

# Contributing to Task 10.4: Atomistic Modelling for Muon Spectroscopy (UNIPR)

*Theme: Making  $\mu$ SR accessible through improved data analysis*

*Current Status: Staff Appointed...*

- 1st Nov.: Ph.D. student: Ifeanyi John Onuorah
  - Experience:
    - Master degree @ International Centre for Theoretical Physics
    - Thesis: Ab-initio Simulations of Sodium Superoxide
  - Work:
    - DFT & code development and deployment under the supervision of Prof. Roberto De Renzi (RDR).
    - RDR will charge 300 h over 3 year to the project.
  - RDR charged hrs. + IJO PhD project will fulfil Parma task.
- 16th Jan.: Postdoc Research Fellow: Pietro Bonfa
  - Fund provided from University of Parma
  - Working full time on DFT+ $\mu$



## Objectives of the Task...

- Developing DFT methods as a predictive tool for muon sites, contact hyperfine fields and evaluating stability of candidate sites.
- Evaluating the reliability of DFT methods as a predictive tool through an investigation of model systems with reliable experimental data.
- Developing subroutines for site refinement through dipolar sums and contact hyperfine fields.
- Development of methods to visualise results.

## Context of the Task...

- Developing interoperability by using Mantid as a platform for hosting ...
  - a Python subroutine library for site refinement
  - visualisation tools
- Bringing together  $\mu$ SR groups currently working on DFT /dipole methods by ...
  - sharing ideas and strategies
  - establishing standards for a subroutine library for sharing codes

A Workshop late 2016 is suggested ( $\mu$ SR groups incl. Parma, Oxford and Durham)
- Potential for sharing DFT knowledge/skills/resources through (for example) ...
  - links with STFC Scientific Computing (PDRA working on muon problems)
  - use of CASTEP and HPC as appropriate