

Supporting Information

Spontaneous desorption of protein from self-assembled monolayer (SAM)-coated gold nanoparticles induced by high temperature

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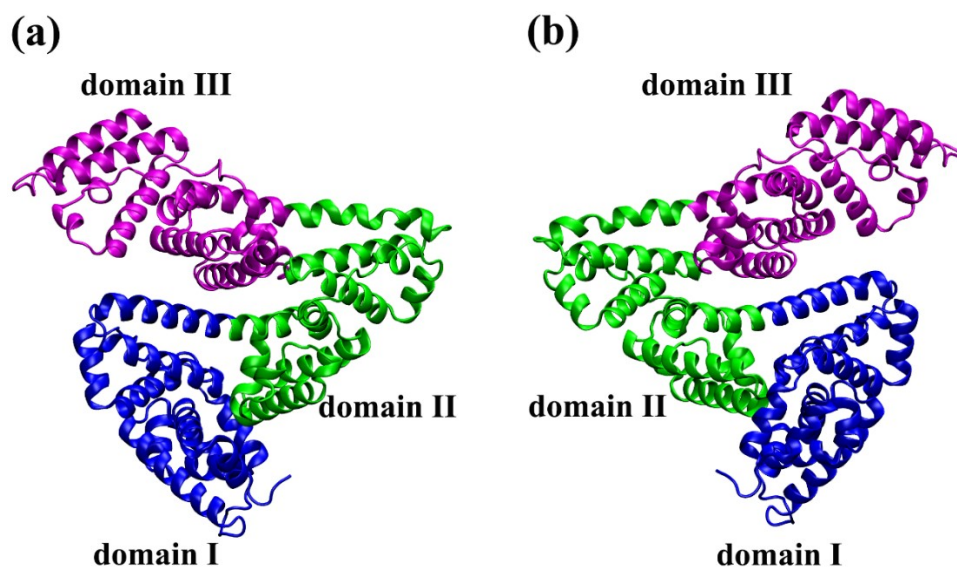


Fig. S1: The bottom view of plane A (a) and plane B (b) of HSA. The three domains of HSA are colored in blue (domain I: residues 2–195), green (domain II: residues 196–383) and magenta (domain III: residues 384–583).

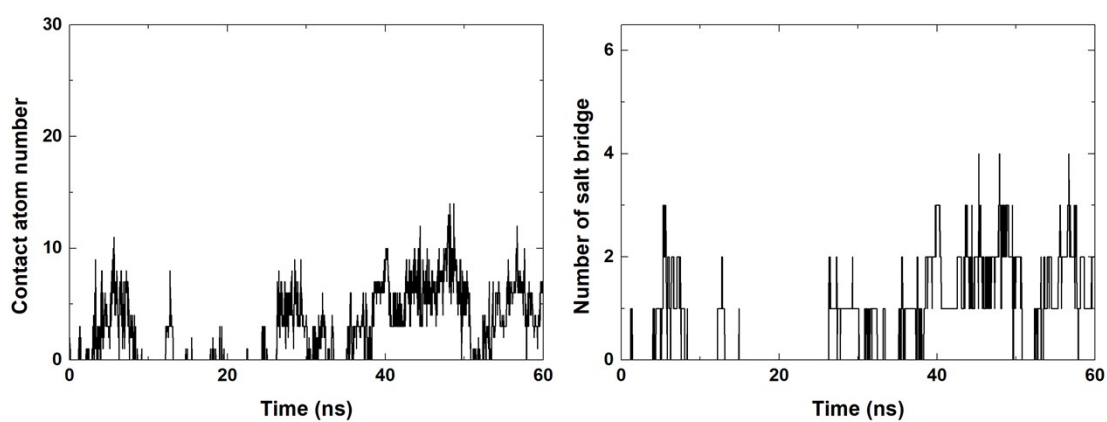


Fig. S2 The number of contact atoms of plane B of HSA with SAM at 300K, and the number of salt bridges formed between plane B of HSA and SAM at 300K.

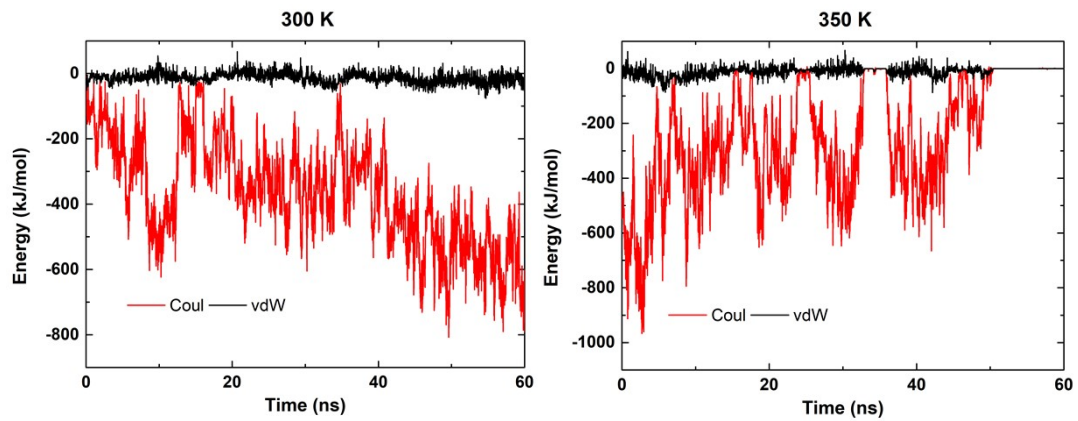


Fig. S3 The Coulomb interaction potential (Coul) and van der Waals interaction potential (vdW) between HSA and SAM at the temperature of 300K and 350K.

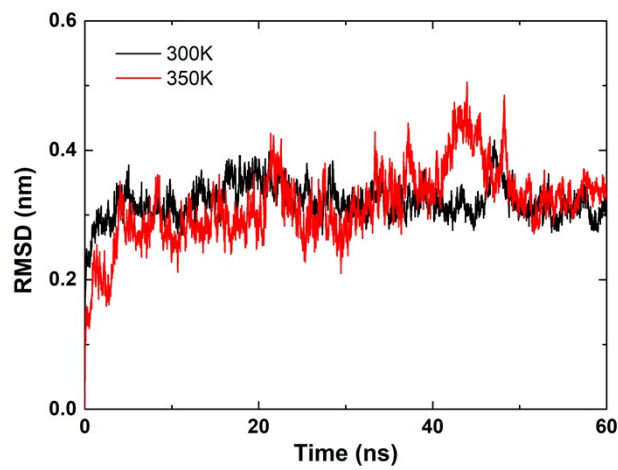


Fig. S4 The comparison of RMSD of HSA during its binding process with SAM between 300K and 350K.

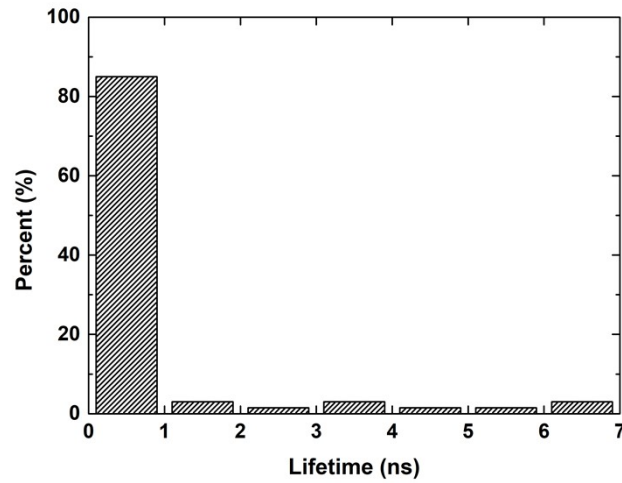


Fig. S5 The distribution of lifetime of HSA adsorption on SAM after $t = 6.8$ ns at 350K.

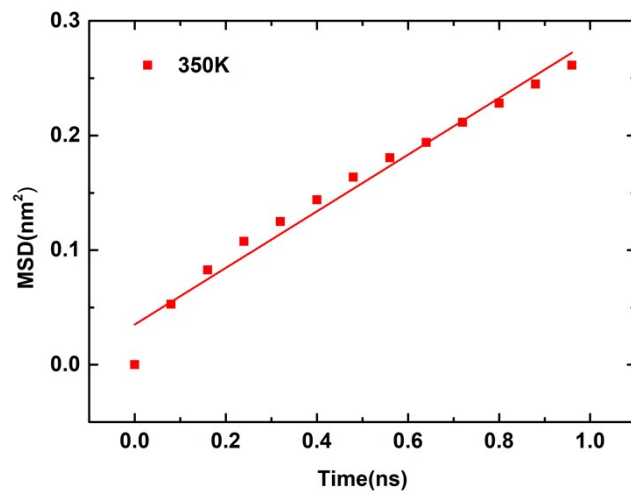


Fig. S6 The mean square displacement (MSD) of HSA before $t = 6.8$ ns at 350K.

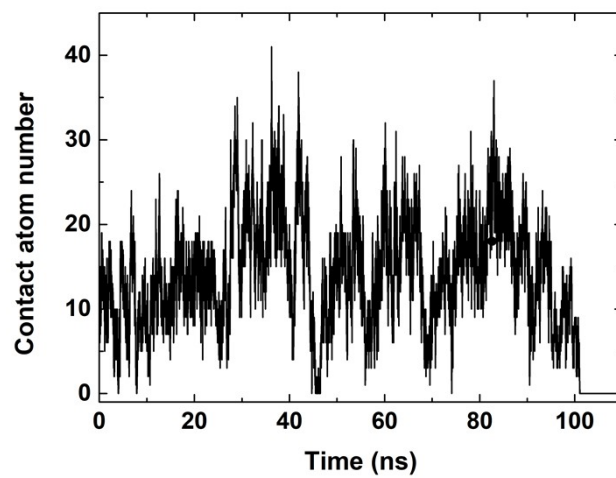


Fig. S7. The number of contact atoms of plane A of HSA with SAMs for another simulation at the temperature of 350K.