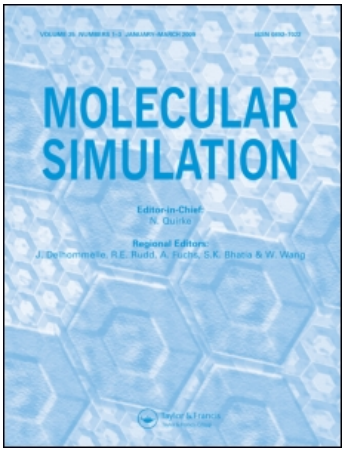

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Guest Editorial

P. Clancy

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GUEST EDITORIAL

This special issue is a selection of papers from the sessions on Molecular Simulation that were presented at the annual American Institute of Chemical Engineering meeting in Miami Beach, Florida, in November 1992. It reflects the great diversity of research that is now underway using atomic-level computer simulation methods and the progression to simulations of more complex systems. In this issue, for instance, the materials studied range from electrolytes (Chialvo and Cummings) to polymers (Broadbelt, LaMarca, Klein, Andrews and Colter) to precursors to exotic natural gas hydrates (Long and Sloan). The study of solid/fluid interfaces is an emerging theme. Wang and Fichthorn have studied the adsorption of EAM-modeled Pt on Pt substrates. Ravi and Murad have produced an interesting new method of studying the adsorption of fluids, here nitrogen in pores. Uttormark *et al.* have studied the kinetics of growth and dissolution processes in solid/liquid systems.

Research interest remains strong in the traditional areas of fluid property evaluation. Hauschild and Prausnitz, along with Chialvo and Cummings report calculations of vapor-liquid equilibria. Prickett and Mavrovouniotis describe a method to determine the properties of organic compounds. Kavassalis, Chou and Rudin present a method of calculating solubility parameters. Broadbelt, La Marca, Klein, Andrews and Colter give a novel method of modeling polymer fragmentation using Monte Carlo techniques. It is heartening to note that novel algorithm development remains strong and that nascent efforts in *ab initio* treatments will have a growing impact on this field in the next few years; no doubt such efforts will be reflected in Molecular Simulation in the future.

P. Clancy
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