

# Meeting to discuss techniques for calculation of the Muon Site

12:00pm, 19<sup>th</sup> March, 2014

CR16 and 17, R80, Rutherford Appleton Laboratory

- 12:00 Buffet Lunch (conference room)
- 12:55 Welcome (Adrian Hillier)
- 13:00 Presentations (maximum 15 minutes + 5 minutes questions)  
(session chair: Adrian Hillier)
- Re-examination of muon sites in  $\text{La}_2\text{CuO}_4$*  (Isao Watanabe, RIKEN)
- Muon Sites in  $\text{V}_4\text{S}_9\text{Br}_4$*  (Mohamed Ismail Mohamed-Ibrahim, USM)
- DFT investigation of muon sites in  $T'$   $\text{La}_2\text{CuO}_4$*  (Pietro Bonfa, Parma)
- Muon site estimation in  $\text{Ce}(\text{Ru}_{1-x}\text{Rh}_x)_2\text{Al}_{10}$*  (Aina Adam, RIKEN)
- Playing quantum Hyde-and-seek with the muon* (Johannes Moeller)
- 15:00 Coffee
- 15:30 Presentations (continued) (session chair: Paul McClarty)
- 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