Electronic Supplementary Material (ESI) for RSC Advances.

Contrasting effects of nanoparticle-protein attraction on amyloid aggregation

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Supplementary Figures

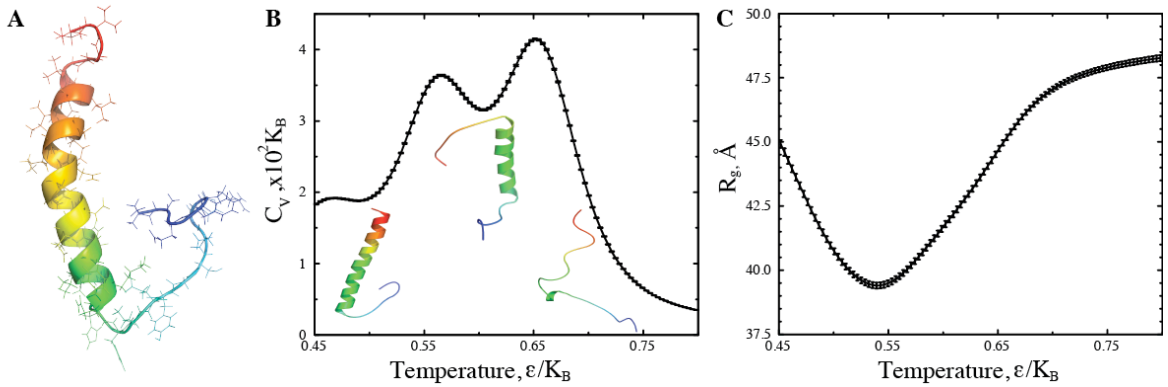

Figure S1. Folding thermodynamics of Aβ monomer derived from DMD simulations. (A) The native state of Aβ (PDB: 1BA4) is shown in cartoon representation. The backbone trace form N- to C-terminal is colored in rainbow for blue to red, respectively. (B) Specific heat (C_v) and (C) Radius of gyration (R_g) and corresponding g statistical uncertainties (as error bars) were computed from replica exchange DMD simulations using the WHAM analysis. Typical structures of Aβ in the simulations, corresponding to native-like, intermediate, and unfold states, are shown in the inset of panel B.

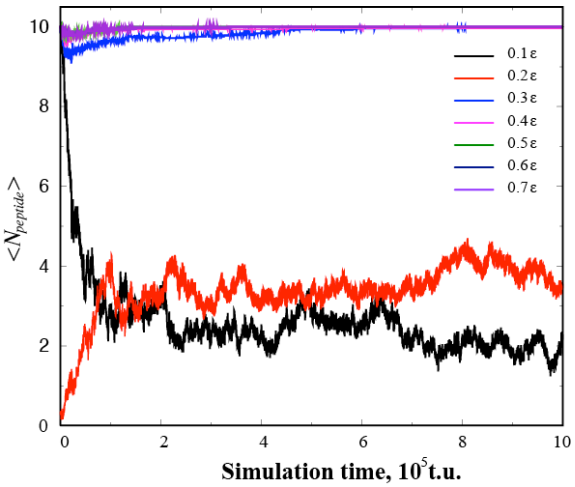

Figure S2. For different values of NP-protein interaction strength, the average number of Aβ peptides on the NP surface was computed as a function of simulation time. The average was taken from 50 independent simulations, each of which was performed for a total 1×10^6 time units (t.u.).

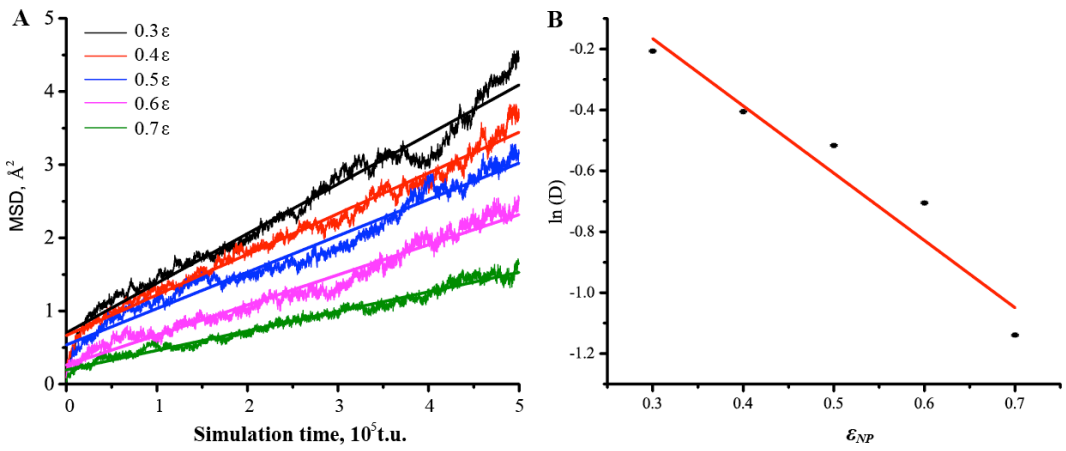

Figure S3. Peptide diffusion on the NP surface. (A) Mean square deviation (MSD) of the peptides was computed as a function of its diffusion time on the NP surface. The analysis was done for simulations with a single peptide bound to the NP surface. We only performed simulations with $\boldsymbol{\varepsilon_{NP}} \geq 0.3\ \boldsymbol{\varepsilon}$ such that the peptide stayed as bound (e.g. Fig. S1). Linear-fit results in the diffusion coefficients, D. (B) The diffusion coefficients follow a linear dependence on NP-protein interaction potential $\boldsymbol{\varepsilon_{NP}}$ in the log-linear plot, suggesting an exponential-like dependence $D \sim exp(-c\boldsymbol{\varepsilon_{NP}})$.

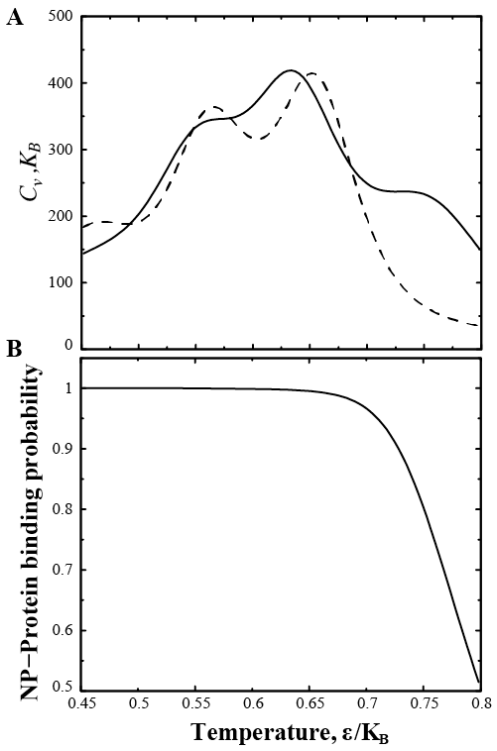

Figure S4. (A) Heat capacity of Aβ monomer in the presence of the NP (solid line), compared to the corresponding heat capacity in the absence of the NP (dashed line). (B) The binding probability of the peptide to the NP surface.

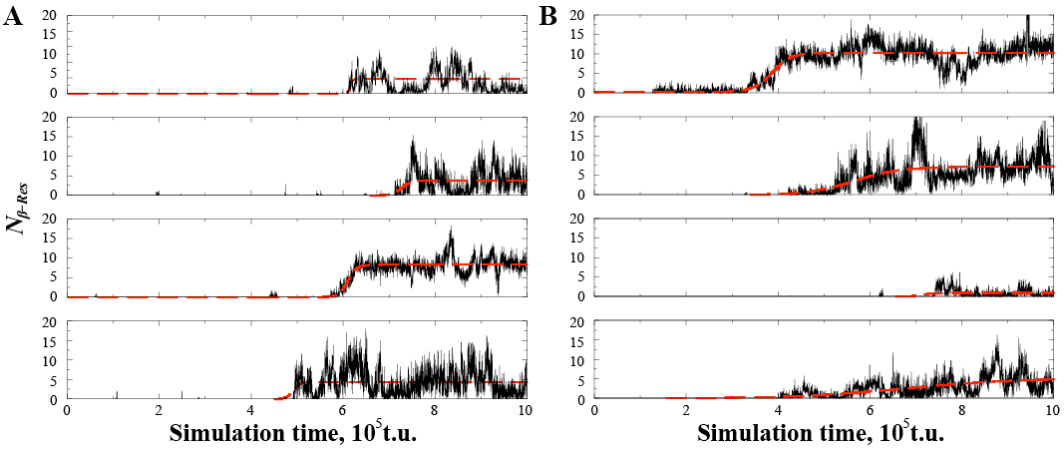

Figure S5. Typical trajectories (4 out of 50 independent simulations) of $N_{\beta\text{-}res}$ for proteins in solution (not NP-bound) as a function of simulation time, in the absence (A) and presence (B) of NP-protein attraction. For each trajectory, the sigmoidal fit was shown as a red dashed line.

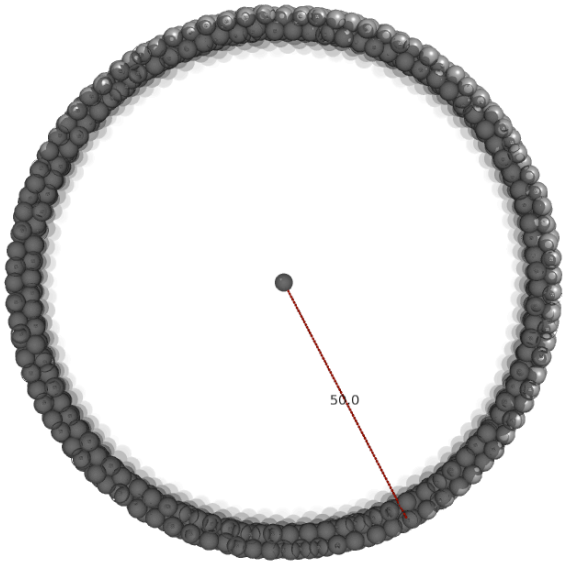

Figure S6. The cross-section of the NP model indicates the two layers of closely packed surface atoms.