

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London

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Friday 18th July 2014

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 Archer Phase 2
- 3 Report on MCC usage of ARCHER
- 4 Distribution of ARCHER resources: management of new proposals
- 5 eCSE funding: brief update
- 6 SLA support
- 7 Any other business, including date for next meeting

UCL CHEMISTRY, 20 Gordon Street, University College London, LONDON

11:10 Scientific Programme – (Christopher Ingold XLG1 Chemistry LT)

For all members – scientific presentation and justification of requests 10M AU and above

11:10 Modelling of TiO₂ nanotubes for lithium-ion microbatteries (Marine Riesenmey, Maria Alfredsson, requested 10M AU)

11:20 Computer simulations of lead interactions with the zeolite-A unit cell (Rebecca Tanney, Maria Alfredsson, requested 10M AU)

11:30 The defect chemistry of dilute nitride and bismide antimonides (John Buckeridge, David Scanlon, Richard Catlow, requested 12M AU)

11:40 Na-ion batteries: transport, voltage and electronic properties of new phosphate & titanate electrodes (Alexander Whiteside, Stephen Wood, Saiful Islam, requested 12M AU)

11:50 Dopants and vacancies in rocksalt metal oxides for CO₂ catalysis (Chris Downing, Andrew Logsdail, Richard Catlow, requested 12.5M AU)

12:00 Ab initio DFT Study of CVD Graphene growth: Defects in graphene on Ir(111) surface (Holly Tetlow, Andrea Floris, Lev Kantorovich, requested 13M AU)

12:10 Walking molecules with a directional and oriented motion on Cu(110) (Andrea Floris, Lev Kantorovich; requested 15M AU)

12:20 Covalent assembly of Co-methyl-di-phenyl and Co-di-phenyl porphyrins on Cu(110) (Andrea Floris, Lev Kantorovich; requested 20M AU)

12:30 Divalent metal impurities in GaN (John Buckeridge, Richard Catlow, requested 20M AU)

12:40 Surface phase transition driven by dehydrogenation reaction (Chiara Paris, Andrea Floris, Lev Kantorovich; requested 23M AU)

13:00 Pack Lunch (just outside lecture theatre)

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

13:30 MCC Meeting (Christopher Ingold XLG1 Chemistry LT)

Main meeting for all members – particularly those requesting additional ARCHER time

- 1 Matters arising from the Minutes
- 2 ARCHER phase 2
- 3 Report on e05 usage of ARCHER
- 4 Distribution of ARCHER resources: new proposals
- 5 Any other business, including date for next meeting

16:00 Refreshments (location TBA)

For all members