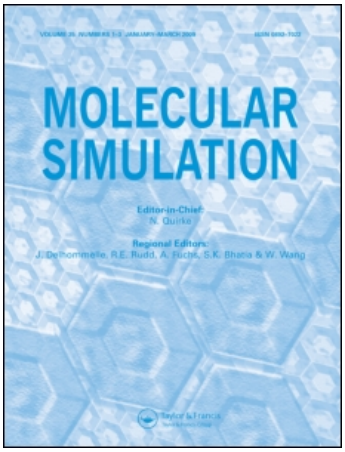

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Guest Editorial

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Guest Editorial

Computer modelling techniques are now influencing almost all areas of Chemistry and Physics. The rapid growth of the field has been enabled not only by developments in theory, algorithms and software, but also by the continuing exponential growth in the power of computer hardware.

The modelling of surfaces and interfaces often involves very wide time and length scales. From picosecond to sub-picosecond, motions of molecules at surfaces to the global motion of membranes at the micrometre scale require timescales that go well beyond those characterising atomic motions. The development of coarse-grained models has enabled the investigation of morphological changes in membranes and biomolecules, opening a computational approach to investigate complex biological processes in the cell. Similarly, first principle methods, namely density functional theory, are advancing considerably our understanding of the physical behaviour of interfaces in polycrystalline materials, as well as gas adsorption on surfaces at an unprecedented level of detail. A detailed understanding of the properties of surfaces and interfaces is vital to many important fields of technological interest, such as nanomaterials.

The UK's Collaborative Computational Project 5 is a network group for computer simulation of condensed phases. In the 2008 CCP5 annual conference on *Surfaces and Interfaces* we saw an impressive range of work. Two of the plenary lectures *Modelling of biomimetic membranes: Budding, adhesion, and fusion processes* (Prof. Reinhard Lipowsky) and *Coarse grained simulations of membrane proteins and peptides* (Prof. Mark Sansom) discussed the applicability of coarse-grained models to investigating complex biological processes such as protein assembly and membrane fusion. Prof. Mike Gillan showed how to use density functional theory to simulate long-time irreversible processes in surface science, such as gas desorption rates. The challenges associated to the modelling of grain boundaries in polycrystalline materials were discussed by Prof. Adrian Sutton. Prof. Steve Parker's plenary lecture focused on atomistic simulations of surface and interfaces, showing the ability of current atomistic methods to model complex surfaces such as those in nanoparticle solutions and the free energy of absorption of molecules on surfaces.

This special issue contains articles that show both methodological advances as well as applications of computer simulations to understand the behaviour of complex interfaces and surfaces. Goujon and co-workers discuss methodological advances on the calculation of long-range interactions of interfaces. Quigley and Rodger present a thorough discussion on how the metadynamics approach can be efficiently used to sample crystallisation processes. Binnie et al.'s article illustrates the applicability of the Quantum Monte Carlo method to investigating surface energies. Structural, dynamic as well as ion adsorption studies of mineral surfaces are presented in the works by Bruska et al., Mulheran et al. and Galea et al., whereas Yang et al., Mulheran et al. and Grafmüller et al.'s articles nicely illustrate the potential of computational approaches to investigate the properties of biological interfaces with materials, as well as complex membrane fusion processes.

We would like to thank the Institute of Physics Publishing, Taylor and Francis Publishing and the EPSRC project 'Structural Modelling of the Biological Interface with Materials' (grant number GR/S80103/01) for kindly sponsoring the conference. We would also like to thank the CCP5 executive committee, particularly Prof. Bill Smith, Dr John Purton and Prof. Mark Rodger, for giving us the opportunity to host a conference in this key area. Finally, we want to acknowledge and thank the support we received from the staff at Bankside House, London School of Economics and Political Sciences where the conference took place.

We hope that the issue illustrates the range and impact of computer simulations in the very important area of surfaces and interfaces.

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