

Supporting Information

A novel form of β -strand assembly observed in $A\beta_{33-42}$ adsorbed onto graphene

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The structure of $A\beta_{33-42}$ in solution

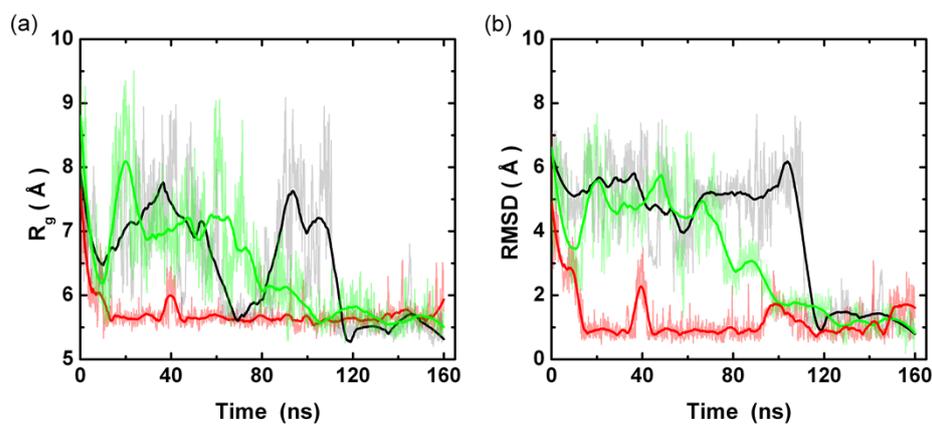


Fig.S1. The radius of gyration, R_g (a) and the RMSD with respect to the β -hairpin structure (b) of $A\beta_{33-42}$ peptide in solution. There are three independent 160 ns MD simulations (black, red, green) and the smoothed data (thicker lines) are added.

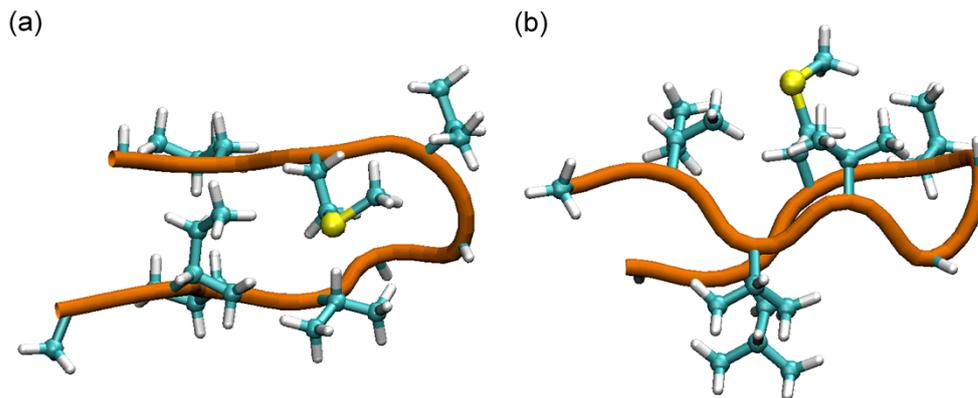


Fig.S2. The representative structures of A β ₃₃₋₄₂ peptide in solution. (a) top view and (b) side view.

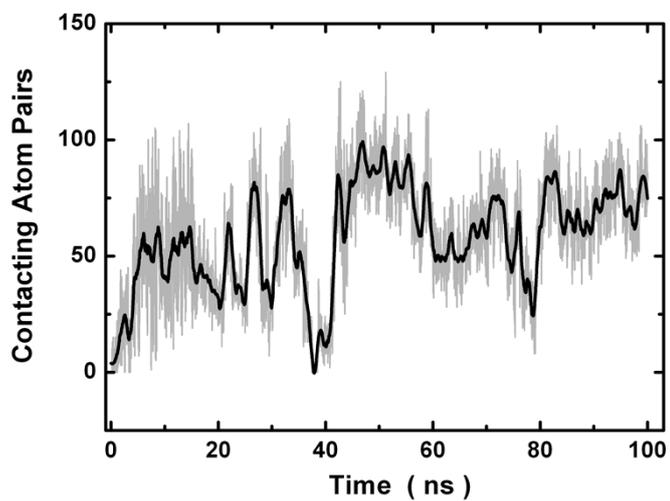


Fig.S3. (a) The number of contacting atom pairs of five peptides adsorbed on graphene (100 ns REMD simulation), together with the smoothed data (thicker lines). The average number of total contacting atom pairs for the last 20 ns is 71.21

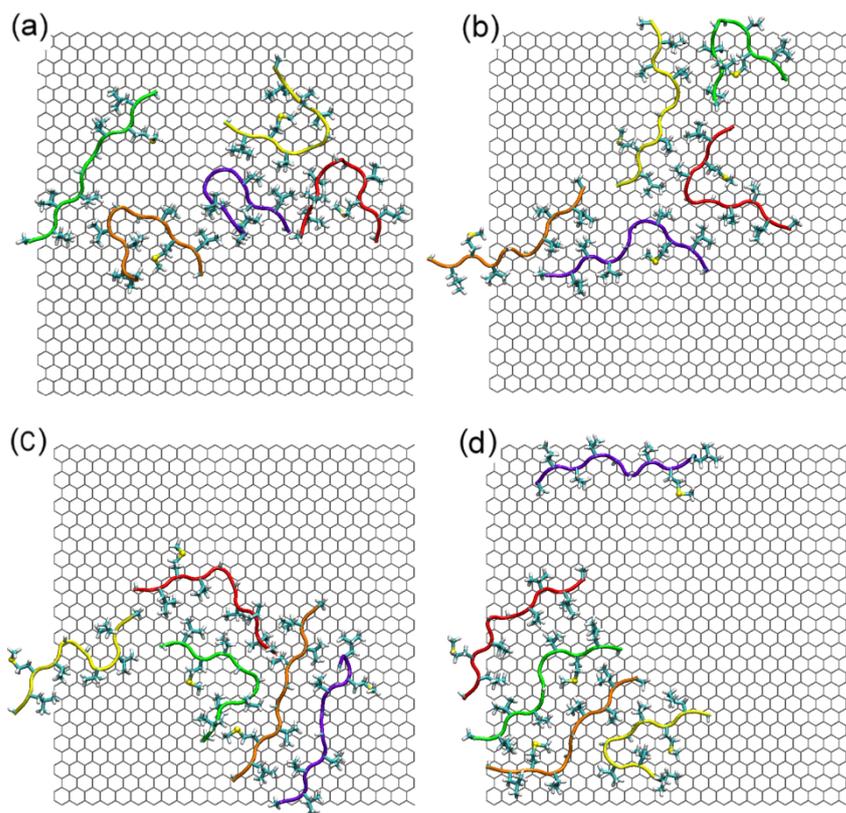


Fig.S4 The structures of five $A\beta_{33-42}$ peptides on graphene at $t = 20$ (a), 40 (b), 60 (c) and 80 ns (d): REMD simulation

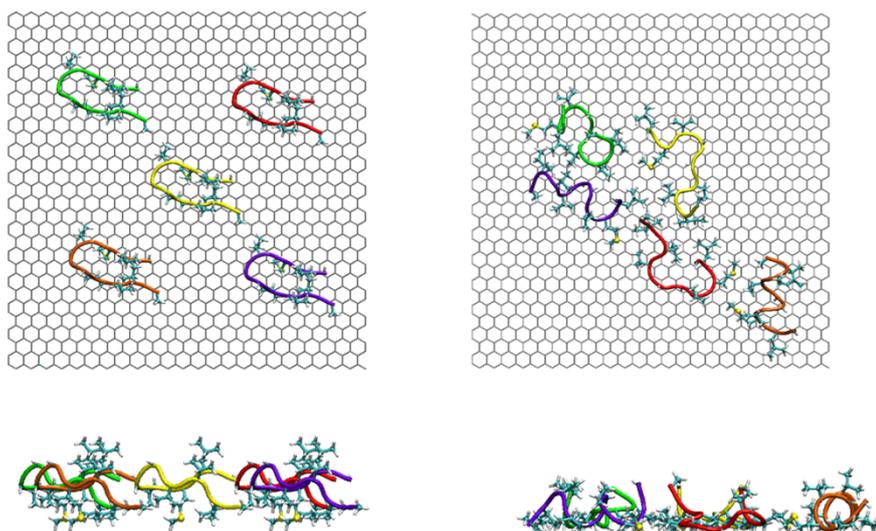


Fig.S5 The initial (a) and final structures (b) of five $A\beta_{33-42}$ peptides on graphene: the conventional MD simulation

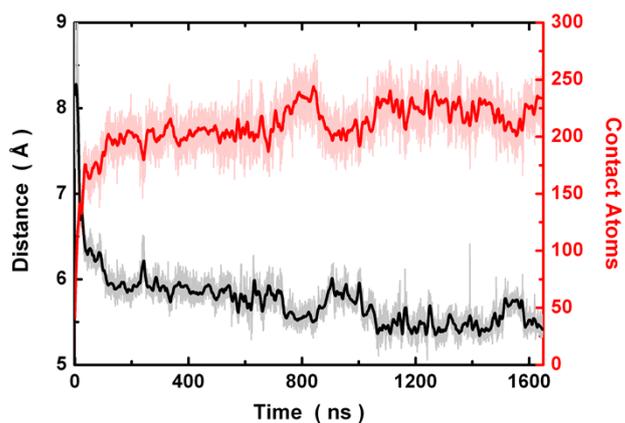


Fig.S6 The distance between the center of mass (COM) of peptides and the graphene (black) and the number of peptide heavy atoms in direct contact with graphene (red) (1640 ns simulation), together with the smoothed data (thicker lines).

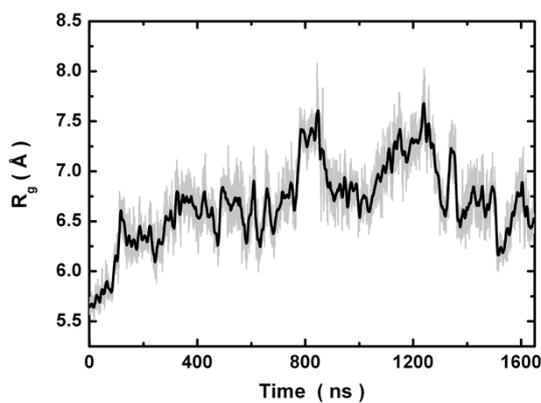


Fig.S7 The average radius of gyration of the five peptides adsorbed on graphene (1640 ns simulation), together with the smoothed data (thicker line).

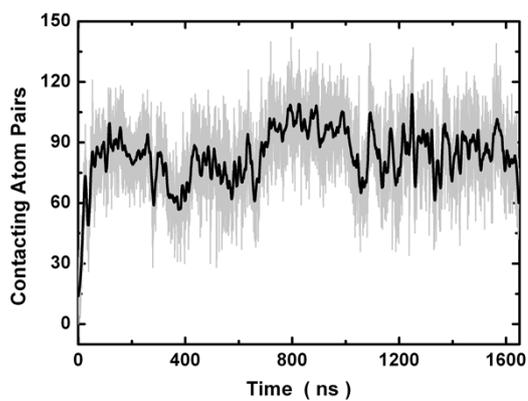


Fig.S8 The number of contacting atom pairs between five peptides adsorbed on graphene (1640 ns simulation), together with smoothed data (thicker line).

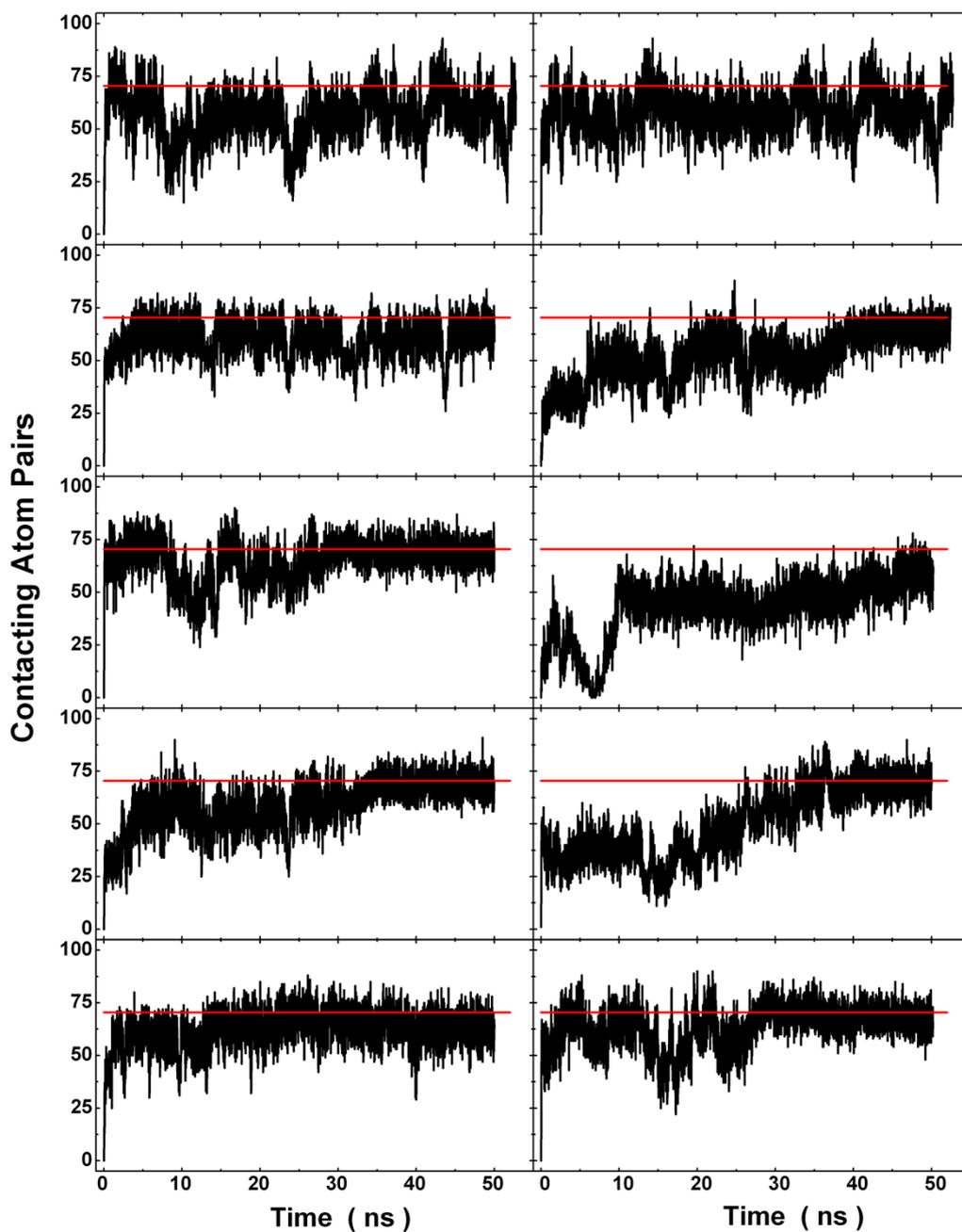


Fig.S9 The number of contacting atom pairs between peptides A-B and D-E in the systems with initial inter-peptide separation of 12.5\AA . The red line denotes the average number of contacting atom pairs between the peptides in the middle region: peptides B-C and C-D. The left/right panel corresponds to the parallel/antiparallel packing assembly, respectively. There are five independent runs for each system (from top to bottom).

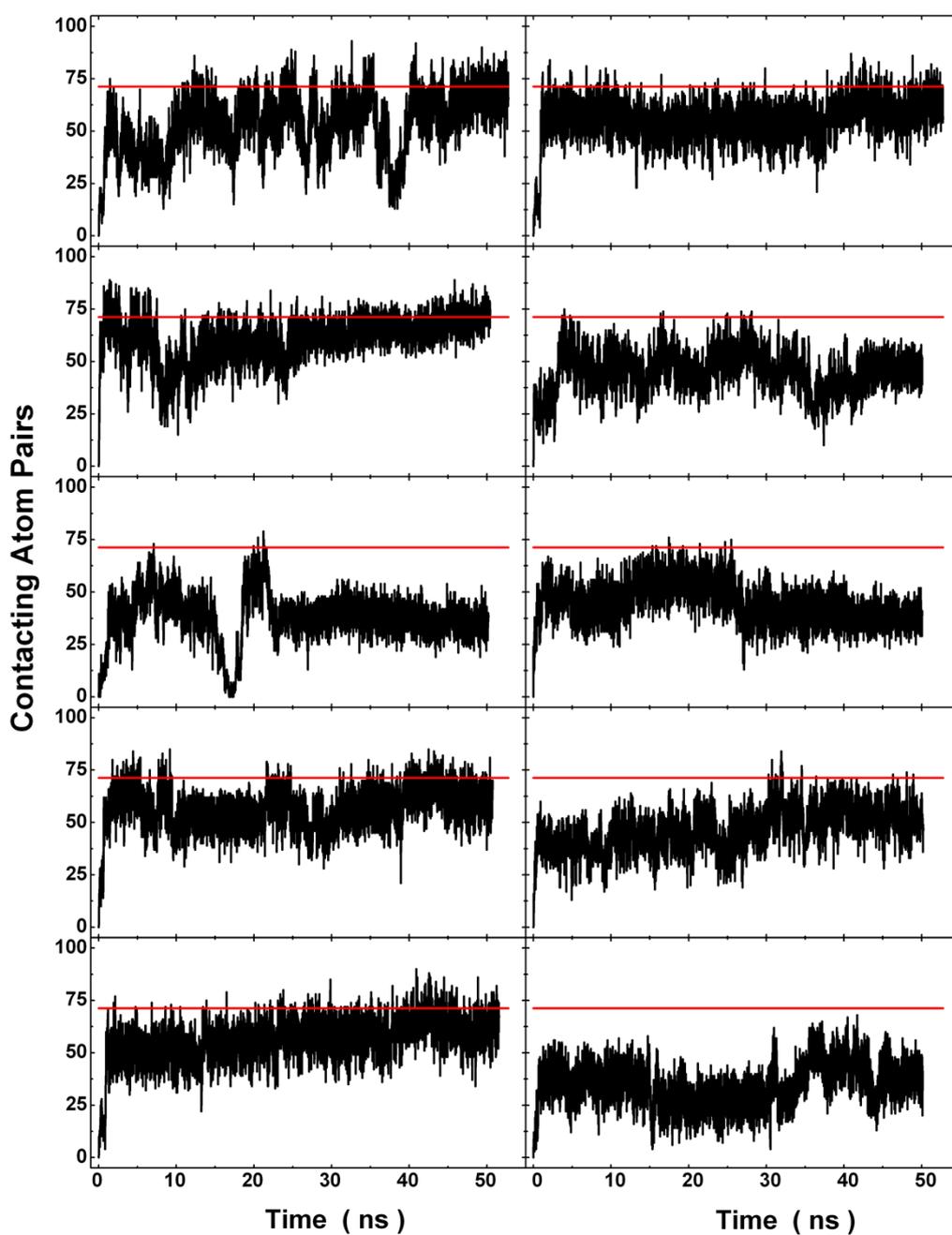


Fig.S10 The number of contacting atom pairs between peptides A-B and D-E in the systems with initial inter-peptide separation of 14.5\AA . The red line is the average number of contacting atom pairs between the peptides in the middle region: peptides B-C and C-D. The left/right panel corresponds to the parallel/antiparallel packing assembly. There are five independent runs for each system (from top to bottom).

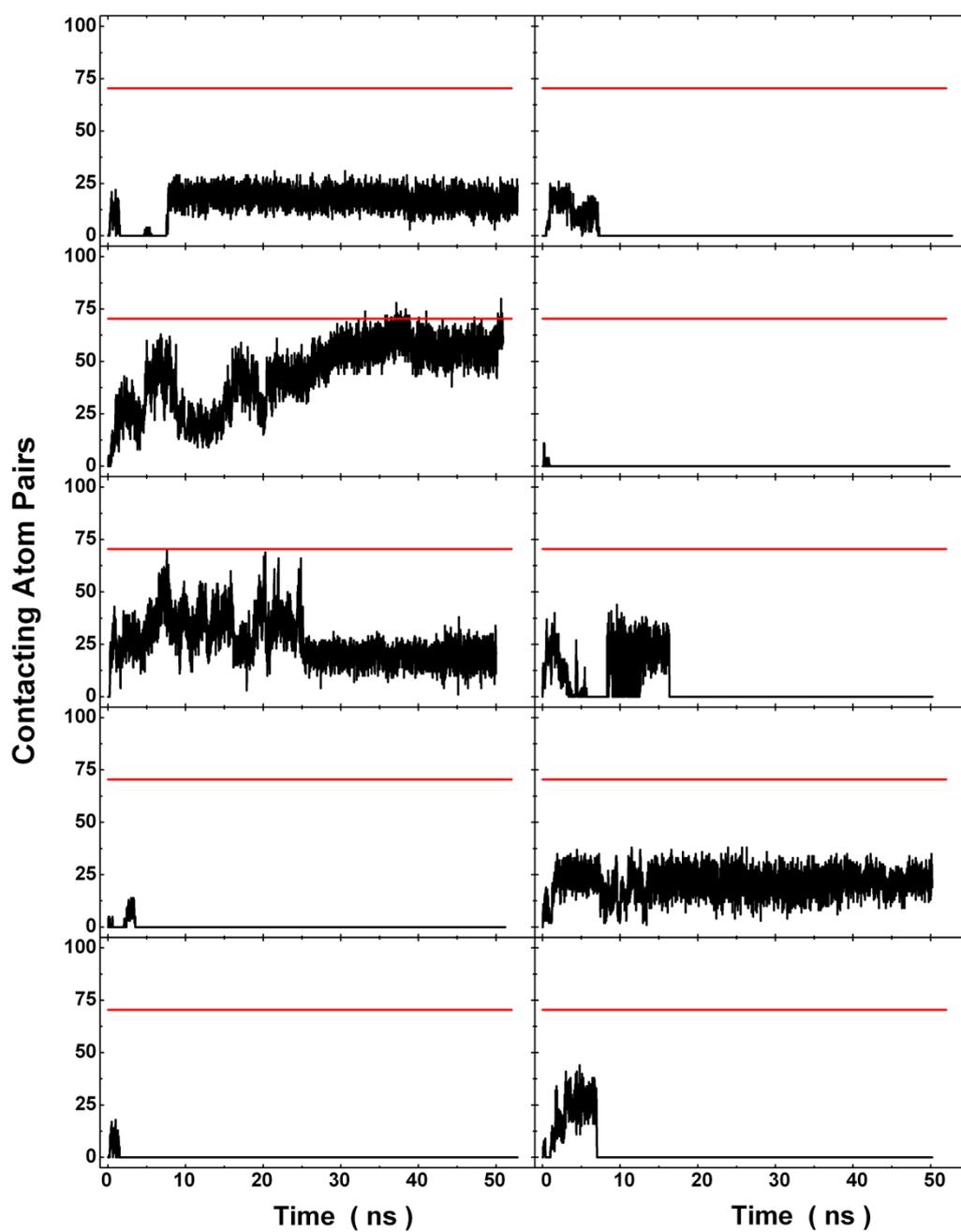


Fig.S11 The number of contacting atom pairs between peptides A-B and D-E for the systems with initial inter-peptide separation of 16.5\AA . The red line is the average number of contacting atom pairs between the peptides in the middle region: peptides B-C and C-D. The left/right panel corresponds to the parallel/antiparallel packing assembly. There are five independent runs for each system (from top to bottom).

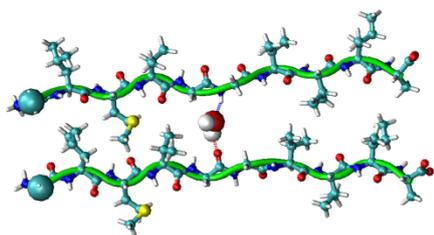


Fig. S12. The representative configuration about water-mediated hydrogen bonds.

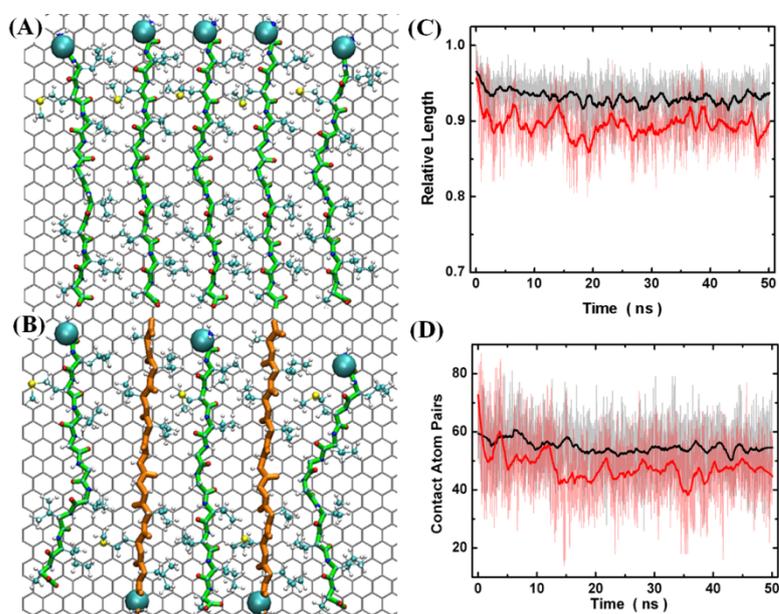


Fig.S13 (A, B) Representative configurations of peptide assemblies (featuring parallel and anti-parallel packing structures) taken from the final 1 ns trajectories of the REMD simulation where the three peptides in the middle (i.e. peptide B, C, D) were restrained to their initial positions and the peptides A and E were free to move. (C) The relative length of peptides A and E in parallel (black) and antiparallel (red) complex. (D) The number of contacting atom pairs between peptides A-B and D-E in parallel (black) and antiparallel (red) complex.

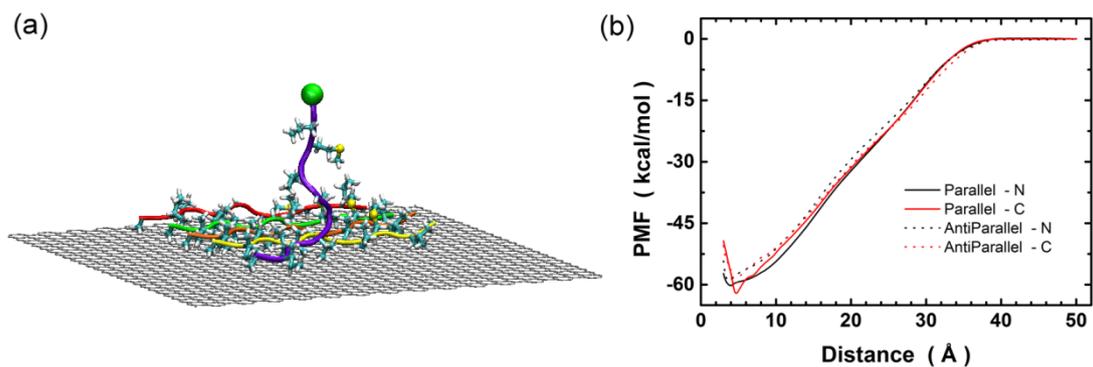


Fig. S14. (a) Representative configuration of Adaptive Biased Force (ABF) simulation of peptide dissociation (in this example, the peptide was detached from graphene surface via its N-terminus). (b) Free energy profiles (potential of mean force, PMF) of peptide detachment in the cases of both parallel (solid line) and antiparallel assemblies (dot line). In addition, both N- (black) and C-terminus (red) detachment were studied separately.

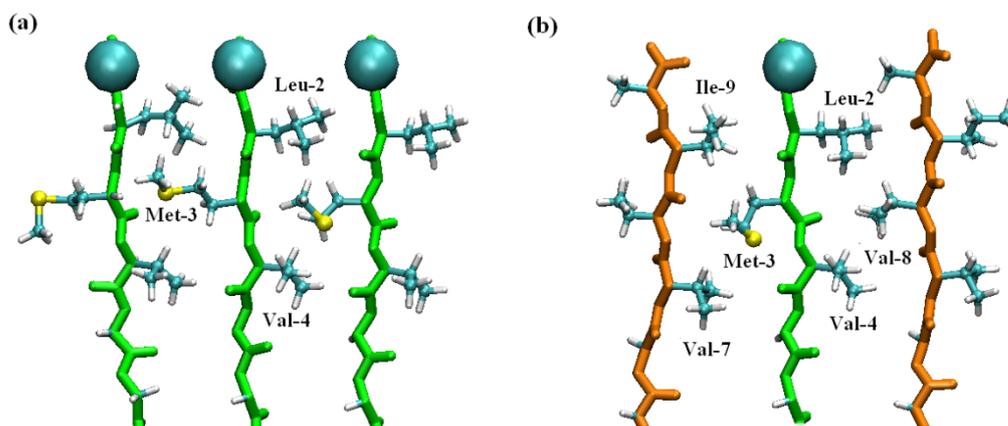


Fig. S15. The schematic draw of parallel (a) and antiparallel packing assembly.