Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Supracolloidal Fullerene-Like Cages: Design Principles and Formation Mechanisms

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Table S1: The corresponding relation between the strength of attraction α_{ij}^{A} and the adhesion energy G. In the simulations, increasing α_{ij}^{A} corresponds to the increase of the adhesion energy G in a reasonable range from 2.00 k_BT to 6.77 k_BT, which may represent hydrophobic or hydrogen bond interactions between attractive patches, and can also be tuned by altering salt concentration, pH, or temperature in experiments. The parameters α_{ij}^{R} and α_{ij}^{A} are given in reduced units, and the reduced unit of length r_c in the model is assumed to approximately correspond to 10 nm.

α_{11}^{R}	α_{11}^{A}	$G\ [k_BT]$
396	88	2.00
396	99	2.48
396	110	3.00
396	121	3.54
396	132	4.13
396	143	4.74
396	154	5.39
396	165	6.07
396	176	6.77

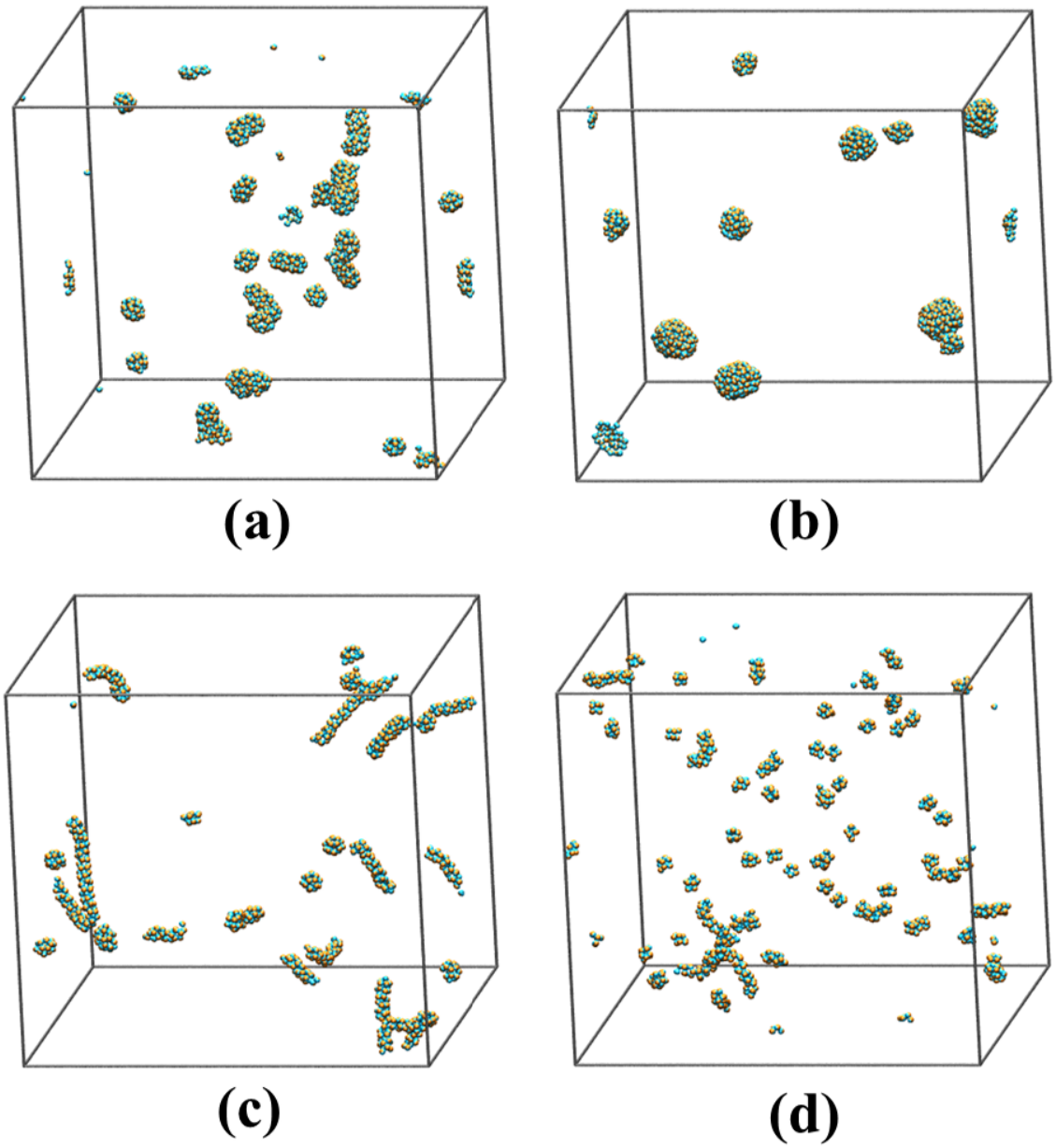

Figure S1: Typical supracolloidal fullerene-like cages observed in Fig.2 with the system size of 1.92×10^5 particles in a $40 \times 40 \times 40$ cubic box at $\alpha_{ij}^R = 396$ ($E = 4.0$ MPa), $\Phi = 0.5\%$. (a) Fullerene-like cages (FLC). (b) Onion-like cages (OLC). (c) Slender nanotube-like structures (S-NT). (d) Small polyhedra (SPH). For the sake of clarity, we only show patchy solute particles in these systems.

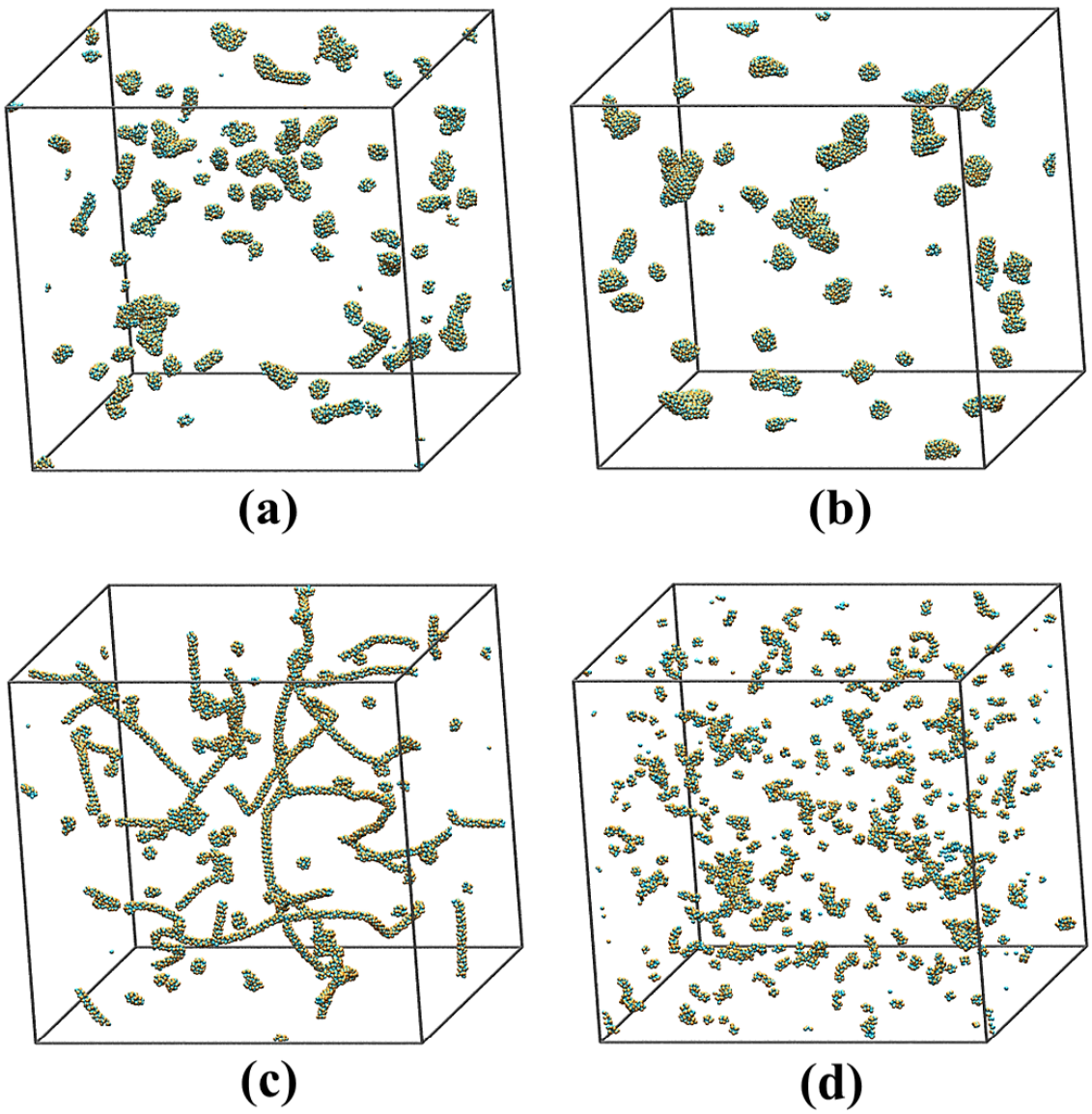

Figure S2: Typical supracolloidal fullerene-like cages observed in Fig.2 with larger system size of 6.48×10^5 particles in a $60 \times 60 \times 60$ cubic box at $\alpha_{ij}^R = 396$ ($E = 4.0$ MPa), $\Phi = 1.0\%$. (a) Fullerene-like cages (FLC). (b) Onion-like cages (OLC). (c) Slender nanotube-like structures (S-NT). (d) Small polyhedra (SPH).

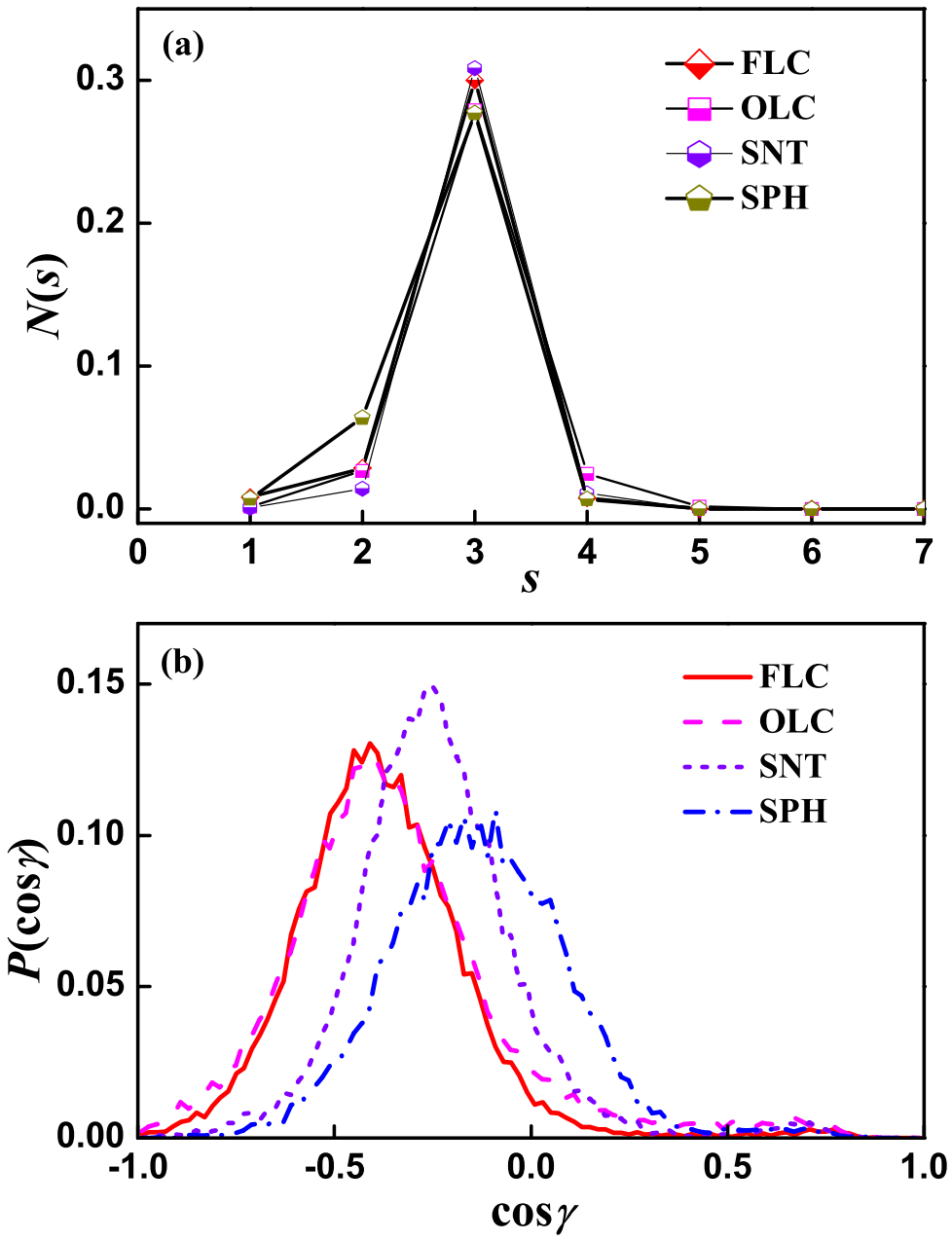

Figure S3: Structural characteristics of typical supracolloidal fullerene-like cages in Fig.S2. (a) Distribution $N(s)$ of the number of bonds (i.e., contacts) between attractive patches per patchy particle s. The distributions $N(s)$ have been normalized so that $\sum_s sN(s) = 1$. (b) Distribution $P(\cos\gamma)$ of the cosine of the angles γ between the edges of the polygons in typical supracolloidal fullerene-like cages. As can be seen in Fig.S3a, for these typical supracolloidal fullerene-like cages in Fig.S2, $N(s)$ shows a narrow distribution at $s = 3$ since the soft three-patch particles are designed to mimic sp^2 hybridized atomic orbitals in C_{60}. For FLCs, $P(\cos\gamma)$ shows a clear peak between $\cos\gamma \approx -0.50$ and $\cos\gamma \approx -0.31$, and the distribution becomes slightly wider for OLCs. For SNTs and SPHs, the distribution $P(\cos\gamma)$ gradually shifts to larger values of $\cos\gamma$.