私は、下記研究課題に係る研究費について、以下のとおり研究成果を報告します。また当該研究費の執行については、規程等を遵守し、適正に使用いたしました。

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<th>1</th>
<th>研究者情報</th>
<th>氏名（職位）：立川 仁典（教授）</th>
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<td>所属：国際総合科学群自然科学系列</td>
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<td>2</td>
<td>研究課題名</td>
<td>Molecular orbital and molecular dynamics simulations for self-assembled nanocubes of gear-shaped amphiphile molecules in aqueous solution</td>
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Gear-shaped amphiphile molecule (1), recently synthesized by Hiraoka et al., is self-assembled into a cubic-shaped hexameric structure, nanocube (1₆), in 25% aqueous methanol (Fig. 1) [1, 2]. However, another gear-shaped molecule (2), in which three methyl groups of 1 are replaced with hydrogen atoms, does not form the nanocube (2₆). Koseki et al. [3, 4] theoretically showed the importance of CH-π interactions in the methylated molecular capsule 1₆ by the ab initio calculation for isolated 1₆ and 2₆ species. However, the mechanism of self-assembly in aqueous solution is not clear, yet. In this study, thus, we have performed molecular dynamics NVT simulations of these 1₆ and 2₆ molecular capsules in aqueous solution, to elucidate the thermodynamic mechanism of the formation of hexameric capsules.

Figure 2 shows the lowest frequency modes of principal components analysis (PCA) for 1₆ and 2₆. This result indicates that the triple π stacking of 3-pyridyl groups in 1₆ is more rigid than that in 2₆ and the structural fluctuations of 2₆ for overall motion are larger than that of 1₆. Thus, the interactions among molecules 1₆ play more important roles than the solvophobic effect due to water molecules and the nanocube 1₆ exists as a more stable species than the nanocube 2₆. Now, we are calculating the nanocube in 25% aqueous methanol under the same conditions of experiment.

References
6 研究発表（投稿準備中、投稿中、発表予定を含む）

※記載にあたっては、例えば発表論文の場合、論文名、著者名、掲載誌名、査読の有無、巻、最初と最後の頁、発表年（西暦）について記入してください。記載の順番は、現在から順に発表年次を過去に遡って記載し、通し番号を必ず付してください。


[13] "Geometric isotope effects on small chloride ion water clusters with path integral molecular dynamics"
[27] "Semiempirical investigations on the stabilization energies and ionic hydrogen-bonded structures of F(H2O)n and Cl(H2O)n (n=1-4) clusters", Q. Wang, K. Suzuki, U. Nagashima, M. Tachikawa, and S. Yan, J.


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<th>発明者名</th>
<th>権利者名</th>
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