Meeting to discuss DFT techniques

9:30, Monday 28th November, 2016

CR16/17, R80, Rutherford Appleton Laboratory

(Presentations: 15 minutes + 5 minutes for questions)

09:30 Session 1 (chair: Adrian Hillier)

Muonic Probe States in Molecular Solids (Francis Pratt, STFC)

DFT+mu:
a step change in muon spectroscopy (Tom Lancaster, Durham)

The magnetic state of MnP under pressure:
a new case for DFT with muons (Roberto de Renzi, Parma)

10:30 Coffee

10:50 Session 2 (chair: James Lord)

Studying the effect of muons in spin ices and liquids
via DFT+mu (Franz Lang, Oxford)

DFT studies of hydrogen in Tin Dioxide:
analogy to muon site problem (Matthew Worsdale, Durham)

Ab-initio calculation of the contact hyperfine fields
for muon spin rotation spectroscopy (Ifeanyi Onuorah, Parma)

Combining μSR and Density Functional Theory:
the case of Benzene (Leandro Liborio, STFC)

12:10 Discussion

12:30 Buffet Lunch and Closed Meetings

14:00 Session 3 (chair: Francis Pratt)

Python automation for muon spectroscopy
with Soprano (Simone Sturniolo, STFC)

Electron-phonon couplings (TBC) (Feliciano Giustino, Oxford)

Electronic structure calculations (TBC) (Stewart Clark, Durham)

Bayesian inference in muSR:
what could it add to DFT? (Steve Blundell, Oxford)

15:20 Coffee, Discussion and Meeting close