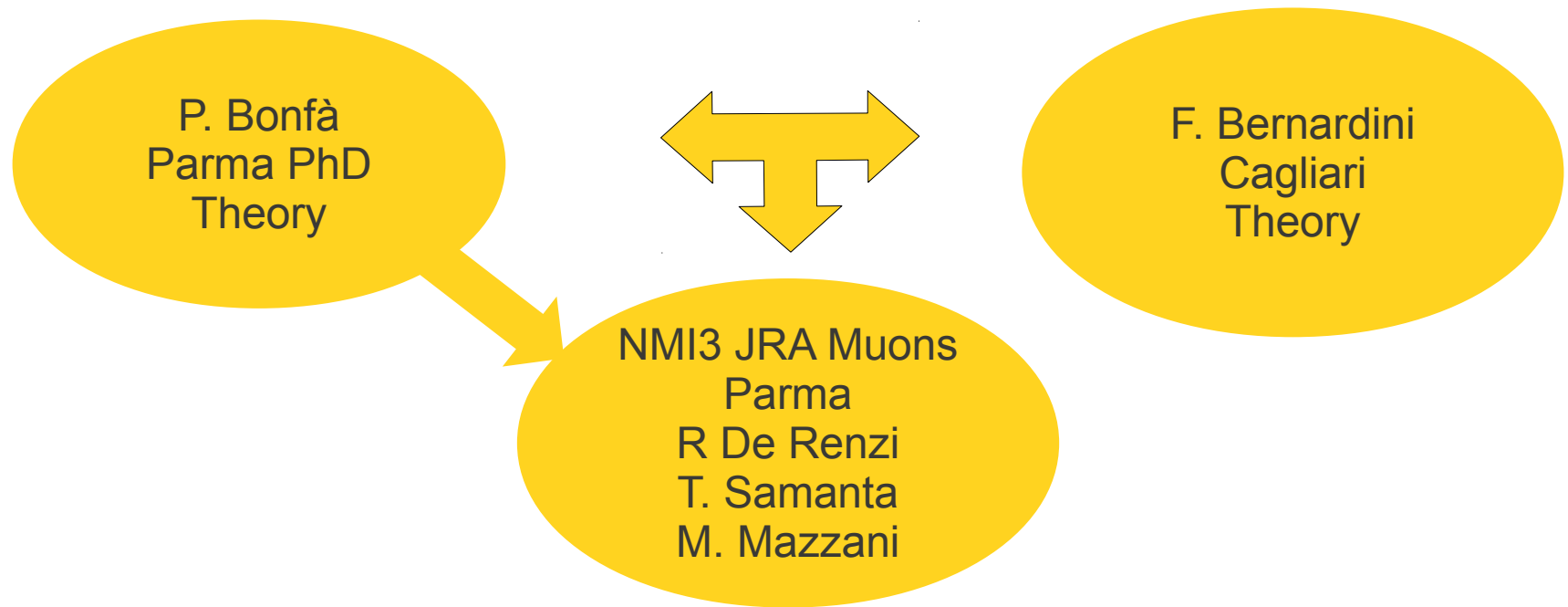


# $\mu$ SR 2.0: a new dimension for implanted muons



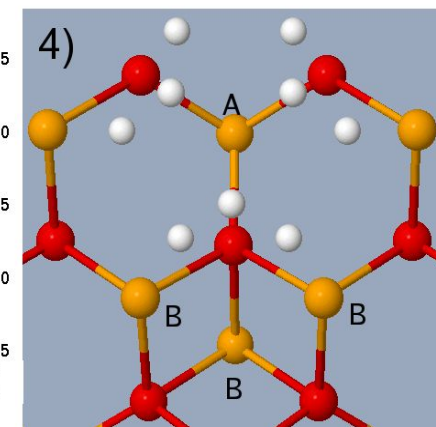
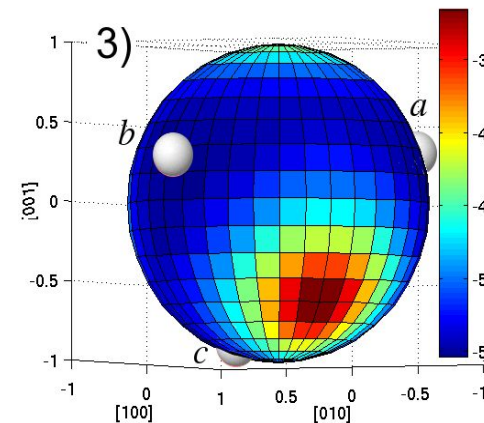
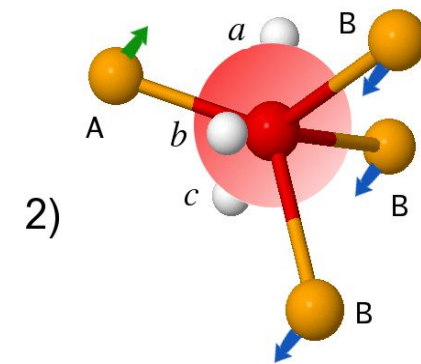
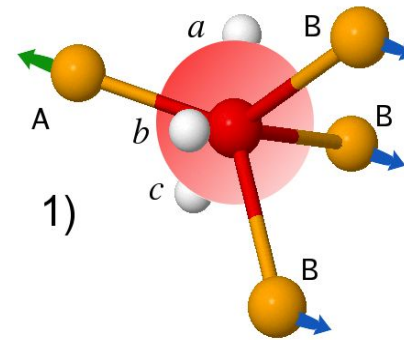
- What is done by experimentalists
- NMI3 plans for muon site
- ASE and python
- DFT
- Perspective, why  $\mu$ SR 2.0?

# The experimentalist approach

- Guess by lattice inspection and wisdom
  - Voids
  - Electrostatic potential for  $\mu^+$
  - Magnets: dipolar field
  - Nuclear dipoles: second moments
- Measure
  - Internal field
  - Nuclear line-widths
  - Paramagnetic shifts

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distant point dipoles

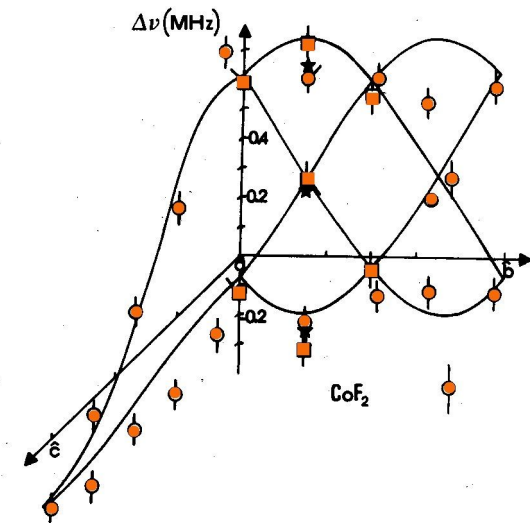
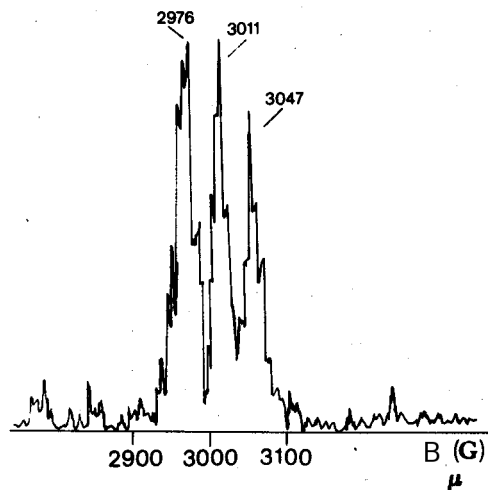
Fermi contact

$$\mathbf{B}_\mu = \frac{\mu_0}{4\pi} \sum_j \frac{3 \mathbf{m}_j \cdot \hat{r}_i \hat{r}_i - m_j}{r_i^3} + \frac{2\mu_0}{3} \mu_B (|\Psi_\uparrow(\mathbf{0})|^2 - |\Psi_\downarrow(\mathbf{0})|^2)$$

( + demagnetization + external field)

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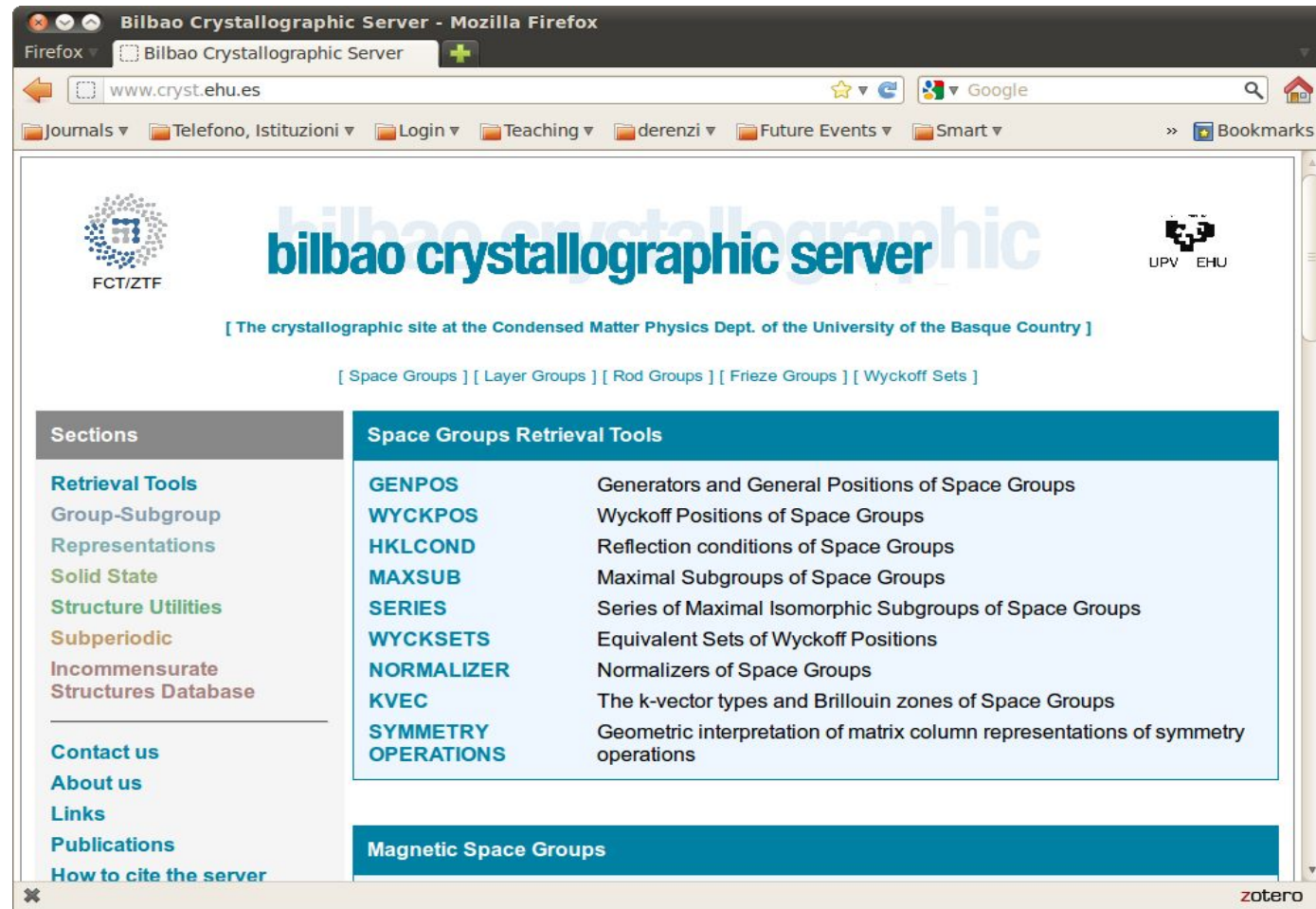


- Help newcomers to calculate dipolar fields
  - Get CIF
  - Define magnetic structure (magnetic CIF?)
  - Dipolar sums

# NMI3 JRA Muons plans

- Help newcomers to calculate dipolar fields
  - Get CIF
  - Define magnetic structure (magnetic CIF?)
  - Dipolar sums

Aim: a web page with Tools, a bit like ...



The screenshot shows the Bilbao Crystallographic Server website. The browser title is "Bilbao Crystallographic Server - Mozilla Firefox" and the address bar shows "www.cryst.ehu.es". The page header includes the logo "bilbao crystallographic server" and the text "[ The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country ]". Below the header, there are links for "Space Groups", "Layer Groups", "Rod Groups", "Frieze Groups", and "Wyckoff Sets". The main content area is divided into two columns. The left column, titled "Sections", lists various tools and resources. The right column, titled "Space Groups Retrieval Tools", lists specific tools and their descriptions.

Sections	Space Groups Retrieval Tools
<a href="#">Retrieval Tools</a>	<b>GENPOS</b> Generators and General Positions of Space Groups
<a href="#">Group-Subgroup</a>	<b>WYCKPOS</b> Wyckoff Positions of Space Groups
<a href="#">Representations</a>	<b>HKLCD</b> Reflection conditions of Space Groups
<a href="#">Solid State</a>	<b>MAXSUB</b> Maximal Subgroups of Space Groups
<a href="#">Structure Utilities</a>	<b>SERIES</b> Series of Maximal Isomorphic Subgroups of Space Groups
<a href="#">Subperiodic</a>	<b>WYCKSETS</b> Equivalent Sets of Wyckoff Positions
<a href="#">Incommensurate Structures Database</a>	<b>NORMALIZER</b> Normalizers of Space Groups
<a href="#">Contact us</a>	<b>KVEC</b> The k-vector types and Brillouin zones of Space Groups
<a href="#">About us</a>	<b>SYMMETRY OPERATIONS</b> Geometric interpretation of matrix column representations of symmetry operations
<a href="#">Links</a>	
<a href="#">Publications</a>	
<a href="#">How to cite the server</a>	

Magnetic Space Groups

- General purpose dipolar sum program
- Input standard CIF

(is ASE stable?)



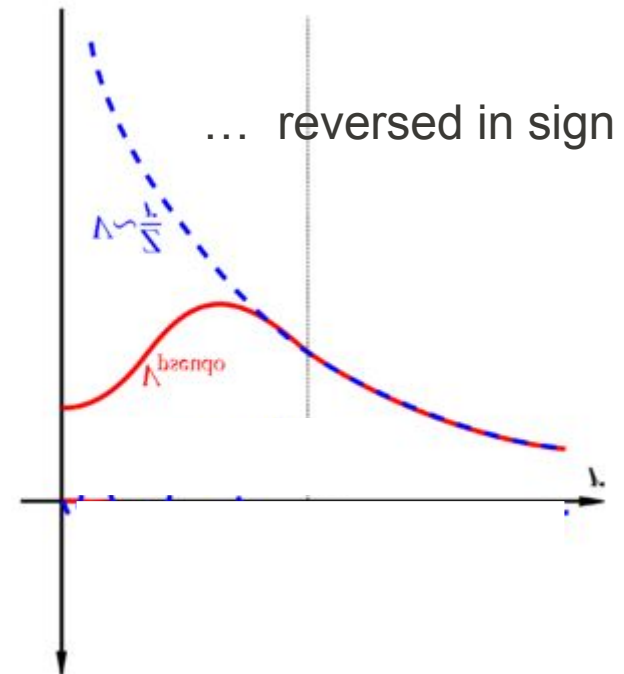
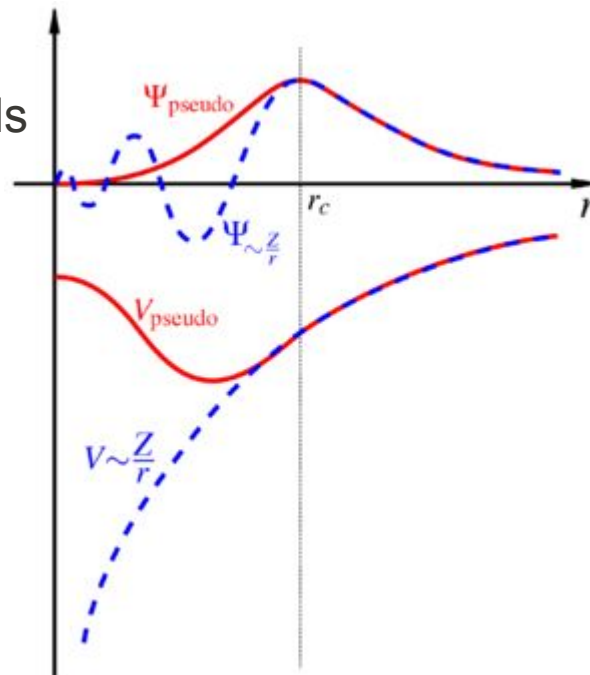
## The three steps of DFT

- Find site (first approximation)
- Refine site (relax lattice + Mu, ...)
- Calculate full local field (also Fermi contact)

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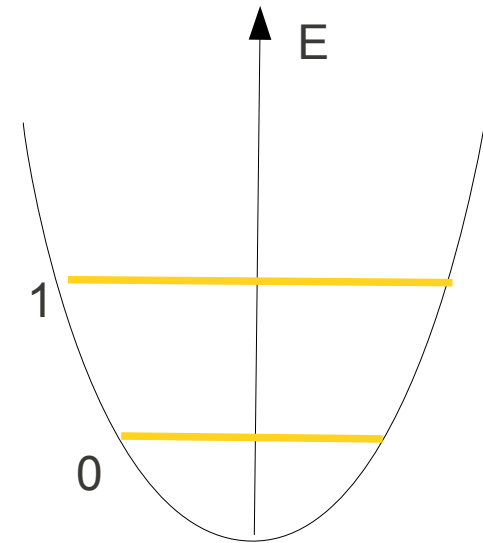
The bare muon feels the  $e^-$  Coulomb potential ...



# The three steps of DFT

- Find site (first approximation)
- Refine site (relax lattice + Mu, ...) Does the site change?
- Calculate full local field (also Fermi contact)

Also: approximate muon as harmonic oscillator and calculate zero point displacement



## The three steps of DFT

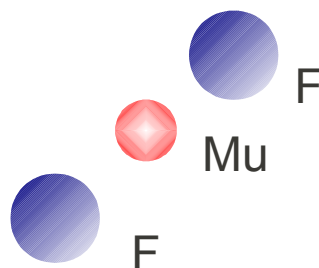
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Fermi contact

# Where $\mu$ SR 2.0 and why?

- Test on textbook cases:
  - $\text{CoF}_2$
  - $\text{LiF}$  (the meaning of  $\text{LiF}$ )
  - $\text{Fe}$
  - $\text{Si}$ ,  $\text{SiO}_2$



Original NMI3 task

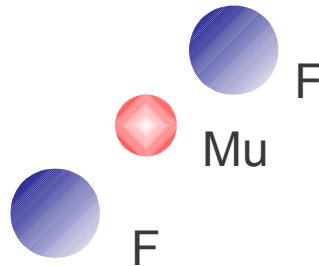
- Build systematics and discover euristics

Metals  
Semiconductors (p-type, n-type)  
Insulators  
Molecular systems  
Magnetic insulators  
Beasts (cuprates, pnictides,

Increasing DFT  
complexity

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- Build systematics and discover euristics

Perhaps:

- Solve old riddles? (e.g. Muon vs. Muonium)
- Tackle “muon-not-a-passive-probe” problems?
- Use muon as a probe of electronic structure?

Original NMI3 task

New scope  
 $\mu$ SR 2.0