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Editorial

Towards accurate calculation of biomolecular recognition and reactivity: A special issue in honour of Professor Ian Hillier

This special issue of the journal draws together articles arising from the 2004 International Meeting of the Molecular Graphics and Modelling Society, held in Manchester, UK. The meeting paid tribute to the scientific contributions of Ian Hillier, Professor of Theoretical Chemistry at The University of Manchester for over twenty years. The theme of the meeting was current progress in computational calculations of biomolecular recognition and reactivity, areas in which Ian's work has impacted over the last four decades. The excellent oral and poster contributions highlighted the considerable inroads that computational chemistry continues to make into unravelling the fundamental principles of complex covalent and non-covalent interactions in biology. Although progress is being driven in part by the seemingly inexorable increase in computing power and structural biology data, innovations in theory, methodology, algorithm and interpretation were also highlighted as key to improving our understanding of these processes. The meeting was a memorable occasion, with a stimulating breadth of topics covered, including development of intermolecular potentials, applications of electronic structure calculations to reactivity, dynamics and thermodynamics, and design of molecular interactions, as reflected by the nine articles in this issue. A number of contributors at the meeting paid tribute to the enduring benefits of their interactions with Ian, as postgraduate students, postdoctoral researchers, colleagues or collaborators.

Ian's early work was on polymer chemistry; he was awarded the degree of Doctor of Philosophy in 1964 at Imperial College London for work on ''Transition in Bulk Polymers.'' At a time when computational chemistry was an emerging discipline, he then went on to a two-year postdoctoral position with the distinguished chemical physicist, Professor Stuart Rice at the University of Chicago. On his return to the UK, he took up a lectureship at the University of Manchester, where he established himself as one of the early pioneers of computational chemistry, in particular through his quantum mechanical studies on transition metal systems, and in 1983, Ian was appointed Professor of Theoretical Chemistry. To date, he has published over 400 papers using theoretical and computational methods to elucidate the relationship between molecular structure, physical properties, and chemical reactivity for a wide range of chemical systems. In particular he has led the UK in the use of hybrid or embedding methods to study the condensed phase, and has applied these methods to study the solid state, solution chemistry and enzyme reactivity. In recognition of his work, he received the Royal Society of Chemistry 1998 Award in Theoretical and Computational Chemistry.

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