

## Electronic Supplementary Information

### **Charge Effects at Nano-Bio interfaces: A Model of Charged Gold Nanoclusters on Amylin Fibrillation**

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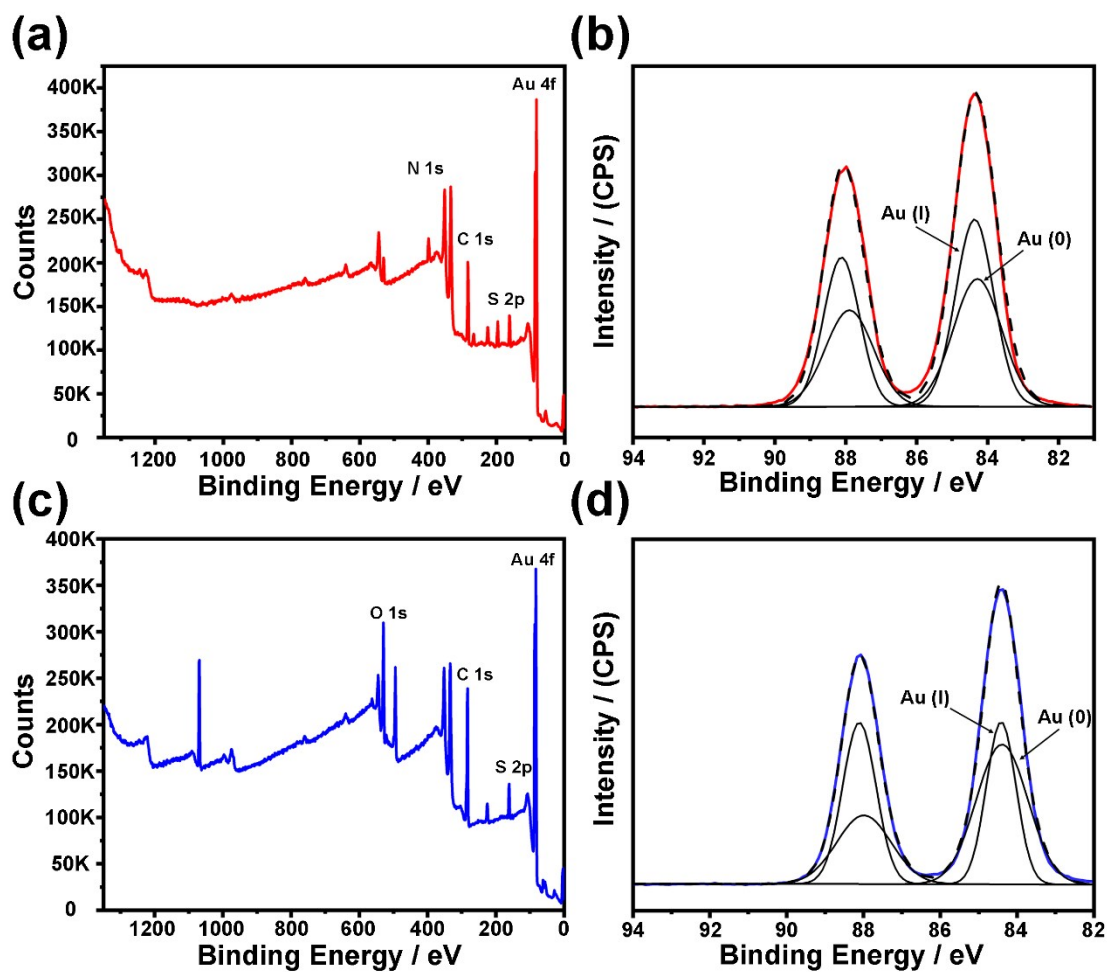
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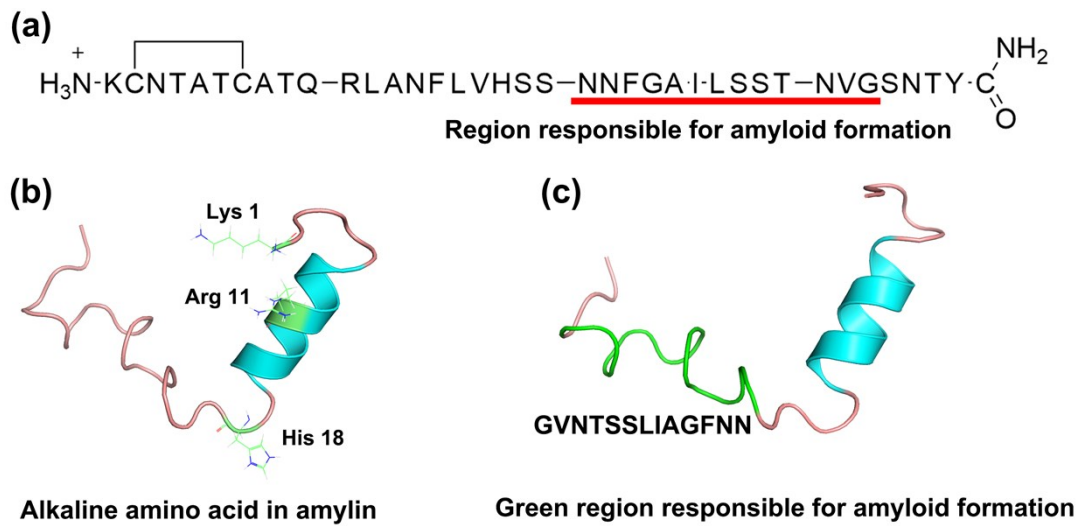
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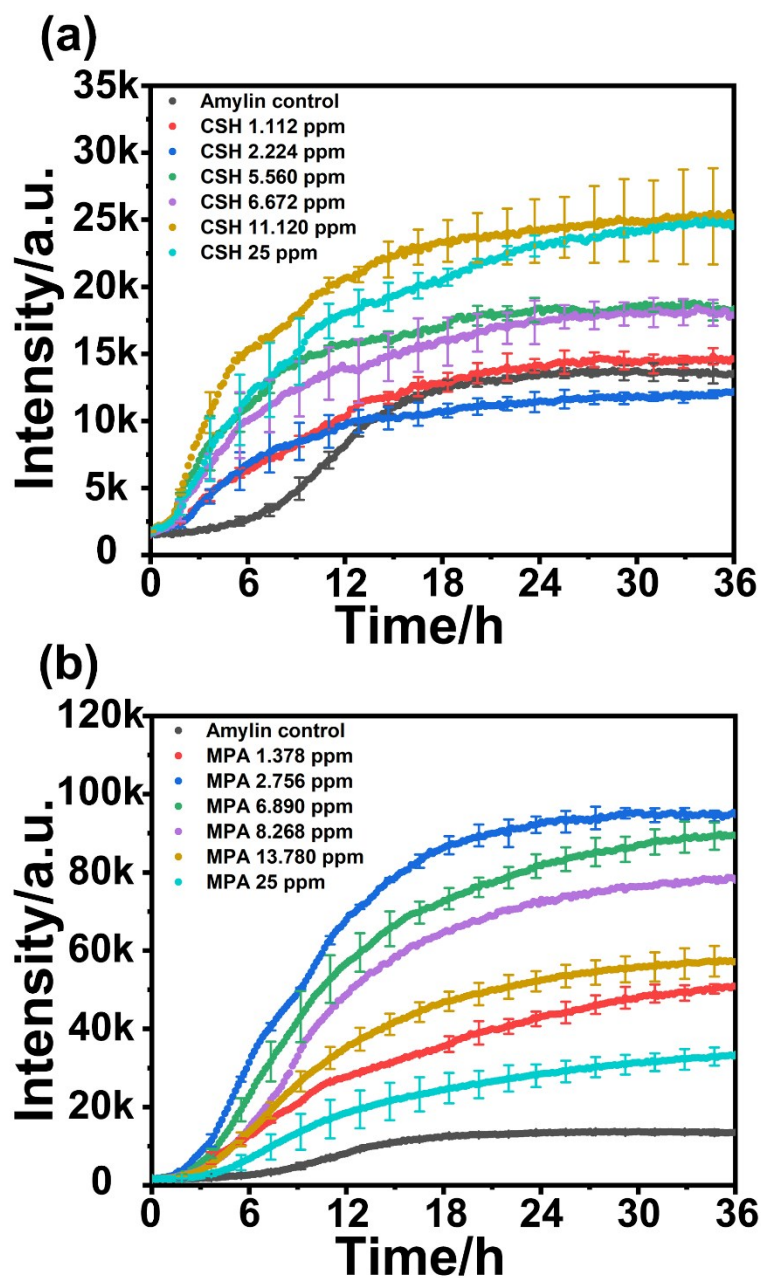
## Supplementary Figures and relevant discussion



**Figure S1** (a) The XPS spectrum of CSH-AuNCs. (b) High-resolution Au 4f peaks of CSH-AuNCs. (c) The XPS spectrum of MPA-AuNCs. (d) High-resolution Au 4f peaks of MPA-AuNCs.

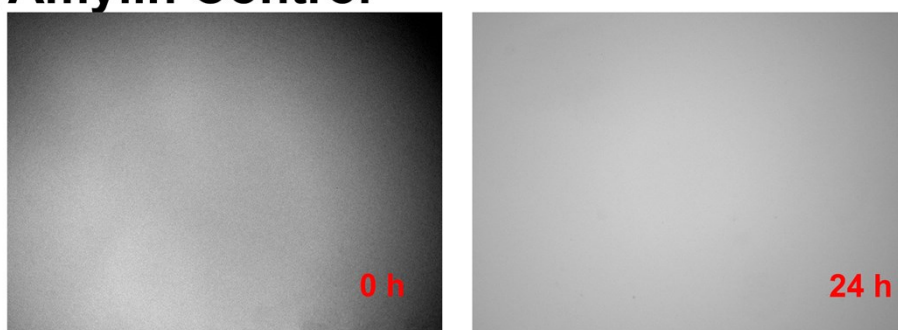


**Figure S2** (a) The primary structure of amylin peptide. (b) Alkaline amino distribution in amylin. (c) The main region responsible for amyloid formation.

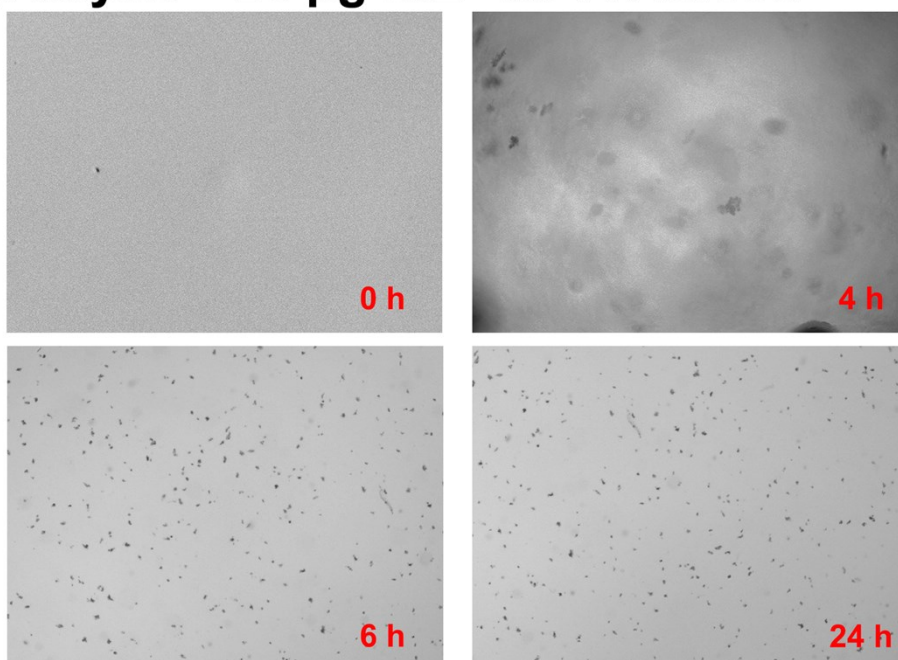


**Figure S3** Fibrillation kinetics of Amylin protein ( $20 \mu\text{mol}\cdot\text{L}^{-1}$ ) incubated with different concentration of (a) ligands CSH and (b) ligands MPA. The ligands concentration gradient used was set based on the concentration of the AuNCs in the kinetic experiment to calculate the content of the ligand with the molecular formula of  $\text{Au}_{18}(\text{SR})_{25}$ .

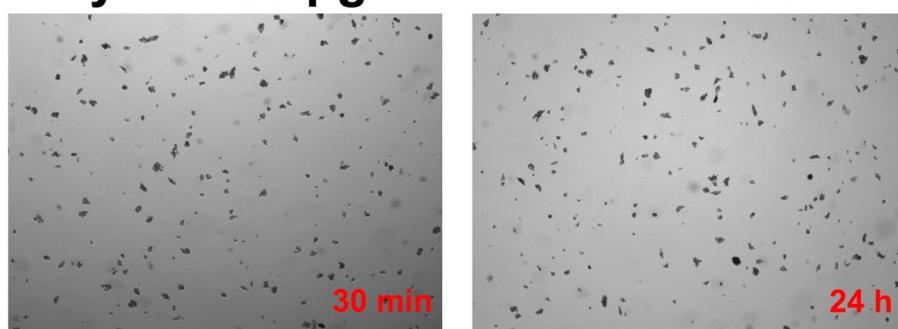
**(a) Amylin Control**



**(b) Amylin + 25  $\mu\text{g}\cdot\text{mL}^{-1}$  MPA-AuNCs**



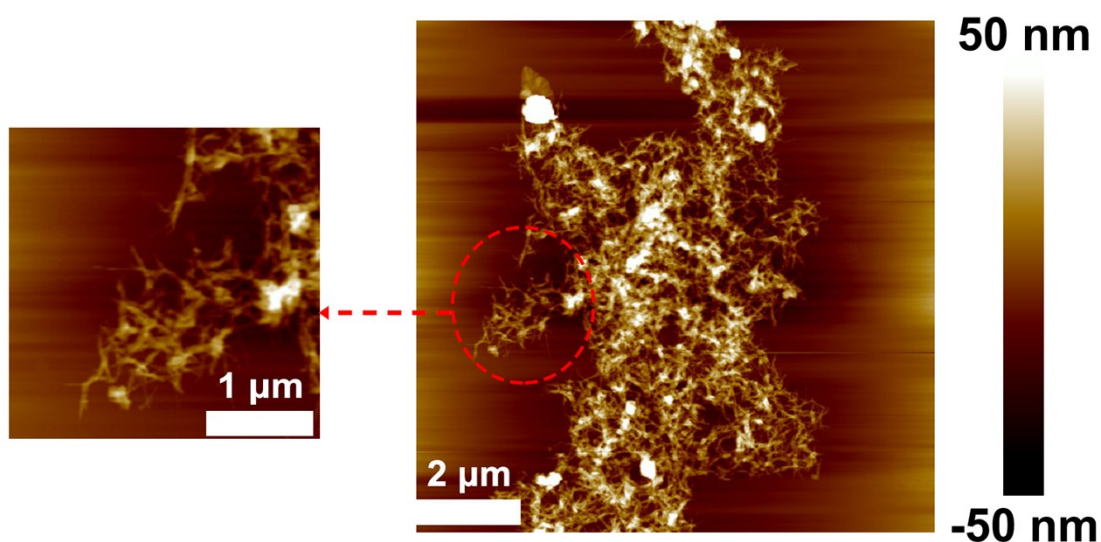
**(c) Amylin + 50  $\mu\text{g}\cdot\text{mL}^{-1}$  MPA-AuNCs**



**Figure S4** The bright field image of 20  $\mu\text{mol}\cdot\text{L}^{-1}$  Amylin incubated at 37 °C in the absence (a) and presence of 25  $\mu\text{g}\cdot\text{mL}^{-1}$  (b) or 50  $\mu\text{g}\cdot\text{mL}^{-1}$  MPA-AuNCs (c) were obtained by Inverted optical micro 0020scope at different time points.

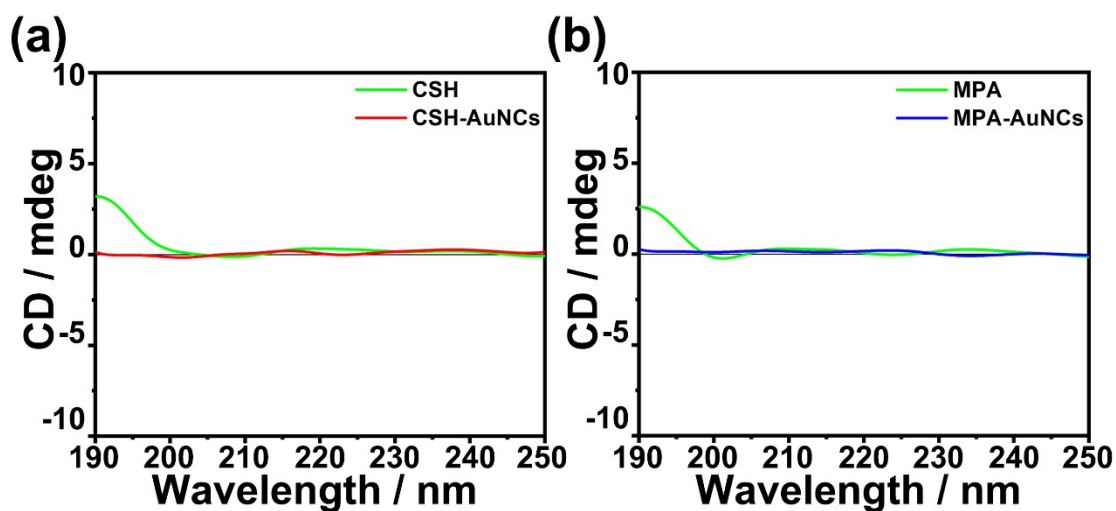
For the sample of amylin co-incubating with MPA-AuNCs lower than 25  $\mu\text{g}\cdot\text{mL}^{-1}$ , no

flocculation floccule could be found under the inverted optical microscope with magnification of X4, which is same as the amylin control group. However, when  $25 \mu\text{g}\cdot\text{mL}^{-1}$  MPA-AuMCs was added, the flocs floating in the system were clearly observed after 6 hours of incubation. With the increase of MPA-AuMCs, the flocculent precipitation rate was faster. As can be seen from figure S3 (c), when the concentration of MPA-AuMCs reached  $50 \mu\text{g}\cdot\text{mL}^{-1}$ , visible flocs appeared in solution less than 30 minutes.



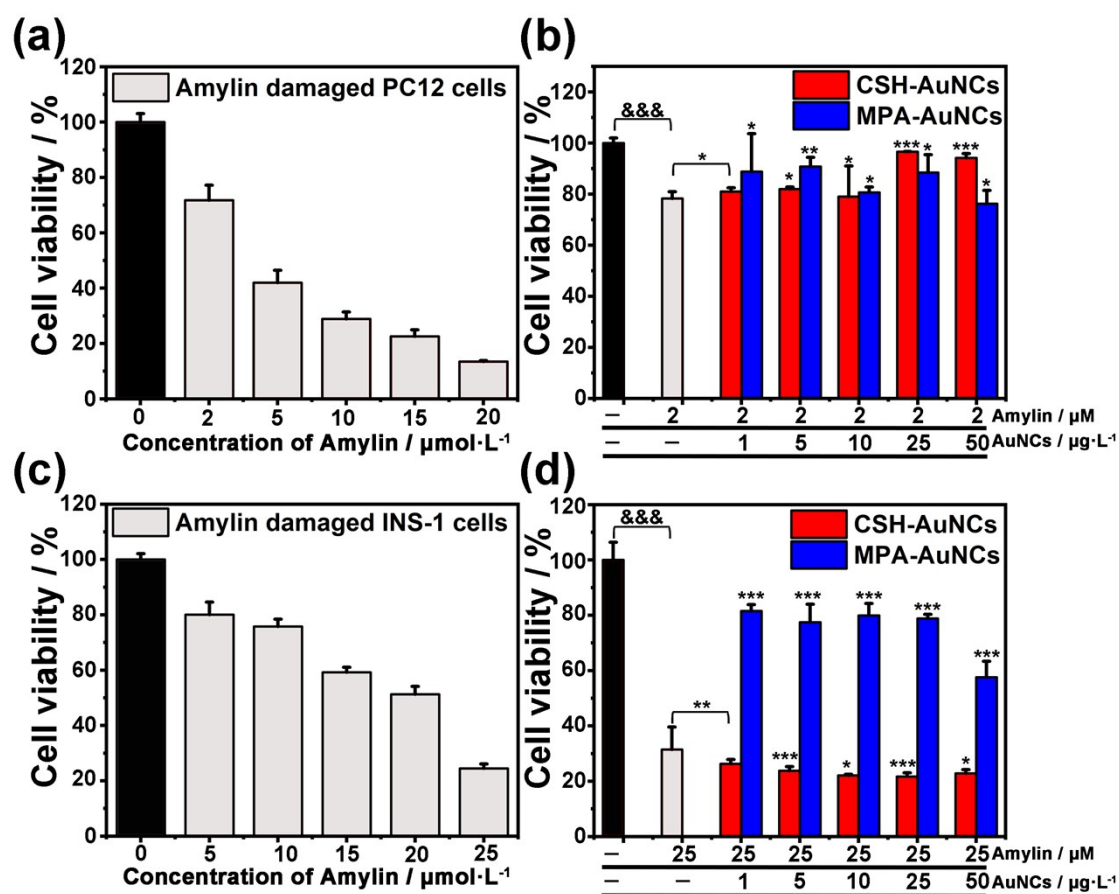
**Figure S5** AFM images of  $20 \mu\text{mol}\cdot\text{L}^{-1}$  Amylin incubated with MPA-AuNCs ( $25 \text{mg}\cdot\text{L}^{-1}$ ) at  $37 \text{ }^\circ\text{C}$  for 24 hours.

From the AFM details images (left), agglomeration floccules from the sample with MPA-AuNCs are consisted of shorter fibers.



**Figure S6** CD spectra of  $50 \mu\text{g mL}^{-1}$  CSH-AuNCs (a) and  $50 \mu\text{g mL}^{-1}$  MPA-AuNCs (b) with and their ligands.

As shown in Figure S6, both  $50 \mu\text{g mL}^{-1}$  CSH-AuNCs and  $50 \mu\text{g mL}^{-1}$  MPA-AuNCs have no CD signal at the range of 190-250 nm.



**Figure S7** CCK-8 assay for PC12 cell and insulinoma INS-1 cell viability (percentage). (a, c) Amylin induced cell damage model. PC12 cells (a) and INS-1 cells (c) incubating in the absence (black) and presence of different concentration of amylin for 24h. (b, d) Amylin induced cell damage experiment. (b) PC12 cells incubating with  $2 \mu\text{mol}\cdot\text{L}^{-1}$  amylin only (gray column), amylin + MPA-AuNCs (blue column) and amylin + CSH-AuNCs (red column) for 24h. (d) INS-1 cells incubating with  $25 \mu\text{mol}\cdot\text{L}^{-1}$  amylin only (gray column), amylin + MPA-AuNCs (blue column) and amylin + CSH-AuNCs (red column) for 24h. Data represented as mean  $\pm$  SD (n = 5). Student's *t*-test, \*\*\**p* <0.001, \*\**p* <0.01, \**p* <0.1 vs amylin group; &&&*p* <0.001 vs control group.