

Associative approach in soft matter theory

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We analyse the possibility of the application of the statistical-mechanical approaches developed in the modern theory of associative fluids for the description of associative phenomena on different properties in soft matter theory [1]. In developed theoretical formalism, the potentials of intermolecular interactions are split into three parts. One of them is the short-range repulsive part responsible for excluded volume effects by molecules. The second one is the short-range strongly attractive part responsible for different clusterization effects, including self-assembly phenomena. The third part is long-range and responsible for the screening and renormalization phenomena. The specificity of the developed approach are connected with the application of the activity diagram expansions for the description of the short-range attractive part of interactions and the density diagram expansions for the description of the last two parts of interactions. Classification and reduction of the obtained diagrams in such expansions leads to the multidensity formalism, whose specificity strongly depends on types of described clusterization phenomena. Special attention is focused on the application of the associative approach in the theory of ionic solutions. The analytical solution of the associative mean spherical approximation (AMSA) and the modified version of the mean spherical approximation - the mass action law (MSA-MAL) approach are used to revise the concept of ion association in the theory of electrolyte solutions. It is shown that AMSA theory is more preferable for the description of thermodynamical properties while the modified version of the MSA-MAL theory is more useful for the description electrical properties [2]. The proposed theory is applied to explain the anomalous properties of the electrical double layer in a low temperature region and for the treatment of the effect of electrolyte on the rate of intermolecular electron transfer. We applied the developed approach for the description of solubilization of biological molecules in reverse micellar systems and the study of biomolecules' influence on the properties of considered systems. As an example, we consider solubilization of cytochrome-c in water in oil reverse micellar system [3] and the solubilization of RNA in water in reverse wormlike micellar systems with lipid covering. The associative approach also gives the possibility to construct the macromolecular systems from chemical functional groups.

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