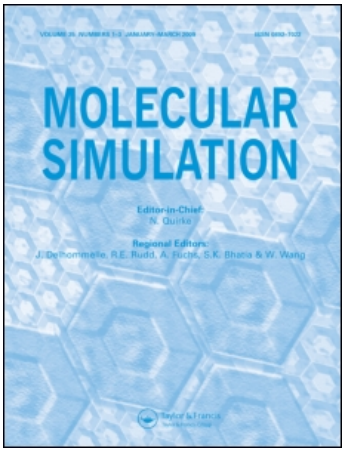

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Editorial

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To cite this Article Gubbins, K. E.(1991) 'Editorial', Molecular Simulation, 7: 5, i — ii
To link to this Article: DOI: 10.1080/08927029108022456
URL: http://dx.doi.org/10.1080/08927029108022456

Molecular Simulation, 1991, Vol. 7, pp. i–ii
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EDITORIAL

There has been a rapid rise in interest in the use of molecular simulation as a research tool in applied chemistry and chemical technology in the last two or three years, particularly in the United States. This has been the result of several factors, including the maturing of the field to a point where useful results can be obtained for applications of industrial, as well as purely scientific, interest, the entry into academic departments of a growing number of young researchers who are well versed in these techniques and in statistical mechanics generally, the availability of supercomputers and fast work stations, and the appearance of books describing the methods in detail. Interest has also grown in industrial research laboratories, and a number of the major oil and chemical companies (Exxon, Shell, Mobil, ICI, BP, etc.) now have active groups using simulations for a variety of applications. This sharpening of interest is apparent at the Annual Meeting of the American Institute of Chemical Engineers, held every November. The first symposium on molecular simulation was organised by myself for the 1977 Annual Meeting, and despite a program that included many of the most prominent researchers, attracted only a handful of people, some of whom mistakenly thought they would be hearing about process simulation! By contrast, similar symposia organised for the Annual Meetings of the last two years have been filled to capacity, and the quality of the presentations has been generally high.

This Special Issue of *Molecular Simulation* contains a selection from the papers presented at the Annual Meeting of the American Institute of Chemical Engineers held in Chicago in November 1990. Two symposia were held on *Molecular-Based Computer Simulations* (chaired by P. B. Debenedetti and L. L. Lee), and one on *Statistical Mechanics of Adsorption* (chaired by P. A. Monson and J. A. O'Brien) that contained a good deal of work on simulations. Simulations to evaluate the physical properties of fluids and mixtures continue to be an area of great interest, due to their importance in chemical processing. The papers of Chialvo and Debenedetti, Kofke, Rowley and Ely, and Ravi and Murad are in this area, the first two concerning thermodynamic properties and phase equilibria, and the latter two papers being on transport properties. There has been a rapid surge in the number of simulations of materials properties. In some cases it is the properties of the materials themselves that is of interest, as in the papers of Richardson and Clancy on solidification in metals and alloys, of Chalam, Gubbins, de Miguel and Rull on liquid crystals, and of Arbabi and Sahimi on disordered materials. In others it is the behaviour of fluids in narrow pores in the solid materials that is simulated, as in the papers of Karavias and Myers (zeolites), Snurr, June, Bell and Theodorou (silicalite), Raghavan and MacElroy (random porous media), and Talu (silicalite). Such porous materials are widely used in the chemical industry for separation and as catalyst supports for reaction of chemicals. Interfacial properties are of great importance, and the paper of Shukla and Robert investigates the vapour-liquid interface in two dimensions.

Several areas of current activity in chemical technology are not represented here. One is simulations of materials of biological or pharmaceutical interest, and another is that of chemical reactions themselves. Much interesting work is underway in these

areas by pure scientists. The work on reacting systems is in its infancy, but is particularly likely to expand rapidly, using both classical and *ab initio* potentials. The simulations currently underway on the etching of silicon by fluorine provides a good example of what is currently possible in this area.

This issue contains the first part of the papers presented at the meeting. The remainder will be published in the next issue of *Molecular Simulation*.

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