

Atomistic Computational Studies of Carbon:

A meeting to celebrate the scientific achievements of Malcolm Heggie

This one day event is a celebration of Professor Malcolm Heggie's scientific achievements and influence, notably in the field of atomistic simulations of carbon materials. His contributions to Carbon Science were manifold, particularly within the UK where he co-founded the British Carbon Group and chaired it for many years, as well as founding and co-organising the annual NanoteC conferences for 20 years. Beyond point defects, Malcolm made important contributions to our understanding of dislocations, surfaces, defect behavior in diverse materials such as ice and diamond.



Programme

- 10:30-11:00 *Arrival*
- 11:00-11:20 Introduction and Welcome (Laura Heggie and others)
- 11:20-11:50 Patrick Briddon, *"Modelling carbon: from 1 atom to 10,000"*
- 11:50-12:20 Ichiro Yonenaga, *"Studies on dislocations in semiconductors with Malcolm"*
- 12:20-12:50 Jim Reed, *"It was just an academic exercise; it meant something to nuclear safety in the UK"*
- 12:50-14:00 *Lunch and Posters*
- 14:00-14:25 Irene Suarez-Martinez, *"Buckle, Ruck and Tuck – the response of graphite to irradiation"*
- 14:25-14:45 Chris Ewels, *"The Heggie story of Ice and Fire"*
- 14:45-15:10 Kenny Jolley, *"Atomistic Modelling of Defects in Graphite"*
- 15:10-15:30 Bernd Eggen, *"The changing face(s) of Fullerenes"*
- 15:30-16:00 *Coffee and Tea break, posters*
- 16:00-16:20 Geoff Fowler and Norman Parkyns, *"Malcolm, the British Carbon Group and the AGM"*
- 16:20-16:40 Philippe Ouzilleau, Sherbrooke, *"Why some carbons may or may not graphitize?"*
- 16:40-17:00 Paul Mouratidis, Loughborough, *"Ab Initio Calculations of Partial Basal Dislocations in Bilayer Graphene"*
- 17:00- *Meeting close*

Posters

- Ben Hourahine: *"Large scale tight-binding models of graphite dislocations"*
- Chris Ewels: *"DFT Modelling of nanoscale carbons"*
- Stephen Lyth: *"Engineering the Work Function of Graphene via Defects and Nitrogen Doping"*
- Hao Xu: *"2D Glassy-Graphene for VOC sensing and optoelectronic applications"*
- Nathalia Martsinovich, *"Photocatalytic Interfaces of TiO₂ with Graphene and Reduced Graphene Oxide: A Computational Study"*

This meeting is kindly supported by

