V-S Monte Carlo Simulation of Molecular Clusters

Physical properties of clusters have attracted much attention. Using Monte Carlo simulation methods, we investigate the properties of clusters and gels, helium in random potential, and other systems.

V-S-1 Boson Localization on the Superfluid-Insulator Transition by Quantum Loop Algorithm

HASHIMOTO, Masahito; TAKASU, Masako

[*Prog. Theor. Phys. Suppl.* **138** 529 (2000)]

For some systems in critical phenomena, Monte Carlo simulations using conventional algorithm is inefficient, because of strong correlation between successive MC configurations. Our system of helium in random potential suffers from this difficulty in critical region between superfluid phase and glass insulator phase. The loop algorithm overcomes this difficulty. We apply this algorithm to soft core boson system, and carry out calculations with random boson Hubbard model. This method is potentially useful for studying molecular clusters.

V-S-2 Monte Carlo Simulation of the Formation of Chemical Gel and Clusters

NOSAKA, Makoto; TAKASU, Masako

Gel is an important material used in everyday life. We focus our attention to the formation process of chemical gel and clusters. By changing the number of monomers, linkers and radicals, we obtain the phase diagram of gel. We also discuss efficient algorithm for determining the percolation of polymers.

V-S-3 Linear-shaped Motion of DNA in Concentrated Polymer Solutions Under a Steady Field

NOGUCHI, Hiroshi; TAKASU, Masako

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We studied the electrophoretic behavior of DNA chains in linear-polymer solutions using Brownian dynamics with an anisotropic friction tensor. We simulated the linear-shaped motion of DNA observed in highly concentrated solutions using a model with a chain segment equal to 1/4 of the persistence length. A linear conformation is seen for a chain with high segment-density regions, which remain at the same positions in space, with a high anisotropy of friction, while a U-shaped conformation is seen for a chain with a low anisotropy of friction.