

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London, Chemistry,
20 Gordon Street, London WC1H 0AJ

Thursday 14th July 2016

10:00 Steering Committee Meeting (room 124d)

- 1 Matters arising from the Minutes
- 2 Report on MCC usage of ARCHER
- 3 New Members (applications and size limit?)
- 4 Software Call
- 5 Reports for allocations above 10M and data collection
- 6 New allocations on ARCHER
- 7 RSC book (chapter per theme)?
- 8 SLA support
- 9 Any other business

Above: for MCC funded staff, the eight theme leaders and SLA representatives
Below: for all MCC members and their group

11:00 Scientific Programme – (XLG2; Auditorium Lecture Theatre)

11:00 Electrochemistry and Ionic Diffusion in Oxide Cathodes and Electrolytes for Rechargeable Batteries ([Hungru Chen](#), e05-isl, Chemistry, University Bath)

11:15 Solar cells; molecular self-assembly; and photocatalysis – new member code nat ([Natalia Martsinovich](#), Chemistry, Sheffield University)

11:30 Covalent assembly of functionalized porphyrins on copper; and Self-assembly mediated by electrostatic interactions – new member code flo ([Andrea Floris](#), Maths & Physics, Lincoln University)

11:45 Understanding and controlling ionic diffusion in thin-film optical coatings – new member code pdb ([Paul Bristowe](#), Materials Science & Metallurgy, Cambridge University)

12:00 Computational calculations of on – surface catalytic coupling; and single atom chemistry with scanning probe microscopy – new member code jar ([Samuel Jarvis](#), Physics & Materials Science, Nottingham > Lancaster University)

12:15 Accident tolerant fuels; breeder blankets for nuclear fusion; and formation of nitrogen-vacancy clusters in diamond by swift heavy ions – new member code mur ([Samuel Murphy](#), Nuclear Materials, Lancaster University)

12:30 Better capacitors for energy storage; improving the design of thermoelectrics for energy conversion; and aiding materials growth at surfaces – new member code hep ([Steven Hepplestone](#), Physics, Exeter University)

12:45 Archer Service: Update ([Andrew Turner](#), EPCC, Edinburgh University)

13:00 Lunch (Just outside Lecture Theatres)

13:30 MCC Meeting (XLG2; Auditorium Lecture Theatre)

- 1 Matters arising from the Minutes
- 2 Messages from Steering Committee Meeting
- 3 EPSRC Consortium Report (for current and future periods)
- 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 [XLG2; Auditorium Lecture Theatre](#)

Proposals under [nandef](#), [gener](#) and [store](#) will be discussed/defended in the [MXLG1; Chemistry Lecture Theatre](#)

Back in the Auditorium Lecture Theatre

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