

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London

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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