

ISIS Crystallography User Group Meeting

PCG/SCMP Winter Meeting

31st October – 1st November 2016

The ISIS Crystallography User Group meeting is held at The Cosener's House, Abingdon, in conjunction with the Physical Crystallography Group of the British Crystallographic Association and the Structural Condensed Matter Physics Group of the Institute of Physics.

Monday 31st October 2016

- 12:00 – 13:00 *Buffet Lunch*
- 13:00 – 13:10 ISIS Crystallography User Group Chair's Welcome
Peter Slater (Birmingham)
- 13:10 – 13:40 ISIS Facility Update
Robert McGreevy (ISIS)
- 13:40 – 14:00 ISIS Crystallography Group Update
Steve Hull (ISIS)

Science Session 1 (Chair: Peter Slater)

- 14:00 – 14:30 Anthony Powell (Reading)
"Structural Investigations of Thermoelectric Materials for Energy Harvesting"
- 14:30 – 14:45 Kent Griffith (Cambridge – *"Atomic and Electronic Structure of High-rate Battery Materials via Diffraction, Multinuclear NMR, and DFT"*)
- 14:45 – 15:00 Karl Hope (Edinburgh & ISIS) – *"High Pressure Studies of Energetic Co-Crystals"*
- 15:00 – 15:30 Simon Clarke (Oxford)
"Chemical Control of iron-based superconductors and related compounds"
- 15:30 – 16:00 *Tea*

Science Session 2 (Chair: Silvia Capelli)

- 16:00 – 16:30 Jacqui Cole (Cambridge & ISIS)
"Understanding the molecular function of working electrodes in dye-sensitized solar cells"
- 16:30 – 16:45 Stephen Argent (Nottingham) – *"Contrasting carbon dioxide and methane absorption behaviours in a metal-organic polyhedral porous molecular solid"*

- 16:45 – 17:00 Ali Shehu (QMUL) – *“Defect structure and ionic conductivity of ytterbium-doped neodymium pyrochlore oxides”*
- 17:00 – 17:30 Ivana Evans (Durham)
“Structural Chemistry of Functional Oxides”
- 18:00 – 19:30 *Posters followed by dinner*

Tuesday 1st November 2016

- 09:15 – 09:20 PCG/SCMP Organiser’s Welcome
Helen Playford (ISIS)

Science Session 3 (Chair: Steve Hull)

- 09:20 – 09:50 Alex Gibbs (ISIS)
“High resolution neutron diffraction studies of $Ba_2M^{2+}Te^{6+}O_6$: interplay between crystal structure and magnetic dimensionality”
- 09:50 – 10:05 Charlotte Kirk (Oxford) – *“Metal imide catalysts for ammonia decomposition applications”*
- 10:05 – 10:20 Robin Perry (UCL & ISIS) – *“Title tbc”*
- 10:20 – 10:50 Howard Stone (Cambridge)
“Understanding alloy stability for more efficient aviation”
- 10:50 – 11:20 *Coffee*

Science Session 4 (Chair: Helen Playford)

- 11:20 – 11:50 Andrew Cairns (ESRF) [2016 PCG Thesis Prize Winner]
“Mechanical and configurational degeneracy in transition metal cyanides”
- 11:50 – 12:05 Seikh M Habibur Rahman (Chalmers) – *“In-situ hydration and neutron total scattering studies of ion conducting $Ba_2In_{2-x}M_xO_5$ (M = trivalent cation) brownmillerites”*
- 12:05 – 12:20 Genoveva Burca (ISIS) – *“The IMAT Instrument”*
- 12:20 – 12:35 Joe Paddison (Cambridge) – *“Emergent Order in the Kagome Ising Magnet $Dy_3Mg_2Sb_3O_{14}$ ”*
- 12:35 – 12:50 Wojciech Slawinski (ISIS) – *“Stacking faults: What can we learn from X-ray powder diffraction data”*
- 12:50 – 13:20 Bill David (ISIS)
“10 decades of powder diffraction”
- 13:20 – 13:30 *Concluding remarks followed by group photograph*
- 13:30 *Buffet lunch*