

Anchoring, Wetting and Symmetry-Breaking Surface Transition in Liquid Crystal Systems

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A nematic liquid crystal in contact with a solid substrate is considered. Three types of surface phenomena are discussed: anchoring, wetting and surface phase transitions, which involve symmetry breaking in the surface layer. Where possible, we reveal relations between these phenomena. We concentrate on the following problems: anchoring on anisotropic substrates, the force balance equation at the nematic-isotropic-substrate contact line, the behaviour of the line tension in the thermodynamic limit, and the onset of the smectic-A order in the surface layer close to the bulk transition to the smectic-A phase. All these problems are studied in the framework of the Landau-de Gennes formalism. Possible directions of future studies are discussed.

Solvation Forces in Near-Critical Fluids. Ising Model Results

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Recent developments in the statistical theory of simple fluids in a film geometry near bulk criticality is reviewed. We summarize results obtained by exact or approximate, but very accurate methods within Ising model. Particular attention is paid to the properties of the measurable solvation force and its relation to the structure of the confined system, in the Ising model given by magnetization profiles. Relevance of the reviewed results for various physical systems is briefly discussed.

Diffusion on a Silicalite Lattice Model

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A lattice model is proposed for describing the diffusion of small molecules in silicalite, as a special example of zeolite. The lattice structure matches the interlacing of the silicalite channels and the molecules hop randomly from site to site according to simple rules. The diffusion of a single molecule is treated exactly. The ability of the model to meet more complicated situations is briefly discussed.

Models of the Hydrophobic Attraction

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Some recently proposed models of hydrophobic attraction, equivalent to the Ising model of ferromagnetism, are described and their properties reviewed. They are such that the accommodation of a hydrophobic solute in the solvent is energetically favorable but even more unfavorable entropically, which is believed to be the basic mechanism of hydrophobicity in water solution. The effective attraction between pairs of solute molecules as mediated by the solvent is calculated, as is the deviation from additivity in the interactions among three or more. The very low solubilities of the solutes in the model solvents are also calculated. In a different model, based on a phenomenological free energy leading to a closed-loop solubility curve in the temperature-composition plane, one finds the same very great increase in heat capacity on dissolving a hydrophobic solute as is found in experiment.

Phase Separation of Binary Mixtures of Symmetric Non-Additive Hard Spheres

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The behavior of a binary mixture of non-additive hard spheres with positive non-additivity parameter is investigated. The coexistence curves are calculated with a high accuracy for a few system sizes. The applicability of semigrand ensemble simulation method to calculation of the coexistence curve and the critical properties of mixtures is compared with other simulation method.

Lattice Cluster Theory for Copolymer Blends: General Theory in the Incompressible System, Long Chain Limit

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The lattice cluster theory is developed for binary blends of two structured monomer copolymers in the simplifying limit of an incompressible system and high molecular weights. The major advance in the present theory is the inclusion of nonrandom mixing effects that lead to a monomer sequence dependence of the Helmholtz free energy without the introduction of new adjustable parameters beyond those present in descriptions of binary homopolymer blends formed from the constituent monomers. Equivalently, the sequence dependent contributions are shown to emerge from a proper determination of the “surface fractions” in individual copolymer chains. The general theory applies to blends of random copolymer, diblock copolymers, alternating copolymers, as well as of copolymers with kinetically controlled monomer sequences. The theory is illustrated for purely random copolymer blends of deuterated and hydrogenated polybutadienes, where the computed phase boundaries depart qualitatively from those predicted by random copolymer Flory-Huggins theory.

Freezing Behavior in Porous Materials: Theory and Experiment

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We report both experimental measurements and molecular simulations of the melting and freezing behavior of simple fluids in porous media. Activated carbon fibers, having a mean pore width of 1.7 nm, were chosen as the porous medium. Differential scanning calorimetry (DSC) and dielectric relaxation spectroscopy (DS) were used to determine the melting point in these materials. The melting point was found to be very sensitive to the relative strength of the fluid-wall interaction compared to the fluid-fluid interaction. Monte Carlo simulations and Landau free energy formalism were used to determine the shift in the melting point, T_m , for simple fluids in pores having repulsive, weakly attractive and strongly attractive walls. The strength of the interaction of the fluid with the pore wall is shown to have a large effect on the shift in T_m , with T_m being reduced for weakly attracting walls. The theory of corresponding states is used to compare the experimental results for several systems to the simulation results. This approach also provides a unified approach in understanding the diverse freezing behavior in porous media.

Application of Histogram Reweighting Monte Carlo Method to Network-Forming Two-Dimensional Lattice Gas Model

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The results of grand canonical Monte Carlo study of two-dimensional lattice gas model of network-forming particles on a triangular lattice are reported. The model takes into account the effects of molecular association, resulting from the orientation-dependent interactions as well as the effects of cooperative interactions, which lead to the weakening of the bond energies. A phase transition between the dilute and the condensed phase is considered. Phase diagrams for different systems are presented and it is shown that the systems studied belong to the universality class of two-dimensional Ising model.

A Generalization of the Smoluchowski Coagulation Equation

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The Smoluchowski equation for irreversible coagulation is generalized by taking both two- and three-particle aggregations into account. The effects of three-particle events are studied through the exact solution of a special model.

Molecular Dynamics Simulations of Kinetic Models for Chiral Dominance in Soft Condensed Matter

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A molecular dynamics model of binary racemic fluid mixtures, consisting of particles which only differ a little with respect to the pair attractions, shows that the isomerization kinetics in condensed states can act as a driver towards a phase separation and a symmetry break so that one of the species finally dominates. The model offers a possible explanation of the origin of biomolecular chirality.

Structure of Proteins: New Approach to Molecular Modeling

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The force field and Monte Carlo sampling method of our recently developed reduced model of proteins is described. Recent applications of the models include *ab initio* structure prediction for small globular proteins, modeling of protein structure based on distantly homologous (or analogous) structural templates, assembly of protein structure from sparse experimental data, and computational studies of protein folding dynamics and thermodynamics. The newest application, described in this paper, enables the prediction of low-to-moderate resolution coordinates of the parts of protein structure that are missed in incomplete PDB files.

Self Similarity, Scaling and Renormalization Group Theory Used to Generate Equations of State for Hard-Particle Fluids

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An approach based on the concept of functional self-similarity is used to derive equations of state for two- and three-dimensional hard-particle fluids. Calculations indicate that this procedure works quite well, producing estimates of the compressibility factor that closely agree with the results of computer simulation.