Introductory remarks

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PREFACE

Introductory remarks

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This special issue contains papers related to the 2009 Thomas Young Centre Workshop at University College London 'Accessing large length and time scales with accurate quantum methods', in celebration of Professor Michael Gillan's 65th birthday.

Mike Gillan won the 2006 Institute of Physics Dirac Medal and Prize, the citation reading: 'For his contributions to the development of atomic-scale computer simulations, which have greatly extended their power and effectiveness over an immense range of applications'. This rightly highlights Mike's seminal work on materials modelling, but misses out some of the many other areas he has enriched.

After taking his PhD at the Department of Theoretical Physics, Oxford University, Mike went as a post-doc to Minneapolis. He then joined the Statistical Physics Group in the Theoretical Physics Division, Harwell, where he stayed for over 20 years, with a brief interlude in Saclay. In the late 1980s, Mike made a transition to become Professor of Physics at the University of Keele, where he stayed for a decade until University College London was fortunate in being able to tempt him to join the Condensed Matter and Material Physics Group, where there was already a significant materials modelling initiative.

Over the years, Mike has made many important contributions, some with impact on other areas of science, others with significance in technology areas such as nuclear safety. Thus, he developed a form of quantum transition-state theory, generalizing Eyring's well-known classical transition-state theory to the case of quantum particles, such as hydrogen, diffusing in condensed matter. He pioneered quantum methods for calculating defect energetics in solids, and then molecular processes on surfaces. He synthesised these approaches into very general ways to calculate thermodynamic free energies of condensed matter from first principles, drawing on his early experience of statistical physics. These methods led to rapid advances in the study of matter under extreme conditions, as in the Earth's core. A further powerful development has been his input to linear-scaling quantum techniques for the properties of very large complex systems. In recent years, his attention has shifted towards increasing accuracy, touching areas such as quantum Monte Carlo and hierarchical quantum chemical techniques.

In this journal issue, we have papers which both reflect topics from the workshop and address a number of areas which are directly in Mike's interests or which have been influenced by his work or assistance. There are papers addressing accuracy in quantum simulations [1–5], methods for applying quantum techniques to large systems [6, 7] and applications of quantum simulations to important problems [8–10]. We also have a viewpoint on magnetism in oxides and carbon [11], prompted by Mike's innovative work on oxides.

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