

Special Evening Session: Muon Site and Related Issues

μSR 2014, Main Conference Hall

20:00, Tuesday 3rd June, 2014

Presentations should be no longer than 10 min, with a further 2 min available for questions

DFT Techniques for Muons

(chair: Adrian Hillier)

Ab initio description of the muon site in T'-La₂CuO₄ (Pietro Bonfa)

Study of Hyperfine Fields and Muon Sites Calculation in Organic-Inorganic Hybrid of
CuCl₄(C₆H₅CH₂CH₂NH₃)₂ and (C₂H₅NH₃)₂CuCl₄ (Edi Suprayoga)

Muon sites via Bayesian inference (Steve Blundell)

Playing Quantum Hyde-and-Seek with the Muon (Johannes Moeller)

Paramagnetic Muon States in Carbonaceous Materials (Rod Macrae)

Theoretical isotropic hyperfine coupling constants in muoniated benzene: Exploring the effects of
anharmonicity, methods and basis sets (Ke Wang)

ALC Spectra of molecular solids: effects of multiple sites, crystalline environment and quantum
delocalisation (Francis Pratt)

Magnetic Polarons in Materials

(chair: Steve Blundell)

Discussion session