

36th MCC Meeting

Online - Tuesday 30th January 2024

11:00 Scientific Programme

11:00 The investigation of ordered carbonaceous frameworks for energy applications – new member code azz (*Alex Aziz*, Department of Natural Sciences, Manchester Metropolitan University)

11:15 The influence of configurational entropy on polymorphic free energy ranking And/Or Landscape Generator and structural similarity – member code sug (*Isaac Sugden*, The Cambridge Crystallographic Data Centre)

11:30 Molecular Glasses - from Fundamentals to Medical Applications – member code gab (*Gabriele Sosso*, Department of Chemistry, University of Warwick)

11:45 The role of DFT and MD simulations in sulphur batteries: my research so far – member code lek (*Constantina Lekakou*, Department of Mechanical Engineering Sciences, University of Surrey)

12:00 Modelling nucleation from solution with seeded and unseeded methods – member code slv (*Matteo Salvalaglio*, Department of Chemical Engineering, UCL)

12:15 Elucidating structure and dynamics of complex interfaces in solution – member code cox (*Stephen Cox*, Department of Chemistry, University of Cambridge)

12:30 HPC Service Updates

12:30 YOUNG service update (*Heather Kelly*, UCL)

12:45 ARCHER2 service update (*William Lucas*, EPCC)

13:00 Lunch break

14:30 – 16:30 Main MCC Business Meeting

[at least one representative for each proposal should be present]