Supporting Information

Molecular Origin of the Self-Assembled Morphological Difference Caused by Varying the Order of Charged Residues in Short Peptides

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As shown in Figure S1, both peptides exhibited high solubility in water. After dissolving them in Milli-Q water at a concentration of 16 mM, the resulting solutions were incubated for 12 days at room temperature prior to TEM characterization. Samples for cryo-TEM characterization were prepared in a controlled environment vitrification system (CEVS). A small volume (~5 μL) of aged peptide solution was dropped onto a TEM copper grid coated with a laced support film and then wicked away with two pieces of filter paper, resulting in a thin film suspended on the mesh holes. After about 3 s, the samples were quickly plunged into a reservoir of liquid ethane (cooled by the nitrogen) at -165 ^{o}C. The vitrified samples were then stored in the liquid nitrogen before transferring to the cryogenic sample holder (Gatan 626) and examined on a JEOL JEM-1400 TEM at about -174 ^{o}C with an accelerating voltage of 120 kV.

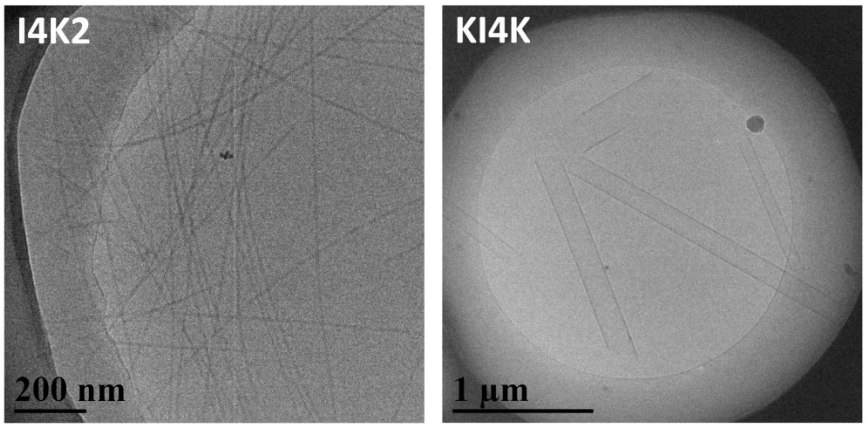

Figure S1. Cryo-TEM images of I4K2 and KI4K self-assemblies in water at 16 mM.

The instantaneous center-of-mass distances between neighboring peptides are shown in Figure S2. It can be seen that the range of ξ is similar for I4K2 and KI4K.

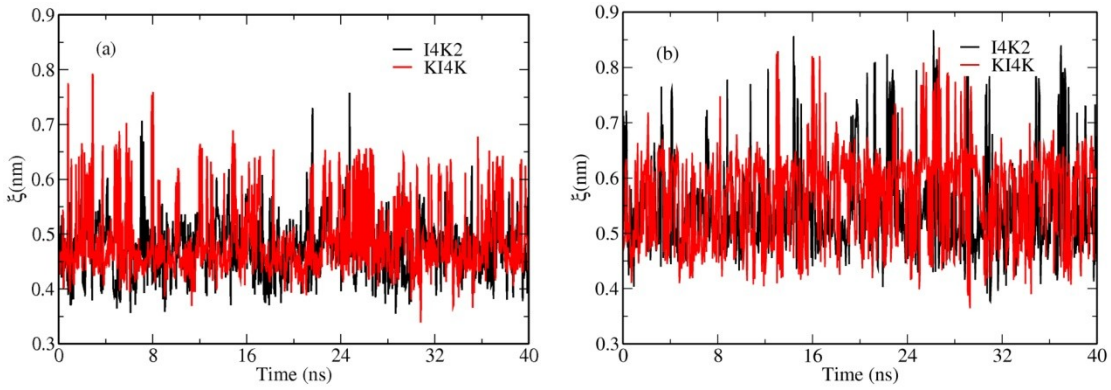

Figure S2. Instantaneous center-of-mass distances between M1 and M2 (a) and between M2 and M3 (b).

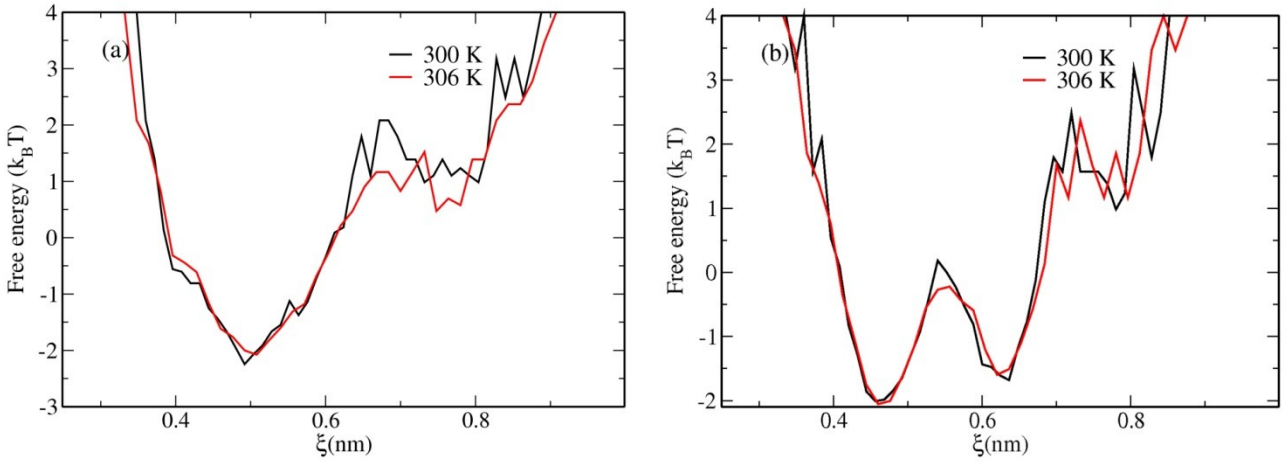

Figure S3. PMFs at for I4K2 (a) and KI4K (b) at T = 300 K and 306 K, respectively.

The PMFs with the reaction coordinate of ξ at T = 300 K and 306 K are shown in Figure S3. I4K2 has obviously different PMFs from KI4K: I4K2 has two local minima at ξ = 0.5 and 0.8 nm, respectively, but KI4K has three local minima at ξ = 0.47, 0.62, and 0.8 nm, respectively.

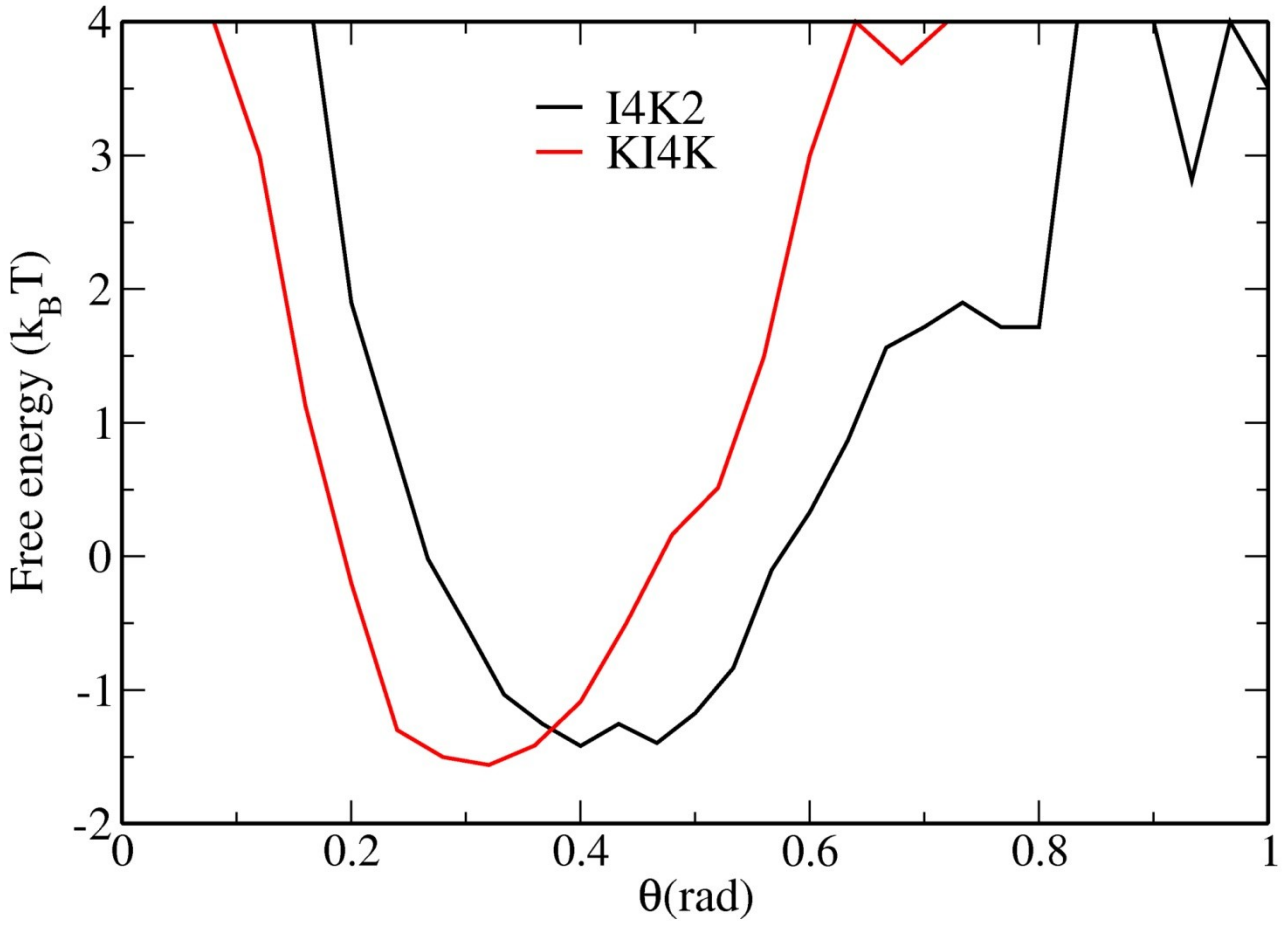

Figure S4. PMFs for I4K2 and KI4K with the reaction coordinate of twist angle.

The PMFs with the reaction coordinate of twist angle θ between two peptides are shown in Figure S4. The I4K2 PMF minimum is located at 0.42 rad and KI4K is 0.3 rad.

The hydrophobic surfaces calculated for the instantaneous configurations in the REMD simulations are shown in Figure S5, and the hydrophobic surface distributions of two peptides are shown in Figure S6. Both results demonstrate that the two peptides differ very little in hydrophobic surfaces.

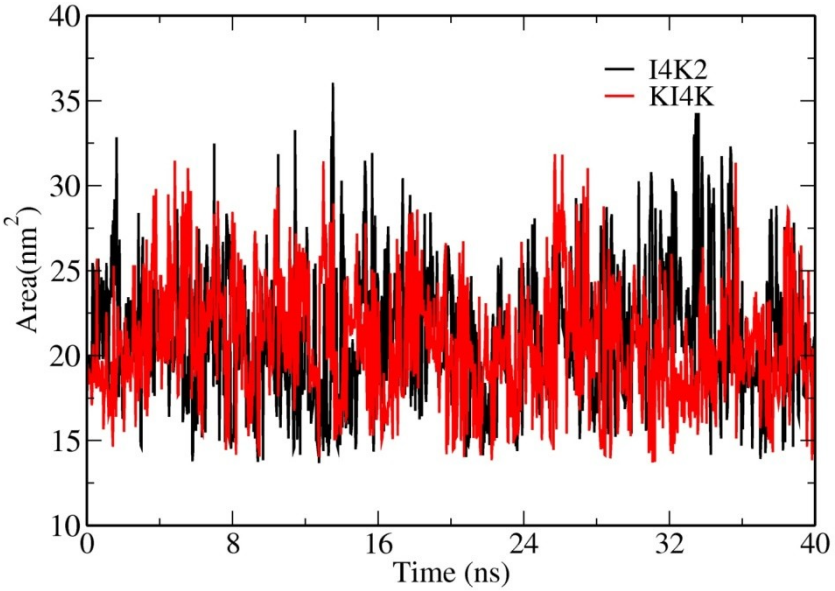

Figure S5. Instantaneous hydrophobic surfaces for I4K2 and KI4K.

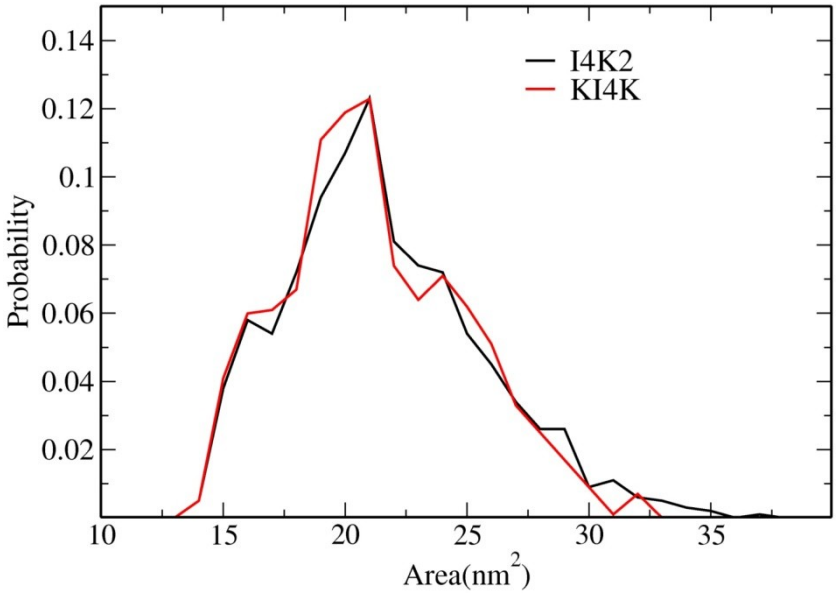

Figure S6. Hydrophobic surface distributions for I4K2 and KI4K.