Supporting Material

Triphenylalanine peptides self-assemble into nanospheres and nanorods that are different from the nanovesicles and nanotubes formed by diphenylalanine peptides

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This supporting material contains 4 tables and 10 figures.

Tables

Table S1. The average contact number of each MC-MC pair in each MD run of the FFF system. The number in the parentheses is the standard deviation.

Contact pair		Number of MC-MC contacts									
		Nanosphere							Nanorod		
		Run1	Run2	Run3	Run4	Run5	Run6	Run7	Run8	Run9	Run10
F1	F1	0.40 (0.02)	0.41 (0.02)	0.39 (0.02)	0.38 (0.02)	0.39 (0.02)	0.40 (0.02)	0.37 (0.02)	0.39 (0.02)	0.42 (0.02)	0.37 (0.02)
F1	F2	1.40 (0.03)	1.45 (0.03)	1.36 (0.03)	1.36 (0.03)	1.40 (0.03)	1.43 (0.03)	1.36 (0.03)	1.35 (0.03)	1.47 (0.03)	1.34 (0.03)
F1	F3	2.13 (0.02)	2.16 (0.02)	2.10 (0.02)	2.09 (0.03)	2.11 (0..02)	2.15 (0.03)	2.08 (0.02)	2.06 (0.03)	2.14 (0.03)	2.06 (0.03)
F2	F2	0.71 (0.02)	0.74 (0.02)	0.68 (0.02)	0.69 (0.02)	0.73 (0.02)	0.72 (0.02)	0.69 (0.02)	0.70 (0.02)	0.74 (0.02)	0.68 (0.02)
F2	F3	1.38 (0.03)	1.43 (0.03)	1.35 (0.03)	1.34 (0.03)	1.37 (0.03)	1.39 (0.03)	1.33 (0.03)	1.34 (0.03)	1.42 (0.03)	1.33 (0.03)
F3	F3	0.43 (0.02)	0.43 (0.02)	0.41 (0.02)	0.41 (0.02)	0.40 (0.02)	0.42 (0.02)	0.40 (0.02)	0.40 (0.02)	0.45 (0.02)	0.39 (0.02)

Table S2. The average contact number of each SC-SC pair in each MD run of the FFF system. The number in the parentheses is the standard deviation.

Contact pair		Number of SC-SC contacts									
		Nanosphere							Nanorod		
		Run1	Run2	Run3	Run4	Run5	Run6	Run7	Run8	Run9	Run10
F1	F1	1.13 (0.03)	1.13 (0.02)	1.15 (0.03)	1.14 (0.02)	1.14 (0.03)	1.13 (0.03)	1.15 (0.03)	1.15 (0.03)	1.12 (0.03)	1.16 (0.03)
F1	F2	2.45 (0.04)	2.46 (0.04)	2.47 (0.04)	2.49 (0.03)	2.47 (0.04)	2.48 (0.04)	2.46 (0.04)	2.47 (0.04)	2.47 (0.04)	2.48 (0.04)
F1	F3	2.93 (0.03)	2.87 (0.03)	2.93 (0.03)	2.94 (0.03)	2.94 (0.03)	2.92 (0.03)	2.91 (0.03)	2.94 (0.03)	2.92 (0.03)	2.95 (0.03)
F2	F2	1.58 (0.03)	1.58 (0.03)	1.56 (0.03)	1.53 (0.03)	1.56 (0.03)	1.55 (0.03)	1.56 (0.03)	1.57 (0.03)	1.56 (0.03)	1.57 (0.03)
F2	F3	2.43 (0.04)	2.43 (0.04)	2.48 (0.04)	2.47 (0.04)	2.45 (0.04)	2.47 (0.04)	2.48 (0.04)	2.48 (0.04)	2.47 (0.04)	2.45 (0.04)
F3	F3	1.15 (0.03)	1.13 (0.03)	1.14 (0.03)	1.13 (0.02)	1.14 (0.03)	1.13 (0.03)	1.14 (0.02)	1.13 (0.03)	1.12 (0.03	1.17 (0.03)

Table S3. The average contact number of each MC-MC pair in each MD run of the FF system. The number in the parentheses is the standard deviation.

Contact pair		Number of MC-MC contacts							
		Nanovesicle				Nanotube			
		Run1	Run2	Run3	Run4	Run5	Run6	Run7	Run8
F1	F1	0.60 (0.02)	0.60 (0.02)	0.60 (0.02)	0.61 (0.02)	0.61 (0.02)	0.60 (0.02)	0.63 (0.02)	0.62 (0.02)
F1	F2	1.86 (0.03)	1.86 (0.03)	1.80 (0.04)	1.88 (0.03)	1.87 (0.03)	1.85 (0.04)	1.88 (0.03)	1.84 (0.04)
F2	F2	0.60 (0.02)	0.60 (0.02)	0.59 (0.02)	0.61 (0.02)	0.61 (0.02)	0.60 (0.02)	0.63 (0.02)	0.62 (0.02)

Table S4. The average contact number of each SC-SC pair in each MD trajectory of the FF system. The number in the parentheses is the standard deviation.

Contact pair		Number of SC-SC contacts							
		Nanovesicle				Nanotube			
		Run1	Run2	Run3	Run4	Run5	Run6	Run7	Run8
F1	F1	2.03 (0.03)	2.02 (0.03)	2.02 (0.03)	2.02 (0.03)	2.04 (0.03)	2.03 (0.04)	2.04 (0.03)	2.03 (0.03)
F1	F2	3.98 (0.04)	3.97 (0.04)	3.98 (0.04)	3.97 (0.04)	4.03 (0.04)	4.00 (0.04)	4.04 (0.03)	4.02 (0.04)
F2	F2	2.02 (0.03)	2.02 (0.03)	2.02 (0.03)	2.01 (0.03)	2.04 (0.03)	2.02 (0.03)	2.04 (0.03)	2.03 (0.03)

Figures

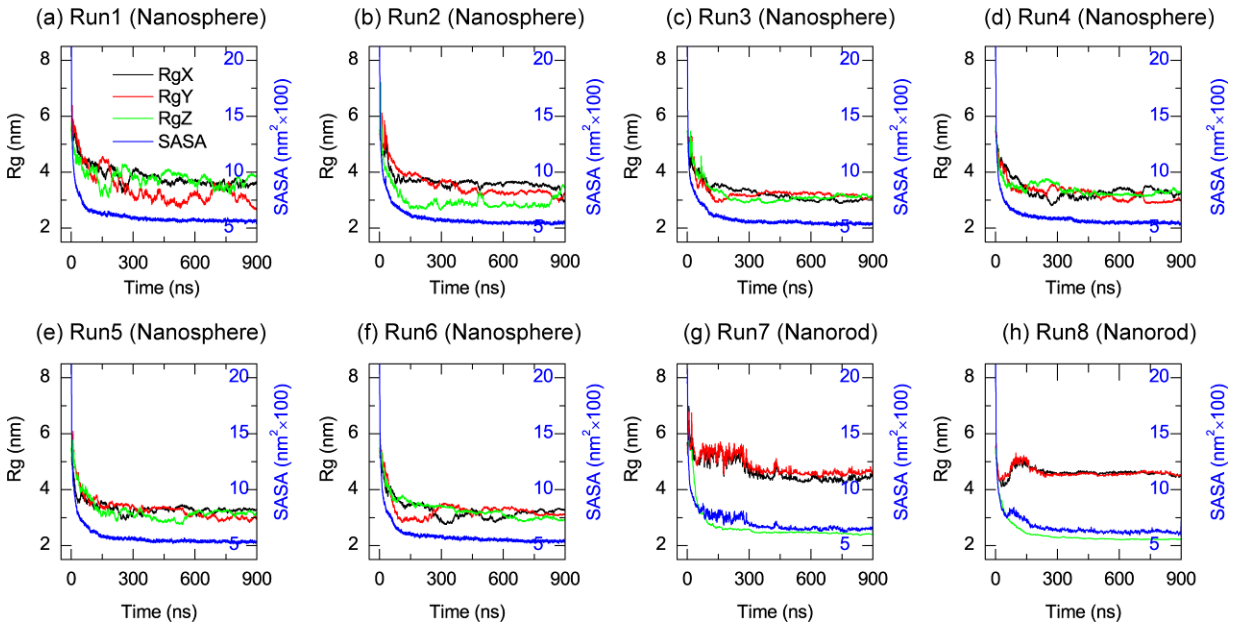

Figure S1: Time evolution of the radius of gyration (Rg) and solvent accessible surface area (SASA) in the left eight MD trajectories. Six MD runs ((a) ~ (f)) lead to the formation of nanospheres and the other two runs ((g) and (h)) lead to the formation of nanorods.

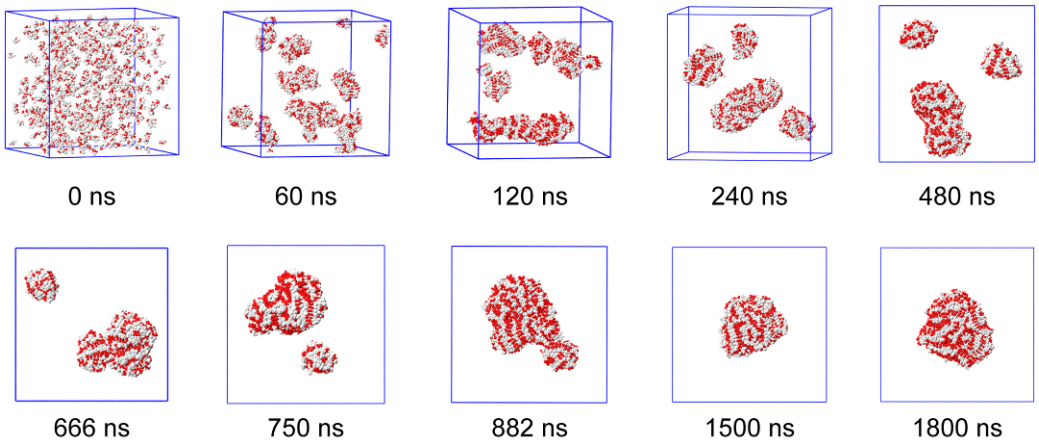

Figure S2: The MD trajectory of FFF peptides leading to the formation of a nanosphere starting from an initial random state with a peptide concentration of 45 mg/mL. There are 600 peptide chains and 76 616 water beads in the cubic simulation box (box length = 22.04 nm). The main chain beads are shown in red and the side chain beads in white. The simulation box is shown by the blue frame in the snapshots.

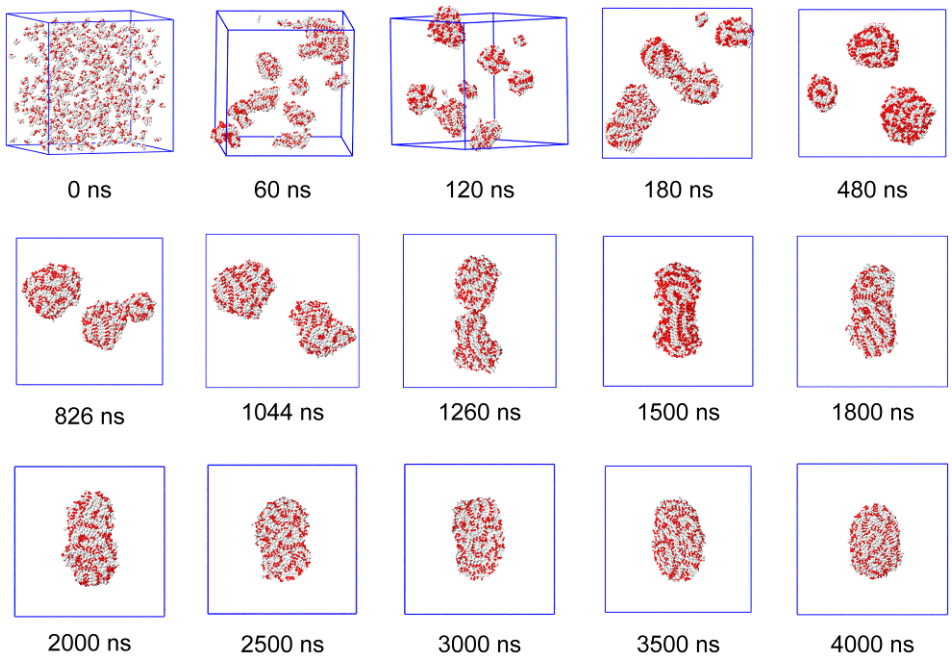

Figure S3: Representative snapshots in a MD trajectory leading to the formation of FFF nanosphere-like structure through a nanorod-like intermediate at a lower peptide concentration of 45 mg/mL. The initial state is the same as shown in Figure S2. A nanorod is formed at 1500 ns, but is not stable. It gradually evolves into a nanosphere-like structure.

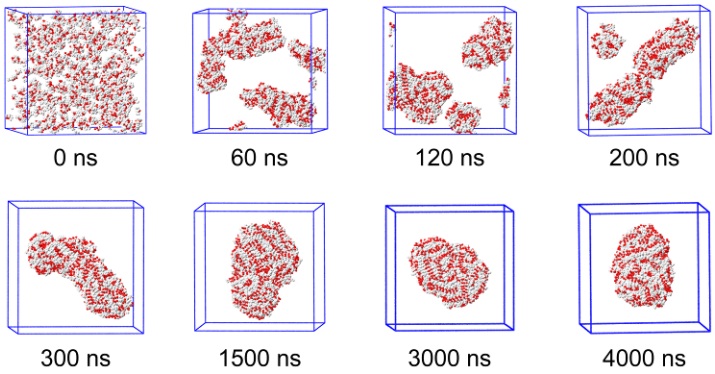

Figure S4: The trajectory of FFF peptides assembling into a nanosphere starting from an initial random state at 80 mg/mL. There are 600 peptide chains and 36 624 water beads in a box with the box length of 17.48 nm. The main chain beads are shown in red and the side chain beads in white. The simulation box is shown by the blue frame in the snapshots.

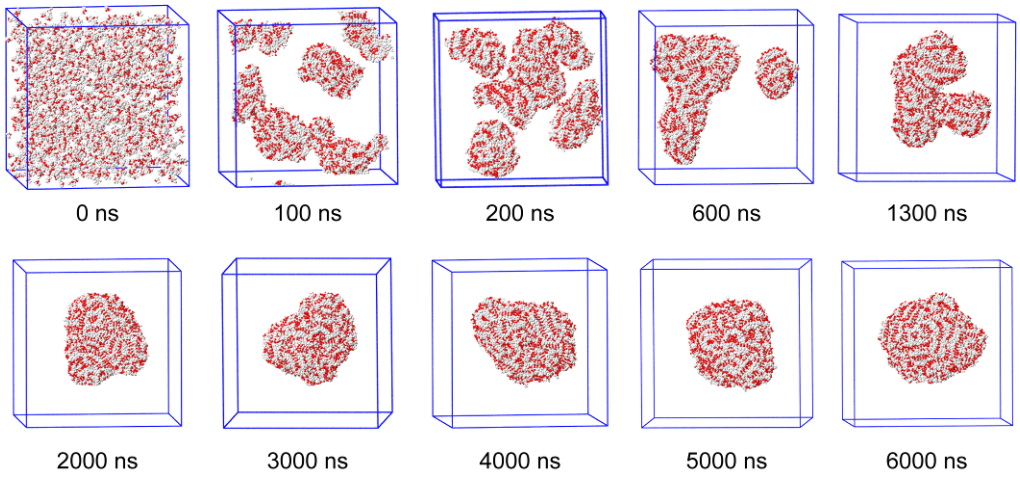

Figure S5. The MD trajectory of 1800 FFF peptides assembling into a nanosphere starting from an initial random state with a peptide concentration of 80 mg/mL. There are 118,580 water beads in the cubic simulation box with a box length of 25.78 nm. For the main chain beads and side chain beads of the peptides, we used the same representations as shown in Fig. S4.

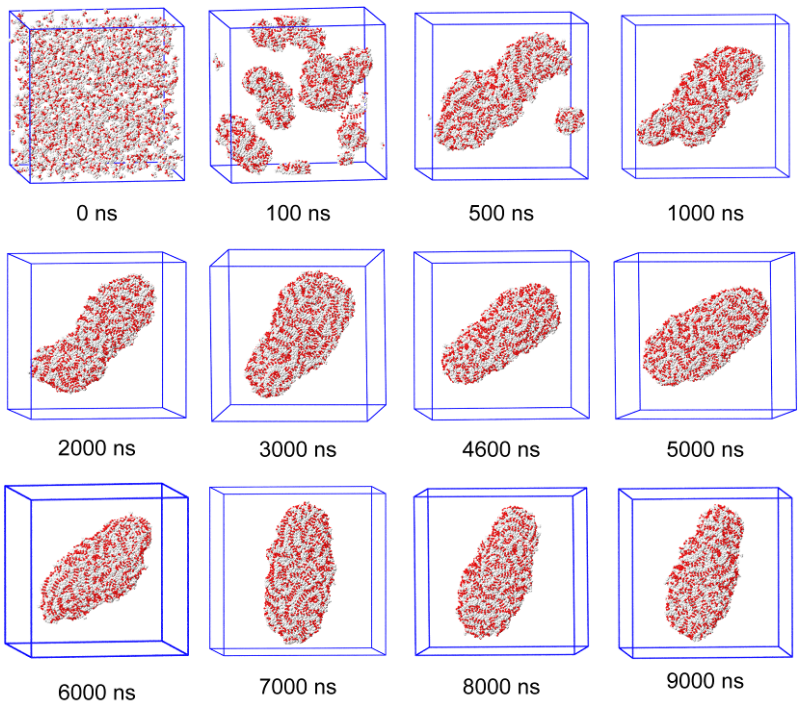

Figure S6: The trajectory of FFF peptides assembling into a nanorod starting from an initial random state at 80 mg/mL. There are 1 800 peptide chains and 118 580 water beads in a box with the box length of 25.78 nm. The main chain beads are shown in red and the side chain beads in white. The simulation box is shown by the blue frame in the snapshots. The length of the nanorod is ~22 nm, and its diameter is ~10 nm. The nanorod maintains its shape from 4600 ns to the end of the simulation (9000 ns).

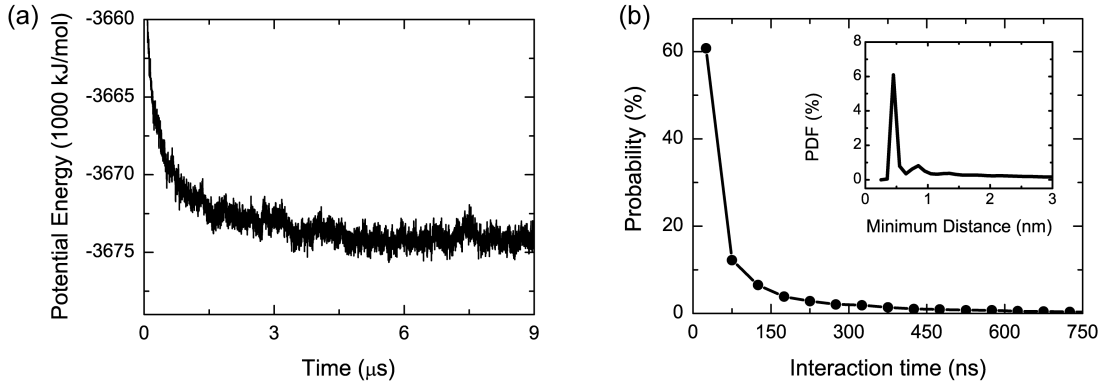

Figure S7: (a) The time evolution of potential energy during the assembly of 1800 FFF peptides at 80 mg/mL. (b) Distribution of the interaction time between adjacent peptides in nanorods. The potential energy converges after 4.6 μs, which indicates that the simulation reaches equilibrium. The interaction time between adjacent peptides is less than 450 ns, much shorter than the simulation time of 4.4 μs, indicating that the FFF nanorod structure is well relaxed within the simulation time duration of 4.4 μs after the nanorod was formed. We define that two peptides are in contacts when their minimum distance is smaller than 0.7 nm. The selection of this cutoff distance is based on the distribution of minimum distance among all the peptide pairs, where the first peak ends at 0.7 nm (see the inset in (b)).

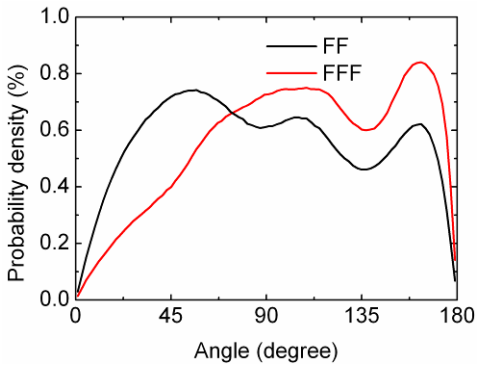

Figure S8: The probability distribution of the angle between two interacting peptide chains. The angle between two chains is calculated by the angle between the vectors from the main chain bead at N-terminus to the one at C-terminus. Angles between two peptide chains are considered when they have at least one main chain-main chain contact. Two main chain beads are in contact if their distance is less than 0.65 nm.

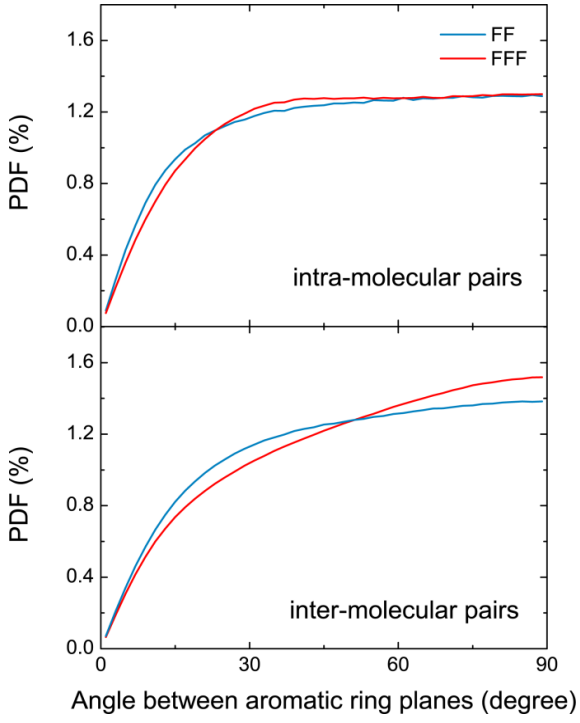

Figure S9: The probability distribution of the angle between two interacting aromatic rings. The angle between two rings is considered when their center-of-mass distance is less than 0.75 nm for intra-molecular aromatic rings and 0.8 nm for inter-molecular aromatic rings.

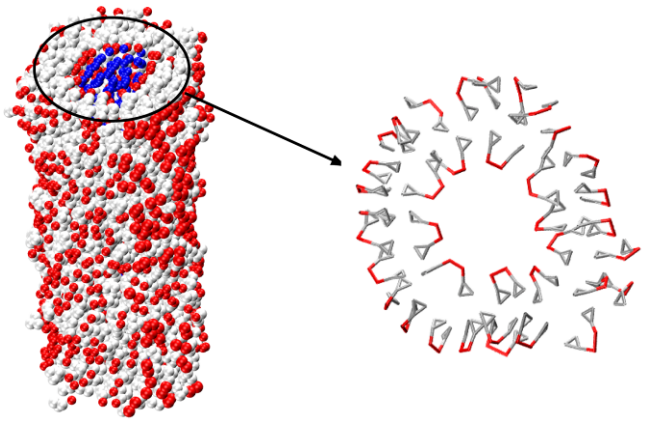

Figure S10. The nanotube formed by 600 FF peptides at 120 mg/mL. The packing of FF peptides in bond representation is also shown on the right. There are ten FF peptide chains in the inner layer of the nanotube wall. Main chain beads are shown in red and side chain beads in white. Water beads inside nanotubes are shown in blue.