Molecular Modeling of Self-Assembly and Transport in Amphiphilic Systems

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Dynamics of self-assembly, structural transitions, and transport in amphiphilic systems play a key role in various technological and biological processes. Understanding these processes is of immense importance in development of new nanostructured materials, drug delivery methods, and novel separation techniques, as well as in deciphering of intracellular transport mechanisms. One of the challenges toward fundamental understanding of self-assembly processes is that theoretical and computational investigations are complicated by a non-trivial interplay between different length- and time-scales. In this talk, we present a theoretical method which allows one to probe the self-assembly dynamics at different scales. We demonstrate an application of this method to formation and disintegration of spherical micelles in solution and predict relative stabilities of spherical aggregates for a model non-ionic surfactant. Moreover, we discuss detailed dynamics of self-assembly and demonstrate an important role played by collective dynamics of amphiphilic molecules in the self-assembly processes.

In the second part of the talk we will discuss mass transport across densely packed surfactant covered oil-water interfaces in microemulsions. This process plays a key role in numerous applications such as separations, reactions, drug delivery, and detoxification. We investigate the role of the surfactant monolayer microstructure on the solute transport and discuss effects of such parameters as solute size and degree of hydrophobicity, as well as the length of surfactant molecules on the transport properties. In particular, we demonstrate that a usual Langevin equation model is not adequate for the solute transport across the monolayer due to a non-trivial behavior of the stochastic force acting on the solute. This phenomenon is related to density fluctuations of the surfactant as well as water and oil molecules around the solute. Possible implications of this phenomenon on solute transport mechanisms will be discussed.