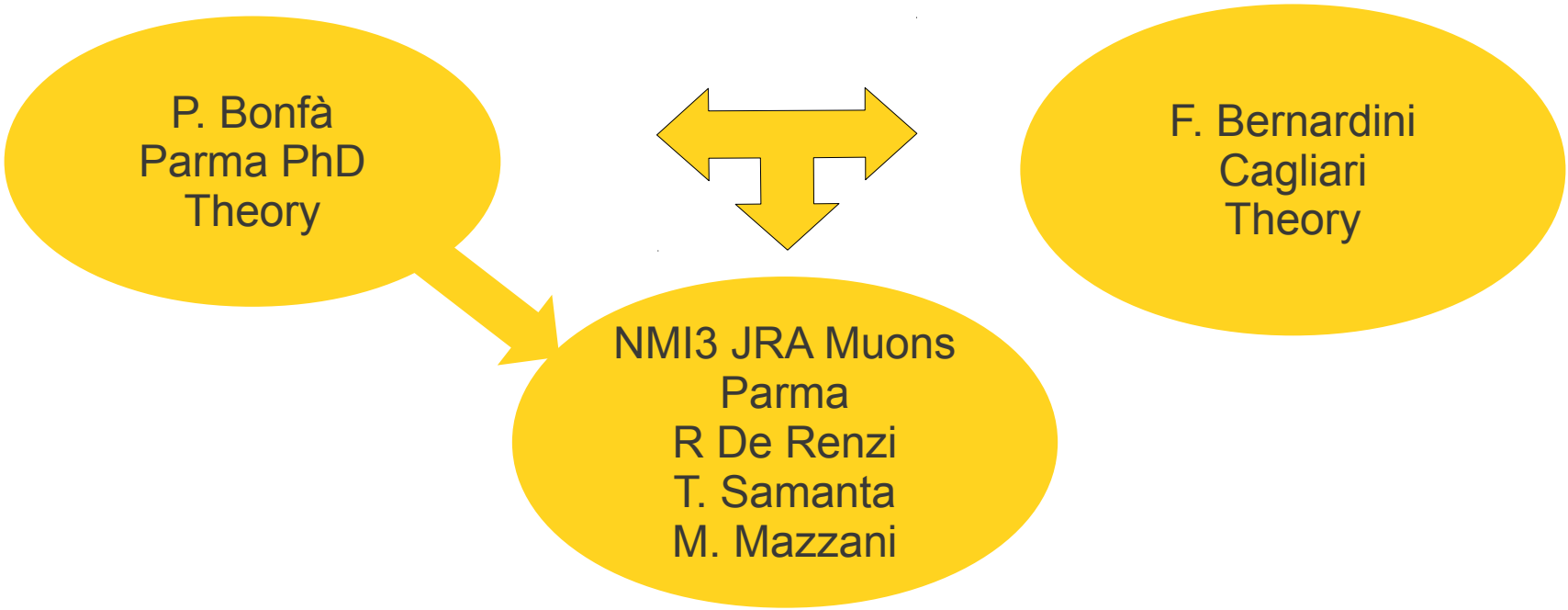
μSR 2.0: a new dimension for implanted muons



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

The experimentalist approach

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

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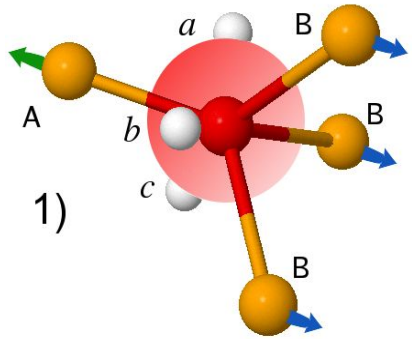
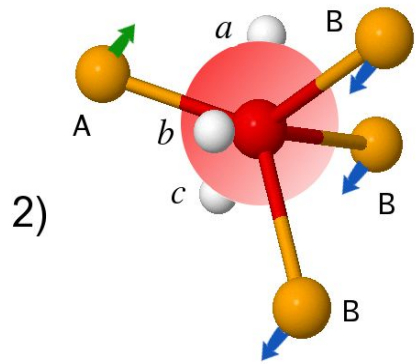
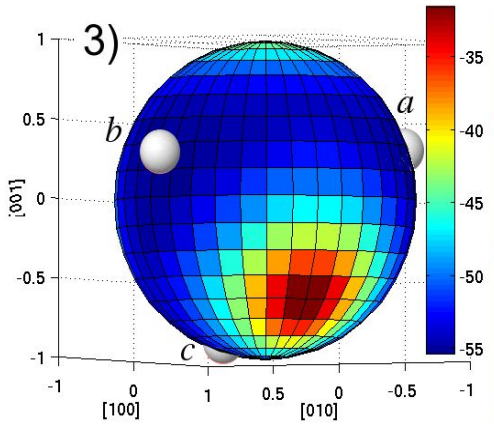
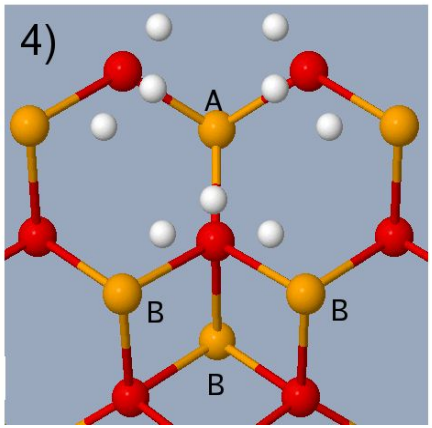




Fe_3O_4





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distant point dipoles

Fermi contact

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

(+ demagnetization + external field)

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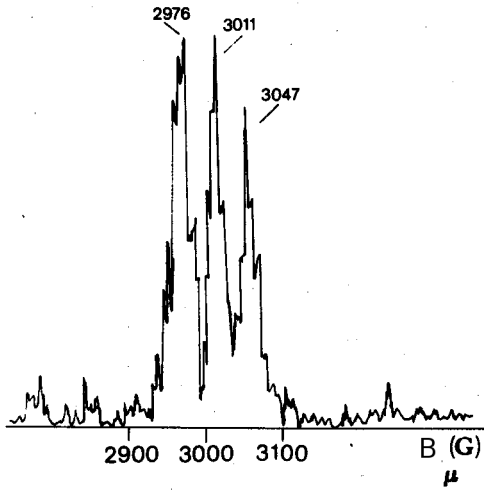

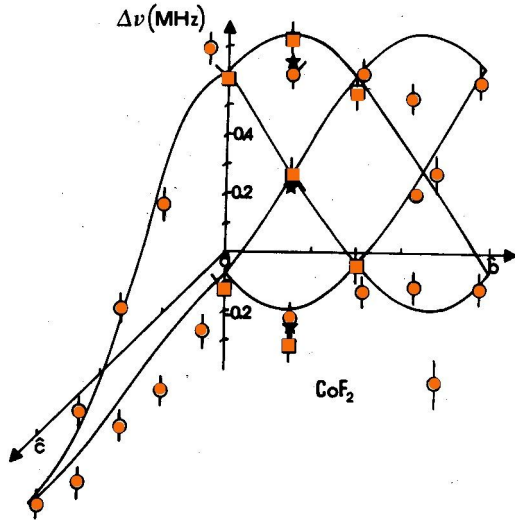

NMI3 *JRA Muons* plans

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

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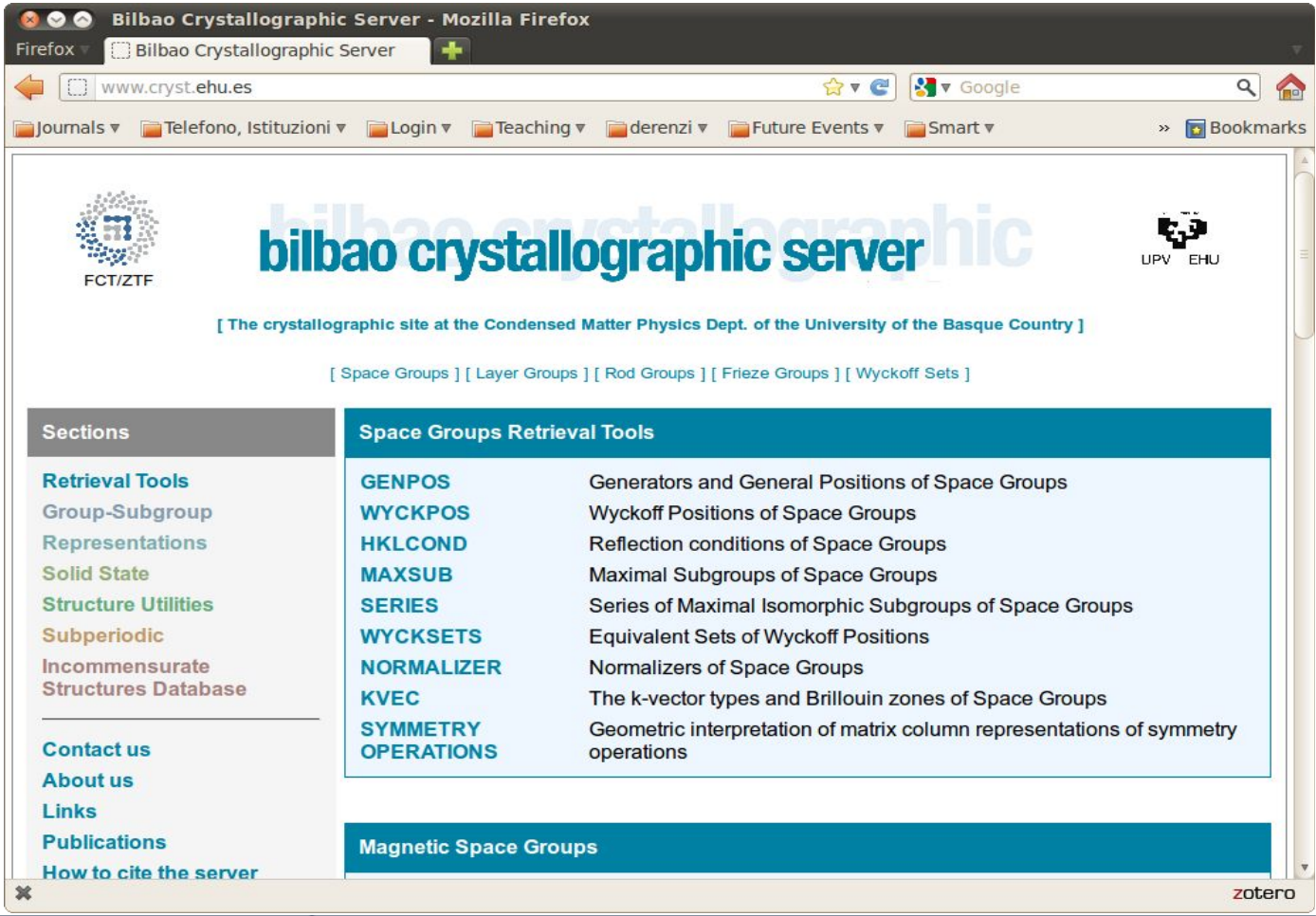
Aim: a web page with Tools, a bit like ...



ASE + python

- General purpose dipolar sum program
- Input standard CIF

(is ASE stable?)

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- Find site (first approximation)
- Refine site (relax lattice + Mu, ...)
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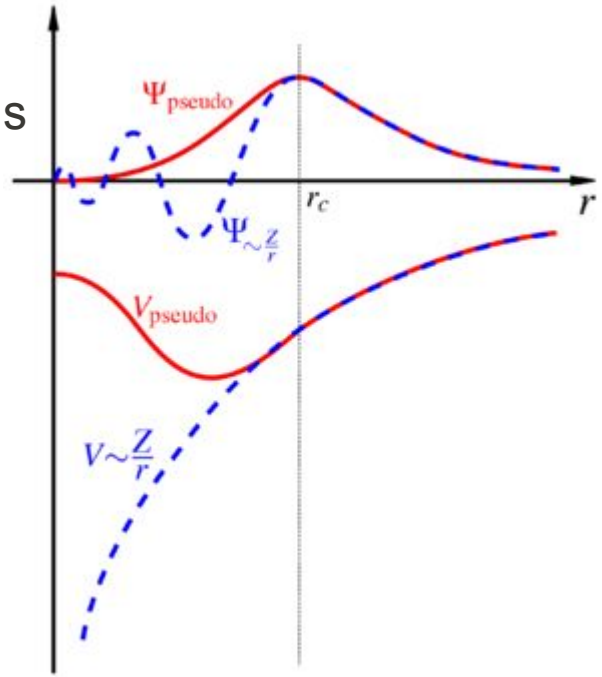
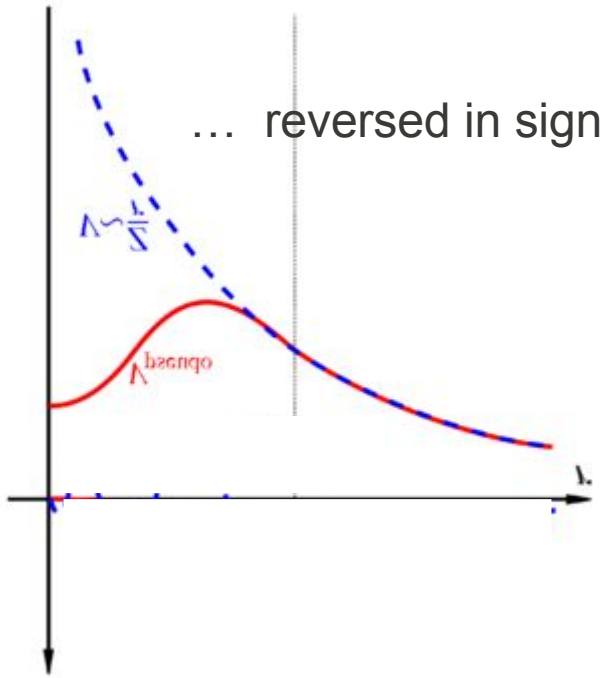
The bare muon feels the e^- Coulomb potential ...



… reversed in sign



The three steps of DFT

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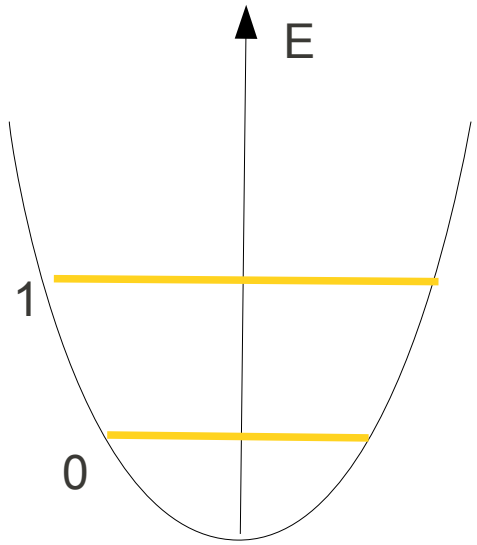
- Refine site (relax lattice + Mu, ...)

Does the site change?

- Calculate full local field (also Fermi contact)

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



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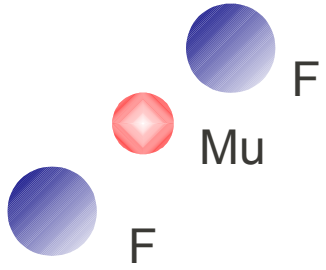
  - CoF_2
  - LiF (the meaning of LiF)
  - Fe
  - Si, SiO_2



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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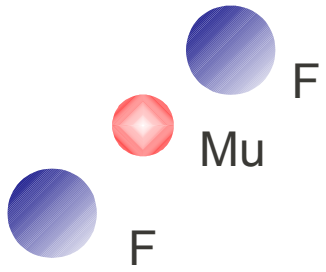

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Perhaps:

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

New scope
μSR 2.0