Supporting Information

Amphiphilic peptides A_6K and V_6K display distinct oligomeric structures and self-assembly dynamics: a combined all-atom and coarse-grained simulation study

Yunxiang Sun, Zhenyu Qian, Cong Guo, and Guanghong Wei*

State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (MOE), and Department of Physics, Fudan University, 220 Handan Road, Shanghai, 200433, China

This material contains the temperature list of REMD simulation for A_6K and V_6K systems and six supplementary figures.

Temperature lists of REMD simulation:

The temperature list for A_6K system is: 300.20, 302.63, 305.07, 307.53, 310.00, 312.49, 315.00, 317.52, 320.05, 322.61, 325.17, 327.76, 330.36, 332.97, 335.60, 338.25, 340.92, 343.61, 346.31, 349.02, 351.76, 354.51, 357.28, 360.07, 362.88, 365.70, 368.54, 371.39, 374.27, 377.17, 380.08, 383.02, 385.97, 388.94, 391.93, 394.94, 397.97, 401.02, 404.09, 407.18, 410.29, 413.41, 416.56, 419.73, 422.91, 426.12, 429.35, 432.60 K. The temperature list for V_6K system is: 300.00, 302.54, 305.10, 307.68, 310.27, 312.88, 315.44, 318.08, 320.74, 323.42, 326.11, 328.83, 331.56, 334.30, 337.07, 339.85, 342.65, 345.47, 348.31, 351.16, 353.98, 356.87, 359.78, 362.71, 365.66, 368.63, 371.62, 374.63, 377.66, 380.71, 383.78, 386.87, 389.98, 393.12, 396.27, 399.43, 402.62, 405.84, 409.08, 412.34, 415.62, 418.91, 422.24, 425.56, 428.93, 432.32, 435.73, 439.16 K.

Six supplementary figures:

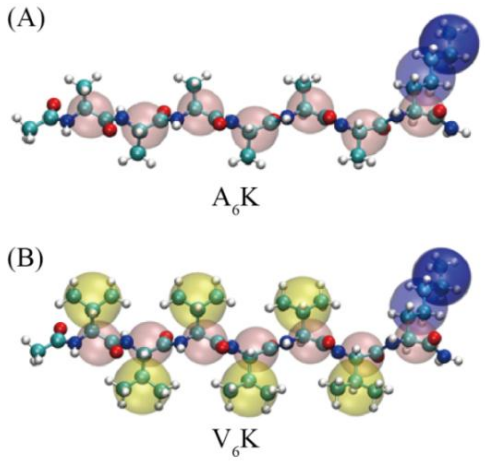

Figure S1. All-atom and coarse-grained models of A_6K (A) and V_6K (B) peptides. Color codes for all-atom model: N, blue; O, red; C, cyan and H, white. Color codes for coarse-grained model: backbone beads of all residues: pink; side chain beads of valine: yellow; side chain beads of lysine: blue. There is no side chain bead for alanine.

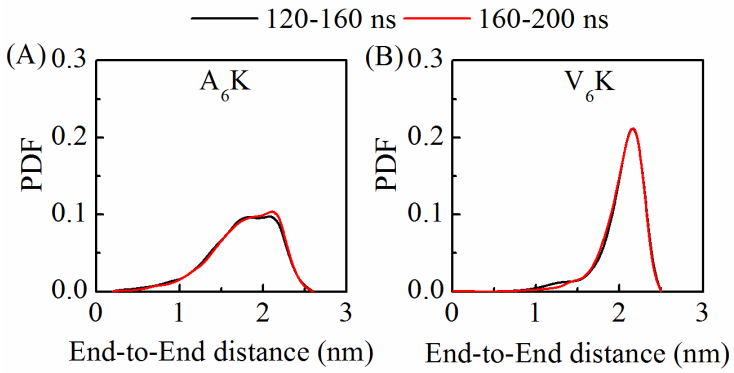

Figure S2. The distributions of end-to-end distance within the two independent time intervals（120-160 ns and 160-200 ns) at 300K.

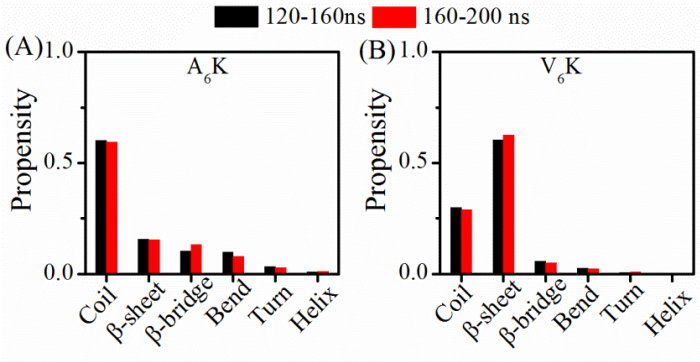

Figure S3. Secondary structure propensity as a function of each each secondary structure (including coil, β-sheet, β-bridge, bend, turn and helix) in both systems at 300 K using two time windows, 120−160ns, 160−200 ns.

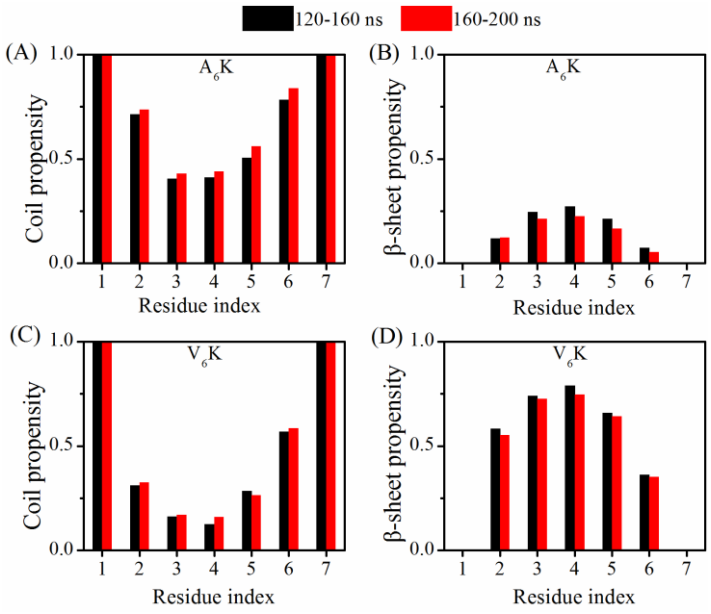

Figure S4. Coil and β-sheet propensity as a function of amino acid residue for both systems at 300 K using two time windows, 120−160 ns, 160−200 ns. (A) (B) A_6K system; (C) (D) V_6K system.

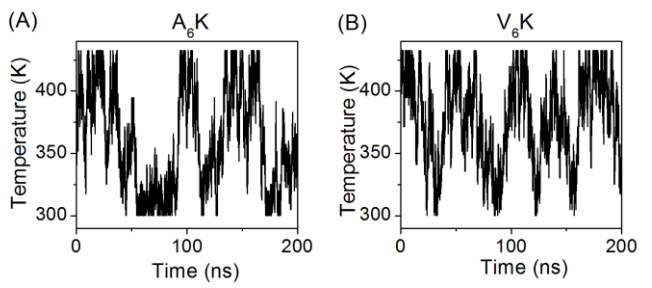

Figure S5: The time evolution of temperature swapping of one representative replica in temperature space for (A) A_6K and (B) V_6K system.

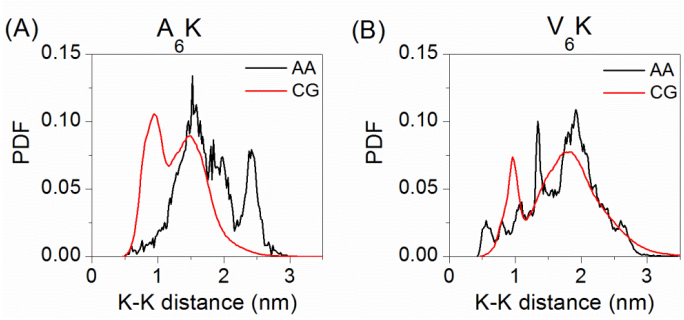

Figure S6. The K-K distance distribution for (A) A_6K and (B) V_6K aggregates generated in all-atom (AA) and coarse-grained (CG) simulations. For AA system, the K-K distance refers to the C_α-C_α distance between lysine residues of β-sheet peptides. For CG system, the K-K distance refers to the distance between lysine backbone beads of two peptide chains.