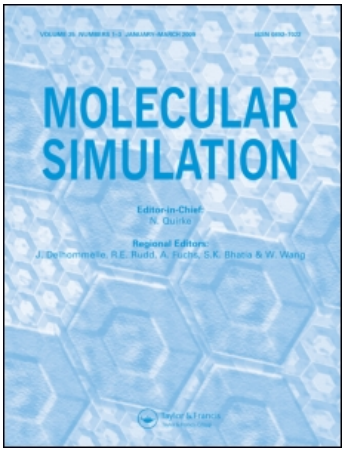

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Note

THE FOURTH SYMPOSIUM ON MOLECULAR SIMULATION

The following is the programme of papers presented at the Fourth Symposium on Molecular Simulation held at Kyodai-Kaikan, Kyoto, Japan on the 18th and 19th of December 1990.

Oral Session

1. Shift and Splitting of Absorption due to Interaction among Transition Dipoles
   S. Hayashi, M. Oobatake[A], and K. Machida
   (Kyoto Univ. and Protein Engineering Research Institute[A])
2. Molecular Dynamics Simulation of Liquid N_2O_4
   T. Kato, M. Oobatake[A], K. Machida[B], and S. Hayashi[B]
   (Seibo Jogakuin Jr. College, Protein Engineering Research Institute[A], and Kyoto Univ.[B])
3. Rotational Isomerism of Molecules in Condensed Phases
   T. Sakka and M. Iwasaki (Kyoto Univ.)
4. Molecular Dynamics Simulations of Charged Polymers Chains
   M. Hasegawa, M. Takasu, and Y. Hiwatari (Kanazawa Univ.)
5. Molecular Dynamics Calculations on Ferroelectric Polymers. III
   Method of Cavity Field and Polarization Fluctuation
   N. Takahashi (Hokkaido Univ. of Education)
6. Dynamics of Charged Polymers in Gel
   M. Matsumoto and M. Doi (Nagoya Univ.)
7. Two Phase Coexistence of String and Liquid Phases:
   Nonequilibrium Molecular-Dynamics Simulations of Couette Flow
   T. Yamada and S. Nose (Keio Univ.)
8. Molecular Dynamics Simulation of Diffusion of Small Molecules in Polymers:
   Effect of Local Structure of Polymers
   H. Takeuchi (Mitsubishi Kasei Corporation)
9. Molecular Dynamics Simulations of Hydrogen in Palladium
   K. Uehara, T. Muranaka, M. Takasu, and Y. Hiwatari (Kanazawa Univ.)
10. Molecular-Dynamics Simulations and Force-Field Parameters of Alkanes
    S. Kuwajima and H. Noma (Century Research Center Corporation)

11. Partial Molar Volumes of Chain Molecules.
Calculations by the RISM-PY Theory
M. Ooba and H. Nomura[A] (Kawai-Juku and Nagoya Univ.[A])

12. Role of Repulsive Force in Condensed Systems
A. Ueda (Kyoto Univ.)

13. The Structure of NH_4^+ $(NH_3)_n$ Cluster Ions (n = 1, 12), a Theoretical Study
T. Shoda and K. Kitaura[A] (Mitsubishi Kasei Corporation Research Center and Institute for Molecular Science[A])

14. Phase Transition of SiO_2 of the Rutile Structure Associated with Softening of Phonons: An MD Study
Y. Matsui and S. Tuneyuki[A] (Okayama Univ. and Tokyo Univ.[A])

15. Band Broadening of Vibrational Spectrum of Polyatomic Ion in Coulombic Liquid
S. Okazaki and I. Okada (Tokyo Institute of Technology)

16. Dynamic Structure and Relaxation around Liquid–Glass Transition of Alkali Halide Mixture
K. Kinugawa, K. Kadono, and H. Tanaka (Government Industrial Research Institute Osaka)

17. Molecular Dynamics Simulation on Fluoride Glasses (II)
M. Keitora (Asahi Glass Company Research Center)

18. Molecular Dynamics Simulation of the Perovskite family of Crystals
I. Fukuda and M. Mikami (Fujitsu Limited)

19. Central Force Potential Models of O–H Interaction for Molecular Dynamics Simulation of Multi-Component Oxide Systems
K. Kawamura, N. Kumagai, N. Sawaguchi, and T. Yokokawa (Hokkaido Univ.)

20. Numerical Solution of Pair Distribution Functions for a Binary Fluid-Supercooled Liquids, Glassy States and Phase Separation
S. Kambayashi and Y. Hiwatari[A] (Information System Center JAE and Kanazawa Univ.[A])

21. Dynamics of Glass Transitions – Residence Time Distribution
T. Odagaki and Y. Hiwatari[A]
(Kyoto Inst. Tech. and Kanazawa Univ.[A])

22. The Effects of Hydrophobic Interactions on the Complex Formation of β-Cyclodextrin-D,(L)Methyl Mandelate
H. Okazaki, T. Yamashita[A], T. Akaike, and T. Yasukawa[A] (Kanagawa Academy of Science and Technology and Tokyo Univ. of Agriculture and Technology[A])

23. Conformational Deformation by Hydrostatic Pressure in Deoxymyoglobin
T. Yamato (Kyoto Univ.)

24. Molecular Dynamics Simulation of the Lipid Bilaye: Membrane
K. Sakai and M. Mikami[A]
(Fujitsu Kyusyu System Engineering and Fujitsu Limited[A])

25. Rapid Simulation of a Protein in Water
M. Saito (Protein Engineering Research Institute)

26. Calculation of Thermostability by Hydration of Proteins
M. Oobatake and T. Ooi[A] (Protein Engineering Research Institute and Kyoto Women's Univ.[A])

Poster Session

P1. Certain Molecular Dynamics
T. Oyabu (Kyoto Univ.)

P2. Conformational Excitations that propagate along the chains in polymer crystals
T. Yamamoto (Yamaguchi Univ.)

P3. An MD Simulation Study on a Mixing Effect in the Molten System (Li,Cs)Cl
Y. Miyamoto, S. Okazaki, and I. Okada (Tokyo Institute of Technology)

P4. An MD Simulation Study on the Structure and Dynamics of Lauric Acid Bilayer
T. Fukada, S. Okazaki, and I. Okada (Tokyo Institute of Technology)

P5. Computer Simulation and Atomic Consideration of Crack Propagation Processes
K. Hata, K. Nishioka, and T. Takai[A]
(Univ. of Tokushima and Kagawa Univ.[A])

P6. Molecular Dynamics Calculation of Heat of Transfer in Mixture Liquid of Inert Gases
T. Ikeshoji (The Government Industrial Research Institute, Tohoku)

P7. Monte Carlo Simulations of Inclusion Phenomena and their Visualization with Computer Graphics
A. Noda, T. Takagi, H. Maezaki, S. Nagai, K. Murano, K. Matsumura, N. Hojo, and H. Fujiwara (Osaka Univ.)

P8. Molecular dynamics simulation on Atomic Diffusion in Supercooled Liquids for Binary Soft-Cores
H. Miyagawa and Y. Hitwatari (Kanazawa Univ.)

P9. Phase Separation Mechanism of Methane and Tetrafluoromethane Mixture
M. Matsumoto, H. Tanaka, and K. Nakanishi (Kyoto Univ.)

P10. Three-Body Effect in Argon Clusters
K. Nomura and K. Nakanishi (Kyoto Univ.)

P11. Thermodynamic Quantities of Triatomic Molecule Model Systems
H. Ohji, S. Murakami, and I. Fujihara[A] (Osaka City Univ. and Osaka Sangyo Univ.[A])

P12. Unification of Thermodynamics and Mechanics
T. Oyabu (Kyoto Univ.)

P13. Deleted

P14. Change of packing topology and diffusion process in liquid water
Y. Kataoka and N. Go (Kyoto Univ.)

P15. Contact-Complex Formation Reaction in 1-,2-, and 3-Dimensional Square-Well Fluids: Density Dependence of the Equilibrium Constant
Y. Yoshimura (Kyoto Univ.)

P16. Rotational States of Single Molecule in the Interacting Two CH4 Molecules
Y. Ozaki (Nagoya Institute of Technology)

P17. Molecular Dynamics Study of Diffusion of Li in Li_2SiO_3 System in Liquid and Glassy States
J. Habasaki, I. Okada, and Y. Hiwatari[A] (Tokyo Institute of Technology, and Kanazawa Univ.[A])

P18. Refinement of Molecular Mechanics Parameters XXXVI Basic Set Effect on the Calculated Intermolecular Interaction Energies of Small Hydrocarbons Including Methane, Ethane and Ethylene
S. Tsuzuki, K. Tanabe, and T. Uchimaru (National Chemical Laboratory for Industry)

P19. Dynamic Process of Ion Diffusion on the Glass Transition of LiI by Molecular Dynamics Method
S. Itoh, H. Miyagawa[A], and Y. Hiwatari[A] (The Nishi-Tokyo Univ. and Kanazawa Univ.[A])

P20. Molecular Dynamics Simulation of n-Butane Solution
H. Hayashi, H. Tanaka, and K. Nakanishi (Kyoto Univ.)

P21. Dynamic Process of Argon Clusters
O. Kitao, I. Ohmine[A], and K. Nakanishi (Kyoto Univ. and Institute for Molecular Science[A])

P22. On the Time Variation of Network Structures in Molten Sodium-Borosilicates
H. Ogawa (Tohoku Univ.)

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