

CCP3/CCP5 Joint Meeting on "Modelling and Simulation of Nanostructures"

This was a two-day meeting (6-7th January 2003), held at Queens' College Cambridge, sponsored jointly by CCP3 and CCP5. The meeting also received support from the Nanoscience IRC based at Cambridge, Bristol and UCL, from the Nanotechnology Network and from the Thin Films and Surfaces Group of the Institute of Physics.

An important objective of the meeting was to confront both theorists and modellers with experimental facts and problems, as well as the latest developments in their own fields. We therefore adopted the format of having entirely invited talks, with plenty of time for discussion. There was also a poster session (in the bar) for people to present their own work. This worked out very well. Indeed, we could have done with more time for discussion than we had. A major strength of the meeting was the diversity of different fields and interests present. A number of participants commented that it would be valuable to have another meeting of this kind in a couple of years time.

There were 45 participants, 9 invited speakers and 16 posters in the poster session. A copy of the titles of the talks, and of the posters is given below.

Talks	
Malcolm Green (Oxford):	The chemistry of carbon nanotubes
Alan Windle (Cambridge):	Modelling of nanotube structures: relevance to technology and biology
Richard Palmer (Birmingham):	Nanostructured surfaces: from clusters to proteins
Mike Payne (Cambridge):	The role of first principles calculations in biology
Andrew Horsefield (UCL):	Making sense of nano-biology to physicists
Mervyn Miles (Bristol):	New methods in scanning probe microscopy
Mads Brandbyge (Tech. University, Denmark):	First-principles simulations of quantum transport in nanoscale systems
Tchavdar Todorov (Queens, Belfast):	Current-induced mechanical effects in atomic wires
Richard Friend (Cambridge):	Organic electronics, a status report
Posters	
M. Persson (Chalmers):	Modelling of inelastic and elastic tunnelling spectra from adsorbates on metal surfaces

D. R. Bowler (UCL):	Formation of clean dimers during gas-source growth of Si(001)
C. Schumacher and N. Seaton (Edinburgh):	Kinetic Monte Carlo simulation of the synthesis and calcination of structured mesoporous silica
D.C. Sayle (Cranfield):	Simulation of oxide nanoparticles: exploitation of teraflop HPC
S. J. Martin and A. B. Walker (Bath) and A. Kambili (Regensburg):	Temperature and field dependence of the mobility in liquid-crystalline conjugated polymer films.
P.C.H. Mitchell (Reading):	Inelastic neutron scattering studies of hydrogen on carbon-supported catalysts.
G. Goldbeck-Wood (Accelrys):	Molecular modelling applied to nanotechnology: field emission from nanotubes, polymer-clay nanocomposites and nanoscale drug delivery
J. A. Elliott, J. Cranshaw, P. R. Claiden and A.H. Windle (Cambridge); J. Starijow (Berlin):	Nucleation of thermodynamically stable structures for polyglutamine amyloid fibres modelled using molecular dynamics
J. A. Elliott, J. Sandler, M. S. P. Schaffer and A. H. Windle (Cambridge):	Hydrostatic compression and collapse of carbon nanotube bundles modelled using constant-stress molecular dynamics.
E. M. Haines, T. Rayment, J. Goodman and C. Abell (Cambridge):	Chiral discrimination by chemical force microscopy; simulations
B. Montanari and N. M. Harrison (Imperial):	A pressure-induced ferroelectric instability in bulk TiO ₂ rutile
L. D. Lloyd, T. V. Mortimer-Jones, C. Massen, R. L. Johnston and S. Salhi (Birmingham):	Structures and segregation of Pt-Pd nanoalloys
B. G. Walker and C. Molteni (Cambridge); N. Marzari (MIT):	Structural properties of liquid sodium surfaces from ab initio molecular dynamics.
A. A. El-Barbary, R. H. Telling, C. P. Ewels and M. I. Heggie (Sussex) :	The defect physics of graphite and its implications for nanotechnology
D. Antypov, C. M. Care and D. J. Cleaver (Sheffield-Hallam):	Supramolecular periodic structures formed by rod-sphere aggregates.

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