Theoretical Models in Biochemical and Related Systems

Solvent–Solute Interactions by Quantum-Mechanical and Statistical Mechanical Simulations

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Quantum-mechanical computations are used to obtain the interaction potentials (two-body, three-body and many-body) between solute–solvent, and between solute–solute for multi-solute, one-solvent systems. *Statistical mechanics simulations* are used to obtain the structure and energy-related parameters of the solute–solvent system at a given temperature. This methodology is applied to a vast number of problems, like the structure of water around DNA, RNA and enzymes, ionic solutions, *etc.* The comparison between simulated and experimental data indicates the need to include temperature parameters, the reaction field, and many-body corrections in order to obtain realistic simulations of quantitative predictive value.

Ion Distributions and Energetics in Lamellar Liquid Crystals. A Comparison between Different Theoretical Approaches

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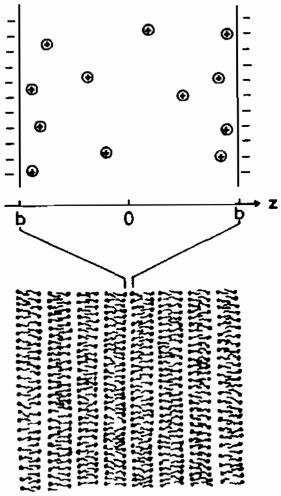

Fig. 1. The amphiphilic molecules form bilayers which are intercalated with aqueous lamellae also containing the counterions. The upper figure shows the schematic model of the aqueous region used in the MC simulations.

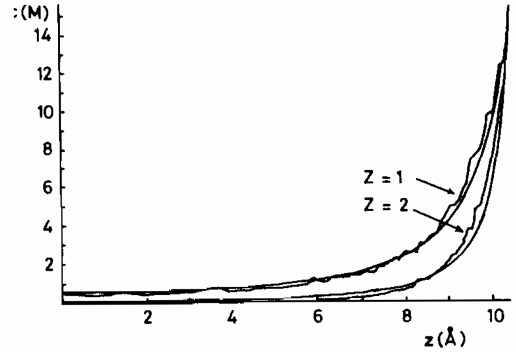

Fig. 2. Concentration profiles between the two charged plates for mono- and divalent ions. The plate distance 2b = 21.0 A. The smooth curves are taken from the PB equation and the two other are obtained from MC-simulations.

Monte Carlo (MC) simultations have been performed for an ionic system between two parallel uniformly charged plates modelling the conditions found in lamellar lyotropic liquid crystals [1] (Fig. 1). The results are used to assess the accuracy of the statistical mechanical approximations leading to the Poisson–Boltzmann (PB) equation. In general there is a good agreement between the MC simulations and results obtained from the PB equation [2], both in the system studied here and in analogous systems [3]. This applies to the ion distribution (Fig. 2) and to a lesser extent to the energy. In particular the PB equation predicts the correct asymptotic behaviour as the distance between the plates is increased. In the MC simulations there is a slight increase in the ion concentration close to the walls compared to the PB solution. This is due to the fact that in the MC simulations one allows for correlations between the ion while the PB equation is