

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

Chemistry Building (ground floor) UCL

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Friday 7th May 2010

Steering Committee Meeting (KLB Seminar Room M304)

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

11:00 Scientific Programme – (Ramsay Lecture Theatre)

11:00 ONETEP: current status (Arash A Mostofi, IC)

11:20 CASTEP: current status (Keith Refson, STFC)

11:40 Magnetic Organic Materials from first principles (Barbara Montanari, new group code “mon”, RL)

12:00 CP2K: Summary of Recent Performance Enhancements & Quantum Espresso (Iain Bethune, EPCC)

12:30 Optimising VASP Γ -point parallel performance & Current status/upgrade path on HECToR (Andrew R Turner, EPCC)

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

13:10 Lunch (Nyholm Room)

14:00 MCC Meeting (Nyholm Room)

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

16:30 Refreshment (Nyholm Room)