Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Mechanical and vibrational characterization of amyloid-like HET-s nanosheets based on the skewed plate theory

Author information

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Material and Methods

Determining the basic geometric unit of HET-s angled layers through equilibrium simulations using HET-s fibril segments

The simulation was conducted by using NAMD 2.8 package with CHARMM27 force field under explicit solvent conditions using TIP3P water molecules.[43] We created a water box around two HET-s fibril segments with a padding thickness of 1.5 nm in all directions. Because the shape of HET-s nanosheet is formed at pH levels higher than 4.0, the pH of the system was set as 7.0 for analyzing the structural stability of the basic nanosheet structures. The system was energy minimized based on 10,000 times of the conjugate gradient method, and the equilibration dynamics simulation was performed for 50 ns with the NVT ensemble. As shown in Figure. S1, we found the structural stability at contact region of HET-s nanosheets after 50 ns. The simulation results were visualized via VMD software.[44]

Supporting Figures and Figure Captions

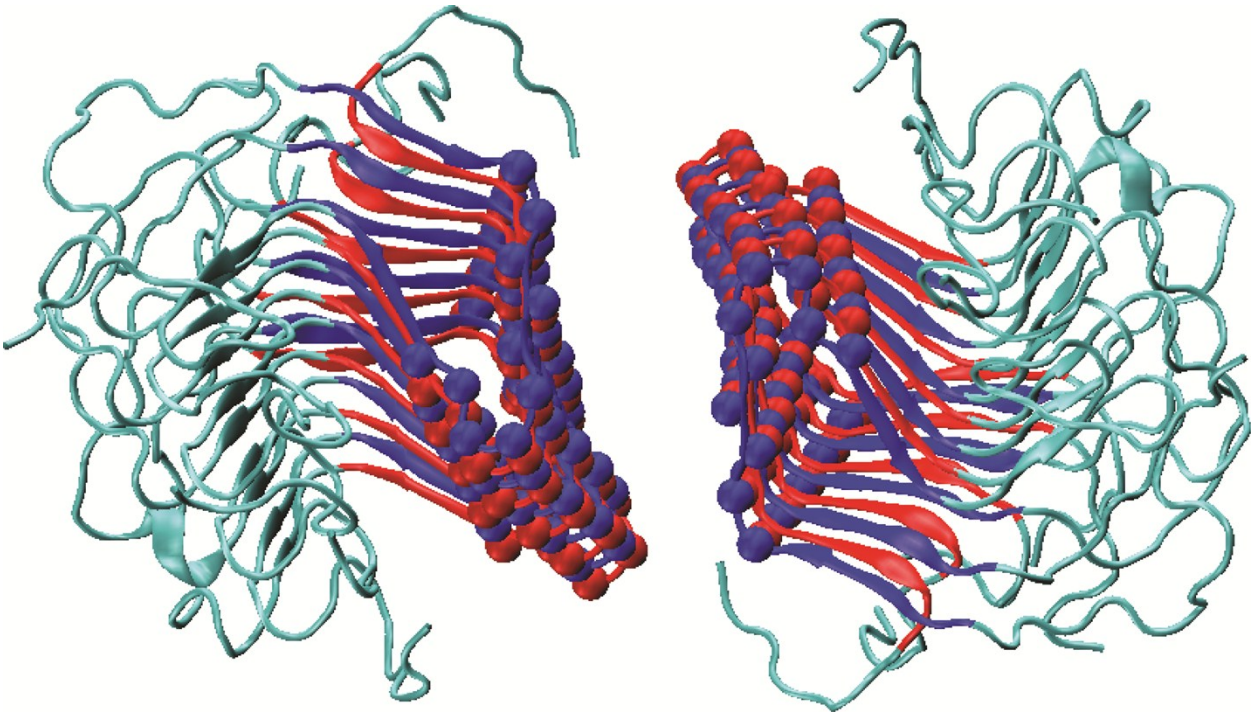

Figure S1. Final conformation of HET-s fibril segments after 50ns MD simulation represented in New Cartoon representation. The backbone region are residue 225-242 (red), and residue 261-278 (blue). Within the backbone region, the nucleation site are assumed to be residue 229-238 (red VdW beads) and residue 265-274 (blue VdW beads).

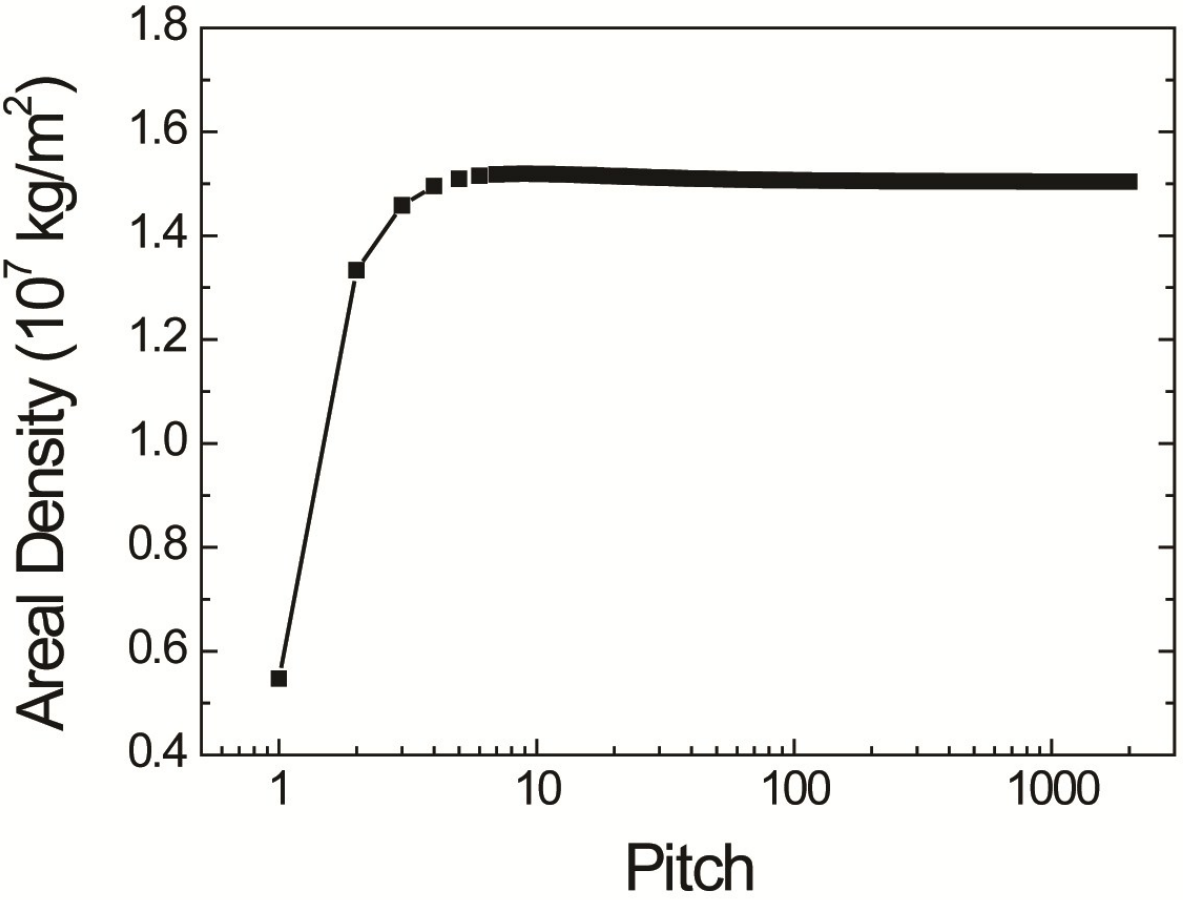

Figure S2. The areal density of HET-s nanosheet structure with respect to pitch-wise fibril length drawn with marker-line representation. Each areal density values are shown with a black filled square (■).

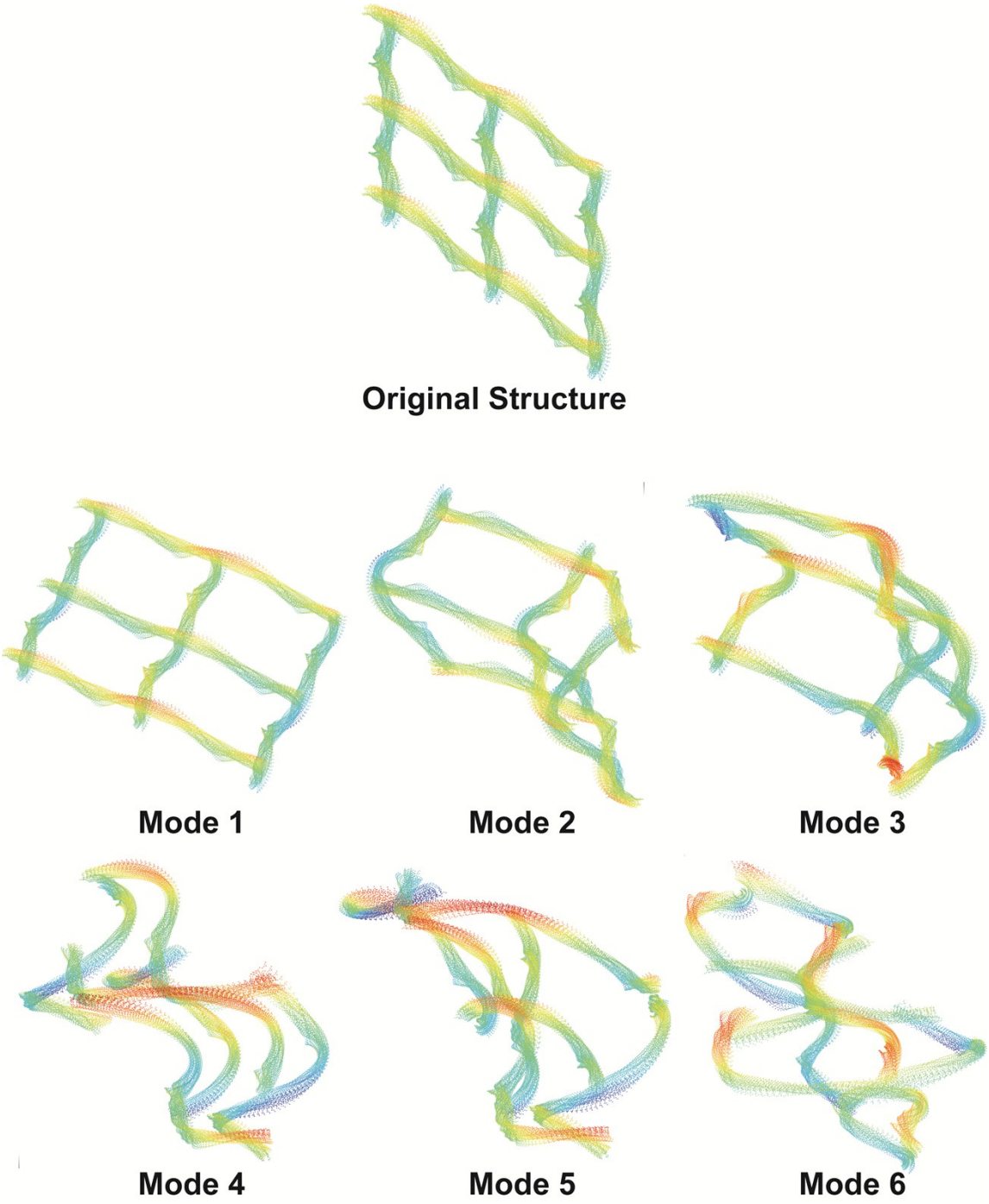

Figure S3. Dominant in-plane modes of Model 2 HET-s nanosheet structures. The color of the structure was represented with respect to the height of the z-position, where yellow ~ red colors indicate a positive z-displacement and light blue ~ indigo colors indicate a negative z-displacement. Green color indicates a z-displacement close to 0.