SUPPORTING INFORMATION

## Peptide conformation and oligomerization characteristics of surface-

## mediated assemblies revealed by molecular dynamics simulation

## and scanning tunneling microscopy

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**Figure S1** High resolution STM images of G8 co-assembled with 4Bpy. Tunneling conditions: (A) 675.1 mV and 299.4 pA. (B) Statistical histograms of the peptide length of G8 measured from the STM images. The statistical histograms were fitted by Gaussian distribution (red lines) with the most probable length of the measured strands ca. 3.8 nm. (C) The supposed model for G8 assembly.



**Figure S2** (A) The cluster analysis of conformations of G8 (B) Side view of the G8graphite system at 0 ns (top) and 60 ns (bottom) respectively.



**Figure S3** (a) STM image of G9 co-assembled with 4Bpy. Tunneling conditions: I = 299.1 pA, V = 699.8 mV. (b) Statistical histograms of the peptide length of G9

measured from the STM images in (a). Statistical histograms were fitted by Gaussian distribution (red lines) with the most probable length of the measured strands ca. 3.9 nm.



**Figure S4** (a) STM image of G11 co-assembled with 4Bpy. Tunneling conditions: I = 286.9 pA, V = 607.6 mV. (b) Statistical histograms of the peptide length of G11 measured from the STM images in (a). Statistical histograms were fitted by Gaussian distribution (red lines) with the most probable length of the measured strands ca. 4.0 nm.