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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2 研究課題名
Theoretical and computational study on functional species by quantum multi-component molecular theories

3 交付額
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4 研究成果
Gear-shaped amphiphile molecule (1) recently synthesized by Hiraoka et al. self-assembles into a hexameric structure, nanocube (1₆), in 25% aqueous methanol by solvophobic effect. Here we have carried out molecular dynamic simulation to elucidate the stability of these hexameric capsules 1₆ and 2₆ in water, 25% aqueous methanol, and methanol. In all solvents, the nanocube 1₆ for all trajectories are maintained. On the other hand, 2₆ in water for one trajectory and seven trajectories in 25% aqueous methanol are collapsed. In methanol solvent, 2₆ for all trajectories are collapsed. The number of collapsed trajectories of 2₆ increased with the ammount of methanol in the solvent. We focus on the nanocube structure of the π-π stacking between pyridyl groups and CH-π interactions between the methyl and pyridyl groups. Our study clearly shows the role of methanol solvent molecules for the nanocube in term of the substituent effect and solvent effect at the molecule level, and these substituent and solvent effects are important for the self-assembly of the nanocubes.

Fig. 1 Chemical formulae of gear-shaped amphiphile molecules, 1 (R = Me) and 2 (R = H). The carbon atoms (C1 and C2) are on central benzene ring of 1 (or 2). The nitrogen atoms (N1, N2, and N3) are on 3-pyridyl groups (Pys). In 25 % aqueous methanol solvent, the molecule 1 can be self-assembled into nanocube 1₆, which has a C₃ axis and the conformation of the triple π stackings for all Pys. N1 is the middle of the triple π stacking. N2 and N3 are near the C₃ axis side and another side, respectively. R1, R2, and R3 are the carbon atoms for 1 (or the hydrogen atoms for 2) of the second nearest substituent (= Me or H) from N1, the nearest C₃ axis, and the nearest substituent (= Me or H) from N1, respectively. Furthermore, N3 sandwiches between R1 and R2.
研究発表(投稿準備中、投稿中、発表予定を含む)


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