Supporting information for:

Changing amyloid nucleation process by small molecule and substrate: a way to build two-dimensional materials

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Fig. S1. Morphologies of FG small molecules deposited on mica surface. **a**. AFM image of fresh mica surface. **b**. AFM image of FG molecules on mica. **c**. AFM image of fresh HOPG surface.



Fig. S2. Packing mode between filaments and HOPG. **a**. The filaments (blue) were in parallel with HOPG (green). **b**. The filaments (blue) rotated 30° with HOPG (green).



Fig. S3. Co-assembly of peptides and FG on HOPG surface. The incubation time was 48 min. **a**. The AFM image of ordered filaments, with its Fourier transform image. **b**. The height distribution of the filaments from **a**. **c**. The distribution of filament orientation in **a**. **d**. The length distribution of filaments from **a**.



Fig. S4. AFM image of $A\beta_{16-22}$ mature fibrils. The concentration of $A\beta_{16-22}$ were 40 μ M.

Secondary structure



Fig. S5. Secondary structure evolution map in 500 ns. Thirty $A\beta_{16-22}$ peptide chains were placed on a graphene substrate for simulation.



Fig. S6. MD simulation of $A\beta_{16-22}$ peptides absorbed on Mica. **a-c**. The snapshots of growth state (0 ns, 50 ns, 100 ns, respectively) on Mica surface. 30 chains were used in the system. **d**. Typical snapshot in 100 ns was exhibited with different postures of $A\beta_{16-22}$.



Fig. S7. MD simulation of $A\beta_{16-22}$ peptides/FG molecules nucleation on Mica surface. a. The snapshots of growth state (0 ns, 100 ns, 200 ns and 300 ns, respectively) on Mica surface. Together with a side view of state in 300 ns. b. Time evolution of the contact number between $A\beta_{16-22}$ peptides/FG molecules and Mica surface. c. Analysis of the contact number between the substrate surface and each residue of $A\beta_{16-22}$. The inset show the interaction between one peptide and two FG molecules on Mica surface.