Supporting Information

An *In Silico* study of TiO_2 nanoparticles interaction with twenty standard amino acids in aqueous solution

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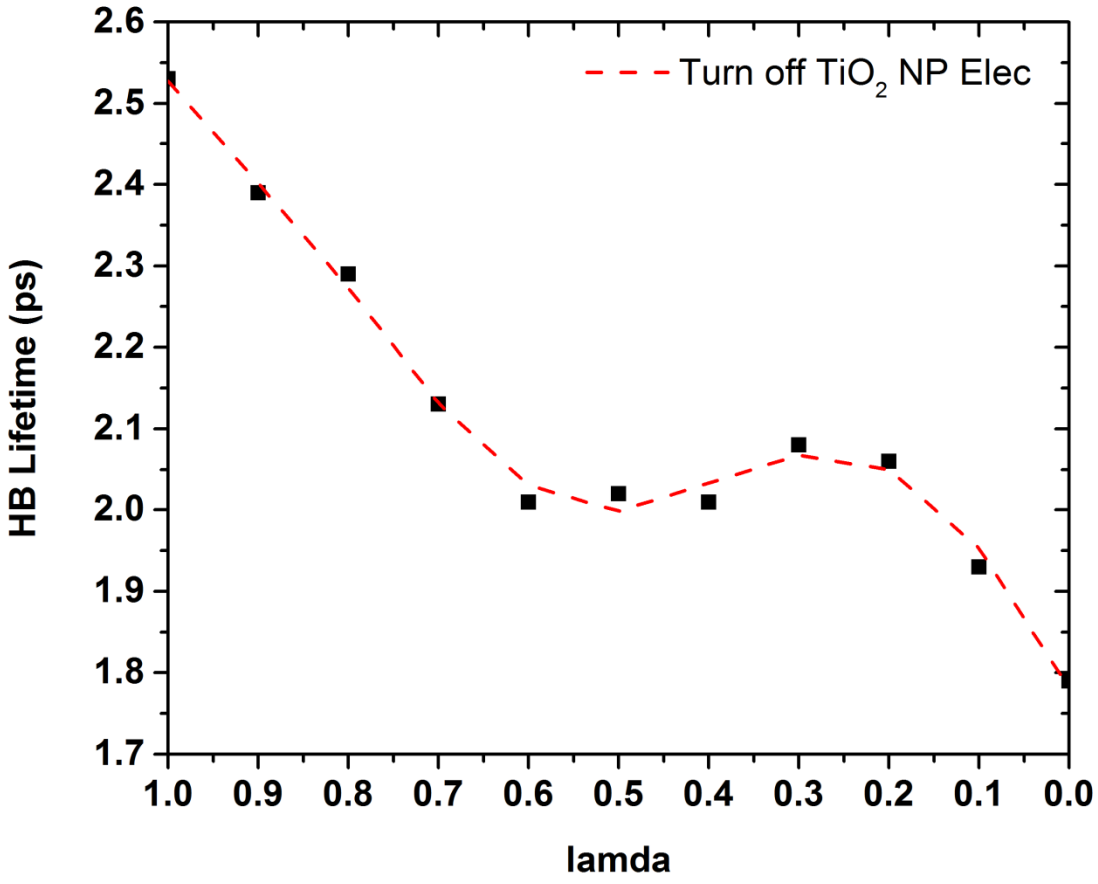

Fig. S1. Hydrogen bond lifetime profile when turning off TiO_2 NP atomic partial charges. The lamda is coefficient applied to TiO_2 atomic charge, lamda=1 stands for turning on atomic charge totally, lamda=0 means completely turning off the charges.

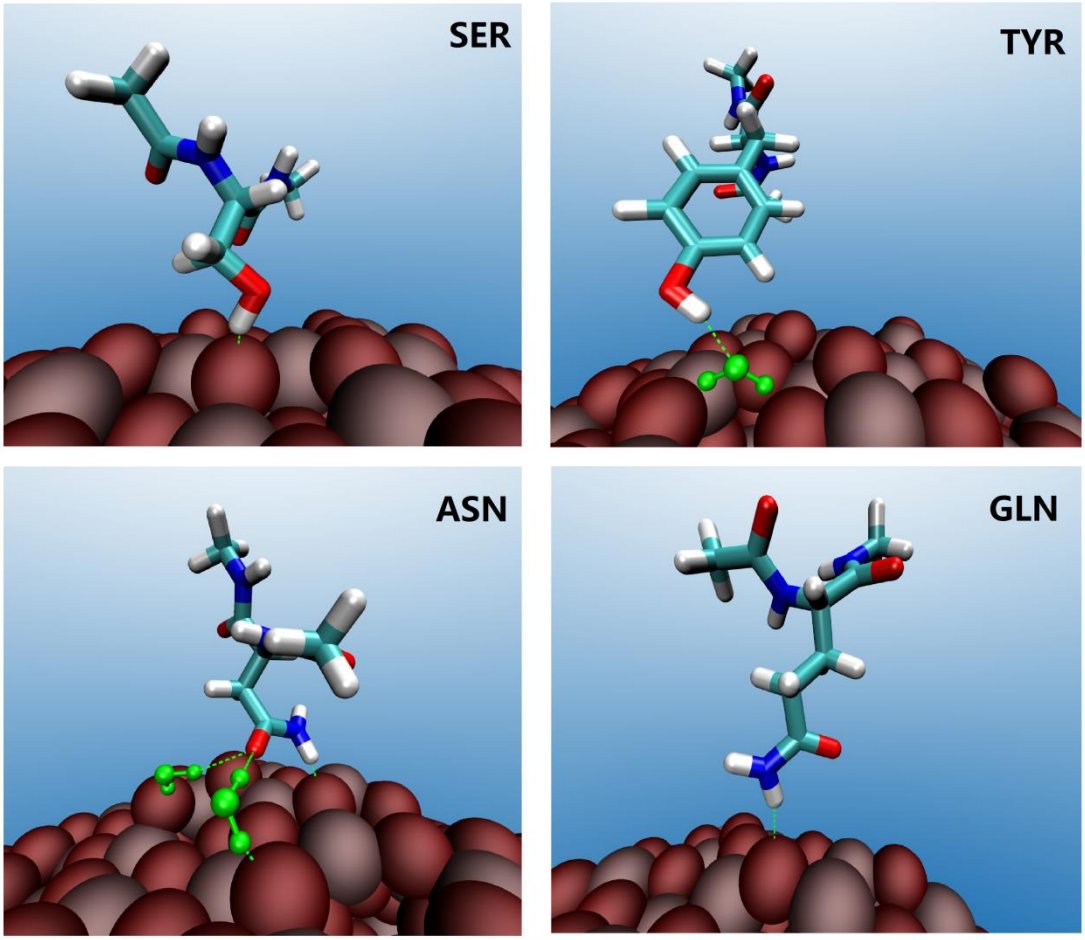

Fig. S2. Representative configuration of Ser, Tyr, Asn, Gln adsorbed onto the TiO_2 nanoparticle surface.

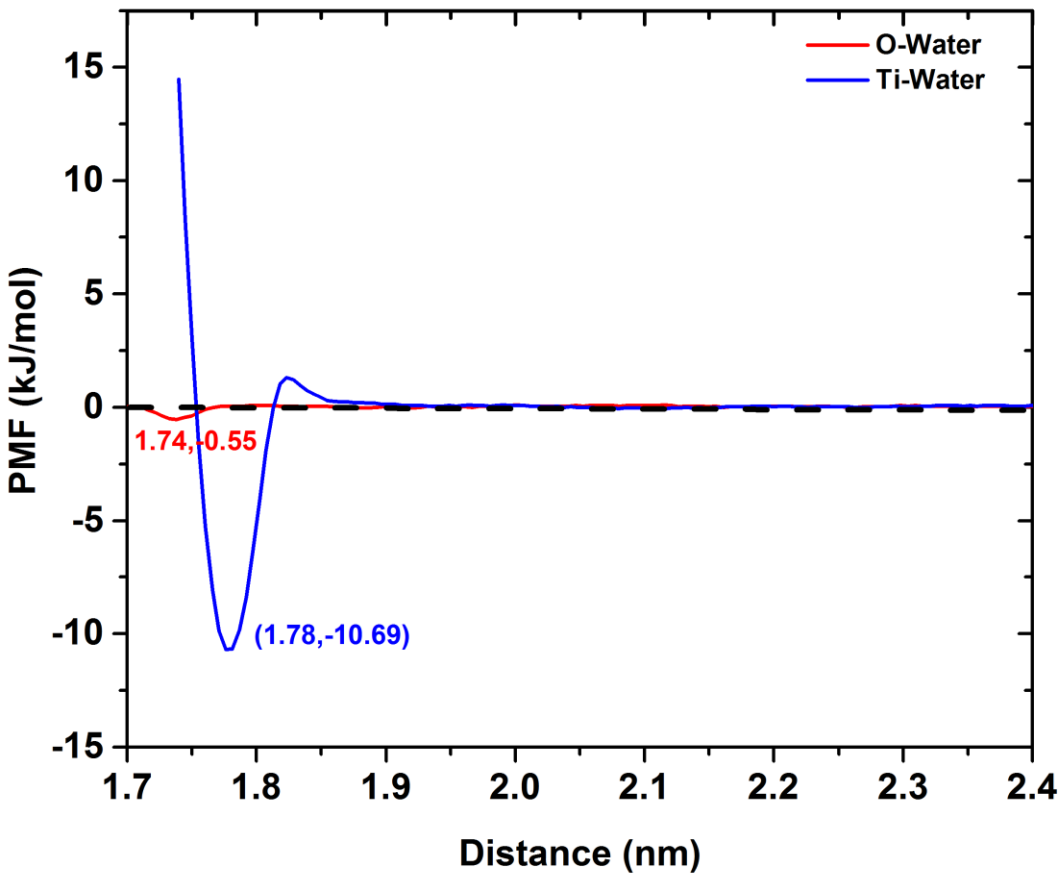

Fig. S3. Free energy profile of the adsorption of Ti-Water and O-Water.

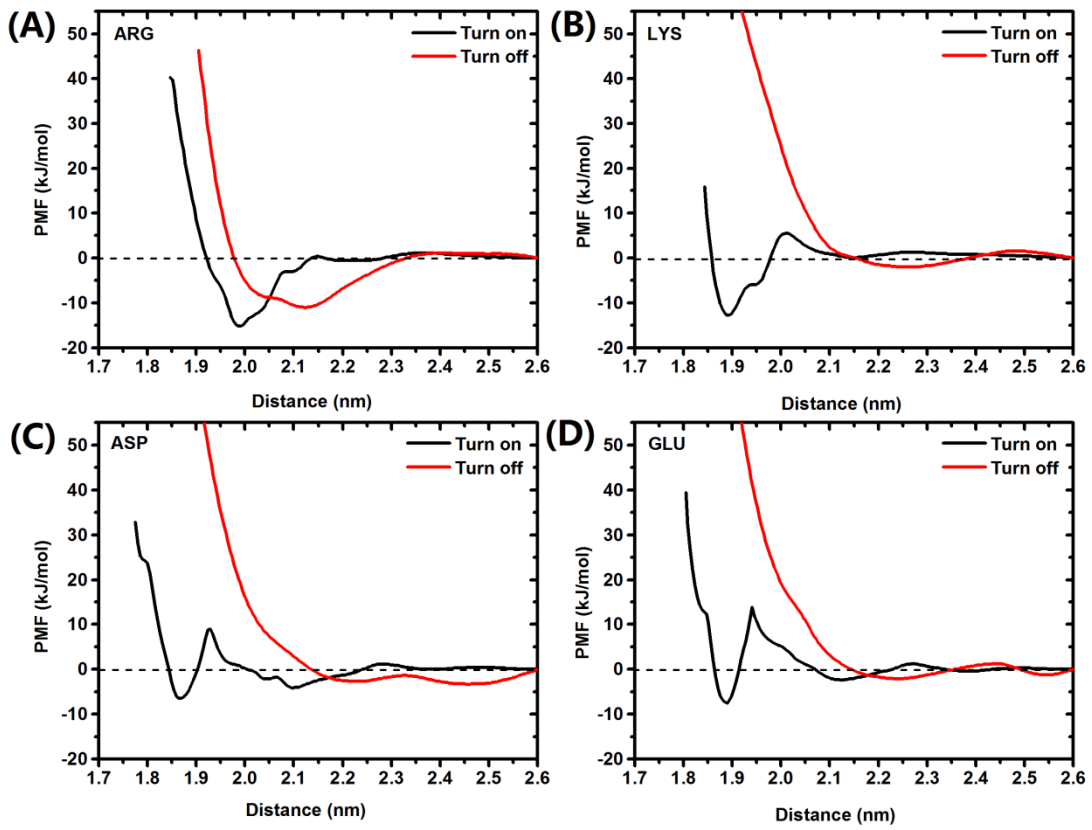

Fig. S4. Free energy profile of charged amino acids in the states of turn-on and turn-off TiO_2 NP atomic partial charge.

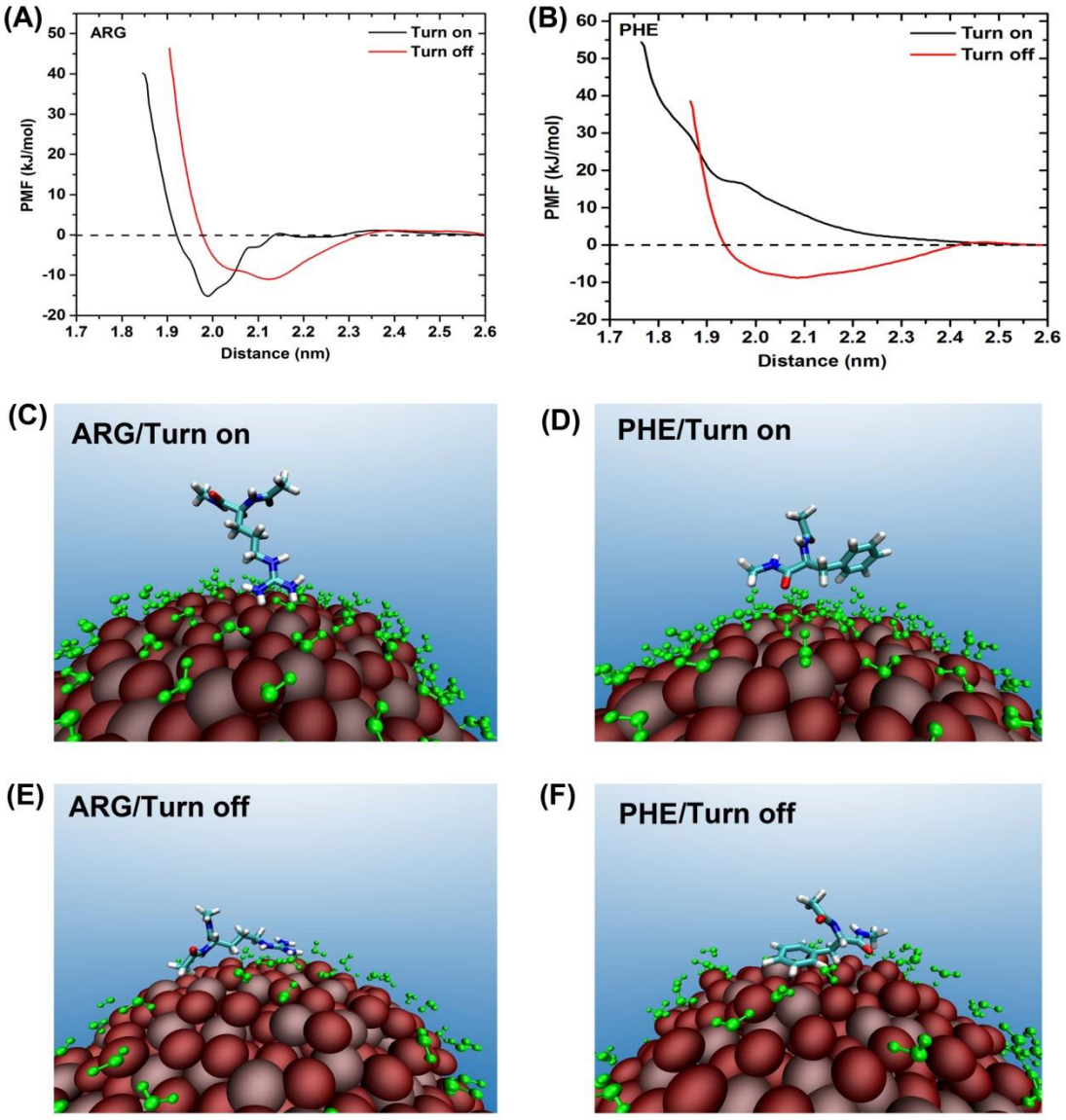

Fig. S5. Free energy profile of Arg and Phe when turning off TiO2 NP atomic charge (**A**-**B**), and their representative configurations (**C**-**F**).