

Supporting Information

**Spontaneous protein desorption from self-assembled monolayer
(SAM)-coated gold nanoparticles**

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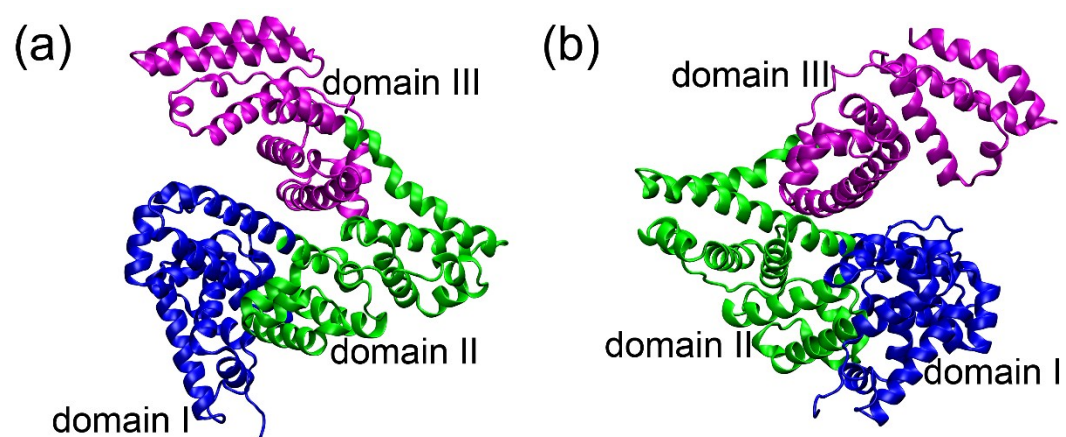


Fig. S1: The bottom view of two binding surfaces of HSA: plane A (a); plane B (b).

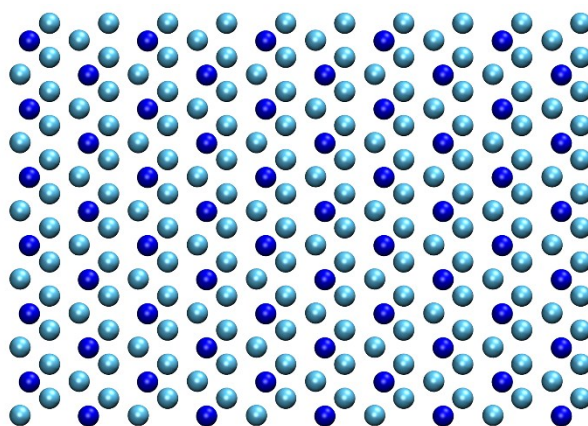


Fig. S2: The sketch of the 25% protonated SAM, the amine (-NH_2) and protonated amine (-NH_3^+) groups are shown as light blue and blue spheres, respectively.

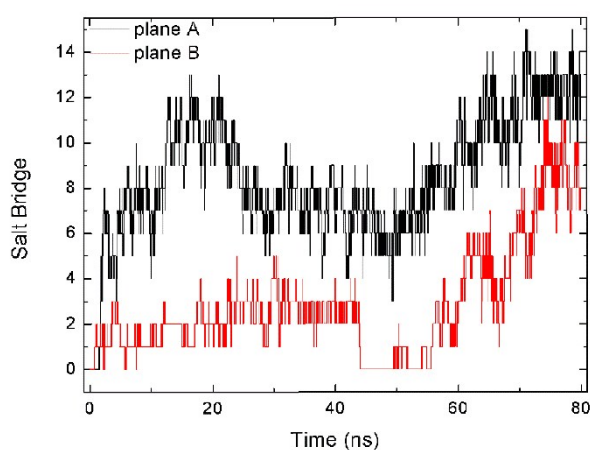


Fig. S3: The number of salt bridge between HSA and SAM in *adsorption-50%*.

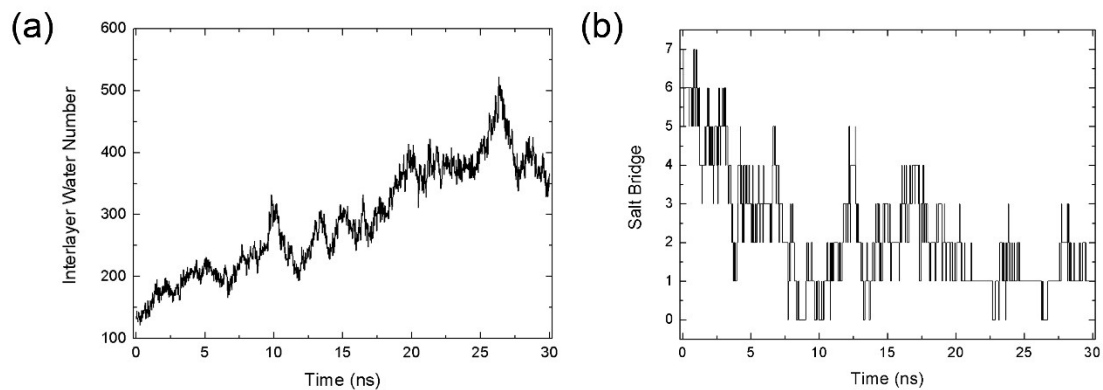


Fig. S4: The number of *interlayer water* (a) and salt bridge between HSA and the SAM (b) in *adjustment-25%*.

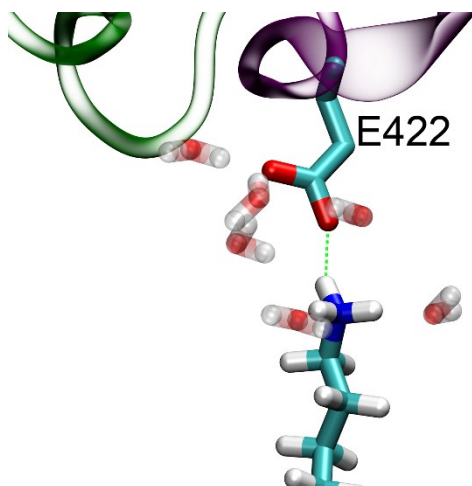


Fig. S5: Some water molecules are in the vicinity of salt bridges formed by E422 with - NH_3^+ groups, and they form hydrogen bonds with the salt-bridge groups.

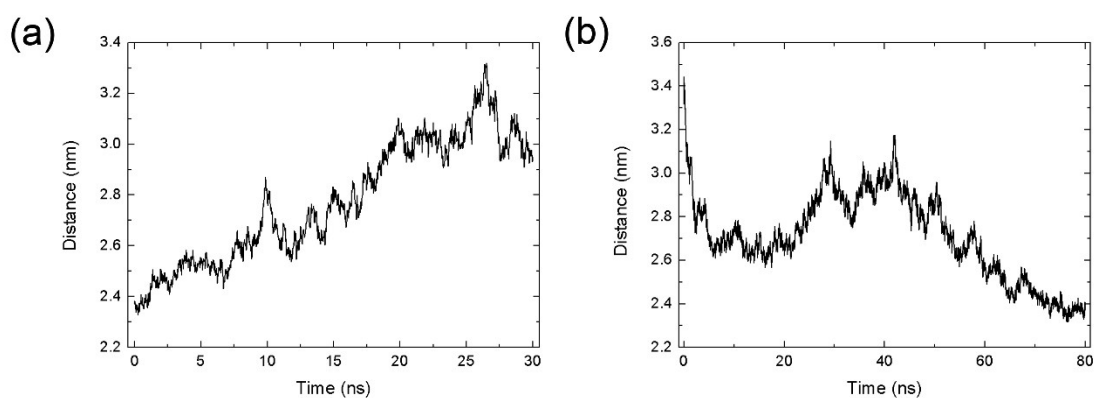


Fig. S6: The distance between the mass center of HSA and SAM surface in *adjustment-25%* (a) and *adsorption-50%* (b).

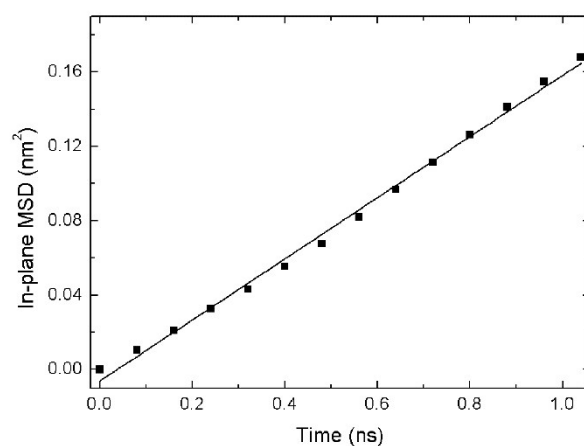


Fig. S7: The in-plane mean square displacement (MSD) of HSA in *adsorption-25%*.

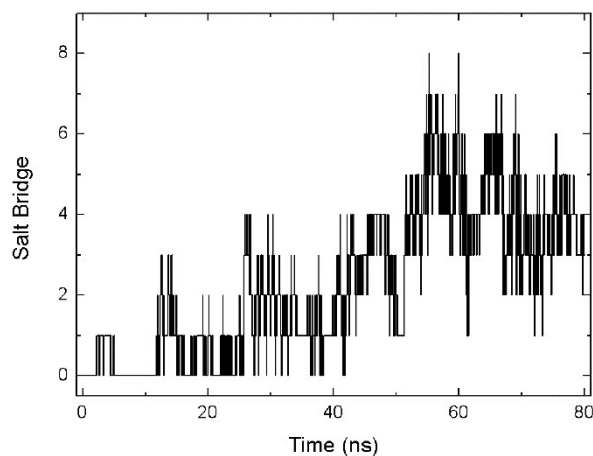


Fig. S8: The number of salt bridge between HSA and SAM in *adsorption-25%*.

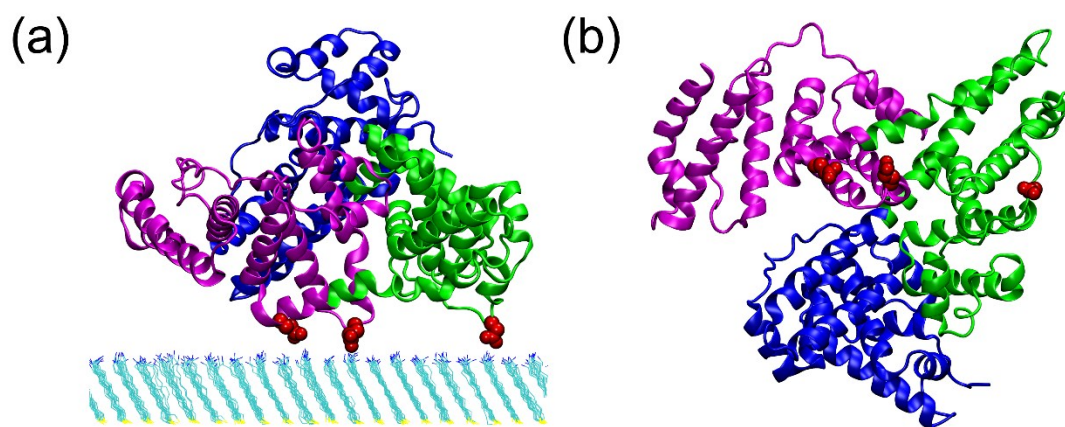


Fig. S9: Final configuration of HSA in *adsorption-25%*: side view (a); bottom view (b). Domains I, II and III are in blue, green and magenta, respectively. Acidic residues that

form salt bridges with SAM are colored in red.

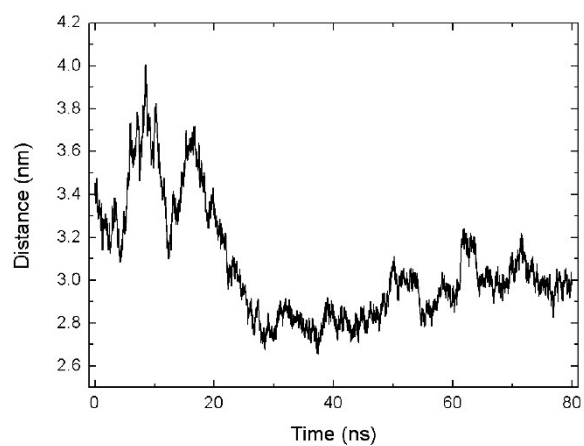


Fig. S10: The distance between the mass center of HSA and SAM surface in *adsorption-25%*.

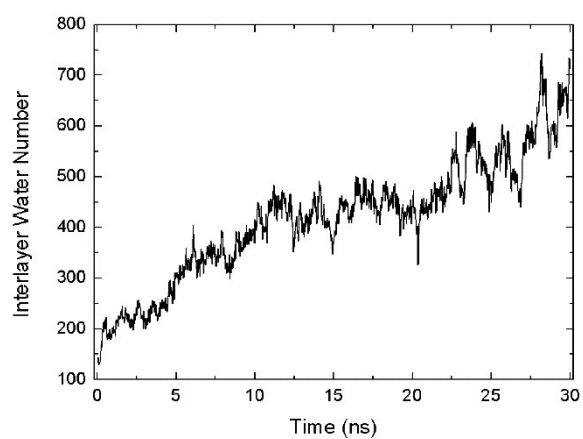


Fig. S11: The number of *interlayer water* during protein desorption.

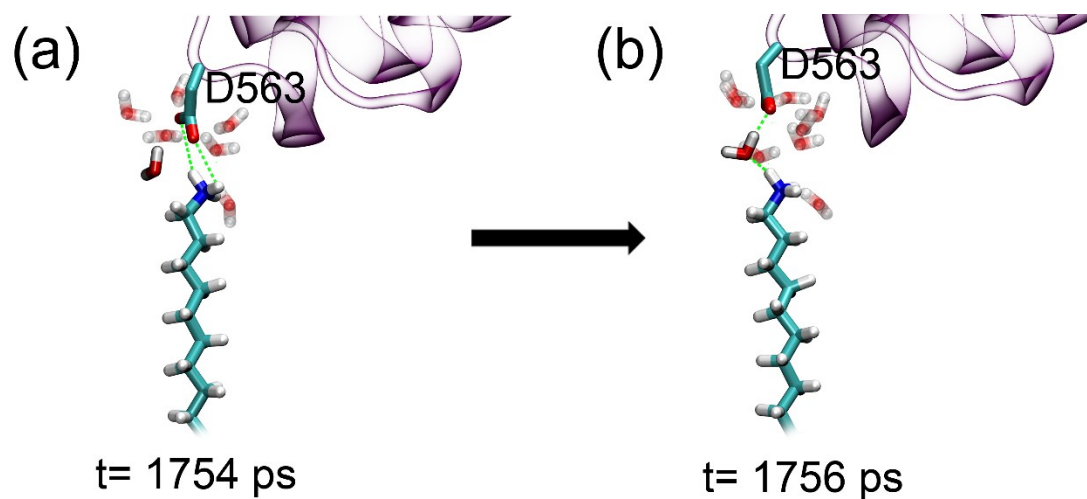


Fig. S12: Water-mediated breakage of salt bridge. There are multiple water molecules around the salt bridge formed by Asp563 with -NH_3^+ group (a). Once the salt bridge is broken, the water molecule inserts in-between the salt-bridge groups, forming a water bridge (b).

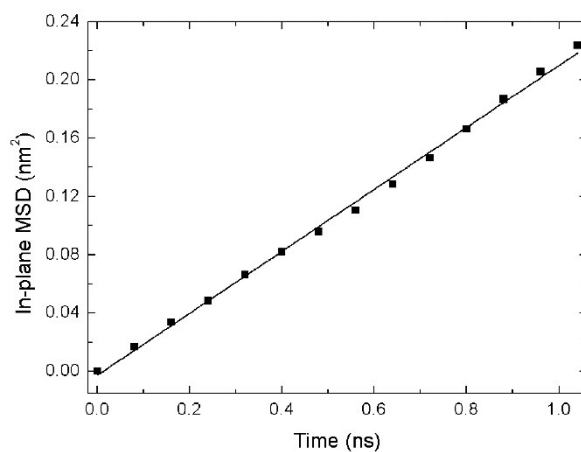


Fig. S13: The in-plane mean square displacement (MSD) of HSA in *adjustmen-6.3%*.

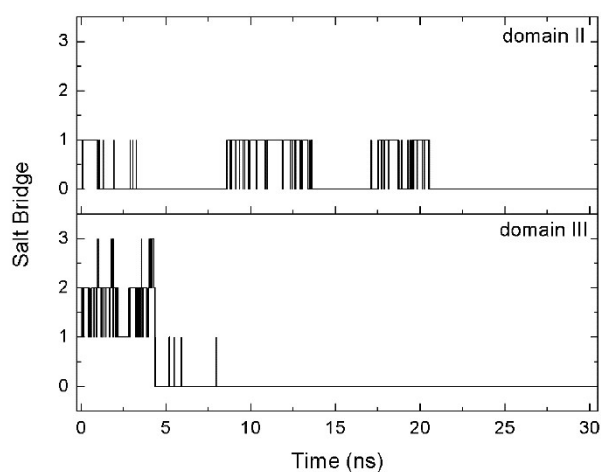


Fig. S14: The number of salt bridge formed by domains II and III with SAM during protein desorption.