Syncronization Modes in Spaghetti-like Nanoclusters

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Spaghetti-like nanoclusters can be found in small clusters of amphiphiles [1]. They have interesting properties such as self-assembly, flexible structures, complex fluids, and irregular shape fluctuations [2]. However, their dynamics show some classification modes such as sphere-like, rod-like, monolayer-like, and cone-like [3]. In previous work, we introduced Aperture, Symmetry, Isotropy, and Compactness dynamics parameter to analyze their shape fluctuations [4]. The method can be used to investigate the transition behavior among certain geometrical pattern [5]. These transition phenomena imply stability information and the factors influencing their instability. In this study, we simulate 16 lipids of POPC (1-palmitoyl-2-oleoyl- phosphatidycholine) and POPE (1-palmitoyl-2-oleoyl- phosphatidylethanolamine) in 300 K and 340 K respectively by using Molecular Dynamics (MD) simulations and AMBER. In the same ways, we simulate in salty water condition. From power spectra analysis, we investigate the frequency for the possibility of soft mode and strong or weak collective behavior in these clusters. Moreover, they show non-Gaussian distribution implying certain random vibration [6]. Each distribution can be more than one stable structure implying synchronization modes in choosing a shape during self-assembly processes. Here, we discuss synchronization modes in spaghetti-like nanoclusters including the explanation of behavior from brownian dynamics aspects as a comparison.

References

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