MODELING OF ADSORPTION LAYERS ON NANOPARTICLES IN AQUEOUS SOLUTIONS OF NONIONIC SURFACTANTS

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Adsorption on solid nanoparticles is at the heart of many advanced technologies, including drug delivery, nanoreactor engineering and separation of chemicals. Of key importance is knowledge of structure of the adsorbed layers because it provides the insight in the molecular mechanisms that control adsorption and desorption in dependence on the characteristics of the nanoparticles and external conditions.

The major limitation of the well-known theoretical approaches proposed for adsorption systems [1,2] is that they do not take into account correlations between interacting functional groups of molecules, even though such correlations definitely play an important role in many cases, e.g., in aqueous and other hydrogen bonding fluids.

In this work, we apply the multilayer quasilattice model (MQuM) [3,4] to describe the details of local structure for adsorption layers on solid hydrophilic or hydrophobic particles submerged in aqueous mixtures that contain amphiphilic chainlike molecules. Within MQuM, the correlations between interacting functional groups are described within the Guggenheim quasichemical approximation; spatially nonuniform fluid around a spherical particle is represented by concentric spherical layers that accommodate segments of chainlike molecules in different orientations. Apart from mimicking adsorption in model systems, we also apply MQuM to a number of real aqueous solutions using the model interaction parameters estimated from vapor-liquid equilibrium data. We discuss the model predictions for the structure of solution around hydrophilic and lipophilic solid particles of varying curvature. We conclude by summarizing the advantages and limitations of MQuM.

1. Fleer, G. J.; Scheutjens, J. M. H. M.; Cohen Stuart, M. A. Colloids Surf., 1988, 31, 1−29.
2. Nap, R. J.; Szleifer, I. J Chem. Phys., 2018, 16, 149.
3. Sorina, P. O.; Victorov, A. I. Langmuir, 2024, 40 (3), 1577–1593.
4. Sorina, P. O.; Victorov, A. I. J. Molecular Liquids, 2024, 414, 126229

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