

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London

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Tuesday 4th October 2011

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

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

CHANDLER HOUSE, 2 WAKEFIELD STREET, LONDON, WC1N 1PF

11:00 Scientific Programme – (G10 Lecture Theatre, Chandler House)

11:00 Ab initio prediction and band gap engineering of novel semiconductors for renewable energy applications (David Scanlon, UCL – requested 8M AUs)

11:15 Structures and dynamics of water on defective rutile TiO₂(110) (Changjun Zhang, UCL – used 4.7M AUs)

11:30 Ab initio DFT based AFM simulations of Cu(110)/O c(6x2) surface (Joseph Bamidele, KCL – used 3.6M AUs)

11:45 The importance of Hund's Second rule to the band gap of beta-MnO₂: Towards understanding its role in lithium energy storage (David Tompsett, Uni. Of Bath – used 9M, requested 4.2M AUs)

12:00 Electronic Properties of Polycrystalline Metal-Oxide Materials (Keith McKenna, University of York – new group code “mck”)

12:20 DFT study of an organic radical on a metal surface (Mats Persson, University of Liverpool – new group code “per”)

12:40 Designing porosity through crystal structure prediction on porous organic molecules (Graeme Day, University of Cambridge – new group code “day”)

13:00 Activity of Supported Catalysts For Autocat Applications (Glenn Jones, UCL – new group code “jon”)

13:30 Lunch – (B04 Social Space, Chandler House)

14:30 MCC Meeting (118 Lecture Theatre, Chandler House)

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

16:00 Refreshment (B04 Social Space, Chandler House)