ΕΙΧΗΜΥΘ-ΙΤΕ

ΣΕΜΙΝΑΡΙΟ

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ΘΕΜΑ: How Accurately Can Simulations Predict the Structure of Electrolyte Solutions?

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΕΙΧΗΜΥΘ- ΙΤΕ

ΗΜΕΡΟΜΗΝΙΑ: 8 Ιουνίου 2000

ΩΡΑ: 12:00

ΠΕΡΙΛΗΨΗ

Computer simulations of Monte Carlo and Molecular Mechanics type are increasingly used to investigate structural, thermodynamic and kinetic data for liquids, in particular of solutions and/ or solvated bio-molecules. The results presented in this lecture deal with the predictive ability of such simulations for the structural details of two to four-component electrolyte solutions. It can be shown that, even for rather simple solvates, the use of 3-body and higher terms is required to avoid serious errors concerning co-ordination numbers and solvation energies, and much more for the discussion of exchanged processes and other data relevant for the "chemical behaviour" of the species present in solution. These findings will be illustrated by simulations performed stepwise by classical pair potentials, 3-body corrected potentials and by mixed quantum mechanical/ molecular mechanical MC/MD techniques. Phenomena like the specificity of potassium channels of cell membranes and the Jahn-Teller effect in solution will be discussed on the basis of these results. Preferential solvation of ions in mixed solvents with the inherent complexity of co-existing microspecies in solution will serve as an example to demonstrate, why experimental methods are rather insufficient to reveal the details of the molecular structure of such solutions.