

Abstract Submitted
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Role of Collective Degrees of Freedom in Formation and Disintegration of Spherical Micelles¹ DMITRY KOPELEVICH, YONG NAM AHN, University of Florida, GUNJAN MOHAN — Dynamics of self-assembly and structural transitions in amphiphilic systems play an important role in various technological and biological processes. We recently demonstrated that even such a simple process as addition of a single surfactant molecule to a micelle involves a complex interplay between micellar and monomer configurations. In this talk, we present a quantitative model for collective dynamics of these degrees of freedom during the monomer addition and removal. This is accomplished by reconstruction of a multi-dimensional free energy landscape of the system and identification of the minimal energy path (MEP) on this landscape. Although analysis of MEP allows us to identify collective degrees of freedom relevant to the monomer addition and removal, MEP alone is not sufficient to adequately describe these processes. Comparable time-scales of several independent degrees of freedom during non-adiabatic stages of these processes imply that the system dynamics cannot be described by a quasi-one-dimensional motion along MEP. Therefore, we solve a multi-dimensional Langevin equation to correctly describe the non-adiabatic system dynamics.

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Dmitry Kopelevich
University of Florida

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