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Fourth Liblice Conference on the Statistical Mechanics of Liquids

June 6–10, 1994, Lake Milovy, Czech Republic

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These conferences are held every 4 years, and cover both fundamental and applied aspects of theory and molecular simulation of liquids.

Please note that only the speaker is listed. Others may have been involved in the work. In addition to the oral papers listed below, there were 78 poster papers.

Opening

J. Valleau (Toronto): Teaching an old dog new tricks: Some recent (and useful) Monte Carlo stunts

CECAM Workshop: Novel Trends in the Simulation of Complex Liquids

Chair: D. Frenkel (Amsterdam) and D. Henderson (Mexico City)

A. Panagiotopoulos (Ithaca): Monte Carlo simulations of phase coexistence
D. Kofke (Buffalo): Phase coexistence properties by molecular simulation: Gibbs–Duhem integration
W. R. Smith (Guelph): Chemical and phase equilibria from a new reaction ensemble
J. Fischer (Bochum): MD study of evaporation from a free surface
B. Smit (Amsterdam): Simulation of complex fluids: Recent progress

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E. de Miguel (Seville): Simulation of liquid crystals: An attempt to go beyond hard-core models
J. W. Perram (Odense): The object-oriented development of a parallel application in polymer dynamics
B. Mulder (Amsterdam): Flexible formalism for persistent chains
P. T. Cummings (Oak Ridge): Molecular simulation of phase equilibria in electrolyte systems
I. Snook (Melbourne): Million atom simulations and application to surfaces and colloids
W. A. Steele (University Park): Simulation of fluids confined in pores of complex shape
R. Holyst (Warsaw): Edge dislocations in thin films and near surfaces
E. Piotrovskaya (St. Petersburg): Computer simulation of two-phase coexistence of the LJ fluid in narrow pores
J. Talbot (West Lafayette): Properties of a hard ellipsoidal fluid confined in a slit pore

Theory

Chair: J. Fischer (Bochum)

Y. Rosenfeld (Beer-Sheva): The "ideal" liquid: Definition, properties, and applications
J. K. Percus (New York): Structure of entropy functionals
P. A. Monson (Amherst): A theory of solid solutions
D. Evans (Canberra): Relations between phase space stability and thermophysical properties
S. Labík (Prague): A new geometrically-based integral equation hierarchy for hard sphere fluids

Inhomogeneous Fluids

Chair: W. A. Steele (University Park)

M. L. Rosinberg (Paris): Perturbation density functional theory for inhomogeneous polyatomic fluids
S. Sokolowski (Lublin): The effect of pore closure on capillary condensation using density functionals
G. Stell (Stony Brook): Quenched-annealed systems
E. Glandt (Philadelphia): Molecular fluids in random media
K. E. Gubbins (Ithaca): Molecular simulation of simple fluids and water in well-characterized pores

L. Blum (Rio Pedras): Structured charged interfaces: Theory and experiment
A. D. J. Haymet (Sydney): Water and electrolytes near charged interfaces
G. M. Torrie (Kingston): Recent results for wholly molecular theories of electrical double layers

Polar and Ionic Fluids

Chair: J. W. Perram (Odense)

G. Patey (Vancouver): From dipolar fluids to ferroelectric liquid crystals
M. van Leeuwen (Amsterdam): Polar fluid mixtures
P. Kusalik (Halifax): The dielectric constant and the distribution of the total dipole moment in polar fluids
H. Nishimura (Tokyo): The HNC equation approach to polar liquids

Associating Fluids

Chair: K. E. Gubbins (Ithaca)

M. Mezei (New York): Issues in modeling liquid water
P. G. Debenedetti (Princeton): Supercooled and glassy water: Theory, simulations, and experiments
E. S. Yakub (Odessa): Statistical thermodynamics of fluids with saturative attractive forces
M. F. Holovko (Lwow): Integral equation theory for the effects of association in ionic fluids
L. Blum (Rio Pedras): The solution of the OZ equation for anisotropic sticky spheres: Towards a model of water

Panel Discussion: Perspectives for CECAM Initiatives on Simulation on Complex Fluids

Moderator: N. Quirke (Orsay)

Speakers: P. T. Cummings (Oak Ridge), D. Frenkel (Amsterdam), K. E. Gubbins (Ithaca), J. W. Perram (Odense)

Normal and Chain-Molecule Fluids

Chair: W. R. Smith (Guelph) and E. Glandt (Philadelphia)

M. S. Wertheim (Haughton): Fluids of hard convex molecules
D. Henderson (Mexico City): Bridge functions and correlation functions for hard spheres using inhomogeneous integral equations

T. Boublík (Prague): Hard body fluids: The 3rd virial coefficient and equations of state
R. Lustig (Aachen): Simulating equations of state
B. Borstnik (Ljubljana): Approaching the Baxter's sticky limit by molecular dynamics simulations
J. Vrabec (Bochum): Vapor–liquid phase equilibria of mixtures from the NpT + test particle method
F. del Rio (Mexico City): Theory and simulation of square-well mixtures
C. Hall (Raleigh): Generalized Flory dimer theory for hard chain molecules
Y. C. Chiew (Piscataway): Equation of state for chain molecules: Monte Carlo and perturbation theory results
M. Banaszak (Annendale): Equation of state for Lennard-Jones chains