

MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

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

- Wednesday 21st December 2016

PLEASE NOTE: The steering committee meetings are for MCC funded staff and the eight theme leaders (and SLA representatives for the afternoon). All MCC members and their group are invited to attend the Scientific Programme, Lunch (for those who have notified me they will be coming), and the main MCC business meeting.

10:15 Steering Committee Meeting (room 124c)

- 1 Matters arising from the Minutes
- 2 New Members (applications and size limit?)
- 3 Report on MCC usage of ARCHER
- 4 New allocations on ARCHER

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

11:00 TBA – new member code log ([Andrew Logsdail](#), Chemistry, Cardiff University)

11:15 Functional Materials: The Role of Composition – new member code mol ([Marco Molinari](#), Chemistry, Huddersfield University)

11:30 Ab initio simulations of disordered materials – new member code sre ([Stephen Elliot](#), Chemistry, Cambridge University)

11:45 First principles calculations on the phase stability of calcium carbonate ([David Carrasco de Busturia](#), requesting 42M AU, e05-nic, Imperial College)

12:00 UK Tier 2 – Access for MCC members ([Angelos Michaelides](#), TYC)

12:15 Archer Service: Update ([Andrew Turner](#), EPCC, Edinburgh University)

12:30 Developments from SLA support – the case of CHEMSHELL and DL_FIELD ([Tom Keal](#), STFC, Daresbury Labs)

13:00 Lunch

13:30 Main MCC Business 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

16:00 Steering Committee Meeting (room 124d)

- 5 Software Call
- 6 RSC book (chapter per theme)?
- 7 SLA support
- 8 Any other business