Supporting Information

Peptide amphiphile self-assembly

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**All-atom molecular dynamic simulations**

We solvated the structure in fig 1b in TIP3P water [1] using a simulation box of 120 x 120 x 74 Å³ in x, y and z, respectively. At neutral pH, the lysine groups and the free carboxyl group at the C-terminal of PA chains are ionized. Therefore, each PA chain has a net charge of 2+. To balance the net charge Cl⁻ ions were added in solution. CHARMM36 force field [2-4] was used to model the system. Molecular dynamics simulations were performed with NAMD 2.11 software [5]. Following a 1000 step minimization to remove high-energy contacts, the initial structures were equilibrated for 2 ns with a NPT ensemble at 310 K and 1 atm, increasing the temperature gradually to 310 K. For temperature and pressure control, the Langevin piston [6] and Nose-Hoover method [7] implemented in NAMD was used. The damping coefficient was 5 ps⁻¹ for temperature coupling using Langevin dynamics at 310 K. Pressure was kept at 1 atm with a Langevin piston period of 100 fs with a damping time constant of 50 fs. Full electrostatics was employed using the particle-mesh Ewald [8] method with a 1 Å grid width. Non-bonded interactions were calculated using a group-based cutoff with a switching function and updated every 10 time steps. Covalent bonds involving hydrogens were held rigid using the SHAKE algorithm [9], allowing a 2 fs time step. Atomic coordinates were saved every 10 ps for the trajectory analysis. Periodic boundary conditions were employed in x, y and z directions. In the production run, a 100 ns simulation was run using the same settings.

The simulation protocol above was repeated for 353 K and 400 K by setting the value of temperature coupling to desired temperature in both equilibration and production runs. For the simulations with higher fiber density, we used the same settings as above at 310 K. The initial box dimensions were 120 x 120 x 49 Å³ in x, y and z, respectively.
Visual Molecular Dynamics (VMD) [10] was used for analysis and generating the snapshots of trajectories used in this paper. The secondary structure information for the PAs was calculated using the STRIDE [11] algorithm implemented in VMD. Because the secondary structure of PAs change throughout the trajectory, only the last 60 ns is used to calculate the average number of structures formed. For all secondary structure data presented in this paper, the block averaging method was used to calculate the mean, standard deviation and standard error values.

References