

Workshop to Discuss Techniques for Calculation of the Muon Site

19th May, 2015

Hinckley Island Hotel, Leicestershire

- 11:00 Registration with coffee (Rotunda)
- 12:00 Lunch (Brasserie)
- 13:00 Site Calculation Workshop - Session 1 (CR12)
Chair: Adrian Hillier, STFC
- Muon sites and spin dynamics in the one-dimensional molecular spin chain $\text{Cu}(\text{pyz})(\text{NO}_3)_2$* (Tom Lancaster, Durham)
- Current Status of Muon-Site Estimations in Strongly Correlated Systems* (Isao Watanabe, RIKEN)
- Assessing stable muon sites with the double adiabatic approximation* (Pietro Bonfa, Parma)
- Density functional theory and slowly varying fluctuations at finite temperature to describe alloy and magnetic phase diagrams* (Julie Staunton, Warwick)
- Quantum Nuclear Effects with Path Integral Molecular Dynamics and CASTEP* (Dominik Jochym, STFC)
- 15:30 Coffee (Rotunda)
- 16:00 Site Calculation Workshop - Session 2 (CR12)
Chair: Francis Pratt, STFC
- DFT methods for simulating hyperfine coupling constants of muoniated radicals* (Jamie Peck, STFC)
- Theoretical isotropic hyperfine coupling constants of muoniated radicals: Exploring the effects of anharmonicity, methods and basis sets* (Ke Wang, QMUL)
- A DFT+ μ study of Pr-based pyrochlores: the effect of muon-induced distortions in quantum spin ice* (Franz Lang / Steve Blundell, Oxford)
- 17:30 Concluding Remarks and Meeting Close
- 19:30 Buffet Dinner (Paris Suite)

Information about the Meeting and Venue

The meeting is being held in conjunction with the UK Neutron and Muon Science and User meeting at the Hinckley Island Hotel, Leicestershire, LE10 3JA.

Our Workshop will take place the afternoon of Tuesday 19th May, running in parallel with a student day being organised for and by UK PhD students. The Science and User meeting will continue Wednesday 20th May with a day of science talks, concluding on Thursday 20th May with the User meeting. Links to a detailed programme for the full meeting can be found on the web at <http://www.isis.stfc.ac.uk/news-and-events/uk-neutron-and-muon-science-and-user-meeting-19--21-may-201515286.html>.

The location of Hinckley Island Hotel is shown below. Further information about travel to the hotel can be found at <http://www.thehotelcollection.co.uk/hotels/hinckley-island-hotel-leicestershire/map-and-directions/>.

