

MATERIALS CHEMISTRY HEC CONSORTIUM MEETING

University College London

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Monday 25th January 2021

Contact MCC using klmc.mcc@ucl.ac.uk

10:15 Scientific Programme

10:15 Differences between ARCHER and ARCHER2 – Holly Judge, EPCC

10:45 Electronic structure of low-valent metal oxides and Surface properties of silicon-based materials – new member code mcg ([John McGrady](#), Department of Chemistry, University of Oxford)

11:00 Computational modelling of polymer systems for materials applications – new member code bev ([Beverley Stewart](#), School of Chemistry and Bioscience, University of Bradford)

11:15 Defects and distortions in energy materials – new member code luc ([Lucy Whalley](#), Department of Mathematics, Physics and Electrical Engineering, University of Northumbria)

11:30 Spin dynamics in molecules from first principals – new member code chi ([Nicholas Chilton](#), Department of Chemistry, University of Manchester)

11:45 Feedback from Early Bird Users (Mohammad Ali Al-Badri, Jamal Abdul Nasir, Manesh Mistry, Taifeng Liu, M. Golomb, J. Buckeridge, N. Zibouche, S. Kavanagh)

11:46 FHI-aims – Matthias Golomb (wal) Imperial

11:49 VASP – John Buckeridge (jbu) LSBU

11:52 Quantum Espresso – Nourdine Zibouche (isl) Bath

11:55 VASP – Sean Kavanagh (dos) UCL

11:58 GROMACS – Mohammad Ali Al-Badri (lor) KCL

12:00 Lunch Break

13:30 Main MCC Business Meeting

- 1 Messages from Steering Committee Meeting
- 2 Transition between HPC services
- 3 Excalibur – update from MMM DDWG
- 4 Annual Reports (for members, MMM Hub and MCC)
- 5 Report on e05 usage of ARCHER and MCC THOMAS
- 6 Distribution of Resources: new proposals
- 7 Any other business

15:30 End