

Report on meeting “New Horizons in Materials Modelling” York, January 4th 2019

This one-day meeting was held in the Bar Convent at York, organised by Matt Probert (York), Stewart Clark (Durham) and John Harding (Sheffield). The meeting was divided into three thematic sessions: Magnetic/Electrical Properties, Transport Properties and Structural properties. Invited talks were given by Richard Evans (York), Paul Bristowe (Cambridge) and Keith Refson (Royal Holloway, London), each of which contained a high-level introduction to the topic and then some of the latest results from their groups. This enabled all attendees, especially PhD students from different sub-disciplines, to appreciate and follow the three sessions.

The materials modelling community is large and diverse, and the three featured themes are not often discussed in a single meeting, although there are fundamental scientific and algorithmic overlaps. As well as new students and experienced academics, there were also representatives from industry (such as Dassault) and government labs (such as Daresbury Lab), which helped to maximize the networking opportunities. Overall, a significant aspect of this workshop was that it brought a diverse group together to appreciate the similarities and differences of these themes and the different approaches used, which maximized the impact of the meeting.

There were 58 delegates (including organisers and invited speakers). 9 contributed talks (20 minutes each) were given. Also, there were 14 posters in a session that was held before and during lunch. We particularly encourage PhD students to give a presentation, and this contributes to their training and helps to boost their academic profile. This is the fifth year that this meeting has been held and, as before, it offered a friendly environment for students to give a talk or a poster. Further details of the presentations can be found at <https://n8cir.org.uk/events/new-horizons-in-materials-modelling/>.

The organisers thank N8 CIR (Gillian Sinclair) for help with the administration of the meeting and both the CCP5, CCP9 and UKCP networks for funding. This enabled us to run the meeting at no cost to delegates.

Stewart Clark (Durham)
John Harding (Sheffield)
Matt Probert (York)