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

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`

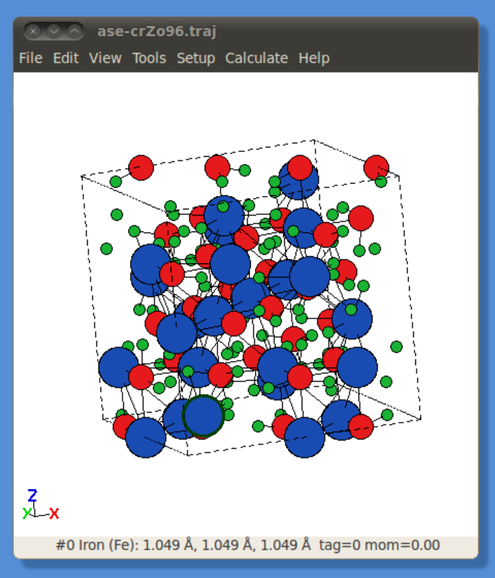
Matlab-like dialect `http://matplotlib.sourceforge.net/`

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

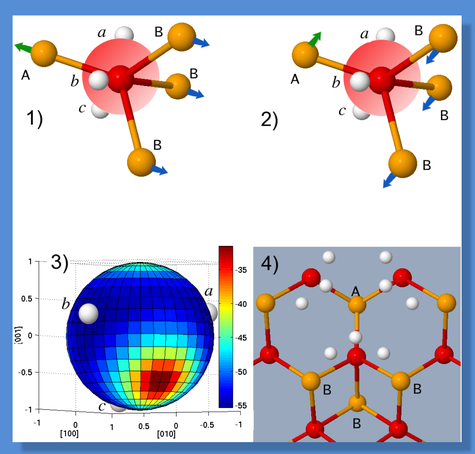
I. Those obtained by simplified strategies, such as $YBa_2Cu_3O_6$ [1] and Fe_3O_4 [2], :
   i. find *point charge potential* V minima,
   ii. check dipolar sums against local field B_μ.

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)

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

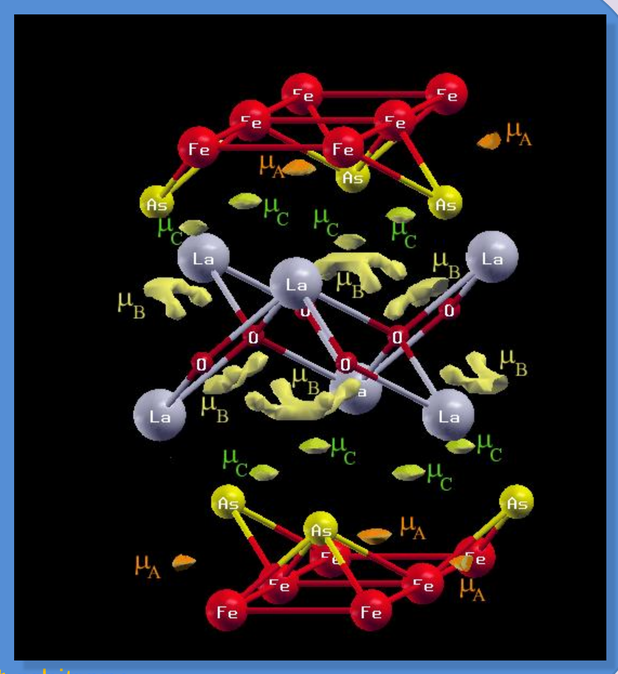
Example, cfr. [3]: **LaFeAsO**

$V = V_\mu = - V_e$ 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(eV)	0*	0.55	0.94
E_0(eV)	0.15	0.12	0.16



* arbitrary

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

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

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