MATERIALS CHEMISTRY HPC CONSORTIUM MEETING
University College London - Monday 6th February 2015

10:00 Steering Committee Meeting (Room 345, 16 TAVITON STREET, LONDON, WC1H 0BW, the building is behind Chemistry booked 10:00-11:30)
Pre-meeting for MCC funded staff, the eight theme leaders and SLA representatives

1. Matters arising from the Minutes
2. Report on MCC usage of ARCHER
3. ARCHER: Phase 2 allocations
4. HEC EPSRC assessment of MCC
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 11:00)
For all members – talks on a selection of projects requesting time; and new members!

11:00 Density Functional Theory Studies of Breathing Transitions in Flexible MIL-53 Metal-Organic Frameworks AND/OR High-Throughput Screening of Hypothetical Mg-MOF-74 for CO2 Capture (Sanliang Ling, University College London, requesting 7M+6M for surfin-ben)
11:15 A DFT study of Free and Supported Au-Rh Nanoalloys (Jack Davis, University of Birmingham, requesting 10M+5M for react-roy and surfin-roy)
11:30 Semiconducting Metal-Organic Frameworks (Christopher Hendon, University of Bath, requesting 15M for nandef-wal)
11:45 Reaction pathways for solvated surface catalysed reactions using molecular dynamics (Liam Thomas, University of Cardiff, requesting 26M for react-wil)
12:00 Molecular scale understanding of structure and behaviour at solid/liquid interfaces – new member code mat (Matthew Watkins, University of Lincoln)
12:15 Water adsorption on actinide dioxide surfaces AND/OR The interaction of brucite surfaces with nuclear fission products – new member code nik (Nik Kaltsoyannis, University of Manchester)
12:30 Chemshell: an update on developments (Tom Keal, Daresbury Labs, SLA support)
12:45 Update on ARCHER (Arno Proeme, EPCC)

13:00 Lunch (outside LT – grab and mingle)
For members/guests that indicated they will be present: sandwiches, crisps, snack & water
13:30 MCC Meeting (Chemistry LT booked until 17:00, Ramsay booked 12:00-15:00)
Main meeting for all members – particularly those requesting new HEC resources

1 Matters arising from the Minutes
2 PM update
3 HEC EPSRC report
4 Report on e05 usage of ARCHER
5 Distribution of HEC resources: new proposals

Meeting splits into two parallel sessions for this agenda item

Proposals under surfin, react, enviro, biomat and softm will be discussed/defended in the Chemistry Lecture

Proposals under nandef, gener and store will be discussed/defended in the Ramsay Lecture Theatre (neighbouring room).

6 Distribution of HPC resources: Summary and matters arising in parallel sessions that need resolving
7 Any other business