

**The Materials and Molecular Modelling Hub Conference & User Meeting 2019,
University College London, 3-4 September 2019**

Name of organizers:

George Booth, TYC, King's College London
Nicholas Bristowe, University of Kent
Georgina Ellis, OCF Plc
Owain Kenway, University College London
Chris Kriton-Skylaris, University of Southampton
Angelos Michaelides, TYC University College London
Andrew Morris, University of Birmingham
Arash Mostofi, TYC Imperial College London
Chris Pickard, University of Cambridge
Matt Probert, UKCP, University of York
Laura Ratcliff, Imperial College London
Elton Santos, Queen's University Belfast
Ms Karen Stoneham, TYC, University College London

Number of participants: 123

Aim of event: The aims of the event were to bring together the UK's materials and molecular modelling community, to expose them to the current state-of-the-art research through a series of high level presentations from national and international leaders in the field, and to celebrate the research that has been made possible by the MMM Hub HPC facility ("Thomas").

Major outcomes: The meeting met its key goals: in terms of the science presented, it was striking how broad the field of materials and molecular modelling has become. Talks covered topics such as the latest developments in density functional theory development (Martin Head-Gordon, Berkeley), modelling of explosive materials (Carole Morrison, Edinburgh), modelling of bacteria (Syma Khalid, Southampton), the spectral properties of correlated materials (Silke Biermann, Paris), and more... There were also two extremely interesting Keynote Talks from experimentalists; specifically, Sharon Ashbrook (St Andrews) talked about latest developments in solid state NMR and Karina Morgenstern (Bochum) on applications of scanning tunneling microscopy to laser driven processes. As for the network and community building there was good representation from many of the key groups in materials and molecular modelling from across the UK. There was also a good balance of established and early career research. Discussions were lively and the room was full throughout the entire meeting.

Impact: We expect that by bringing together so many different people from different subfields of materials and molecular modelling that new ideas and collaborations will have emerged from the meeting.

Conclusions: Overall it was a very successful meeting with a good energy throughout. The presentations were of a high quality and the meeting was very well attended from beginning to end. The responses from our delegate survey were very positive and we expect to run the next edition of this conference in 2020.