

# MATERIALS CHEMISTRY HPC CONSORTIUM MEETING

University College London

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Tuesday 17<sup>th</sup> July 2018

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

## 16:00 Steering Committee Meeting (Part 1, Monday 16<sup>th</sup> Engineering Building (opposite Waterstones) Front Suite 104)

- 1 Current and New Grant Transition
- 2 Method for Redistribution of Resources
- 3 Annual Reports (annual report template)
- 4 CoSeC Support (steering and software champions)
- 5 MCC Membership (size limit and strategies for over demand)
- 6 MCC Workshops
- 7 MCC 3<sup>rd</sup> conference (Lincoln)

## 10:00 Steering Committee Meeting (Part 2; 14 Taviton (behind the chemistry building) room 131; booked between 9:30 and 11:30)

- 8 Matters arising from the Minutes
- 9 New Members (applications)
- 10 Report on MCC usage of ARCHER
- 11 New allocations on ARCHER
- 12 AOB

## 11:00 Scientific Programme – (Gustave Tuck Lecture Theatre, Wilkins Building; room booked from 10:30)

11:00 Computational thermodynamics: how to calculate phase diagrams without the fuss – new member code lbp ([Livia Bartok-Partay](#), Reading University)

11:15 Towards a parameter-free theory of electrochemical phenomena at the nanoscale – new member code clo ([Clotilde Cucinotta](#), Imperial College)

11:30 CoSeC support update, plus “An insight into DL\_FIELD” ([Thomas Keal and Chin Yong](#), CoSeC, Daresbury Labs)

11:50 Controlled chemistry at surfaces: from photocatalysis to nanoarchitecture – new member code rjm ([Reinhard Maurer](#), Warwick University)

12:05 Polycyclic Hydrocarbons, Metal Catalysts and Catalyst Supports – new member code arc ([Arunabhiram Chutia](#), Lincoln University)

12:20 Lattice dynamics for materials modelling– new member code ske ([Jonathan Skelton](#), University of Manchester)

12:35 ARCHER update ([Andrew Turner](#), EPCC)

13:00 Lunch (JBR, UCL main building, booked from 12:30)

13:30 Main MCC Business Meeting (Gustave Tuck Lecture Theatre, Wilkins Building; room booked until 16:00)

- 1 Messages from Steering Committee Meeting
- 2 Reports (for current and future periods)
- 3 Report on e05 usage of ARCHER and THOMAS
- 4 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 [Wilkins Room, UCL main building](#)

Proposals under [nandef](#), [gener](#) and [store](#) will be discussed /defended in the [JBR, UCL main building](#)

Back in the Wilkins Room

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

15:30 Celebratory Drinks (Room: JBR, must end by 16:30)