Shape fluctuation modes and synchronization patterns in self-assembly aggregate bionanoclusters

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ABSTRACT

I evaluate shape fluctuations in self-assembly aggregate bionanoclusters by introducing concepts of aperture-*A*, symmetry-*S*, isotropy-*I*, and compactness-*C*. Each concept has physical meaning and concern with such kind degree of tail fluctuation, shape fluctuation, parallelism, and cluster stability, respectively. Although the dynamics of those parameters exhibit random processes, they show correlation with each other. I mainly discuss the correlation or coupling of *I-C* and *I-S*. The coupling of *I-C* can explain possible stable shape of bioaggregates, while, the coupling of *I-S* can classify them into four cluster modes. In addition, the coupling of *I-S* shows fuzzy cluster regions as smooth transitions of the modes. At different condition such as salty water and different temperature, the parameters consistently show the shape fluctuation modes. Interestingly, the regions of shape fluctuations in the salty water show slightly different and apparently follow a fluctuation line. Furthermore, the wider fluctuation line and jump motions participate in occurring non-Gaussian phenomena for the pure water. Finally, we discuss mutual cluster dynamics. Unlike individual clusters that mainly show random fluctuation, mutual clusters show certain patterns in delayed time analysis such as mutual fluctuations periodically occur for same number of lipids. It indicates that an existence of synchronization patterns occurs.

SUMMARY

In this thesis, I mainly discuss five issues on self-assembly aggregate bionanoclusters. The five issue are as follows: developing method to measure degree of fluctuations, classifying the fluctuation patterns, identifying smooth transitions of the shapes, identifying solvent effects, and investigating simultaneously fluctuation on mutual bionanoclusters. We perform several molecular dynamics simulations for POPC and POPE lipids at various conditions. In first issue, we propose a technique to analyze the dynamics based on the concepts of aperture-*A*, symmetry-*S*, isotropy-*I*, and compactness-*C*. Each parameter has physical meaning. We found some interesting phenomena in the dynamics, density, and correlation among those parameters. Although the dynamics of those parameters exhibit random processes, they have correlation with each other. This analysis can also explain the possible shapes in biological systems such as micelle, vesicle or membrane. In second issue, we classify the irregular shapes by using the coupling of *S-I* (symmetry and isotropy). We find four shape fluctuation modes: sphere-like, rod-like, cone-like, and monolayer-like. In third issue, we investigate smooth transitions of the shapes leading to fuzzy cluster modes. To reveal the transitions, we perform fuzzy c-means clustering. We find not only better classification of micellar cluster modes and their transition regions but also can determine more proper

position to define each mode on fuzzy region. In forth issue, we investigate solvent effects on each parameter. From the results, adding salt and increasing temperature generally change each parameter and contribute on shape fluctuations. Interestingly, the regions of shape fluctuations in the salty water show slightly different than in the pure water. It apparently shows that they follow a fluctuation line. The fluctuation line likely contributes in occurring non-Gaussian distributions for the pure water. In fifth issue, the jump motions likely contribute on the existence of transitions in the non-Gaussian distributions. Additionally, even numbers of lipids show more symmetric than the odd numbers of lipids and the symmetry distributions are shift at higher temperature. From power spectra density analysis, each individual cluster shows nearly random fluctuation. Beside of individual clusters, we also investigate mutual clusters. Surprisingly, although individual clusters fluctuate randomly, mutual clusters show certain direction correlations. Moreover, they show certain patterns in delayed time analysis such as mutual fluctuations periodically occur for same number of lipids. It indicates that an existence of synchronization patterns occurs in shape fluctuations of the bionanoclusters.

学位論文審査結果の要旨

当該学位論文に関して、各審査員が個別に検討し面接調査を行った後、論文内容を詳細に検討した。その後平成２０年８月４日に行われた口頭発表の後に審査委員会を開き、協議の結果以下のように判定した。

本論文は分子動力学シミュレーションにより少数のリン脂質二重膜構成物質からなるミセル状クラスタのダイナミックスに関する研究を行っている。これらの構成分子は分子数密度によって球状・卵状・層状・棒状などの構造になることが実験やシミュレーションにより解析が進められている。１０構成分子までのミセル状クラスタのダイナミックスを解析するために新しい解析方法を提案し、ミセル構造の広がり・対称性・等方性・大きさに関する時間発展を解析した。少数ミセル状クラスタではこれらの特性は、ほぼランダムな構造揺らぎをしていることを見いだした。この構造揺らぎは温度が高くなると大きくなり、イオンを含む水溶液中でも大きくなることも見いだしている。ミセル間の相関を解析し、分子が同数であるクラスタ間では周期的に強い相関あるいは同期を示すことを見いだした。以上の研究はリン脂質二重膜構成物質ミセル状クラスタのダイナミックスにおいて水溶液の重要性を示唆し、今後の実験研究に多くの寄与をもたらすものである。以上により、この論文は博士（理学）に値するものと判定した。