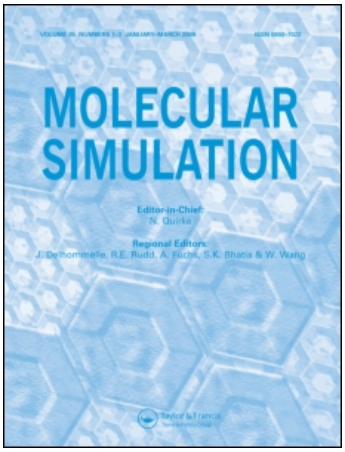

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Guest Editorial: *e*Minerals: an *e*-science project for modelling the environment from the molecular level

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Guest Editorial

*e*Minerals: an *e*-science project for modelling the environment from the molecular level

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Many problems in environmental geochemistry, such as transport of pollutants, development of remediation strategies, weathering and containment of high-level radioactive waste, require an understanding of fundamental mechanisms and processes at a molecular level, as these microscopic processes affect observed behaviour at the macroscopic scale. Whereas, computer simulations at a molecular level can lead to considerable progress in our understanding of these processes, developments in atomistic simulation tools must now be linked with GRID technologies in order to facilitate simulation studies that can be performed with realistic conditions, and which can scan across a wide range of physical and chemical parameters. The *e*-science challenge is then to scale up the length- and time-scales of the simulation techniques from this molecular level, through the mesoscopic scale, towards the length and time scales of human experience.

In 2001, the Natural Environment Research Council awarded one of their newly instigated *e*-Science testbed grants to an interdisciplinary team of computer and computational scientists from a range of UK universities and research institutions. The proposed project 'Environment from the molecular level: An *e*-science proposal for modelling the atomistic processes involved in environmental issues' was soon dubbed *e*Minerals and the expressed aim was to develop new methods for scaling simulations, archiving and mining of simulation output data, and visualisation of critical events.

The work programme of this consortium naturally fell into three parts: (i) computational software development, including linear-scaling quantum mechanical methods, Molecular Dynamics and quantum Monte Carlo simulations; (ii) development of GRID-enabled computing technologies; and (iii) science applications. The science output of the consortium would focus on fluid/surface interfaces, radiation damage, transport of pollutants and adsorption of pollutants to mineral surfaces.

The project is now nearing the end of its third year, which seemed to be an appropriate time to present a comprehensive collection of the work carried out within the *e*Minerals consortium. One of the major factors contributing to the success of the consortium project has been the enthusiastic interplay between scientists from sometimes widely different academic disciplines, comprising earth sciences, chemistry, physics and computer science, which is exemplified by the wide spread of topics and the interdisciplinary nature of the articles presented in this thematic issue of Molecular Simulation.

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