Theoretical study on substituent and solvent effects for nanocube formed with gear-shaped amphiphile molecules

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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 (Figure 1) [1, 2]. On the other hand, another gear-shaped molecule (2), in which three methyl groups of 1 are replaced with hydrogen atoms, does not form the nanocube (2₆). Hiraoka et al. further found that 1 does not assemble in pure methanol, thereby suggesting solvophobic self-assembly. The purpose of this work is to elucidate the stability of these hexameric capsules 1₆ and 2₆ in water, 25% aqueous methanol, and methanol, with the aid of molecular dynamics simulation.

In all solvents, the nanocube 1₆ structure for all trajectories are maintained. On the other hand, the 2₆ structure in water for one trajectory and seven trajectories in 25% aqueous methanol are collapsed. In methanol solvent, the 2₆ for all trajectories are collapsed. The number of collapsed trajectories of 2₆ is raised, as the number of methanol solvent molecules is increased. We focus on the nanocube structure of the π-π stacking between pyridines and CH-π interactions between the methyl group and pyridine. The CH-π network among pyridyl groups and CH₃ groups can be constructed on the 1₆ as shown in Figure 2 because the nanocube structure can be stable by van der Waals force. I will show the detailed results in 25% aqueous methanol, same as the experimental condition, at the poster presentation.