# Global Optimisation Techniques Applied to the Prediction of Structures

"Gordon Conference style" Workshop in the Nyholm Room, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ

## Wednesday 5th July

Check in for accommodation at Butler's Wharf Residence (LSE), 11 Gainsford Street London SE1 2NE.
18:00: The Bridge Tandoori (Restaurant), 214 Tower Bridge Road SE1 2UP. Informal evening meal/get-together (I will reserve a table so please let me know if you intend to join us. Note that this meal is not free).
20:00: Dean Swift (pub with TV for those wishing to watch the second World Cup Football Semi Finals).

## Thursday 6th July

09:45: Morning coffee and biscuits in the Nyholm Room.

10:15: Welcome and introductory information (Scott Woodley)
10:30: GOSPP: a computer program for structure prediction of inorganic solids using the whole space group symmetry and powder diffraction data (Raúl Carbonio, chair: Christian Schön)
11:15: Potential problems with chameleon clusters: the low energy landscape of nanosilica (Stefan Bromley, chair: Christian Schön)

12:00: Lunch (Food and cold drinks) in the Nyholm Room

13:00: Visualization and complexity analysis of multi-dimensional energy landscapes: Relevance to global optimization (Roy Johnston, chair: Michael Treacy)
13:45: Can we predict inorganic-organic hybrid structures (Caroline D-Mellot, chair: Michael Treacy)

14:30: Short Break (cakes, fresh fruit and cold drinks).

15:00: Predicting the low-temperature region of phase diagrams without recourse to input from experiment (Christian Schön, chair: Scott Woodley)
15:45: Global optimization for molecular cluster structures and protein folding (Bernd Hartke, chair: Scott Woodley)

16:30: Afternoon break (coffee and biscuits) and informal open discussions
17:30: Nyholm Room Closed

19:00: Conference Meal, Hing Lee Chinese Restaurant (opposite Butler's Wharf Residence), 32 Curlew Street, London SE1 2ND. Followed by fireworks on the Thames!

## Friday 7th July

09:45: Problems in structure prediction of inorganic particles (Said Hamad, chair: Roy Johnston)
10:30: Weeding and harvesting zeolite graphs; Can we quickly tell the tetrahedral from the merely 4-coordinated? (Michael Treacy, chair: Roy Johnston)

11:15: Morning Break (coffee and cakes) in the Nyholm Room.

11:30: The limitations of global optimisation techniques in organic crystal structure prediction (Sally Price, chair Kenneth Harris)
12:15: Structure prediction by combination of graph theory and quantum mechanics (Bjoern Winkler, chair Kenneth Harris)

13:00: Lunch (Food and drink) in the Nyholm Room

14:00: Development and application of evolutionary algorithms in structure determination from powder diffraction data (Kenneth Harris, chair: Richard Catlow)
14:45: Microporous titanium silicates predicted by GRINSP (Armel Le Bail, chair Richard Catlow)

15:30: Teatime (Food and drink) and informal open discussions
16:00: Closing Remarks (Richard Catlow)
17:30: Nyholm Room Closed

Each presentation allocated 30 minutes plus 15 minutes for an open discussion