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Third Liblice Conference on the Statistical Mechanics of Liquids

May 28–June 1, 1990, Bechyně, Czechoslovakia

Opening Lecture

Henderson, D.: Theory of inhomogeneous fluids

Chairman: M. S. Shaw

Frenkel, D.: Recent development in simulations on liquids

Panagiotopoulos, A.: Molecular simulations of phase equilibria

Goldman, S.: Simulation on polyelectrolytes using a discrete model for the solvent

Pusztai, L.: Reverse Monte Carlo simulation

Chairman: J. Perram

Ben-Naim, A.: Solvent-induced interactions in aqueous solutions

Heinzinger, K.: MD simulations of aqueous electrolyte solutions

Haymet, A. D.: Molecular theory of pH in aqueous solutions

Krienke, H.: Mixtures of dense associated charged liquids

Holovko, M.: On the account of the association effects in the statistical theory of ion-molecular systems

Chairman: E. Glandt

Wertheim, M.: Dimerization, association, and polymerization in fluids

Kolafa, J.: Thermodynamics of primitive models of associated liquids

Boublík, T.: Equation of state of fused-hard-sphere fluids

Rodger, M.: Anisotropic site–site interaction—A flexible and realistic model of intermolecular forces in condensed phases

Kahl, G.: Thermodynamically self-consistent integral equations for the structure of one- and two-component liquid systems

Pospíšil, R.: Integral equation theory for molecular fluids

Sarkisov, G.: Asymptotic behavior of correlation functions

Chairman: M. Neumann

Perram, J.: Theory and simulation of polar liquids

de Leeuw, S. W.: Phase separation in polar/nonpolar fluid mixtures

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Chairman: A. Ben–Naim
Neumann, M.: Computer simulations on water
Brodskaya, E. N.: MD study of water clusters formed around ions
Borstnik, B.: Liquid-water structure at the wall

Chairman: M. S. Wertheim
Glandt, E.: Aggregation and gelation: From liquid theory to percolation theory
Petsche I.: Fluctuation theory of near-critical systems

Chairman: P. Monson
Gubbins, K. E.: The behavior of fluids in micropores
Percus J. K.: Site representation of nonuniform molecular fluid
Diestler, D. J.: Structure and dynamics of molecularly thin fluid films
Levesque, D.: Surface properties of ionic systems
Bleha, T.: Distribution of flexible chains between bulk phase and small pores

Chairman: D. Henderson
Monson, P.: Computer simulation and theory of adsorption at a fluid–solid interface
Sokolowski, S.: Adsorption of binary fluid mixtures on solid surfaces: Theory and simulations
Nezbeda, I.: Molecular fluid mixtures at a hard wall
Rickayzen, G.: Structure at the solid–liquid interface
Rosinberg, M. L.: A free energy functional for inhomogeneous fluids
Lotfi, A.: Kinetics of a fluid at interfaces

Round-table Discussion: Should and could we be more efficient with respect to practical applications?

Moderator: J. Fischer
Panel speakers: A. Ben-Naim, D. Frenkel, K. E. Gubbins, I. Nezbeda

Chairman: D. Frenkel
Shaw, M. S.: A density of state transformation MC method for fluid thermodynamics
Möller, D.: The NPT + test particle method for the determination of vapor–liquid phase equilibria
Vörtler, H. L.: Chemical potential of the LJ fluid from a novel version of the insertion particle method
Aim, K.: On the equation of state of the Lennard-Jonesium
Saager, B.: Predictive power of effective pair potentials

Chairman: K. E. Gubbins
Fischer, J.: On prediction of the thermodynamic properties of real fluids

Kohler, F.: Shape effects on mixtures of linear molecules
Lustig, R.: Perturbation theory and MD results for linear and nonlinear molecules
Mollerup, J.: Determination of hard convex body parameters of real fluids
Winkelmann, J.: Structural and thermodynamic properties of nonspherical molecule fluids from integral equations and perturbation theories