

34th MCC Meeting

Online - Tuesday 18th July 2022

11:00 Scientific Programme

11:00 Deep learning on small datasets and Generative materials discovery – new member code ktb (*Keith Butlers*, School of Engineering and Materials Science, QMUL)

11:15 Gaining Macroscopic Insights on Clathrate Hydrate Growth from Non-Equilibrium Molecular Dynamics Simulations – new member code pha (*Anh Thi Van Phan*, School of Chemistry and Chemical Engineering, Surrey)

11:30 Flash Presentations from 1st Wave of Grand Challenge Projects

The Phase Diagram of the Electron Liquid, *Matthew Foulkes* (bulk-fou; 227M AU)

Modelling Phase Transitions in Functional Materials, *Tifeng Liu* (bulk-sok; 333M AU)

Novel Li-ion Battery Materials: The Structure and Dynamics of Oxygen Species in High Energy Density O-redox Cathodes, *Andrey Poletayev* (power-isl; 379M AU)

Electron and structural dynamics in amorphous oxides, *Jack Strand* (bulk-shl; 473M AU)

Machine Learning Discovery of High Entropy Alloy Catalysts, *Sanliang Ling* (discov-lin; 265M AU)

12:00 HPC Service Updates

12:00 YOUNG service update (*Heather Kelly*, UCL)

12:15 ARCHER2 service update (*William Lucas*, EPCC)

12:30 Flash Presentations from 1st Wave of Grand Challenge Projects

RAFFLE Intercalation of M2gO Graphene, *TBA* (surfin-hep; 379M AU)

First-principles calculations of excitons in moiré superlattices, *TBA* (nano-lis; 363M AU)

Finite-temperature optical properties of photovoltaic materials, *TBA* (discov-wal; 379M AU)

Nanosecond dynamics of electron and hole polarons at hematite/ liquid water interfaces from ab-initio MD-trained Neural Network Potentials, *Jochen Blumberger* (biosoft-blu; 320M AU)

Computational discovery of clathrate thermoelectrics, *Alex Squires* (discov-dos; 419M AU)

13:00 Software Update

13:00 DefAP: A Python code for the analysis of point defects in crystalline solids, *Samuel Murphy* (mur), Lancaster

13:15 Lunch break

15:00 – 16:45 Main MCC Business Meeting