

# MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London

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Friday 4<sup>th</sup> April 2014

09:45 Steering Committee Meeting (KLB Seminar Room, 3<sup>rd</sup> Floor, 357)

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

- 1 Matters arising from the Minutes
- 2 Report on MCC usage of HECToR
- 3 Report on MCC usage of ARCHER
- 4 Distribution of HPC resources: new proposals
- 5 SLA support
- 6 Any other business

**CHEMISTRY BUILDING**, 20 Gordon Street, University College London, WC1H 0AJ

11:00 Scientific Programme – (Christopher Ingold XLG1 Chemistry LT booked from 10:30)

For all members – report from members who requested a significant proportional of time in previous meeting, SLA support and Archer, plus introduction to GPUs and a new member!

11:00 Post Hartree-Fock calculations of Functional Molecules on Bulk Insulating Surfaces (10MAU: Matthew Watkins, Physics, UCL)

11:15 Dopants and Vacancies in Rocksalt Metal Oxides for CO<sub>2</sub> Catalysis (10MAU: Chris Downing, Chemistry, UCL)

11:30 Towards the molecular design of hypothetical porous organic molecules (Kim Jelfs, Chemistry, Imperial College – new group code “kim”)

11:45 Nanostructured TiO<sub>2</sub> for photovoltaic hydrogen production (Early ARCHER request 34MAU: Monica Patel, Chemistry, Imperial College)

12:00 Modelling of uranium oxides and defect structures in UO<sub>2</sub> and Thermoelectric perovskite materials (Total Nov’13 request 13MAU: Stephen Parker, Chemistry, Bath)

12:15 Alternative HPC based on GPUs for running materials software? (Timothy Lanfear; NVIDIA)

12:35 SAFE – update on ARCHER service (Kevin Stratford; EPCC)

12:45 Molecular structure prediction (Sally Price, UCL Chemistry – new group code “sal”)

13:00 Lunch (outside LT – grab and go)

For members/guests that indicated they will be present: sandwiches, crisps, snack & water

13:30 MCC Meeting (Chemistry LT booked until 18:00 but hopefully ends by 16:00)

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

- 1 Matters arising from the Minutes
- 2 SLA support: update and an opportunity for members to make suggestions for future work (Thomas Keal, DL; Barbara Montanari, STFC)
- 3 PM update
- 4 Report on e05 usage of HECToR
- 5 Report on e05 usage of ARCHER
- 6 Distribution of HPC resources: new proposals
- 7 Any other business