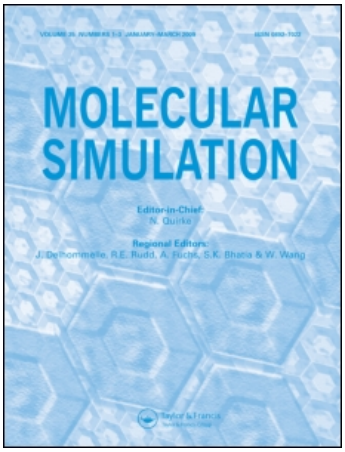

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Guest Editorial

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GUEST EDITORIAL

For many years, computers have been used to model, in an idealized way, the properties of matter. Much insight can be obtained from the study of a simple model, making it easier to interpret the behaviour of more complicated systems. However, increasingly, the emphasis is shifting towards direct practical applications of computer modelling, using realistic rather than idealized models, driven by the requirements of technology. When there is a compelling need to understand certain material properties, or to design materials with prescribed properties, then such barriers as may exist between different computational techniques, and between theoreticians and experimentalists, quickly disappear.

In January 1989, a meeting was held at Bristol University on the subject of 'Computer Modelling of New Materials'. It was sponsored by two Collaborative Computational Projects of the U.K. Science and Engineering Research Council: CCP5, concerned with computer simulation of condensed phases, and CCP9, involved in electronic structure calculations. The aim of the meeting was to bring together people from a range of backgrounds, experts in a variety of computer modelling techniques, to discuss progress and future prospects in this field. The meeting was well-attended, with 55 registered participants.

The subject of the meeting was deliberately kept as open as possible. Obvious areas of current interest were represented in the invited talks, some of which were to provide an overview of a specific field, and some to concentrate on recent results. There was interest in the study of bulk semiconductors, surfaces and atomic clusters using Car-Parrinello, local density functional, and tight-binding approaches. The crystal structures and electronic structures of high-T_c superconductors were also extensively discussed. Finally, challenges in the atomistic simulation of complex systems such as polymers, liquid crystals, and ceramics, were addressed. Contributed talks and posters covered the above topics, and also subjects such as zeolites, electrorheological fluids, and quantum simulations.

The papers in this issue constitute the formal proceedings of the meeting. Not all the talks are represented: some were purely of a review nature, better published in a different format, while others dealt with work still at a preliminary stage, again a valuable part of the meeting but not yet ready for publication. Nonetheless, these proceedings include a representative selection of the topics discussed, and an encouraging set of pointers to future work in this area of research.

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