

HPCx Materials Chemistry Consortium (e05)

Tuesday 2nd December, The Royal Institution of Great Britain

Agenda

10:00 **Coffee** (provided in the Council room)

10:30 **Scientific Programme** (in the BSLT)

Invited presentation

10:35 Gold nanoparticles in a supercritical fluid. M. Lal, W. Smith and M. Plummer.

Current major users 10 minute presentations on the scientific aspects of their projects and to touch upon the utilisation of the facilities

10:50 Mechanisms of ion conduction in nano-porous complex oxides. P. Sushko.

11:00 Formation and growth of ZnS clusters in water solution. S. Hamad.

11:10 Thermodynamics of M_2O_3 (0001) surfaces. A. Wander.

11:20 Atomistic modelling of the electrical double layer. S. Kerisit.

11:30 Investigation of radiation-induced structural changes in oxides. I. Todorov

11:40 Simulation studies of magnetic iron sulphides. S. Wells.

11:50 Computer simulation studies of Newton black films. F. Bresme.

12:00 DFT calculations of chlorine adsorption at silver surfaces. N. de Leeuw.

12:10 Calculation of defect properties in amorphous silica. S. Mukhopadhyay.

12:20 Nucleation and inhibition of clathrate hydrates. C. Moon.

12:35 Quantum monte carlo on bulk and defective MgO. M. Gillan.

13:00 **Lunch** (provided in the Council room)

13:45 **MCC Meeting** (in the Council room)

1. Welcome/introduce Consortium new PDRA(s)
2. Update on resource/machine usage
3. Current Flagship Projects (discuss continuation)
4. New Flagship Projects (peer reviewed based on proposals)
5. Time/Hard-disk allocation for next period
6. Newton proposal
7. Other business (at discretion of chairman)

15:15 **Programme ends**