Abstract for an Invited Paper
for the MAR06 Meeting of
The American Physical Society

Hydrophobic Effects as Seen in Lattice Models

BENJAMIN WIDOM, Cornell University

A class of lattice models incorporating the thermodynamic mechanism of hydrophobicity is defined and its properties derived. The models are equivalent to Ising models in a field. The solvent-mediated part of the potential of mean force between a pair of hydrophobic solute molecules is obtained from the pair correlation function of the underlying one-component lattice gas. The models yield a testable relation between the strength of the hydrophobic attraction between solute molecules and the free energy of solvation of a single one. The properties of the models are obtainable analytically in Bethe-Guggenheim approximation. The local energy density in the solvent is obtained as a function of the distance from an inserted solute. As a consistency check, this energy density, when summed over the lattice, is found to satisfy the required thermodynamic relation between the total energy change due to the solute molecule and the temperature dependence of the solubility.