

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

Kathleen Lonsdale Building (2.5th floor) UCL - Tuesday 16th November 2010

Steering Committee Meeting (usual room next to Scott's office)

Pre-meeting for MCC funded staff and the seven theme leaders will be held at 10am

11:00 Scientific Programme – (Seminar Room)

11:00 Simulating electron transport in soft condensed matter: organic solar cell materials and biological wires (Jochen Blumberger, UCL Physics – new group code “blu”)

11:20 Absorption spectra of inorganic nanostructures (Martijn Zwijnenburg, UCL Chemistry – new group code “zwi”)

11:40 Radiation damage effects in nuclear and thermonuclear power applications (Kostya Trachenko, Queen Mary Physics, new group code “kos”)

12:00 Li-ion battery cathode phases (Derek Middlemiss, Cambridge Chemistry)

12:30 The phase IIc (GEMINI) upgrade and options for Phase III on HECToR (Jason Beech-Brandt, CRAY)

12:50 VASP: k-points parallelism (Asimina Maniopoulou / Ian Bush, NAG)

13:10 Lunch (Library)

14:00 MCC Meeting (Seminar Room)

- 1 Matters arising from the Minutes
- 2 DCSE support
- 3 MCC postdoctoral appointments (update)
- 4 RS Proc A: MCC themed issue
- 5 Report on machine usage
- 6 Distribution of HECToR resources: new proposals
- 7 MCC mid-term meeting
- 8 Any other business, including date for next meeting

16:00 Refreshment (Library)