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Electronic Supplementary Information

Computer simulation study on the self-assembly of tethered nanoparticles with tunable shapes

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Actually, we have considered a generic model for polymer tethered nanoparticles. Say the nanocube is made of SiO_2 with side length equal to 10 nm, the density of SiO_2 is 2.2×10^{-3} kg/cm³, the mass of SiO_2 is m=ρV=2.2×10^{-3} kg/cm³ $\times (10^{-6}\, cm)^3$=2.2×10^{-21} kg. The temperature is room temperature at 300K, the time unit in our simulations is therefore can be estimated as: $\tau = \sqrt{mr_c/k_BT} \approx 0.5 \times 10^{-3}$ s.

In the inset of Fig.S1, we schematically show the packing of two nanocubes. The "hard cores" of beads at the corners of the nanocube are highlighted with green color. In simulations, we have used eight beads in a plane (i.e., a small square is embedded in a large square) to construct one side surface of the cube. In this way, we can ensure that the side surfaces of the nanocube are impenetrable. When two nanocubes are in close packing (as shown in the inset of Fig.S1), their center-of-mass distance d equals to the side length ($l_a = 0.78$) of cubes plus double the radius of hard core ($r_s = 0.3$). Choosing this value ($r_s = 0.3$) for the radius of hard core follows (H. Liu et al., J. Chem. Phys., 2008, 129, 024902), in which the authors showed no bond-crossing in the simulations. We then measure the radial distribution function g(r) for the center of mass of nanocubes in our simulations; the result is shown in Fig. S1. r_{min} indicated by an arrow in the figure represents the minimum center of mass distance between two nanocubes in a course of simulation. When $r_{min} \geq d$, there will be no overlapping between nanocubes in the system.

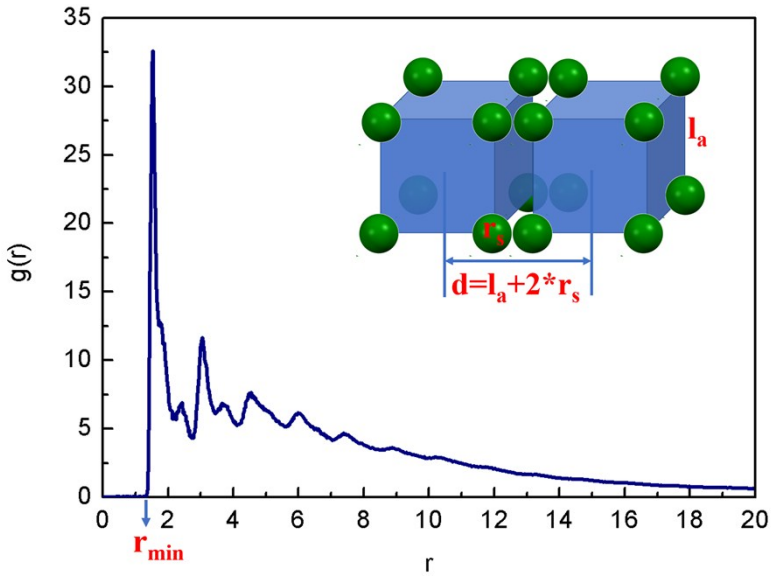

Fig.S1 Radial distribution function between centers of mass of cubes system A_1B_3 in the case of $\alpha_{AS} = 30$. The inset shows the schematic of close packing of two nanocubes. The green spheres represent the hard cores of the beads constructing the nanocube; the blue color highlights the cubic shape, $r_{min} = d = 1.38$.

Table S1. The number of beads in each system. The volume of cube $V_{cube} = (l_a + 2 * r_s)^3 = (0.78 + 2 * 0.3)^3 = 2.63$, the volume of beads in polymer chains and solvent beads bead $V_C = V_S = 4\pi/3 * 0.5^3 = 0.52$.

	The number of cubes N_C	The number of B beads $N_C \times L_C$	The number of S beads N_S
A_1B_3	1174	3522	179215
A_1B_5	943	4715	179845
A_1B_{10}	633	6330	180682
A_1B_{15}	476	7140	181104

Table S2. The interaction parameters of double-layer nested cubic nanoparticles with G particles in the case with $\alpha_{GG} = 0$ and $\alpha_{AS} = 50$.

	A	G	B	S
A	25	0	55	50
G	0	0	0	0
B	55	0	25	50
S	50	0	50	25

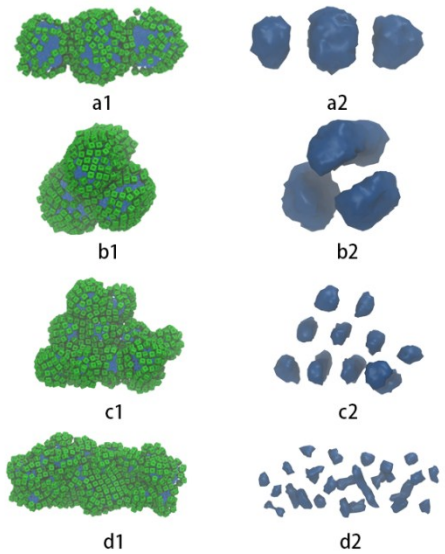

Fig.S2 Pearl-necklace-like morphology with different chain lengths in the case of $\alpha_{AS} = 30$. As the chain length decreases, more compact structures appear. (a1~a2) A_1B_{15}, (b1~b2) A_1B_{10}, (c1~c2) A_1B_5, (d1~d3) A_1B_3.

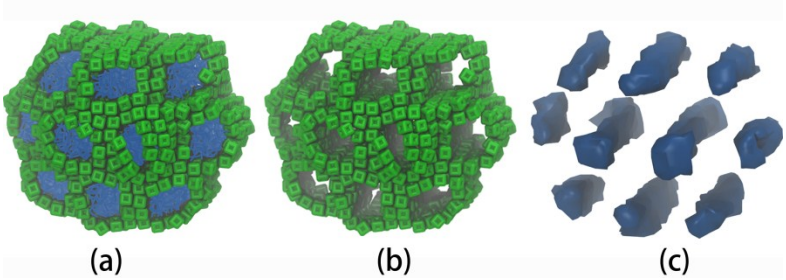

Fig.S3 Cubic columnar phase in hexagonal packing in case of A_1B_5, $\alpha_{AS} = 40$, and $\phi = 0.07$.

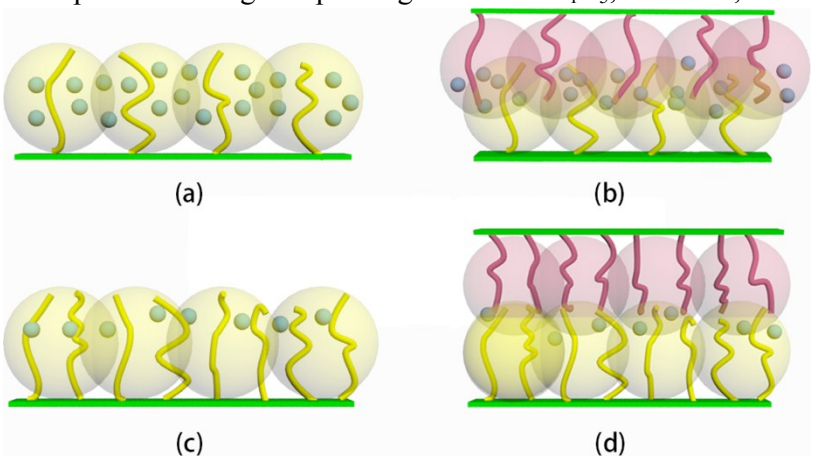

Fig.S4 Schematic of solvents entering ligand chain layer and the packing of ligand chains. (a) Solvents enter ligand chain layer with low grafting density, (b) the packing of ligand chains with low grafting density, (c) solvents enter ligand chain layer with high grafting density, and (d) the packing of ligand chains with high grafting density.