

## **Report on "*Modelling of Materials: Atomistic and Ab Initio Approaches*"**

The meeting "*Modelling of Materials: Atomistic and Ab Initio Approaches*" was held at Mansfield College and the Physical and Theoretical Chemistry Laboratory, Oxford, from 9–10 April, 2003. It was co-organised by the RSC Theoretical Chemistry Group and CCP5. The meeting was concerned with developments in methodology and algorithms for atomistic and *ab initio* simulations of materials, as well as their applications. It consisted of 7 invited lectures, 18 contributed lectures and 19 contributed posters. The meeting was successful and was felt to be timely, with the combination of delegates from different areas of materials modelling working particularly well.

56 people registered for the meeting, of which 43 were residential and 13 non-residential delegates. 17 of the delegates were postgraduate students (most of whom presented either a talk or a poster). The majority of the delegates were based in the UK, though 4 came from overseas (including a postgraduate student from Turkey).

The conference organizers are grateful to CCP5 for the award of £1500 (from the workshop funding programme) to support the meeting. This funding has been used to pay for the accommodation and travel expenses of the invited speakers, to subsidise (partially) the registration and accommodation fees of conference delegates (not including postgraduate students – who were subsidised by a grant from the Angela and Tony Fish bequest of the RSC), to pay for the reception at the poster session and to cover the expenses of producing the conference booklet.

The funding from CCP5 was acknowledged on the conference website (<http://www.tc.bham.ac.uk/~roy/TCG/Materials.html>) and in the conference booklet provided to all delegates.

Dr Roy L. Johnston

Conference co-organiser