

Electronic Supplementary Information

Aggregation of Amyloid Peptides into Fibrils Driven by Nanoparticles and their Curvature Effect

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The hydrogen bonding method and peptide chain stiffness

We adopted the hydrogen bonding approach developed by Olvera de la Cruz et al.^{1,2}. Firstly, we preset that a CG bead could form two hydrogen bonds at most, considering there are one donor N-H and one acceptor C=O in each amino acid. The hydrogen bonds were allowed to form or break during the simulation. We defined the activation energy for forming the first hydrogen bond of the CG bead as

$$U_a = \varepsilon_\beta \cos(\vartheta_{ij}), \quad (1)$$

where $\varepsilon_\beta = 3k_B T$ is the activation energy parameter which determines the probability of forming or breaking hydrogen bonds. ϑ_{ij} is the angle between the bonded CG beads in the two adjacent chains, $\cos(\vartheta_{ij}) = (\Delta\vec{r}_i \cdot \Delta\vec{r}_j) / (\Delta r_i \Delta r_j)$, in which $\Delta\vec{r}_i = \vec{r}_{i+1} - \vec{r}_{i-1}$, the bead i and j belong to different chains. As shown in Figure 1a, the two peptide chains could tend to parallel with each other according to the equation.

For the second hydrogen bond, the CG bead k from the third chain would be supplied and placed along the connection of the CG beads i and j . We added an additional parameter φ_i to describe the angle between the two hydrogen bonds ij and ik , which should be close to 180° (shown in Figure 1a). The angle φ_i was defined as $\cos(\varphi_i) = (\Delta\vec{r}_{ki} \cdot \Delta\vec{r}_{ij}) / (\Delta r_{ki} \Delta r_{ij})$, so the activation energy for the second hydrogen bond was

$$U_a = \varepsilon_\beta \cos(\vartheta_{ij}) \cos(\varphi_i). \quad (2)$$

In addition, once the hydrogen bonds were formed, we added the formation energy of hydrogen bond, as well as the fibril bending energy into the total energy. The formation energy of hydrogen bond was set at $U_h = -3k_B T$ for each hydrogen bond, according to

the previous experimental and simulation works^{3,4}. The fibril bending energy was described as,

$$U_{fib} = g_i(1 + \cos \varphi)^2, \quad (3)$$

which was similar as the equation of peptide intramolecular bending energy described in the main text (Equation 2). The rigidity constant g_i was also set at $100k_B T$. The total bending energy was composed of the fibril bending energy and the intramolecular bending energy.

The probabilities for forming and breaking hydrogen bonds, p_{form} and p_{break} , were determined by the following criterion, respectively

$$p_{form} = \frac{g(U_{a,ij})}{1 + g(U_{a,ij})}, \quad (4)$$

$$p_{break} = \frac{1}{1 + g(U_{a,ij})}, \quad (5)$$

where $g(U_{a,ij}) = \exp(-U_{a,ij}/k_B T)$, $U_{a,ij}$ is the activation energy for forming or breaking hydrogen bond between two CG beads. If the distance between two CG beads was smaller than 1.5σ , a random number R between 0 and 1 could be generated. If R is smaller than p_{form} or p_{break} , we would perform the step of forming or breaking of hydrogen bonds.

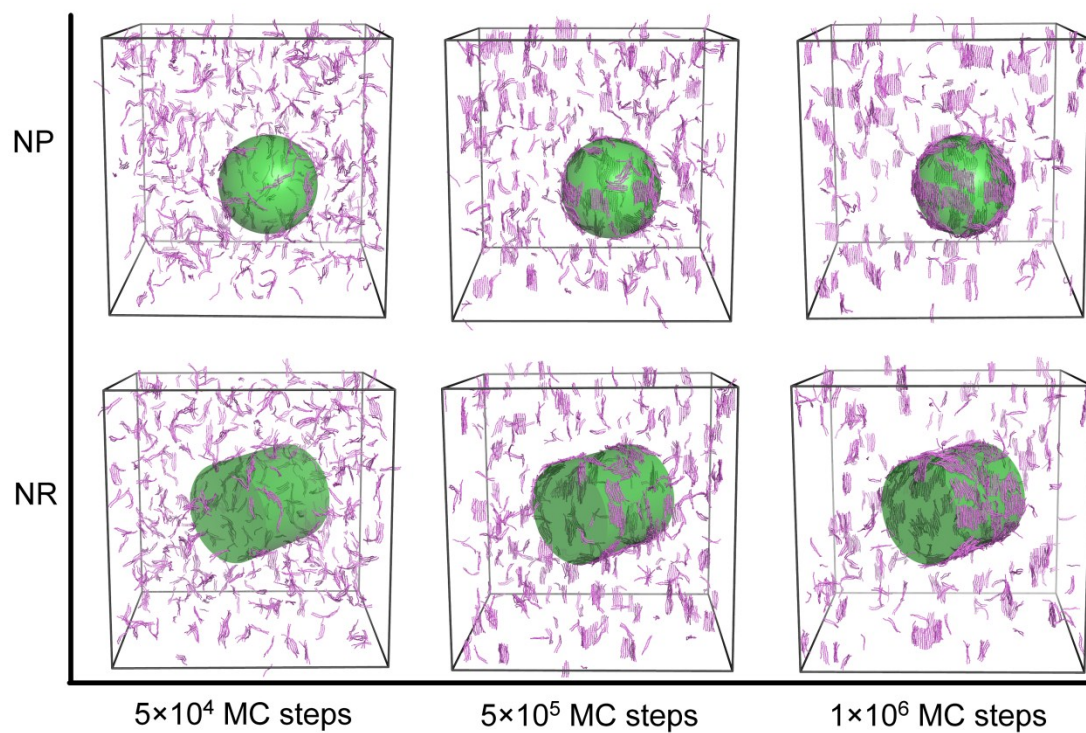


Fig. S1 The kinetic pathways for the formation of fibrillation structures on NP and NR surfaces with diameter 64σ . The top three figures are the snapshots of NP system for 5×10^4 MC steps, 5×10^5 MC steps and 1×10^6 MC steps; the bottom three are the snapshots of NR system at same MC steps.

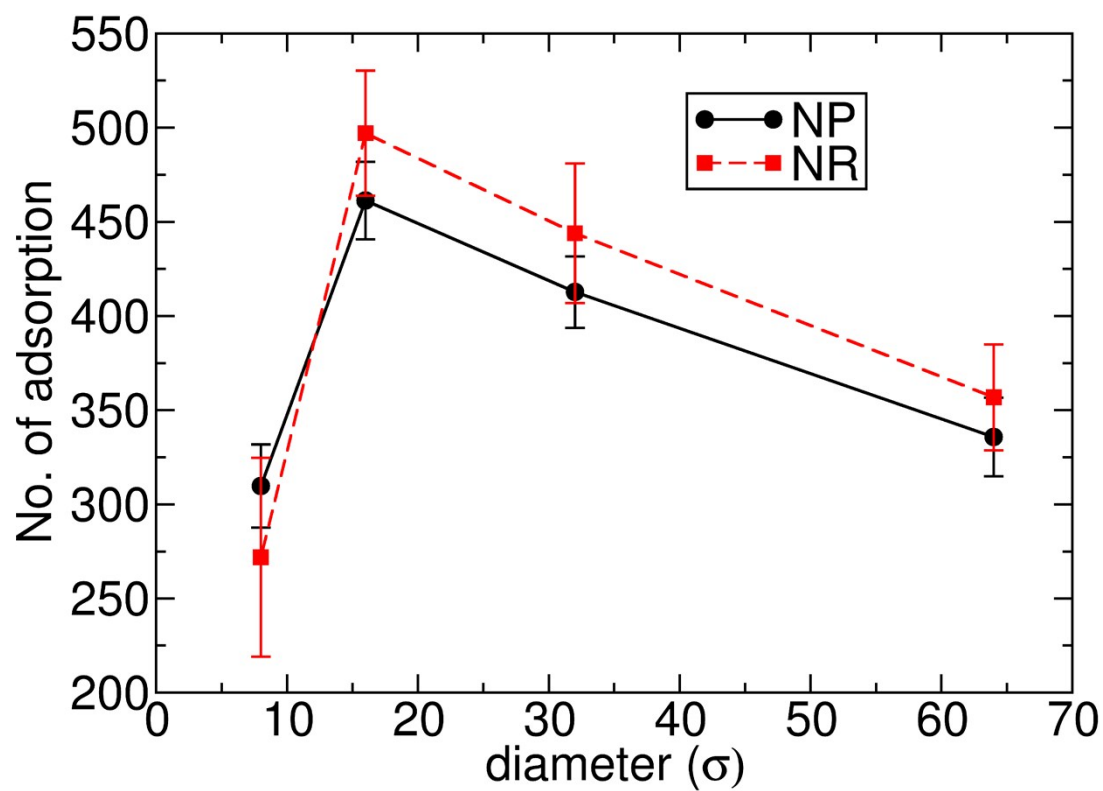


Fig. S2 The number of peptide chains adsorbed on the surfaces of NPs/NRs in lower concentration peptide systems, x axis corresponds the diameters of NPs, as well as diameters and heights in NRs.

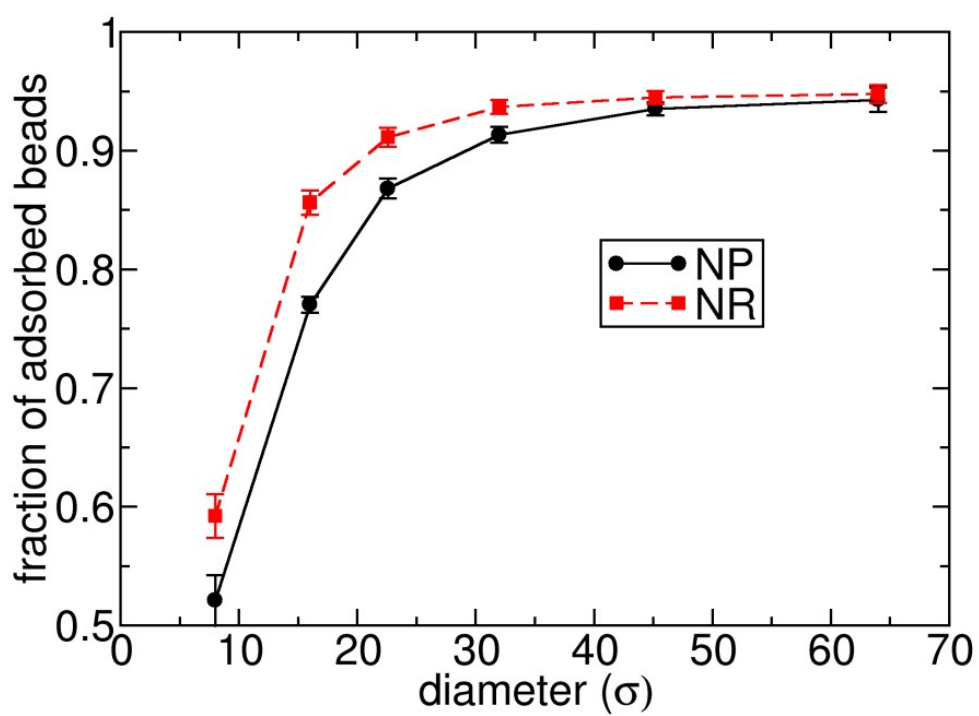


Fig. S3 The fraction of beads adsorbed on NPs/NRs surfaces in each peptide chain.

Table S1 The parameters of NPs with different diameters

diameter (σ)	8.0	16.0	22.6	32.0	45.2	64.0
number of beads in NP	40	160	320	640	1280	2560
number of NPs	64	16	8	4	2	1

Table S2 The parameters of NRs with different sizes

diameter (σ)	8.0	16.0	22.6	32.0	45.2	64.0
height (σ)	8.0	16.0	22.6	32.0	45.2	64.0
number of beads on side surface	40	160	320	640	1280	2560
number of NRs	64	16	8	4	2	1

References

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