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Kinetics of formation and disintegration of ionic and non-ionic spherical micelles[1] GUNJAN MOHAN, PPG Industries, DMITRY KOPELEVICH, University of Florida — Dynamics of self-assembly and structural transitions in amphiphilic systems play an important role in various industrial and biological processes. Main challenge in computational modeling of these dynamics is a complex interplay between various length- and time-scales. In this talk, we discuss development of a multi-scale model for formation and disintegration of non-ionic and ionic spherical micelles. This study is performed under the assumption that the dominant mechanism of micelle formation (disintegration) is a stepwise addition (removal) of individual surfactant monomers to (from) a surfactant aggregate. A series of molecular dynamics simulations is used to develop reduced stochastic models for these elementary processes. It is demonstrated that these processes involve complex interactions of the translational degree of freedom (i.e., distance between centers of mass of the aggregate and the monomer) with degrees of freedom corresponding to the monomer orientation and the micellar shape and microstructure.

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