

Meeting to discuss techniques for calculation of the Muon Site

12:00pm, 19th March, 2014

CR16 and 17, R80, Rutherford Appleton Laboratory

- 12:00 Buffet Lunch (conference room)
- 12:55 Welcome
- 13:00 Presentations (maximum 15 minutes + 5 minutes questions)
- Re-examination of muon sites in La_2CuO_4 (Isao Watanabe, RIKEN)*
Muon Sites in $V_4S_9Br_4$ (Mohamed Ismail Mohamed-Ibrahim, USM)
DFT investigation of muon sites in $T'La_2CuO_4$ (Pietro Bonfa, Parma)
Muon site estimation in $Ce(Ru_{1-x}Rh_x)_2Al_{10}$ (Aina Adam, RIKEN)
Playing quantum Hyde-and-seeK with the muon (Johannes Moeller)
- 15:00 Coffee
- 15:30 Presentations (continued)
- Muon stopping states from first principles calculations using CASTEP (Dominik Jochym, STFC)*
DFT calculations on Cu-based metal-organic hybrid magnets (Edi Suprayog, RIKEN)
Muonium Sites in ZnO (Shukri Slaiman, USM)
Theoretical isotropic hyperfine coupling constants of muoniated benzene: Exploring the effects of anharmonicity, methods and basis sets (Ke Wang, QMUL)
ALC spectra of molecular solids: effects of multiple sites, crystalline environment and quantum delocalisation (Francis Pratt, STFC)
- 17:30 Coffee and Discussion
- 18:00 Meeting close
- 19:30 Dinner