

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London

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Friday 3rd May 2013

09:45 Steering Committee Meeting (KLB Seminar Room, 3rd Floor, M304)

Pre-meeting for MCC funded staff and the eight theme leaders

- 1 Matters arising from the Minutes
- 2 Current and New EPSRC Funding
- 3 Report on MCC usage of HECToR
- 4 Distribution of HECToR resources: management of new proposals
- 5 MCC postdoctoral appointments: brief update
- 6 SLA support
- 7 Any other business, including date for next meeting

MEDICAL SCIENCES AND ANATOMY, University College London, LONDON

11:15 Scientific Programme – (Anatomy G29 J Z Young Lecture Theatre)

For all members – Introduction to new members and possible SLA support

11:15 The functional electronic properties of materials containing transition metal ions; Computational heterogeneous catalysis; and The study of metal-free functional solids (Furio Cora, UCL Chemistry – new group code “cor”)

11:30 Desirable electronic and photophysical properties (Paul Elliott, Huddersfield – new group code “ell”)

11:45 Modelling molecules with amorphous materials (Colin L Freeman, Sheffield – new group code “fre”)

12:00 Electronic Structure Codes (Barbara Montanari, SLA support)

12:15 Atomistic and Hybrid Codes (Paul Sherwood; SLA support)

12:30 Lunch (Social Space within North Cloisters)

For members that have indicated they will be present: sandwiches, crisps, muffin & water

13:30 MCC Meeting (Anatomy G29 J Z Young Lecture Theatre)

Main meeting for all members – particularly those requesting new HECToR resources

- 1 Matters arising from the Minutes
- 2 Current and New EPSRC Funding
- 3 SLA support
- 4 Report on e05 usage of HECToR
- 5 Distribution of HECToR resources: new proposals
- 6 MCC postdoctoral appointments: update
- 7 Any other business, including date for next meeting

16:30 Celebration (KLB Library Area, 3rd Floor, outside M304)

For all members