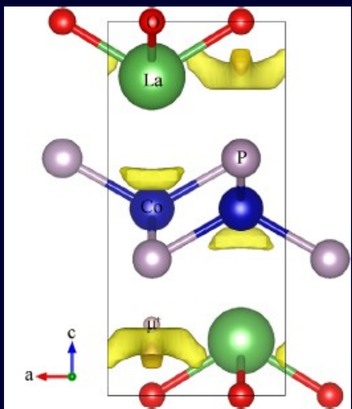
The Muon Site: μSR 2.0

μSR, muon spin spectroscopy, is an important experimental technique, unique in providing very fast turnout information on the properties of magnetic materials, hydrogen reactions, slow local motions (e.g. ionic diffusion). It is extremely easy to implant muons in virtually any material and to detect the muon spin evolution in time, in conceptual analogy with NMR, but with a much faster, broadband experiment. For magnetic materials μSR, neutron scattering and NMR are the techniques of election.

The main drawback of the muon has been until now our a-priori ignorance of where the muon sits when implanted in the lattice. We know that it is most frequently an interstitial site, but we do not know where in the cell. Part of the information remains therefore quantitatively relative, not absolute.

We have recently learnt how to predict the muon site by Density Functional Theory. DFT is an established theory, building on the Nobel Prize discovery of Walter Kohn, and built into a number of codes (e.g. Quantum Expresso) available on our computers.



Candidate muon sites at the center of the yellow energy isosurfaces, in LaCoPO, a relative of the Fe superconductors.

This is the beginning of MuSR 2.0, since it allows the direct measurements of important physical quantities, that could be previously obtained only from extensive single crystal experiments. For instance the muon site assignment allows the precise determination of the ordered magnetic moment in a known magnetic structure, often requiring neutron diffraction experiments, not always feasible. Our new strategy [1] has been shown to work in a steadily growing number of cases [1,2], sufficient to establish the method, but far from having exploited its potentials yet.

The ideal perspective Master/PhD student [4] is not afraid of theory, has a passion for problem solving, some skills in computing, love and respect for experimental data, all qualities that may develop during the journey. The only pre-requisite is a generic background in solid state physics at the Master level. Of course acquired skills in any of these aspects are highly valued.

The task will be to build on what we did until know, by participating in μSR experiments, mostly on magnets and superconductors, and by running the DFT search for the muon site. A growing number of internationally established muon groups, working on cutting edge problems, is interested in collaboration on this subject, with a high perspective paper yield.

Ask any questions to roberto.derenzi@unipr.it, impressions and group life reference to the present PhD students and Post Docs, for DFT, μSR, NMR: pietro.bonfa@fis.unipr.it and for NMR, μSR: sara.bordignon@studenti.unipr.it

References

[1] J. S. Moeller, P. Bonfà, D. Ceresoli, F. Bernardini, S. J. Blundell, T. Lancaster, R. De Renzi, N. Marzari *Playing quantum hide-and-seek with the muon: localizing muon stopping sites* Phys. Scr. 88 068510 (2013)

[2] F. Bernardini, P. Bonfa, S. Massidda and R. De Renzi, Phys. Rev. B 87, 115148 (2013)

[3] P. Bonfà, F. Sartori, R. De Renzi, J. Phys. Chem. C 119, 4278–4285, (2015)

[4] The Parma Doctorate in Physics has at least 7 payed positions for the XXX Cycle, application deadline 4 September 2014, admission 1 November 2014;