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Invitation

LMU-Seminar

Title: **Computer Simulations for Interpreting Muon-spin Relaxation Experiments**

Speaker: **Dr. Leandro Liborio**
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Time: **Tuesday, November 12th 2019, 10:30**

Place: **WBGB/020**

Abstract:

In a muon-spin relaxation experiment (μSR) spin-polarized positive muons are implanted in a sample to probe its local static and dynamic magnetic properties. μSR is a sensitive probe of magnetism, but one of its limitations is not knowing the site of implantation of the muon, which prevents the use μSR for measuring magnetic moments or for comparing different magnetic structures.

In some limited cases, the muon stopping sites can be found using direct experimental approaches. For example, in muonated iron[1]. In other cases, such as LiF[2] and the coordination polymer copper-pyrazine-nitrate $Cu(pyz)(NO)_3$[3], a combination of experiments and calculations was used to determine the muon stopping sites. In these examples, the theoretical calculations are a cheap way of testing potential muon stopping sites. In most of these examples there are a few starting guess sites for the muon, which limits the number of test calculations. However, this limitation is not possible in most species.

So, whenever the candidate muon sites cannot be assigned by an educated guess, we need to explore all the possible interstitial sites using purely theoretical methods. In this talk, I will present the methods that we are developing to tackle this problem and I will discuss their advantages and limitations.

The first of these methods is the unperturbed electrostatic potential method, which relies on the analysis of the electrostatic potential of the host material that is obtained from DFT simulations. The second method is based on a combination of ab initio calculations, random structure searching and machine learning[4], and it provides the basis for our third method, which distinguishes from the second one in that it uses Density Functional Tight Binding Calculations[5] instead of pure ab-initio ones, which accelerates the calculations by, at least, two orders of magnitude. I also will show how our methods have successfully predicted the muon stopping sites in materials as diverse as Si, Diamond, Ge, LiF, the three crystalline phases of TiO_2, La_2LiHO_3 and a series of organic crystalline materials.

Finally, I will also present the software tools that we have already developed to implement these methods and also briefly present some of the new tools that we are currently developing for μSR.

[1] PRB **32**, 293, 1985

[2] PRB **87**, 121108(R), 2013

[3] PRB **91**, 144417, 2015

[4] J. Chem. Phys. **148**, 134114 (2018)

[5] J. Chem. Phys. **150**, 154301 (2019)