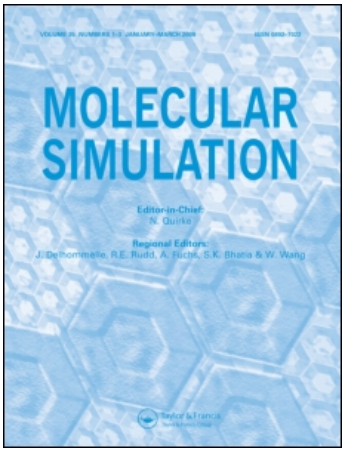

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Editorial

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EDITORIAL

The techniques of molecular simulation now occupy a central place in condensed matter physics and chemistry, and are beginning to assume an important role in chemical engineering and in the study of biological molecules. The uses of molecular simulation range from the provision of exact data for idealised model systems against which approximate theories may be checked, to the prediction of thermodynamic, structural and transport properties of detailed molecular models intended to be realistic representations of natural systems.

There now exists considerable simulation activity in disparate application areas that are not always in communication. There is no one source of advice and literature on new applications of molecular simulation or new algorithms for molecular simulation. This situation can only hinder the rapid exploitation of numerical methods based on statistical mechanics for scientific research.

Molecular Simulation has been created to provide a remedy by encouraging the publication, within a single journal, of papers concerned with the use of molecular simulation to produce new scientific results in a given area *and* with the development of new algorithms and procedures. The expectation is that significant cross-fertilization of ideas will be facilitated. A further major concern has been to insist on proper documentation of simulation work to enable, in principle at least, the work to be repeated in other laboratories.

Molecular Simulation will welcome contributions on all aspects of the subject, in particular:

1 significant new scientific results obtained using molecular simulation methods (including full details of the execution of the simulation);

2 the development of new algorithms and new simulation practices (the latter would include "tricks of the trade" such as equilibration procedures);

3 the derivation of intermolecular potentials (including *ab initio* quantum calculations);

4 new computers and new languages.

We thank the Editorial Board for their advice and support and trust that, together, we will provide a useful service to the research community.

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