Development of water-soluble molecular capsules with fast inclusion and high response assembled from gear-shaped amphiphiles

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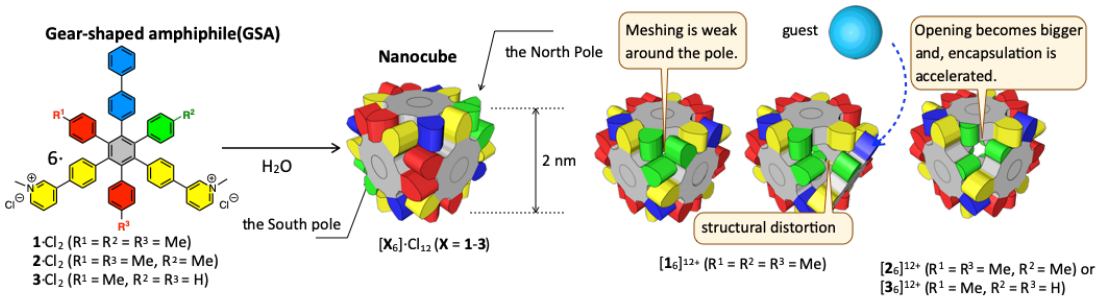
Over years, lots of artificial molecular capsules have been developed, but the artificial capsules displaying fast response as proteins do are rare, because artificial molecular hosts are structurally rigid compared with biological ones.

Previously, our group reported a box-shaped discrete self-assembly, $[\mathbf{1}_6]\cdot Cl_{12}$, i.e. "nanocube" assembled from six gear-shaped amphiphiles (GSAs), $\mathbf{1}^{2+}$, whose thermal stability is extremely high with the disassembly temperature of 130 °C.[1,2] What's more, the nanocube shows great induced-fit property, responding to the size, shape, and charge state of the guest molecules.[3] Furthermore, though the monomer GSA does not fluoresce, the nanocube fluoresces at 450 nm, whose intensity is affected by the change in the size of the nanocube upon binding of guest molecules.[4] This property can be used as sensing LPG with the response time of 15 sec, the low detection limit of 0.1 vol%, and the quantitativity ranging from 0.1 to 100 vol%, demonstrating fast response.[4]

To reveal how the nanocube encapsulates the guest molecule, molecular dynamics simulations were carried out by Tachikawa group (Yokohama City Univ.), suggesting that the guest molecule enters the nanocube through a small opening around the poles made by the structural distortion. Based on this theoretical result, new GSAs ($\mathbf{2}\cdot Cl_2$ and $\mathbf{3}\cdot Cl_2$) with fewer *p*-tolyl methyl groups than $\mathbf{1}^{2+}$ were designed and synthesized to make small openings around the poles in the nanocube. It was found that the nanocubes, $[\mathbf{2}_6]^{12+}$ and $[\mathbf{3}_6]^{12+}$, assembled from the new GSA retained high induced-fit property and the fluorescence, while the encapsulation speed was accelerated.



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