

The muon site: a toolbox

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Aim: put together an easily shearable tool to identify the muon site.

Functions and strategies:

1. Open software with simple mathematics and graphics (matlab like)
2. Access to a crystallographic library, to define and visualize lattice & magnetic structure
3. **Exploration of tentative muon sites:**
 - Simple dipolar sums, with given point-like magnetic moments
 - Point charge electrostatic potential, e.g. constrained on spheres around anions
4. **DFT calculation of muon site**
 - Full muon potential
 - Zero point motion
 - Full hyperfine field (contact and dipolar)
5. Documentation, both embedded and web based

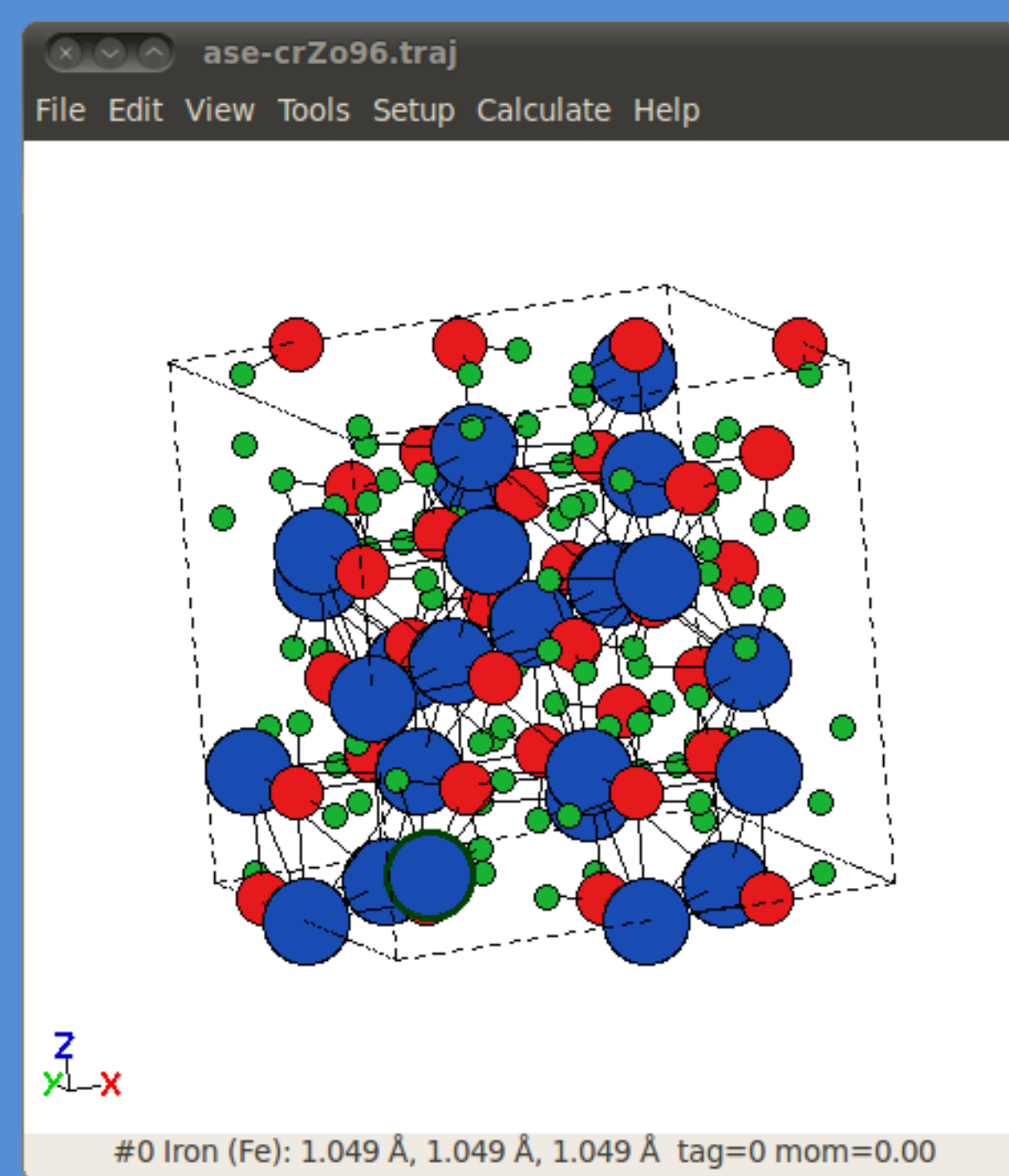
2. ASE: Atomistic Simulation Environment

<https://wiki.fysik.dtu.dk/ase>

Includes

- full crystal symmetry groups
- lattice visualization
- initial magnetic moments and ion charges
- interface to many DFT calculators

```
import ase
import numpy as np
from ase.lattice.spacegroup import crystal
a = 8.3940
fe3o4=crystal(['Fe','Fe','O','H'],
              basis=[(0.12500, 0.12500, 0.12500),
                    (0.5, 0.5, 0.5),
                    (0.25480, 0.25480, 0.25480),
                    (0.285, 0.285, 0.1302)],
              setting=2,
              spacegroup=227, cellpar=[a, a, a, 90, 90,
              90],
              size=(1,1,1),pbc=False)
ase.visualize.view(fe3o4)
```



3. ASE

Zero-order muon site validation. Reproduce two types of published results

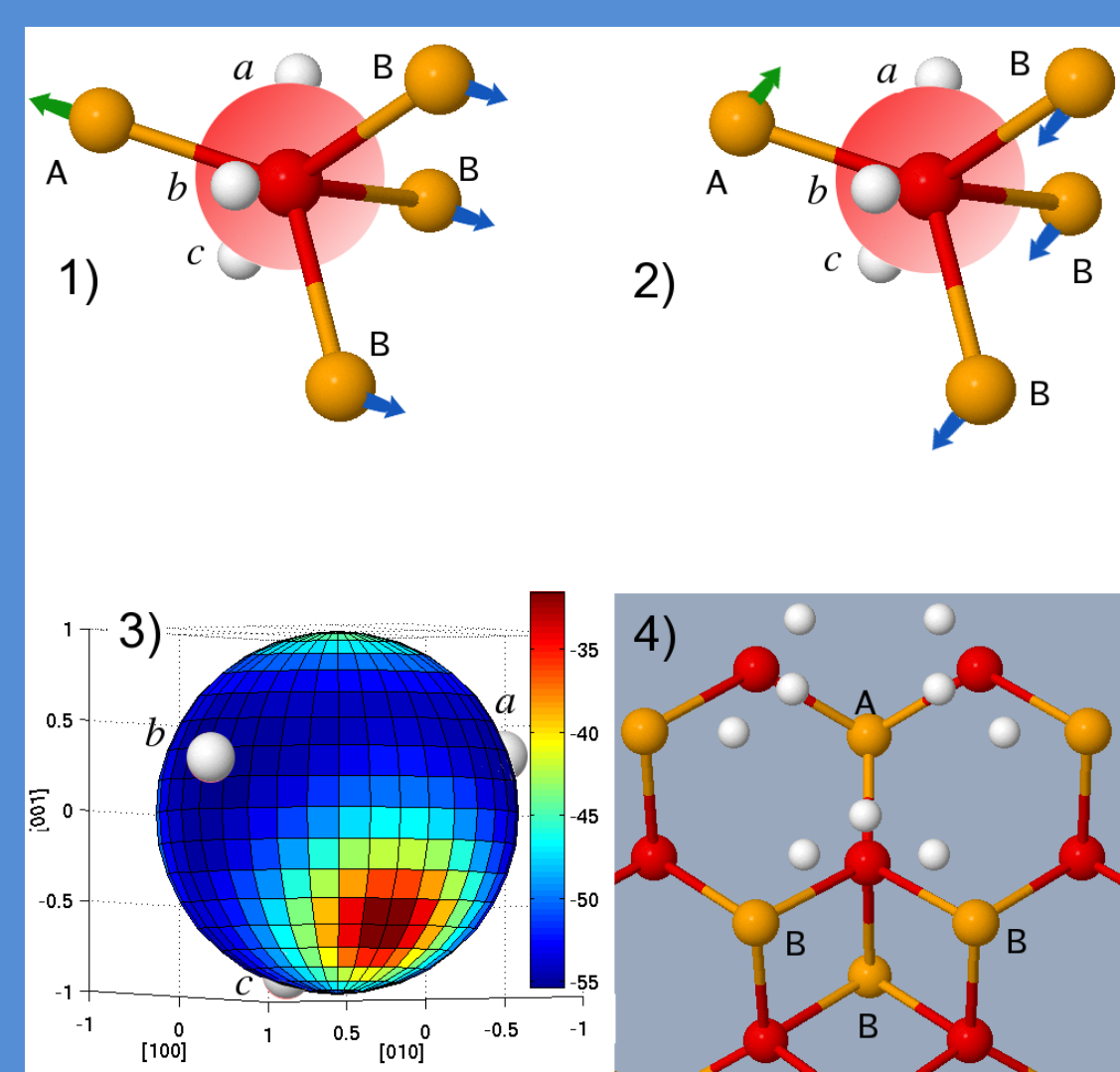
- I. Those obtained by simplified strategies, such as $\text{YBa}_2\text{Cu}_3\text{O}_6$ [1] and Fe_3O_4 [2]. :
 - i. find *point charge potential* V minima,
 - ii. check dipolar sums against local field B_μ

Dipolar sum code
5 declarations
12 lines of code with check of convergence

Point charge potential with Ewald's trick
4 declarations
26 lines of code

See also
<http://www.fis.unipr.it/~derenzi/dispense>

(node pmwiki.php?n=MUSR.ASEStart#potential)



- II. Those obtained by DFT (see box 4. on the right)

5. Documentation

Embedded, ipython provides

- tabbed completion of commands
- interactive help on each available command just by entering command?

Web based, a wiki (under construction) with instructions on

- how to install the various bits
 - Python itself
 - ASE
 - The chosen DFT
 - The toolbox
- examples of how to run the toolbox

1. Python <http://www.python.org/>



Open software, available on all OS

Quick interface to software in any other language, see bona below

ipython, specialized for interactive use, with more extensive help

<http://ipython.scipy.org>

Matlab-like dialect <http://matplotlib.sourceforge.net/>



4. Density Functional Theory calculator

Many different programs can be installed and invoked with a simple python command:



More can be interfaced, including Wien2k



One is already included and allows simple calculations



Finding the muon site by DFT may be anything between *straightforward* (ionic crystal) and a *subtle art* (the muon bond in a lattice with *all-electron* atoms, typically rare earths)

4. Density Functional Theory by F. Bernardini

Example, cfr. [3]: **LaFeAsO**

$$V = V_\mu = -V_e \quad \text{only Coulomb!}$$

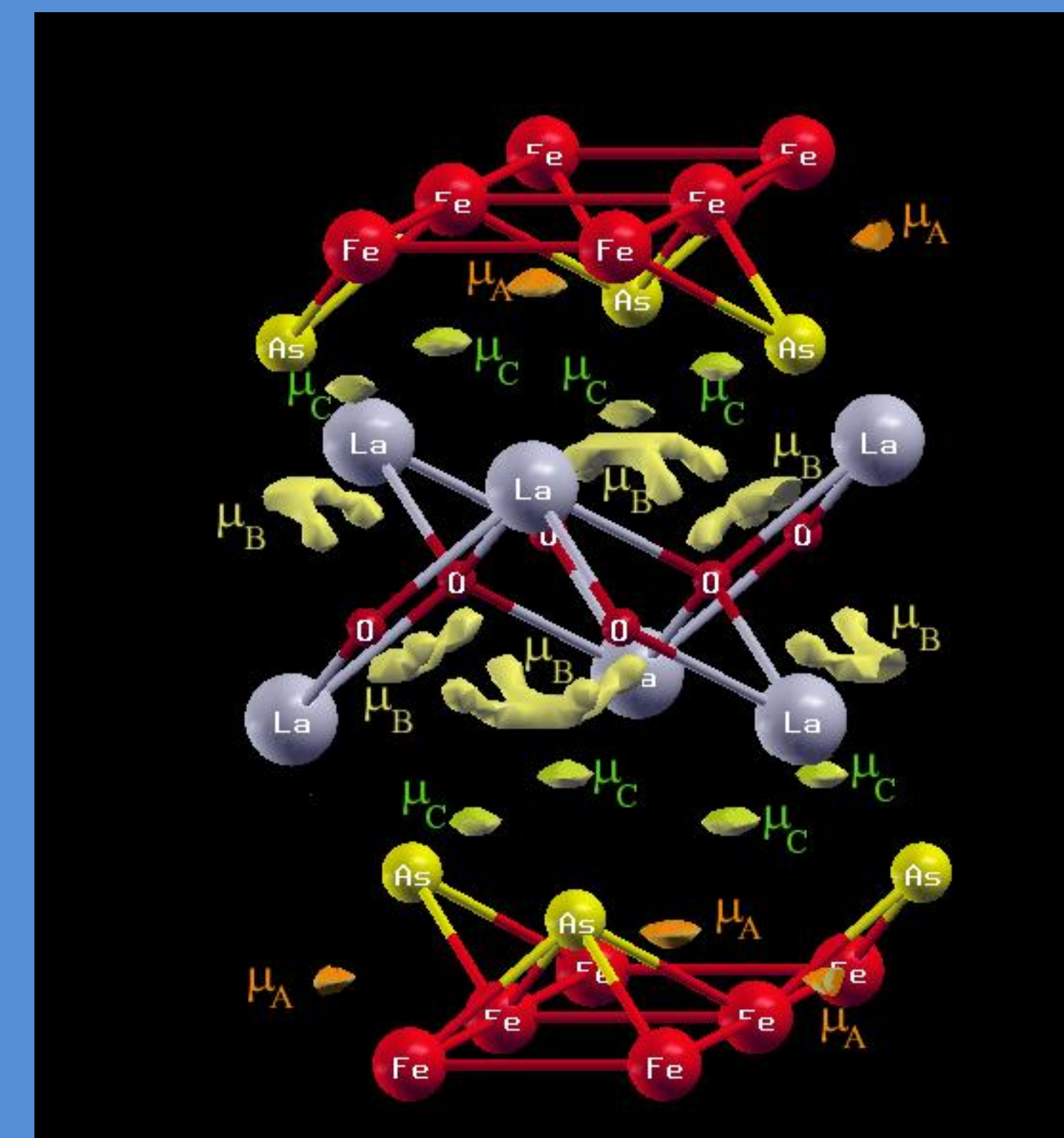
Muon site(s) volume

- centered at **min(V)**
- defined by harmonic **zero energy E_0** within the isopotential surface

$$V = \min(V) + E_0$$

	μ_A	μ_B	μ_C
$V(\text{eV})$	0*	0.55	0.94
$E_0(\text{eV})$	0.15	0.12	0.16

* arbitrary



To be done

- Documentation
- Packaging, distribution, installation instructions
- Choice of suitable DFT for ASE
- Full hyperfine field calculation
- Muon bond
- More extensive validation

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References

- [1] M. Weber, P. Birrer, F. N. Gygi, B. Hitti, E. Lippelt, H. Maletta, A. Schenck, Hyperfine Interactions **63**, 207 (1990)
- [2] M. Bimbi, G. Allodi, R. De Renzi, C. Mazzoli, H. Berger, Phys. Rev. B **77**, 045045115 (2008)
- [3] H. Maeter et al., Phys. Rev. B **80**, 094524 (2009)

