Adsorption of model electrolytes in disordered porous materials. Predictions of the replica integral equation theory

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Partitioning of electrolytes between matrices containing charges and the bulk solution is not only a matter of academic interest, but finds its practical application in many technological, industrial and biological processes (for example: desalination of water, ion exchange, membrane equilibria etc.).

The present contribution will show that the replica Ornstein–Zernike integral equation theory is an adequate theoretical tool for studying preferential adsorption of a mixture of model electrolytes in random matrix media. The latter will be considered as a quenched equilibrium distribution of a size and charge symmetrical electrolyte, while the electrolyte that will be allowed to anneal within the matrix particles will be represented as a mixture of two electrolytes with common ion (for example AX and BX, where A and B are cations that differ in size and/or charge and X is the common anion).

After a short conceptual introduction to the replica theory its predictions will be compared with the exact results obtained by the Monte Carlo simulations in the grand canonical ensemble. It will be shown that the theory is in good agreement with the simulation.

Next, we will present a phase diagram for the given model. We will see that sorption of the electrolyte into the matrix media occurs only at low matrix concentrations and at low concentrations of the annealing electrolyte, whereas at higher concentrations we get exclusion from the porous media.

Ions with smaller radii (*i.e.* larger surface charge density) tend to be preferentially absorbed, since they can come closer to the matrix ions and feel stronger Coulombic force. Replica Ornstein–Zernike theory seems to be appropriate for studying the dependence of different parameters (matrix preparation, concentration, conditions of annealing) on the preferential adsorption of ions from such mixtures.