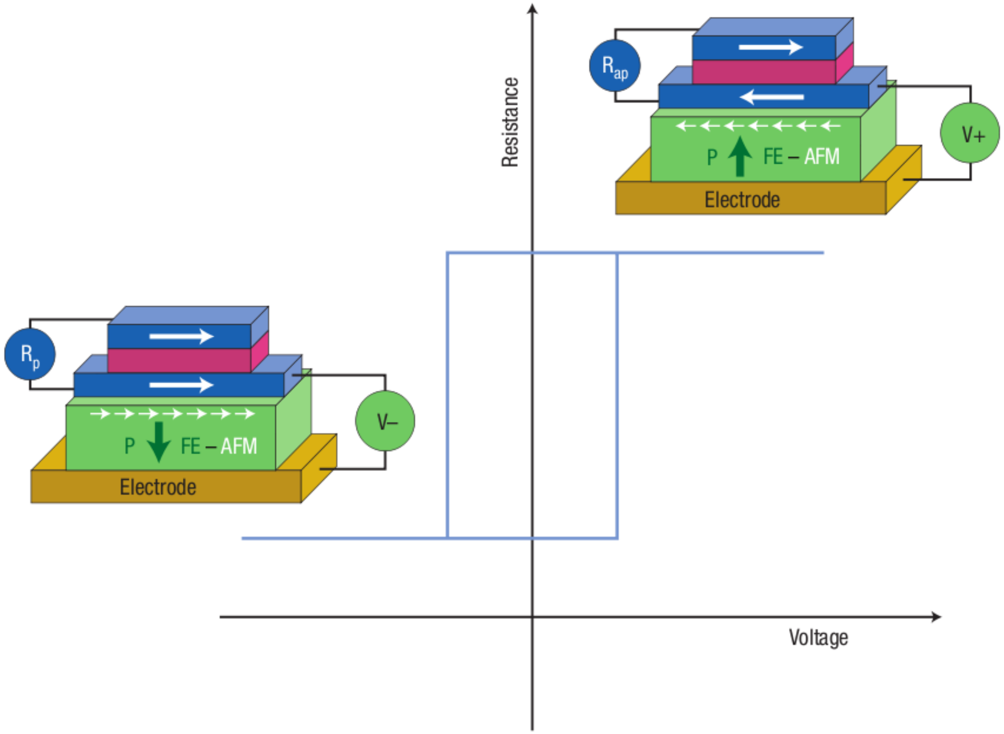
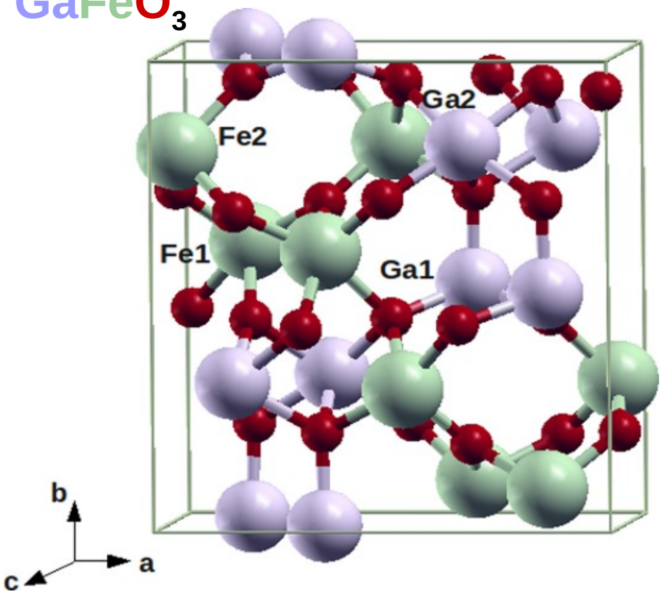
ME device



Manuel Bibes & Agnès Barthélémy, Nature Materials 7, 425 - 426 (2008)

Gallium ferrite (GFO): The magnetoelectric ferrimagnet

$GaFeO_3$



Properties are influenced by the Fe/Ga ratio

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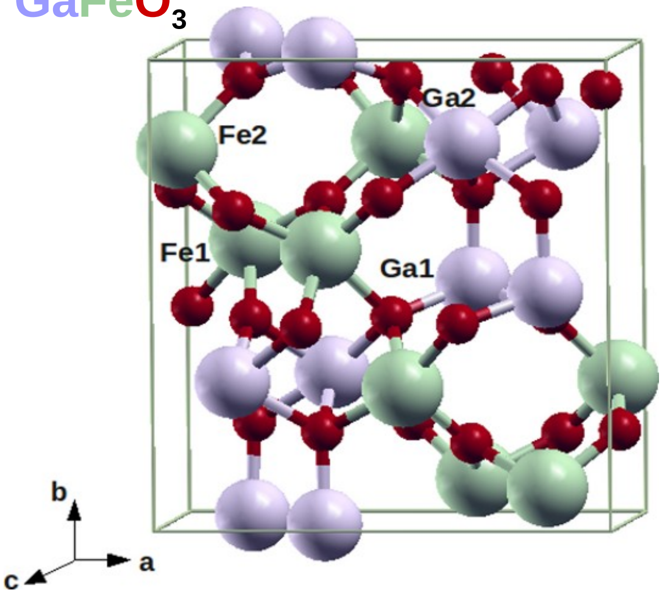

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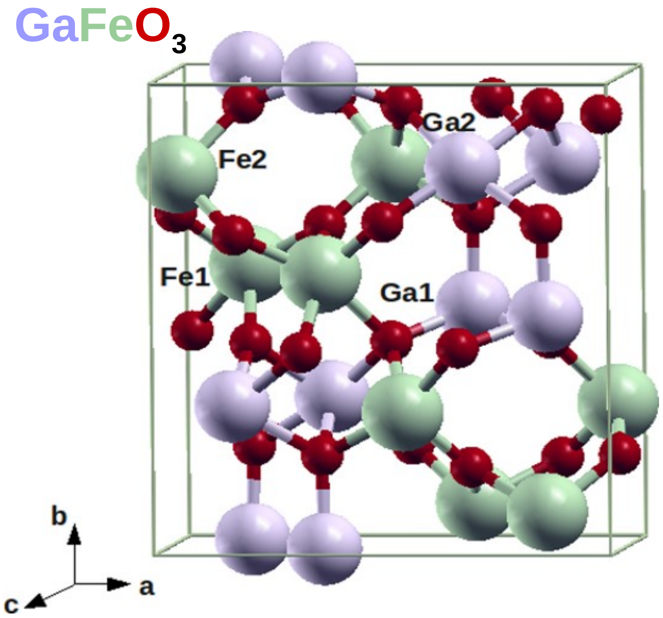
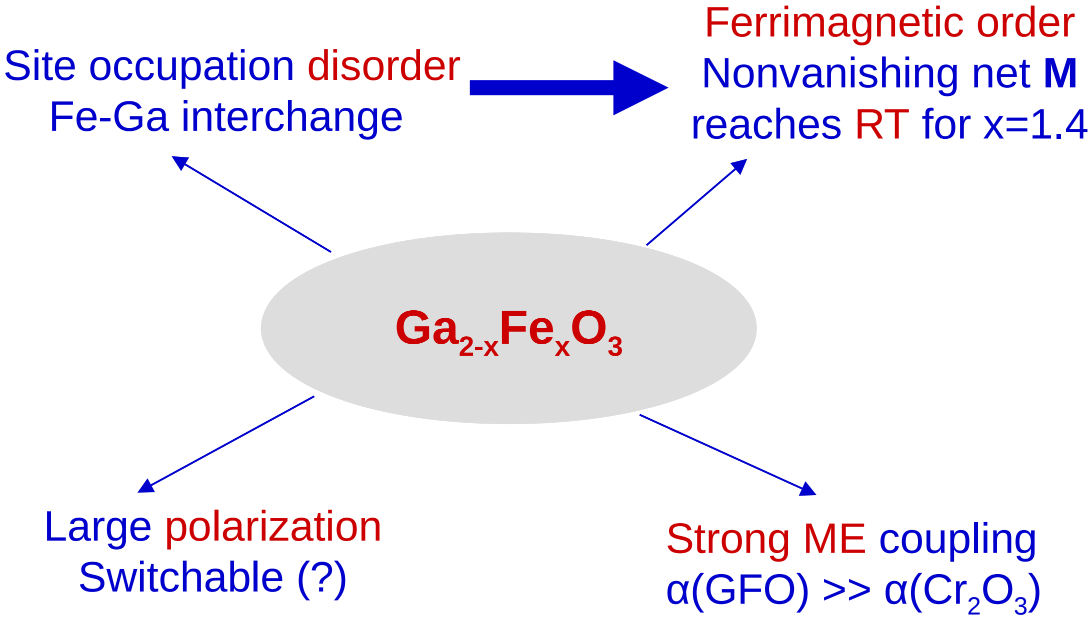


Properties are influenced by the Fe/Ga ratio

Experimentally demonstrated:



Site occupation disorder
Fe-Ga interchange

Ferrimagnetic order
Nonvanishing net **M**
reaches RT for x=1.4

$Ga_{2-x}Fe_xO_3$

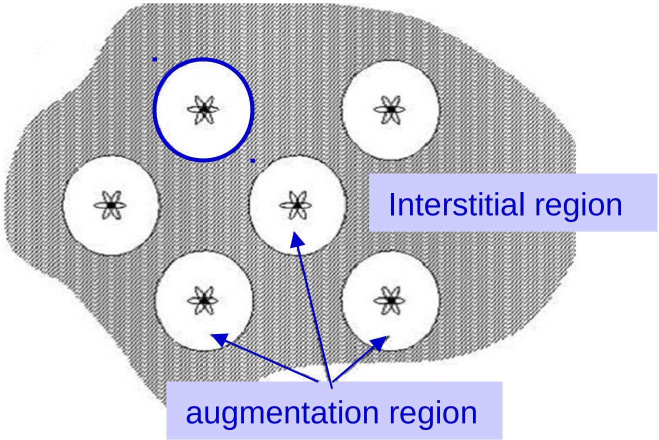
Large polarization
Switchable (?)

Strong ME coupling
α(GFO) >> $\alpha(Cr_2O_3)$

Methodology

Projector augmented wave (PAW)

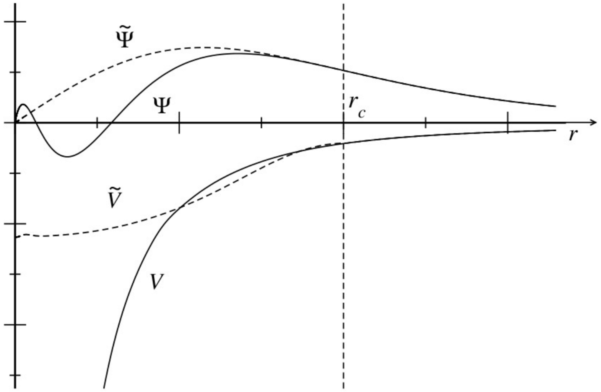
- PAW method based on the following approximations:
  - Frozen-core approximation
  - Dual representation of space
    - plane waves
    - localized basis into the augmentation spheres



Interstitial region

augmentation region

  - Pseudopotential based method



  - Various XC DFT functionals

- P.E. Blochl, PRB 50, 17953 (1994)

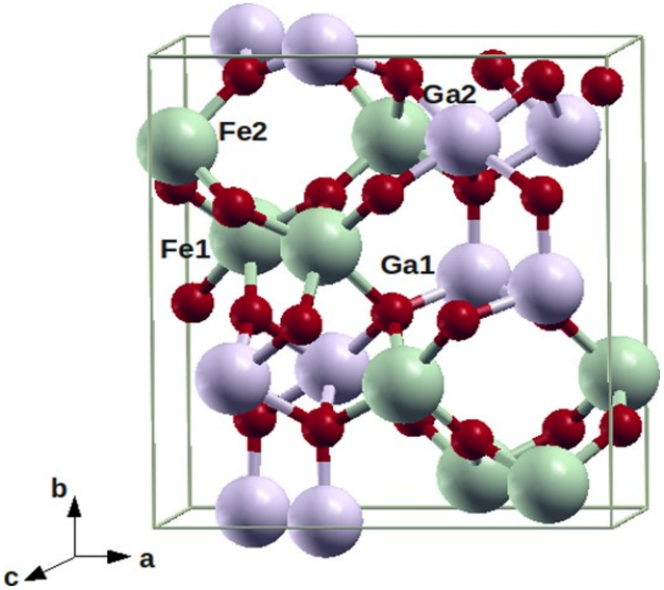
- http://www.cms.mpi.univie.ac.at/vasp/vasp.html

Materials : Gallium ferrite

Previous theoretical studies

F. Ibrahim, Thesis

- ❐ Correlated system → On-site Coulomb interaction (LDA+U)
- ❐ Different levels of approximation:
  LDA and GGA



- ❐ Orthorhombic structure
- ❐ 4 different atomic sites:
  - octahedral: Ga2, Fe1, Fe2
  - tetrahedral: Ga1
- ❐ Modelled supercell: 8 formula units (40 atoms)

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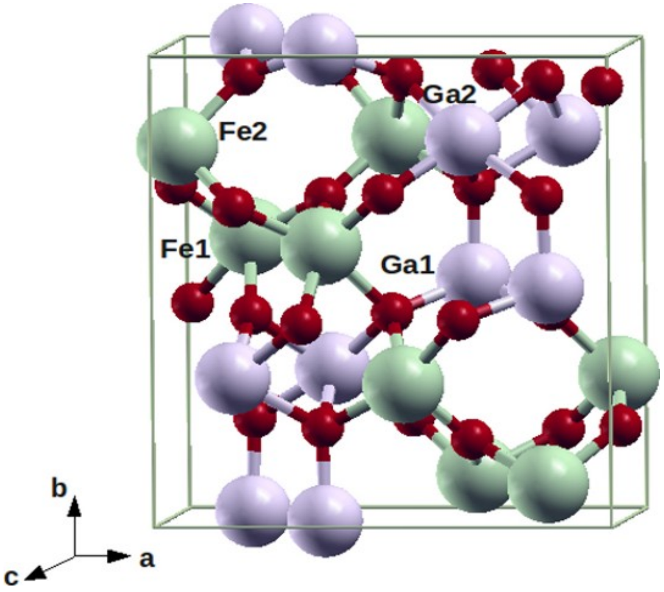

$Ga_{2-x}Fe_xO_3$: (atomic + volume) relaxation

⬇

✓ **Ground state**

✓**- x = 1 : Fe1 and Fe2 are AFM coupled**

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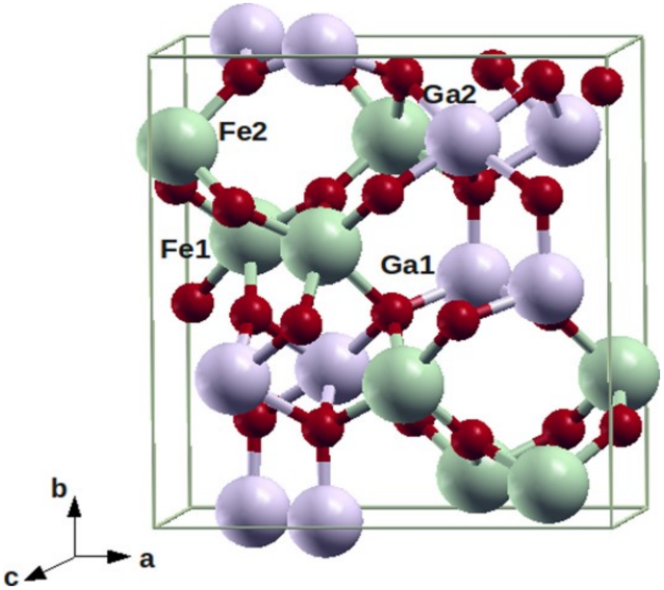

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✓ **Ground state**

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- x > 1 : excess Fe occupies Ga2 site and is FM coupled to Fe2 → **Ferrimagnetism**

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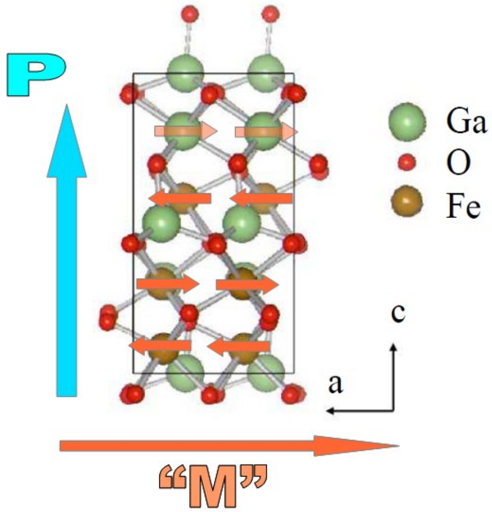
D. Stoeffler, J. Phys. : Condens. Matter **24**, 185502 (2012)
Dixit Anant, Thesis



GFO presents a highly polar equilibrium structure (*Pna*2_1)

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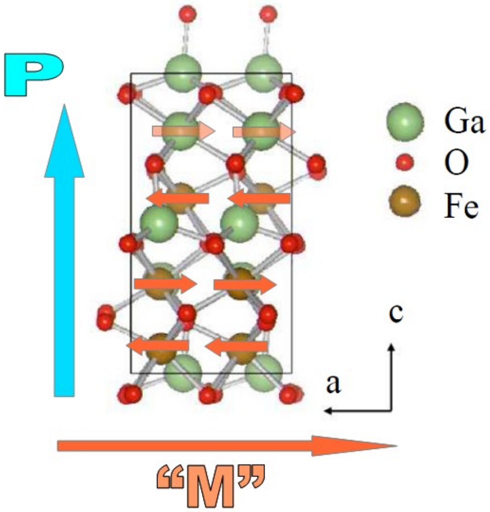

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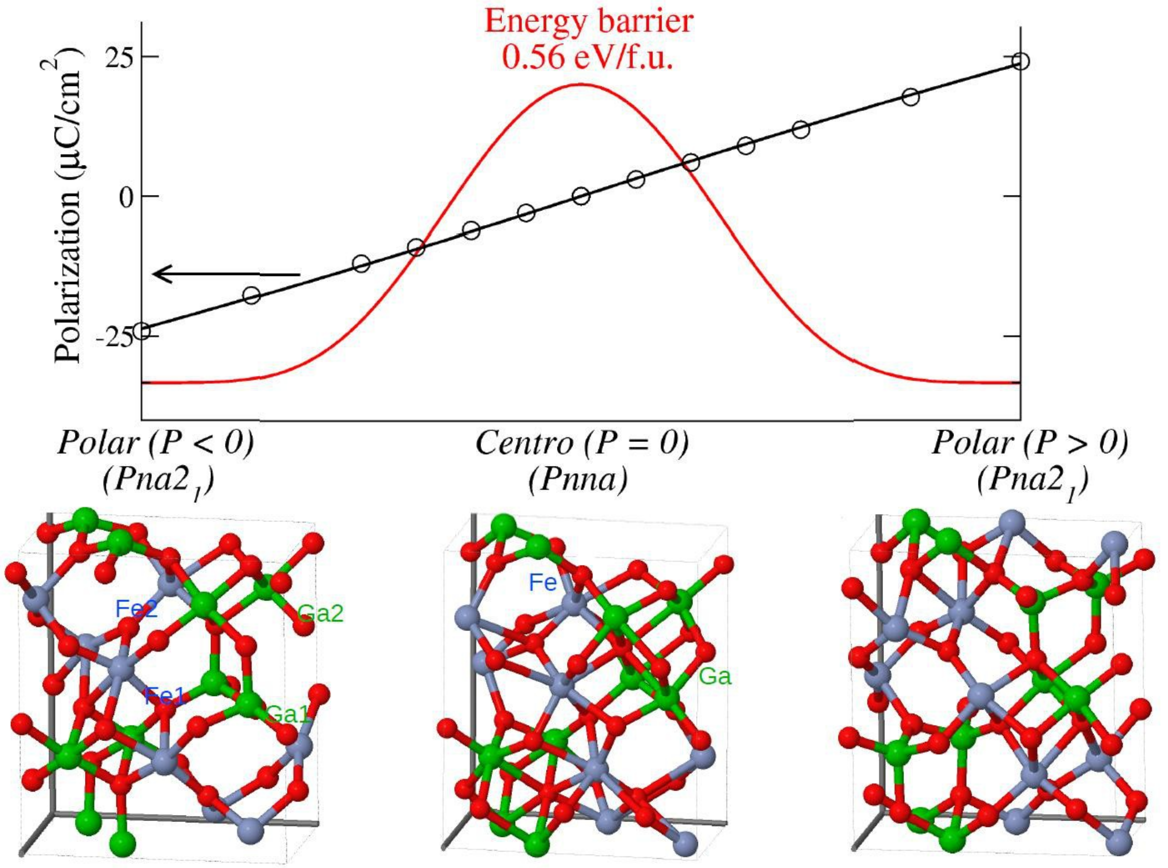

Modern theory of polarization :
P determined relative to a *Pnna* centrosymmetric structure → $P = -25\ \mu C/cm^2$.

The energy barrier to overcome for this homogeneous switching is found very large.

The polarization is weakly affected by variation of *x*

Goal

Magnetoelectric properties of selected oxides

(Cr_20_3, $YFeO_3$ and $GaFeO_3$)

1. Getting familiar with the VASP package on parallel computers.

2. Computing the magnetic properties.

3. Computing the electric polarization.

4. Investigate the relationship between the magnetization and the polarization.

Thank you for your attention!