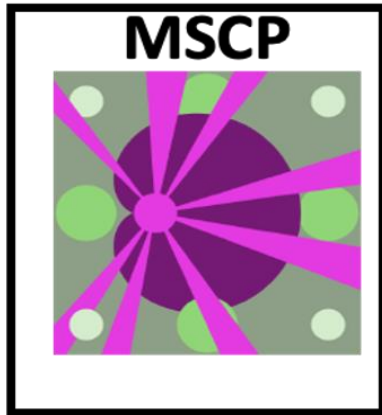


ISIS Muons – LMU Meeting

L. Liborio¹

¹Scientific Computing Department, STFC, UK
21 July 2026



**Science and
Technology
Facilities Council**

Ada Lovelace Centre

Development work and some suggestions

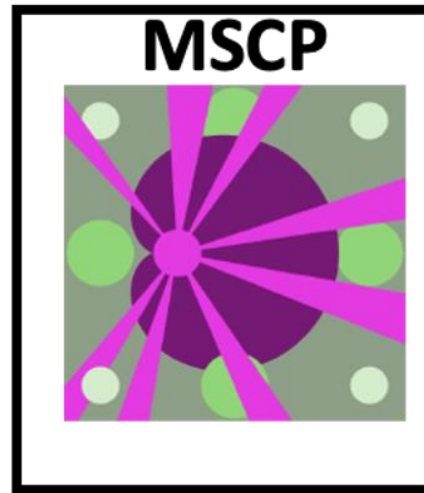
<https://muon-spectroscopy-computational-project.github.io>

Sustainable, User-friendly and Reproducible Software Tools for Interpreting Muon Experiments

pymuon-suite

μ^+ Predicting muon stopping sites.

- Tool used in most **μ^+** experiments
- Built prototype in  **AiiDA**lab
- Working on CASTEP  **AiiDA**lab
- Tutorials and training materials available
- Integrating with PSI muon tools
- Develop plug-in to assist DFT simulations
- Develop Quantum Espresso plug-in



Muspinsim

μ^+ spin dynamics of systems of a muon plus other spins

- ALC PhD working on the fundamentals of the electronic structure calculations.
- Working on adding RF experiments
- Tutorials and training materials available
- Will make plug-in in  **AiiDA**lab
- Use MLIP to simulate dynamical effects



MuDirac

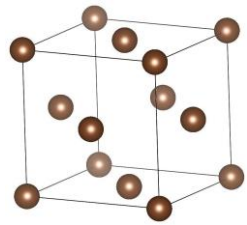
μ^- Modelling muonic x-rays

- Tool used at PSI and J-PARC
- Part of the EVA software at ISIS
- Working on peak-intensities for muonic x-rays
- Tutorials and training materials available
- New MuDirac uses nuclear properties improvements to elemental analysis
- Working on improving EVA+MuDirac -> next MuDirac version with intensities
- EVA for all muon sources

μ^+ workflows in AiiDALab

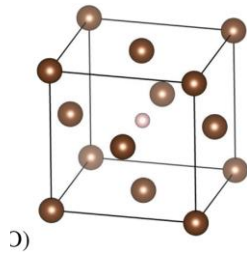
1

DFT
simulation
pure system



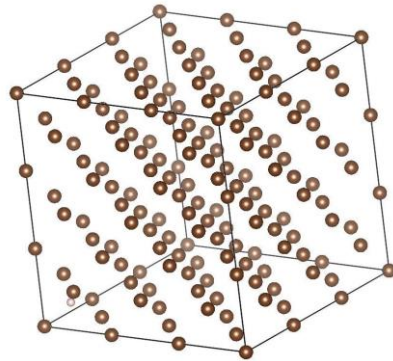
2

Find potential μ^+
stopping sites



3

DFT simulation
muonated
system



LLM assistance

LLM assistance

4



5



Development work and some suggestions

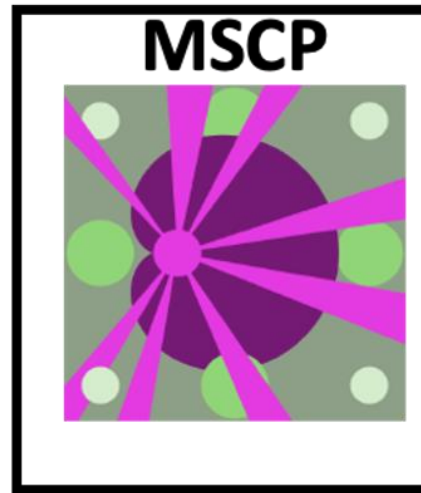
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μ -MuDirac and EVA



- MuDirac 1.0 created a periodic table of muonic atoms that EVA uses.
- New version is MuDirac 1.3.0. Uses experimental data to improve nuclear models.
- Can be used in nuclear muon experiments to estimate nuclear radius. These experiments are done at PSI.
- Developing a method to update periodic table in EVA with MuDirac 1.3.0 and future MuDirac versions.
- Adapt EVA to take PSI experimental data. Which data format is used at PSI?
- SCD is working on a Machine Learning tool to fit negative muon spectra. Could this be extended to PSI?
- New version of MuDirac will have better calculated intensities.
- Develop EVA so that it can be used in several muon sources.