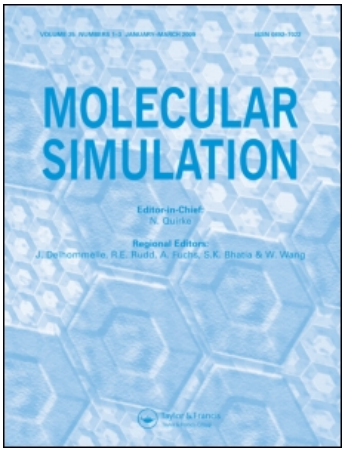

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Guest Editorial

K. Nakanishi

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GUEST EDITORIAL

This issue of *Molecular Simulation* contains papers presented at the 3rd Annual Symposium on Molecular Simulation, Japan, held at Kyoto University from January 24th to 26th 1990. The purpose of this series of symposia is to offer a forum in which scientists may present their research results on the computer simulation of molecular systems and in which interdisciplinary discussions are strongly encouraged. Contributed papers from chemistry, physics, biological science and earth science are solicited. The first symposium of this series was held in Kyoto on December 17th and 18th 1987 (the organisers were Dr. H. Tanaka and Prof. K. Nakanishi; 20 papers) and the 2nd at the Tokyo Institute of Technology on December 9th and 10th 1988 (the organisers were Professor I. Okada and Dr. S. Okazaki; 34 papers).

The present symposium was organized by Professor A. Ueda and Dr. Y. Kaneko and the number of papers presented increased to 39. The number of participants is also increasing reaching 120 from universities, institutions and industry.

As an editorial board member, I suggested to Prof. Quirke that we should publish selected papers presented in this symposium as a special issue of the journal. With the consent of Prof. Quirke and Prof. Ueda, this proposal was accepted and with the present issue it is my pleasure and satisfaction to complete the editing of these proceedings.

Let me give a brief overview of the contributed papers. The first three papers discuss some important problems in molecular physics. While two studies use a Monte Carlo technique to treat a solution of polar molecules with electron polarization (Hatano *et al.*) or two-dimensional polymer molecules with short range interaction (Takashima *et al.*), the other gives an interpretation of the velocity autocorrelation function for molecular motion in liquids with a fluctuating spring model (Morita). We have five papers dealing with oxide melts or molten salts. Molecular dynamics simulations have been carried out for SiO_2 (Tsuneyuki *et al.*), TiO_2 (Matsui and Akahagi), $Na_2O{\cdot}2\text{-}SiO_2 + K_2O{\cdot}2.5SiO_2$ (Kawamura and Yokokawa), LiBr + LiI (Itoh *et al.*) and LiOH (Okazaki and Okada). They are followed by four papers on the liquid and solution states of nonelectrolytes. Thermodynamic properties of hydrogen bonding liquids such as water and hydrogen fluoride are discussed based on simulation and new potential functions (Honda *et al.*). The next three papers deal with mixtures: Monte Carlo study of mixtures of monatomic and diatomic molecules with Lennard-Jones type interactions (Murakami *et al.*), Monte Carlo study of associating structure in benzene + methanol mixtures (Adachi and Nakanishi), and molecular dynamics and quenching studies of aqueous solution of rare gases (Tanaka and Nakanishi). The last four papers present applications of molecular simulation to material design. Monte Carlo or molecular dynamics simulation is used to study the crystal growth of a metal film (Kaneko and Yamomoto), the formation of thin films (Sasajima and Yamamoto), the phenomenon of crack propagation (Hata *et al.*) and the radiation damage of amorphous alloys (Okamoto *et al.*).

Finally the guest editor is grateful to the Editor in Chief, Prof. N. Quirke, Prof. A. Ueda and Prof. M. Tanaka for their suggestions and encouragement.

K. Nakanishi
Kyoto, August 1990