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A closure relation to molecular theory of solvation for macromolecules ALEXANDER E. KOBRYN[1], National Institute for Nanotechnology, National Research Council Canada — We propose a closure to the integral equations of molecular theory of solvation, particularly suitable for polar and charged macromolecules in electrolyte solution. This includes such systems as oligomeric polyelectrolytes at a finite concentration in aqueous and various non-aqueous solutions, as well as drug-like compounds in solution. The new closure (KGK closure) imposes the mean spherical approximation (MSA) almost everywhere in the solvation shell but levels out the density distribution function to zero inside the repulsive core and in the spatial regions of strong density depletion emerging due to molecular associative interactions. We test the performance of the KGK closure coupled to the reference interaction site model (RISM) on the examples of LJ liquids, polar and nonpolar molecular solvents, including water, and aqueous solutions of simple ions, and use the KGK closure to obtain the solvation structure and thermodynamics of oligomeric polyelectrolytes and drug-like compounds at a finite concentration in electrolyte solution, for which no convergence is obtained with other closures. We further test the 3D-version of the KGK closure with 3D-RISM for molecular mixtures as well as oligomeric polyelectrolytes and drug-like molecules in electrolyte solutions.

[1]11421 Saskatchewan Drive, Edmonton, Alberta, T6G 2M9, Canada

Oleksandr Kobryn
National Institute for Nanotechnology, National Research Council Canada

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