Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Complexing Agent Study via Computational Chemistry for Environmentally Friendly Silver Electrodeposition and the Application of Silver Deposit

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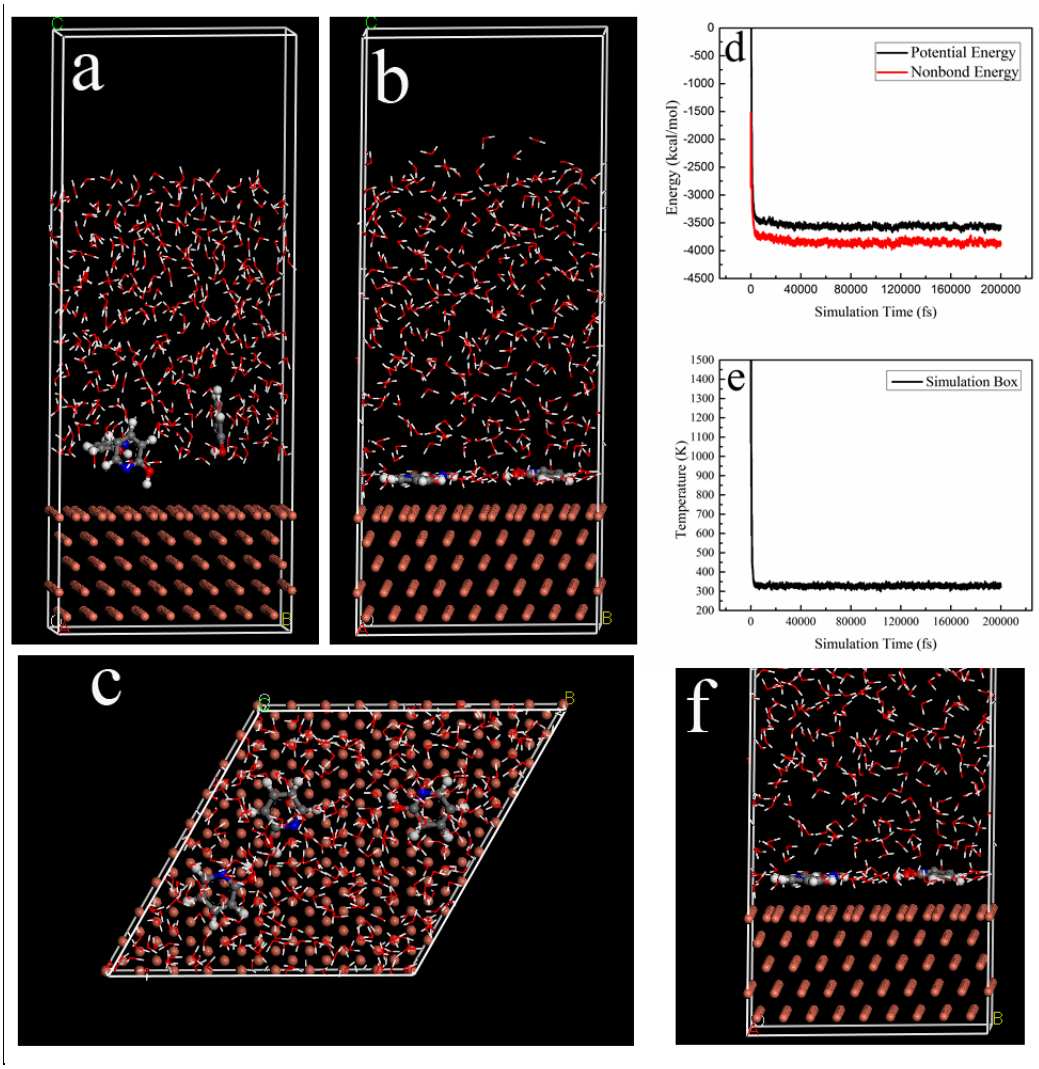

Fig. S1 (a) Initial configuration of the simulation box (2-Hydroxypyridine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of 2-Hydroxypyridine on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of 2-Hydroxypyridine on Cu surface.

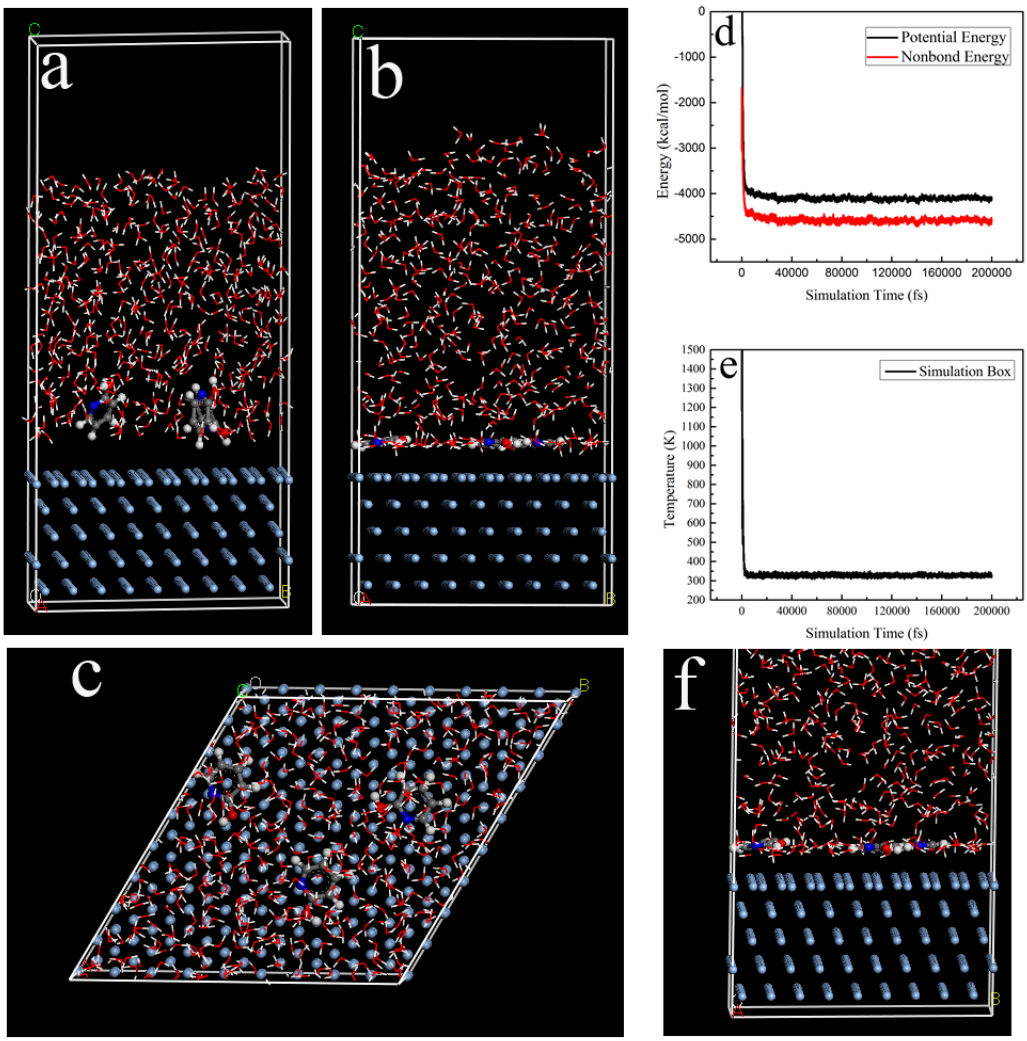

Fig. S2 (a) Initial configuration of the simulation box (2-Hydroxypyridine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of 2-Hydroxypyridine on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of 2-Hydroxypyridine on Ag surface.

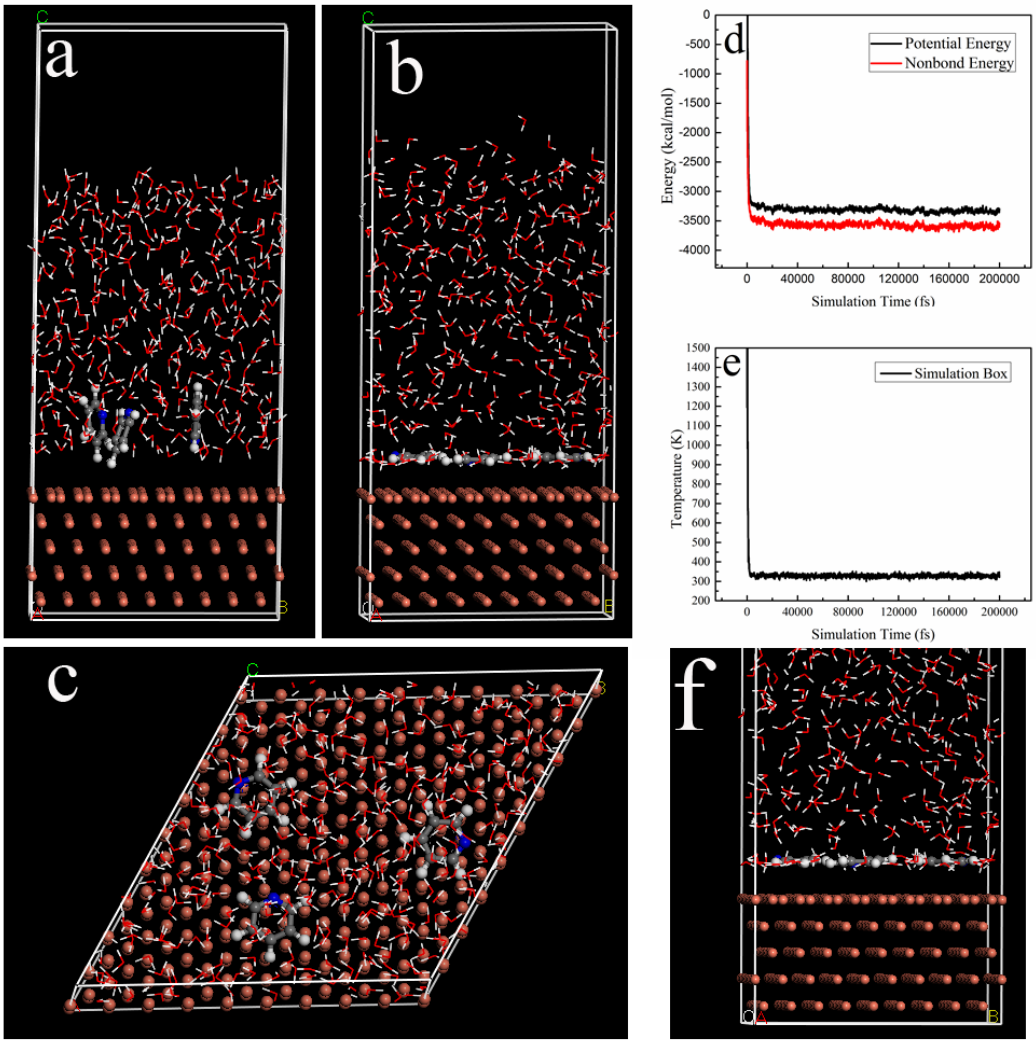

Fig. S3 (a) Initial configuration of the simulation box (Pyridine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Pyridine on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Pyridine on Cu surface.

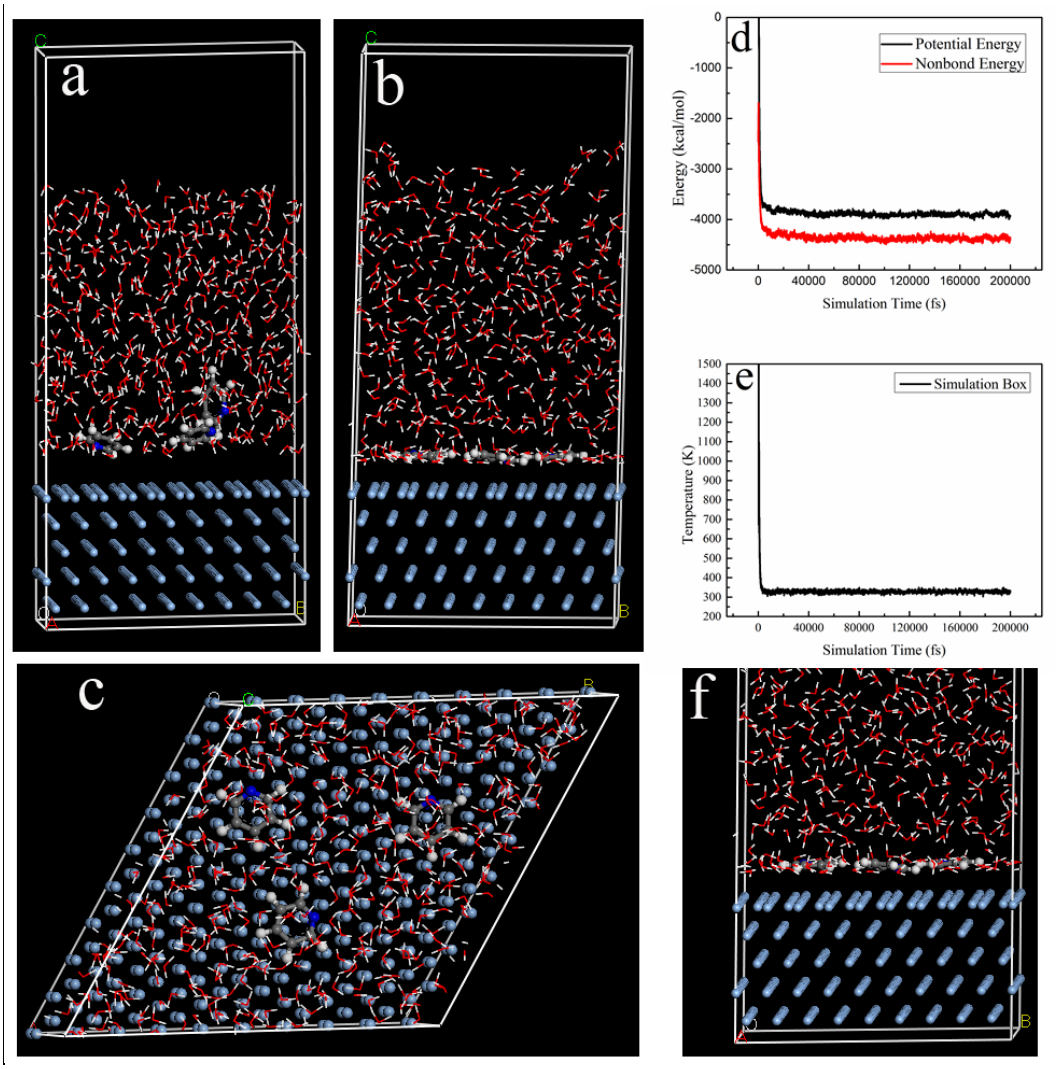

Fig. S4 (a) Initial configuration of the simulation box (Pyridine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Pyridine on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Pyridine on Ag surface.

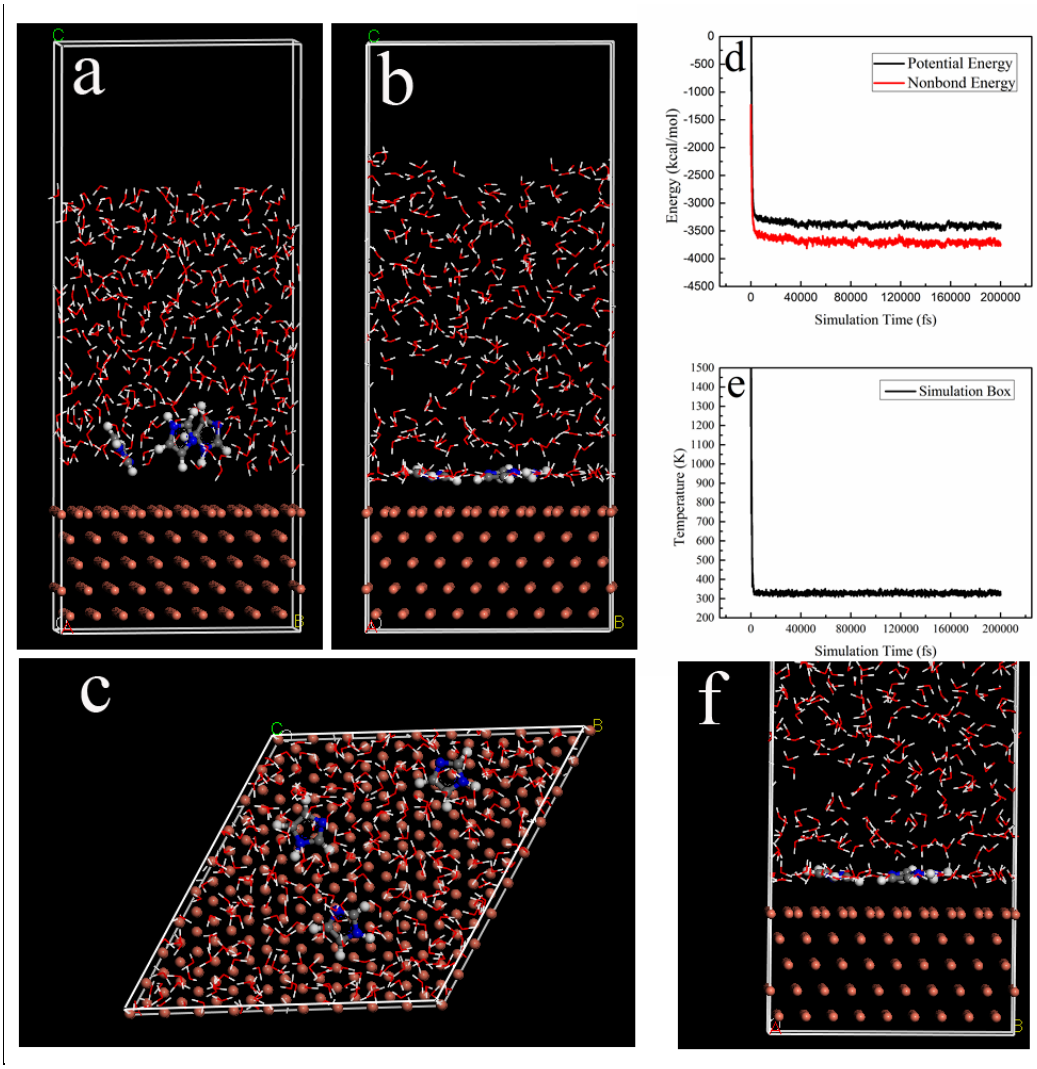

Fig. S5 (a) Initial configuration of the simulation box (Imidazole visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Imidazole on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Imidazole on Cu surface.

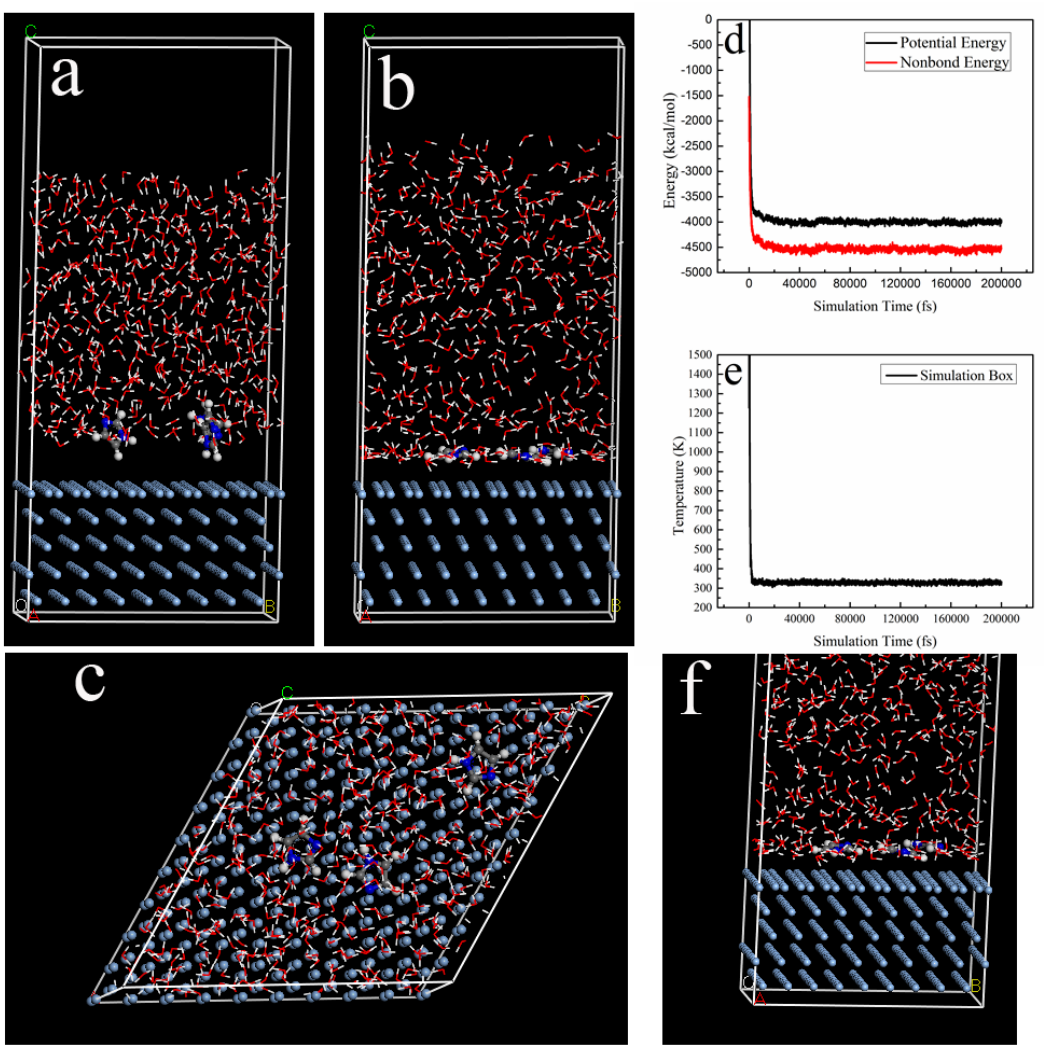

Fig. S6 (a) Initial configuration of the simulation box (Imidazole visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Imidazole on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Imidazole on Ag surface.

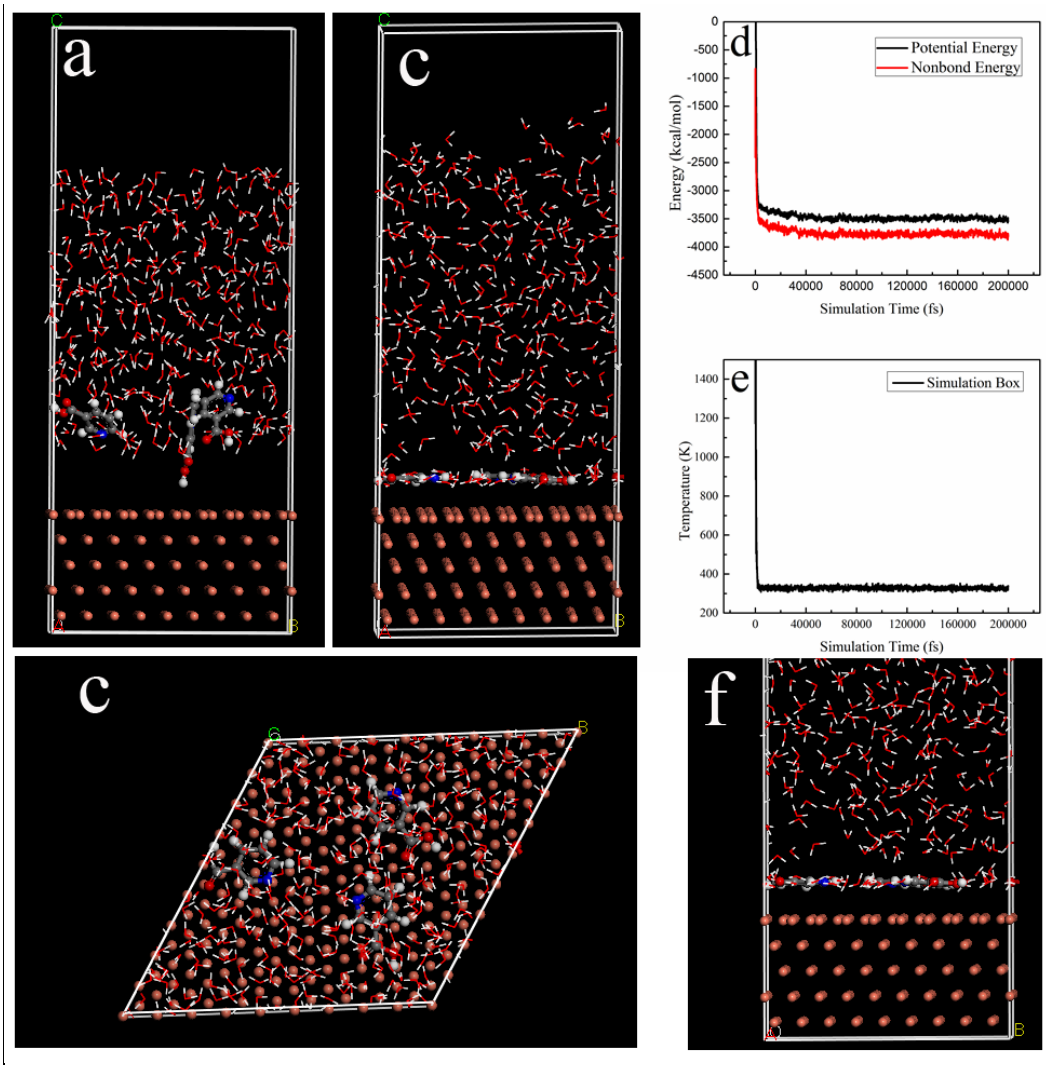

Fig. S7 (a) Initial configuration of the simulation box (NA visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of NA on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of NA on Cu surface.

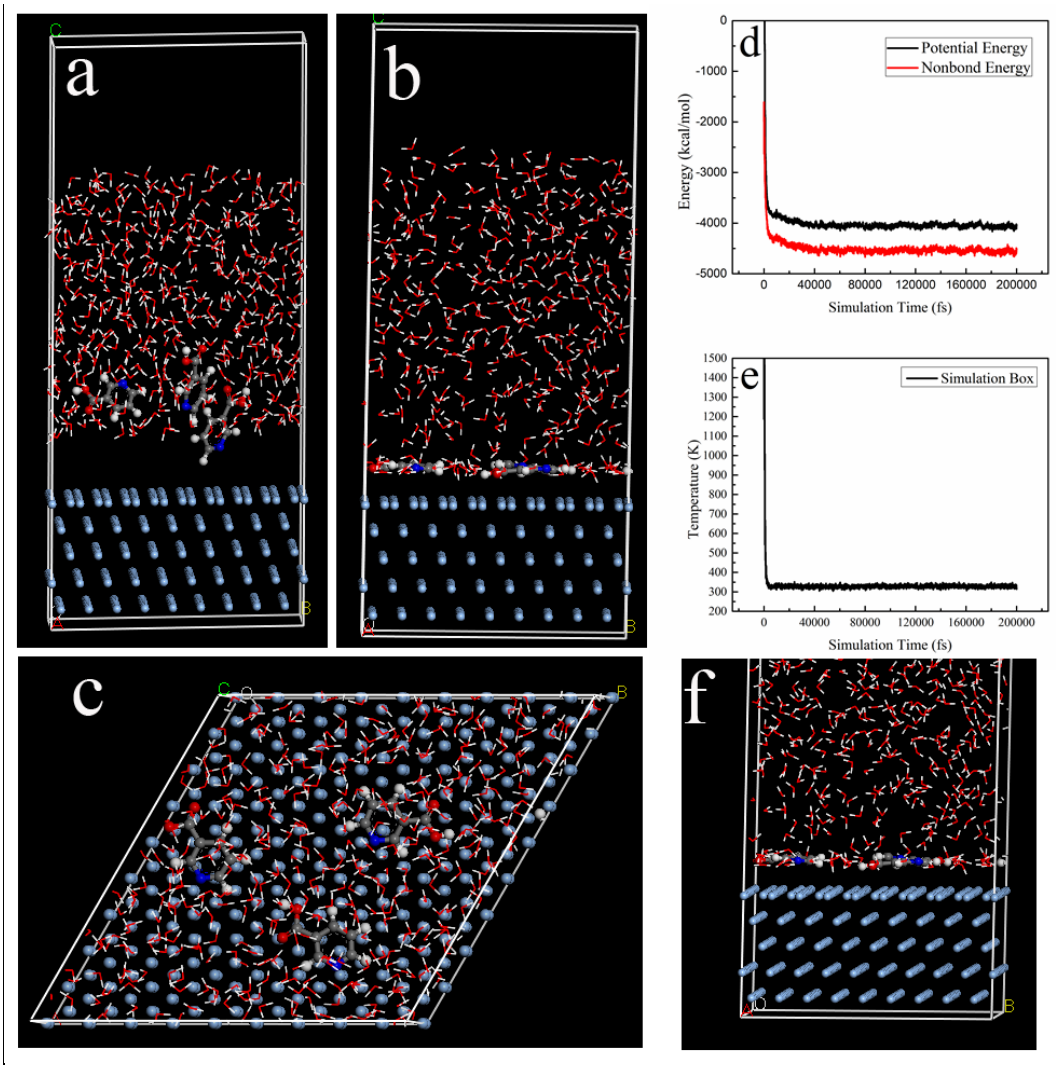

Fig. S8 (a) Initial configuration of the simulation box (NA visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of NA on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of NA on Ag surface.

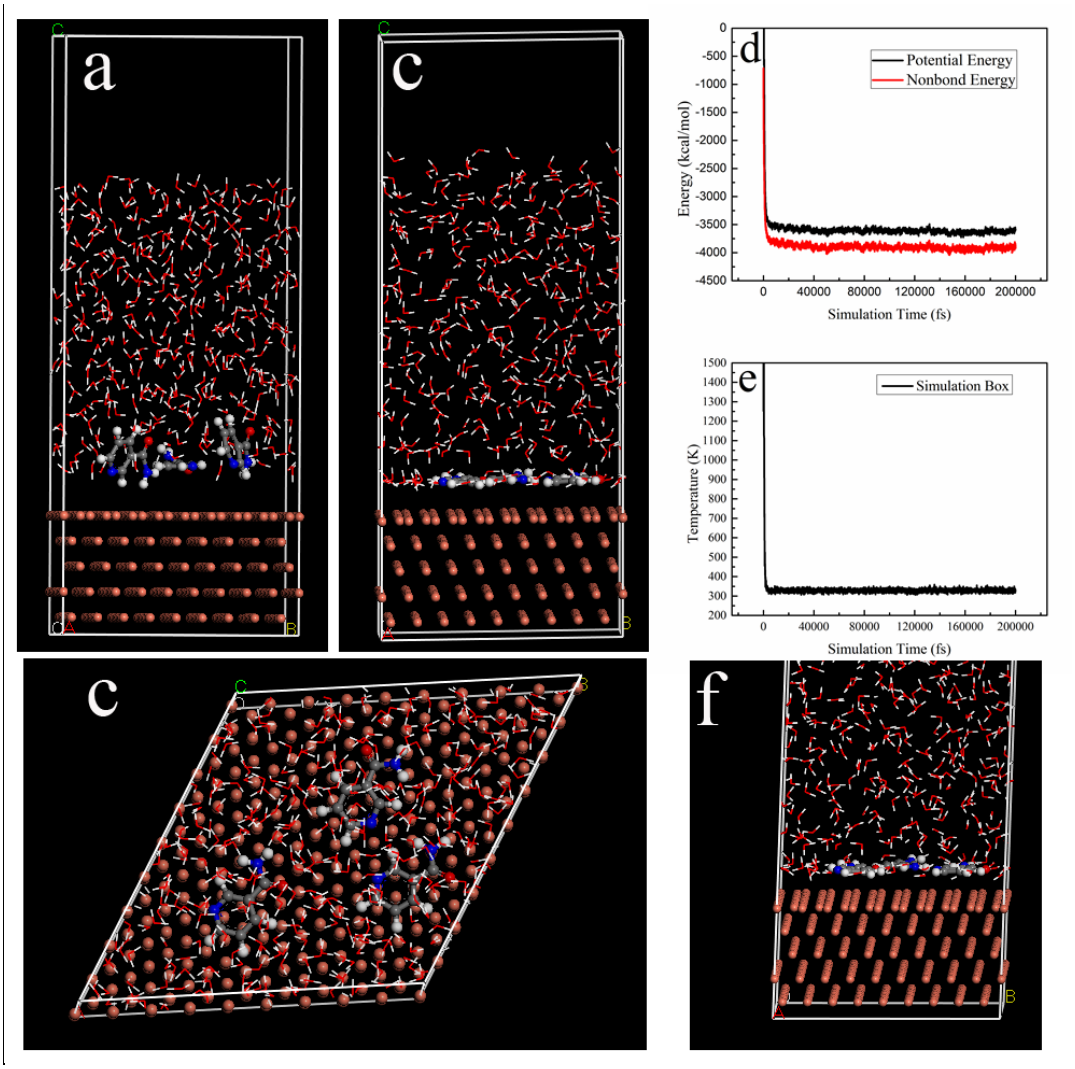

Fig. S9 (a) Initial configuration of the simulation box (Nicotinamide visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Nicotinamide on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Nicotinamide on Cu surface.

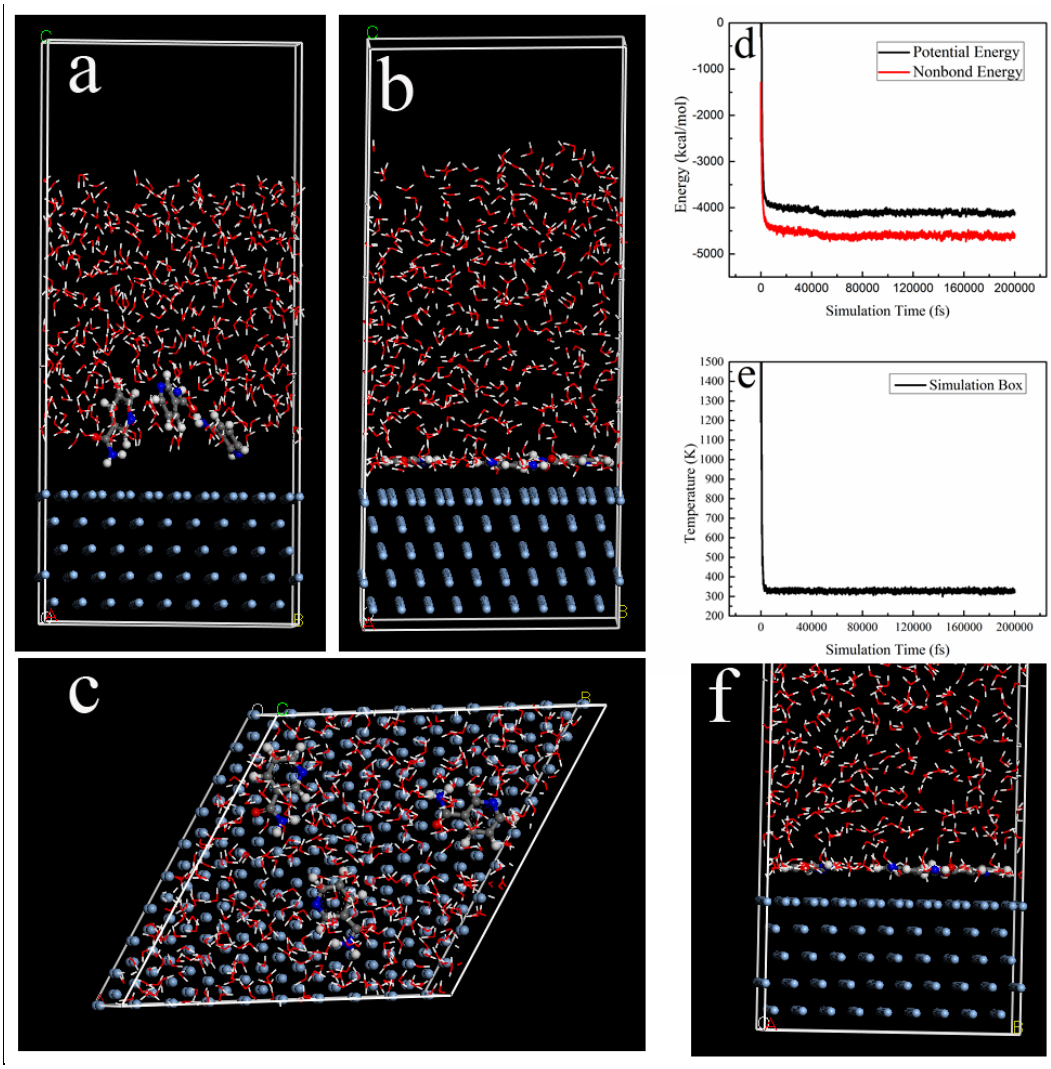

Fig. S10 (a) Initial configuration of the simulation box (Nicotinamide visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Nicotinamide on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Nicotinamide on Ag surface.

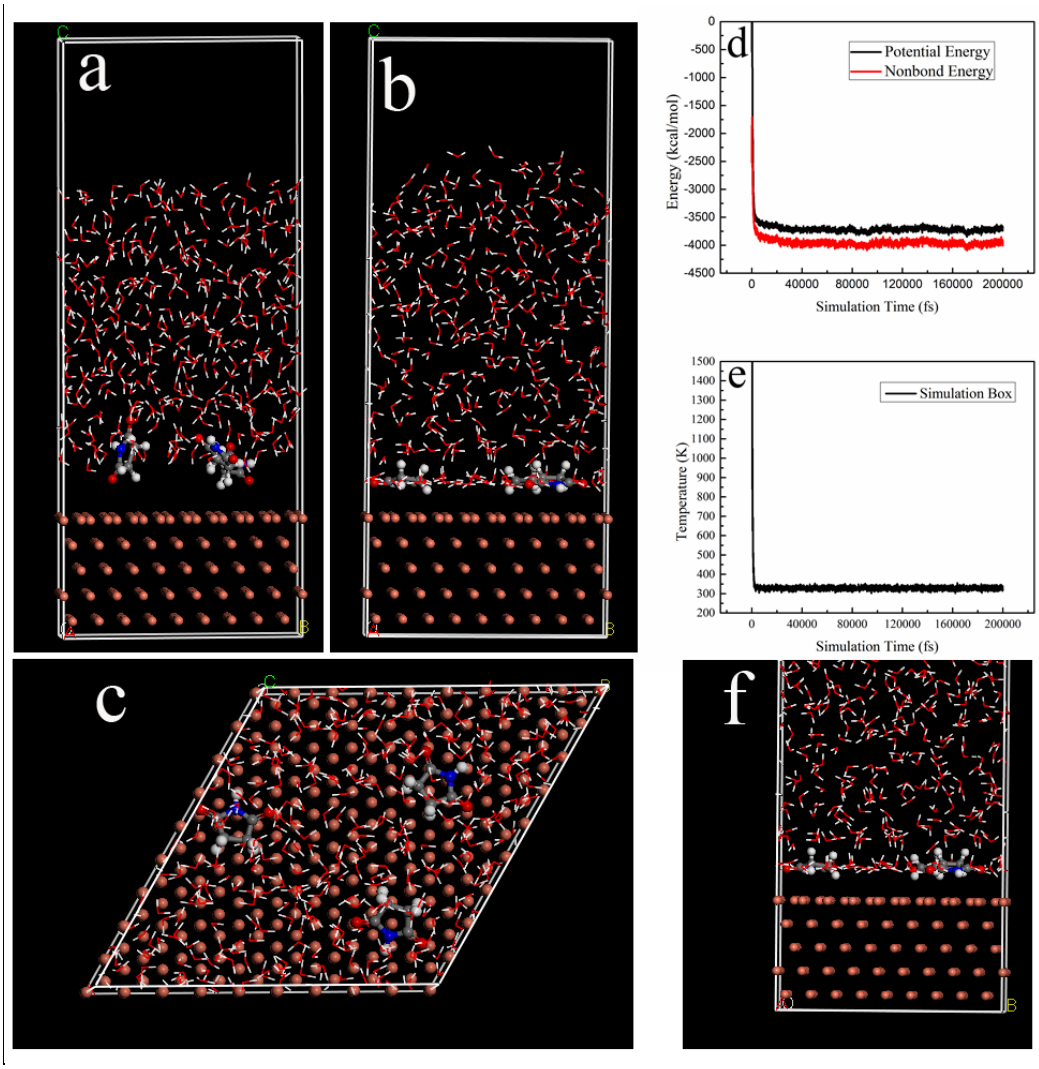

Fig. S11 (a) Initial configuration of the simulation box (Succinimide visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Succinimide on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Succinimide on Cu surface.

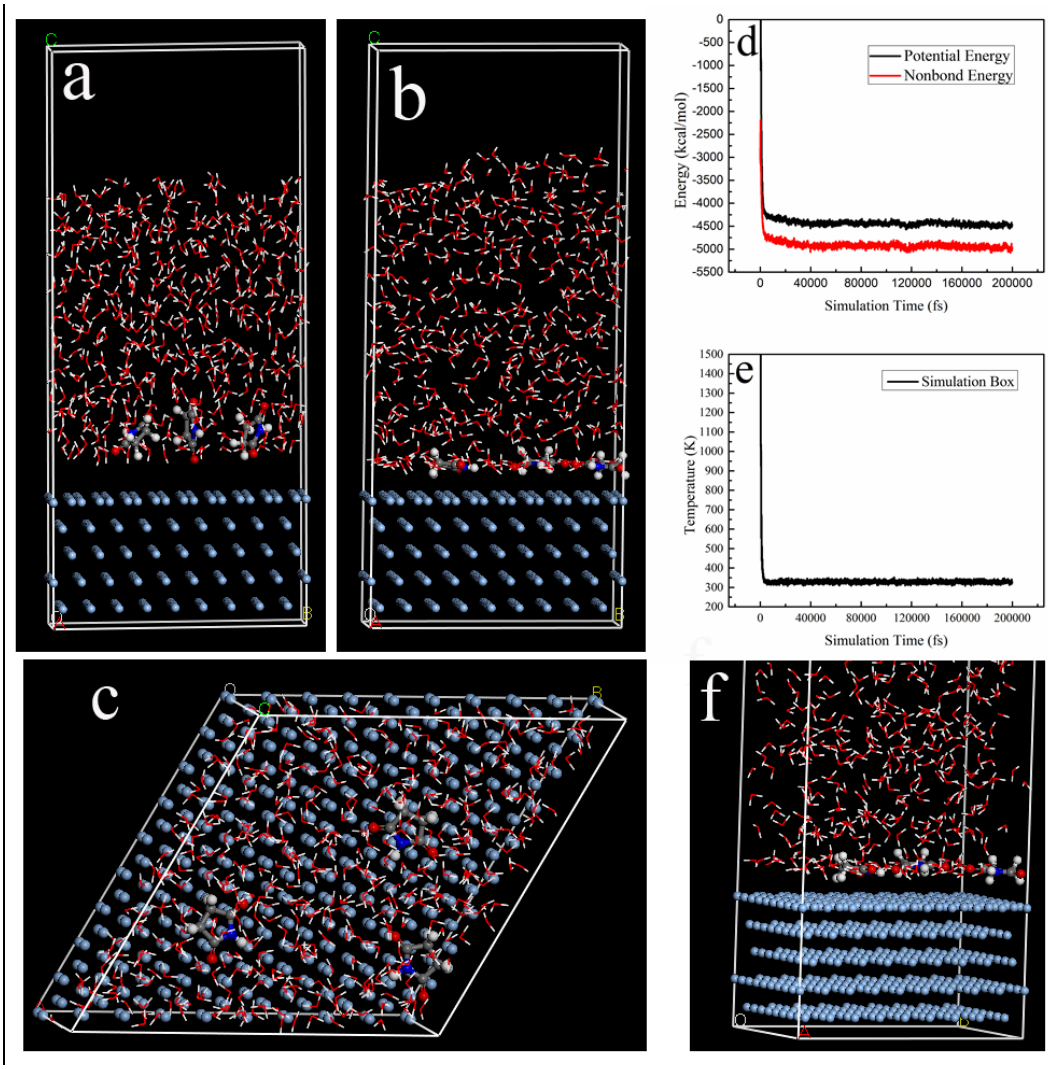

Fig. S12 (a) Initial configuration of the simulation box (Succinimide visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Succinimide on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Succinimide on Ag surface.

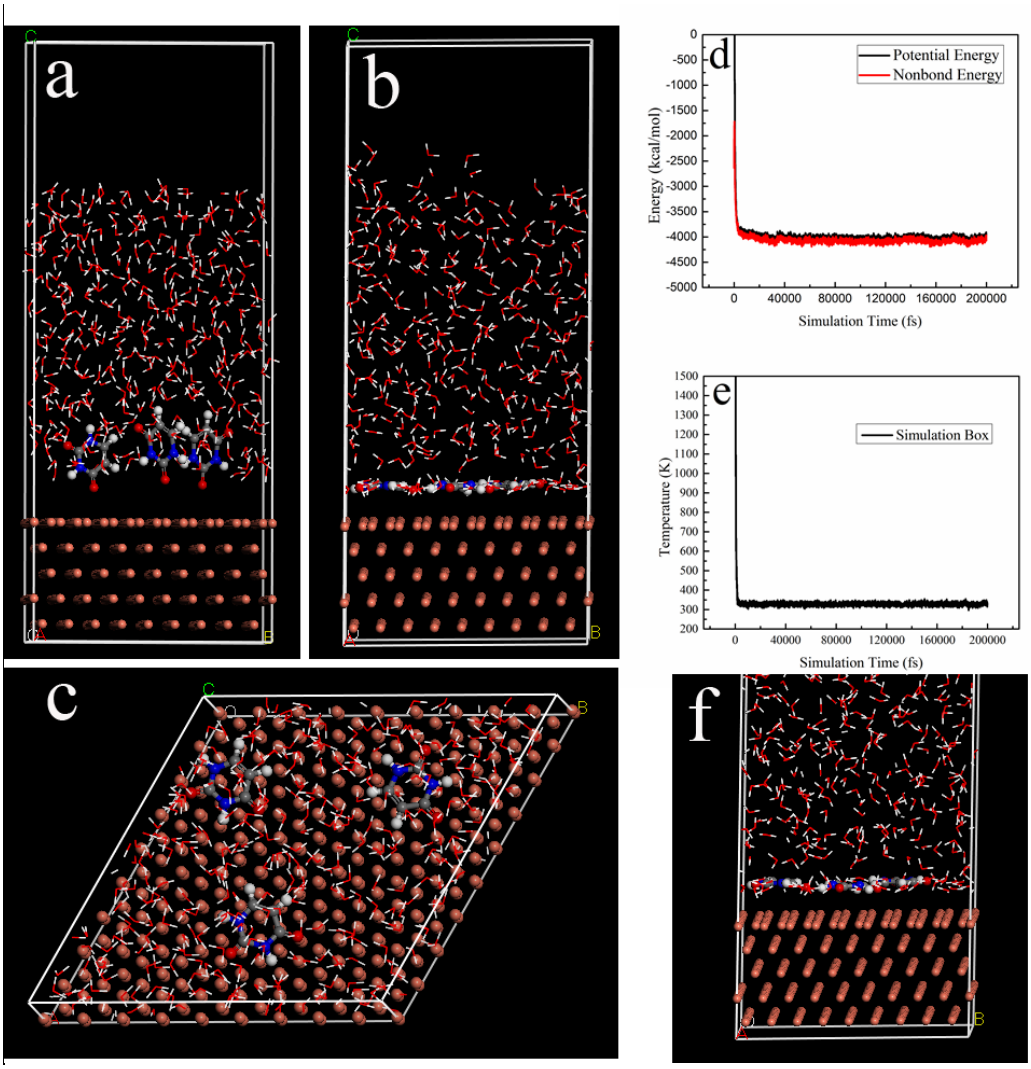

Fig. S13 (a) Initial configuration of the simulation box (Uracil visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Uracil on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Uracil on Cu surface.

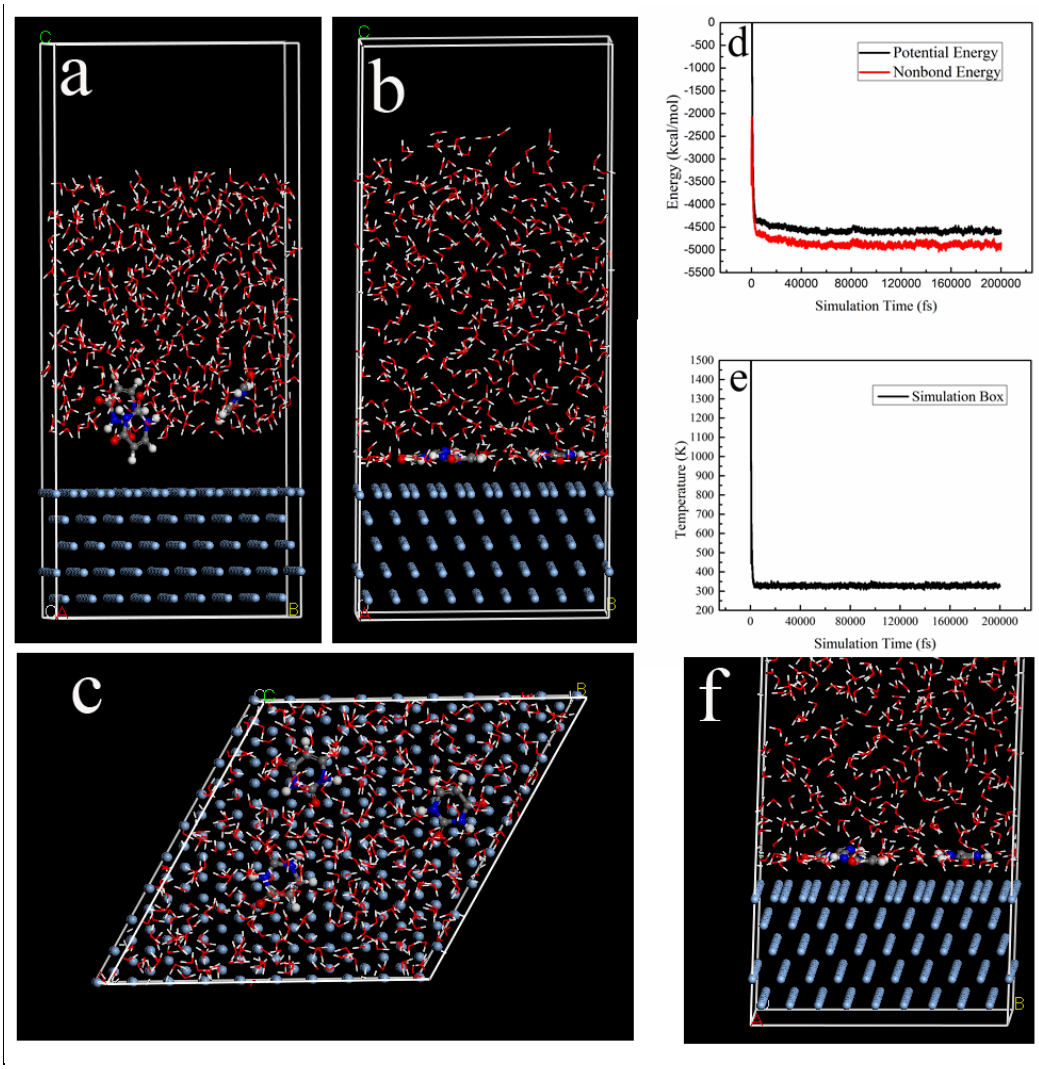

Fig. S14 (a) Initial configuration of the simulation box (Uracil visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Uracil on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Uracil on Ag surface.

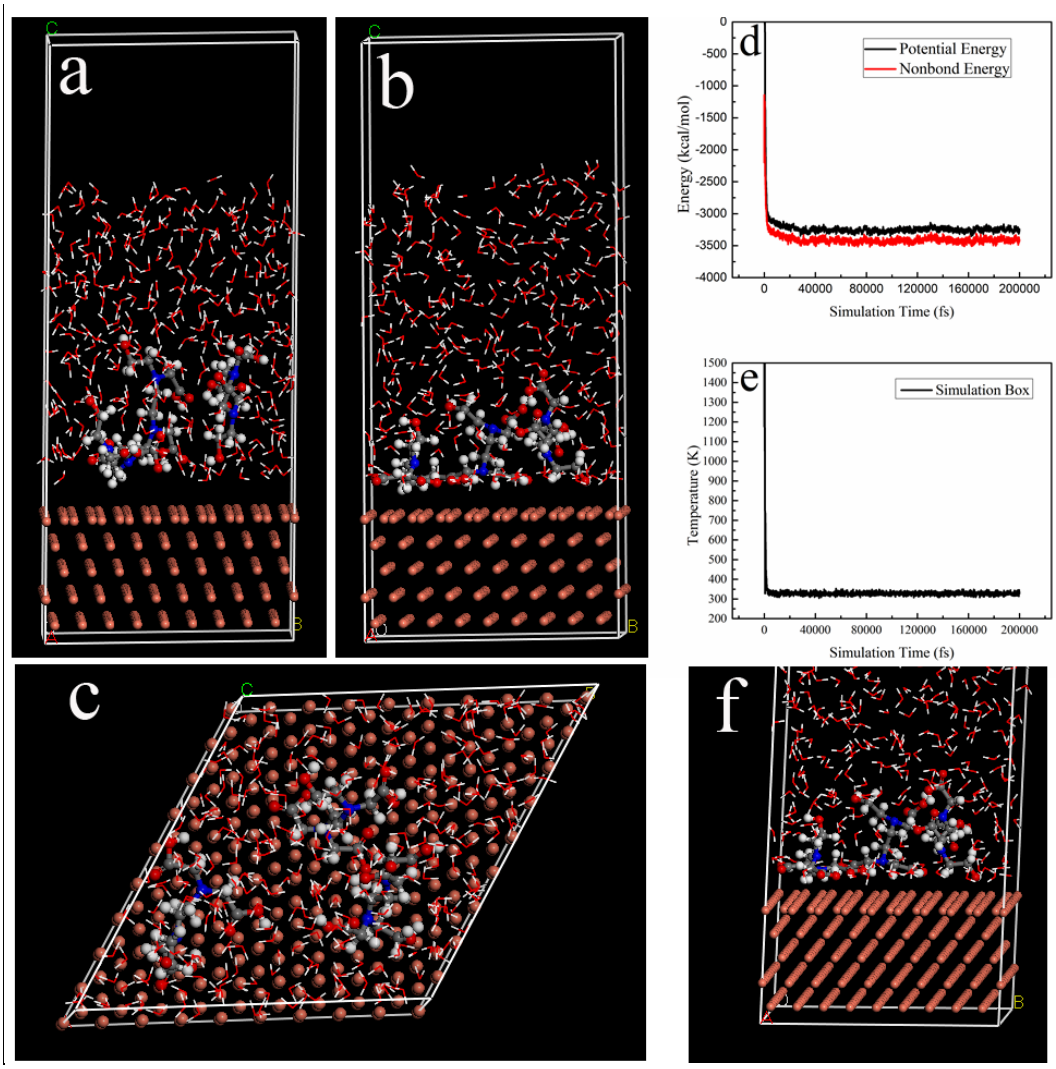

Fig. S15 (a) Initial configuration of the simulation box (HEDTA visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of HEDTA on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of HEDTA on Cu surface.

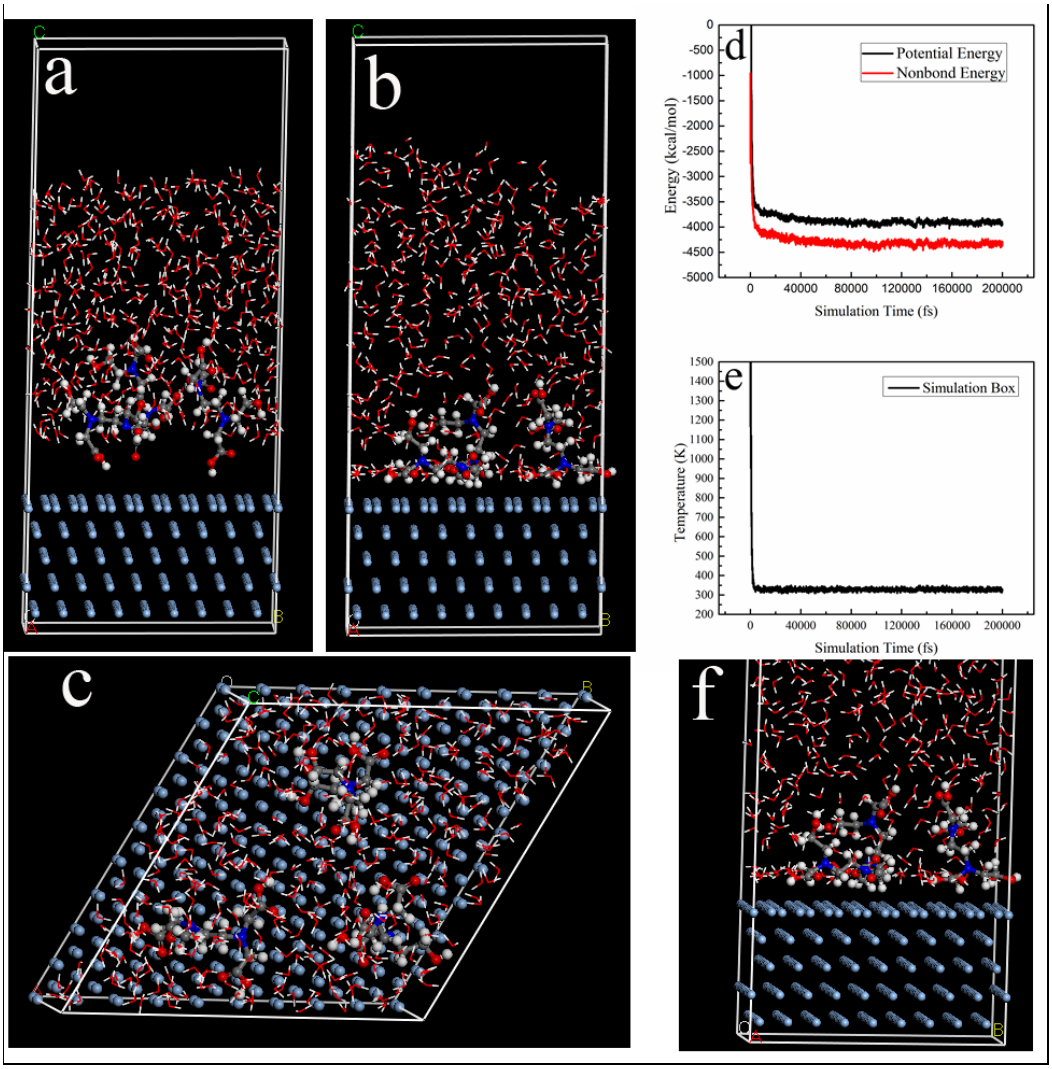

Fig. S16 (a) Initial configuration of the simulation box (HEDTA visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of HEDTA on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of HEDTA on Ag surface.

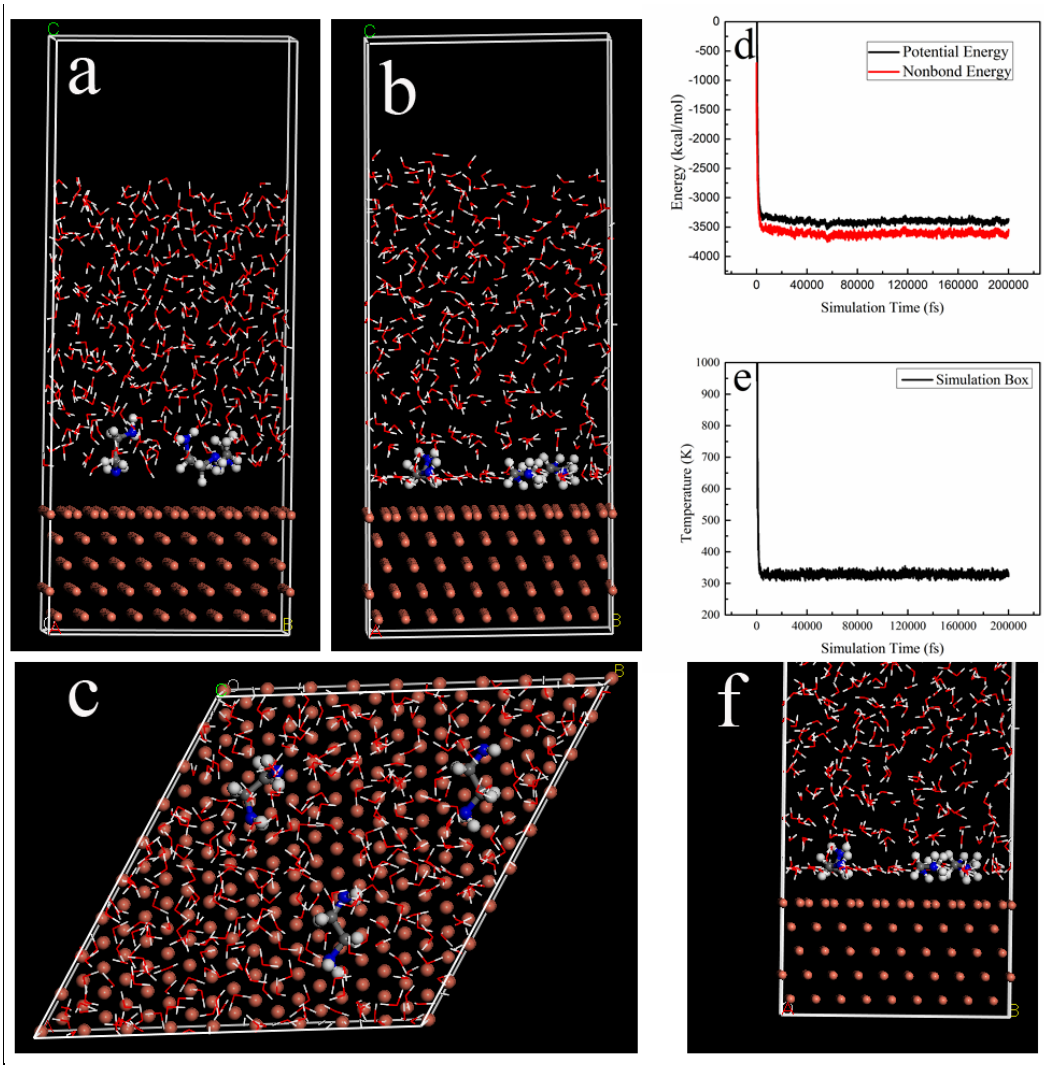

Fig. S17 (a) Initial configuration of the simulation box (Ethylenediamine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Ethylenediamine on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Ethylenediamine on Cu surface.

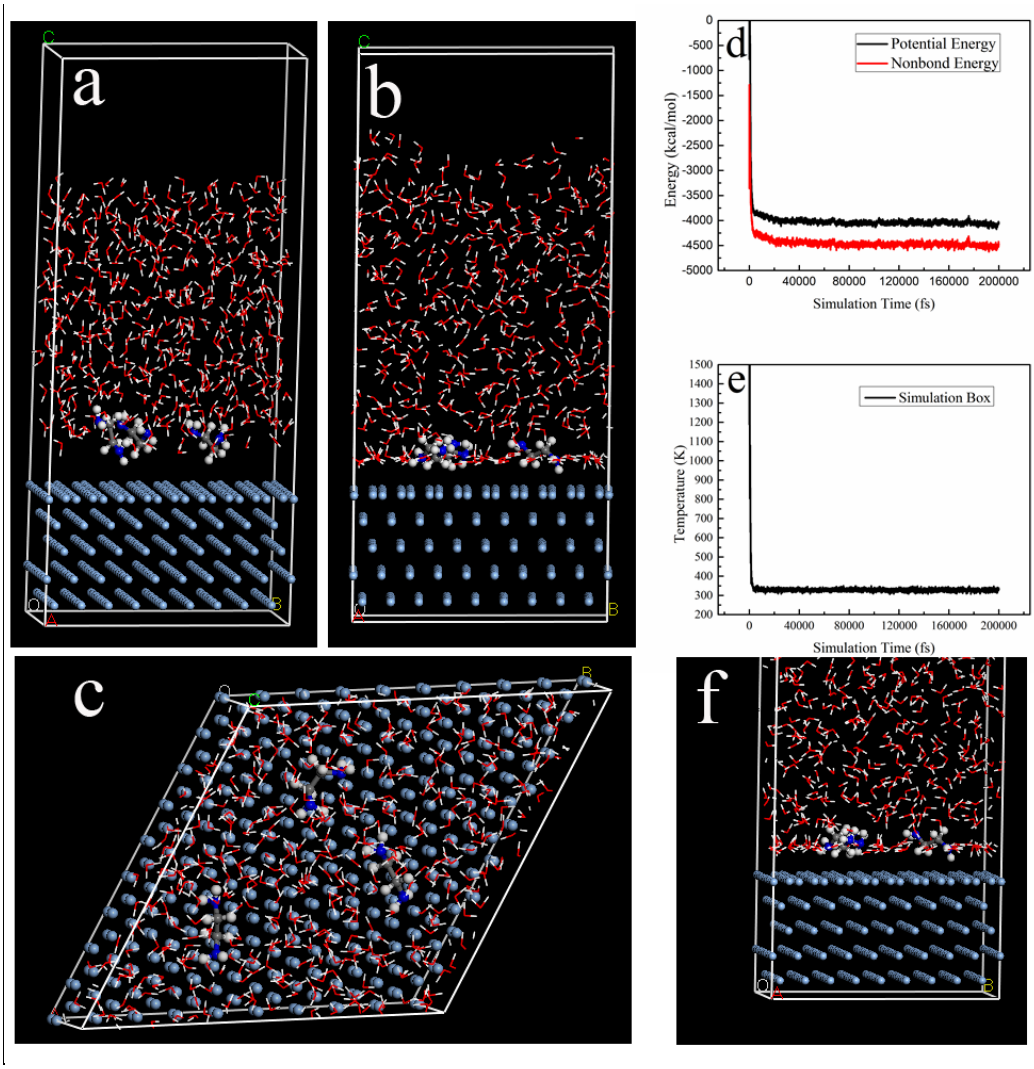

Fig. S18 (a) Initial configuration of the simulation box (Ethylenediamine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Ethylenediamine on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Ethylenediamine on Ag surface.

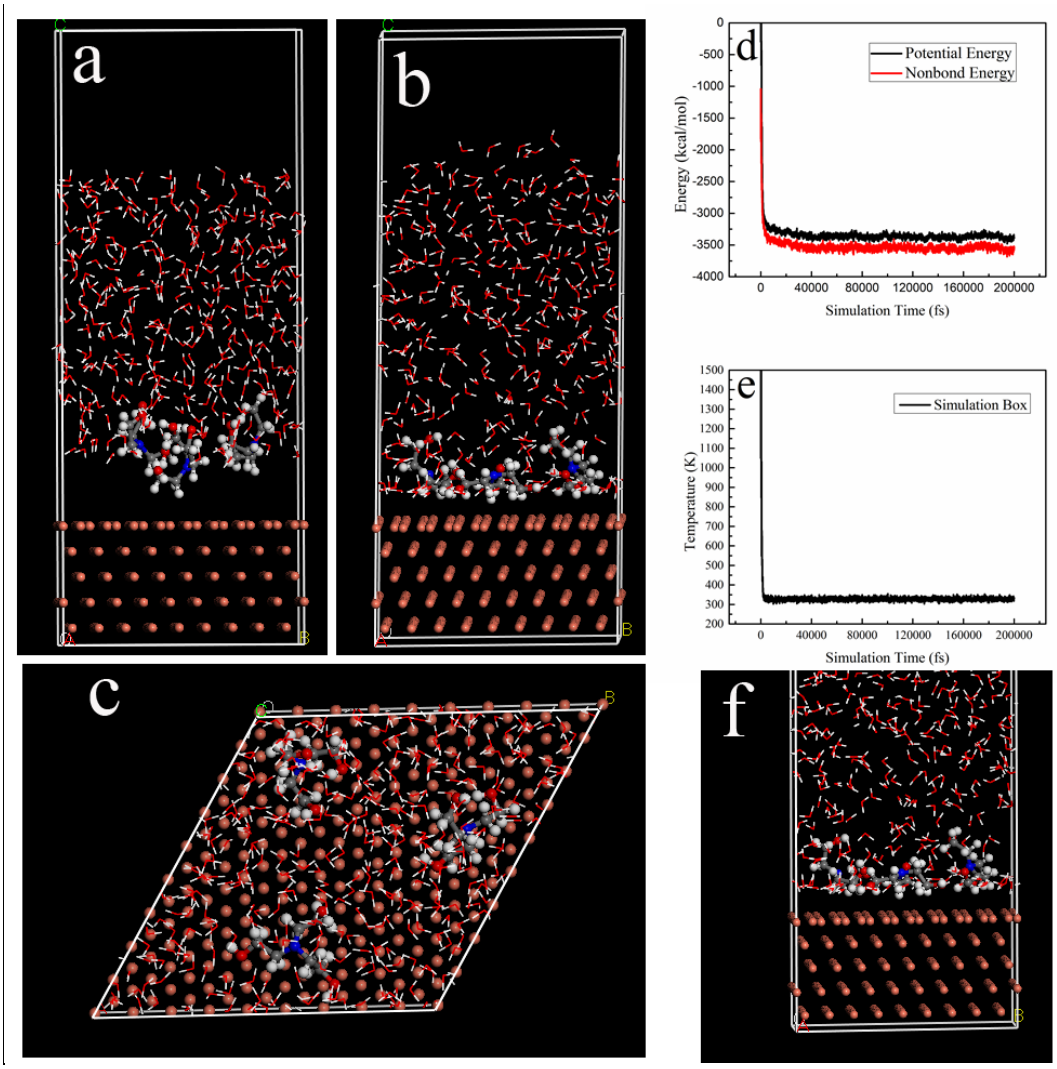

Fig. S19 (a) Initial configuration of the simulation box (Triethanolamine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Triethanolamine on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Triethanolamine on Cu surface.

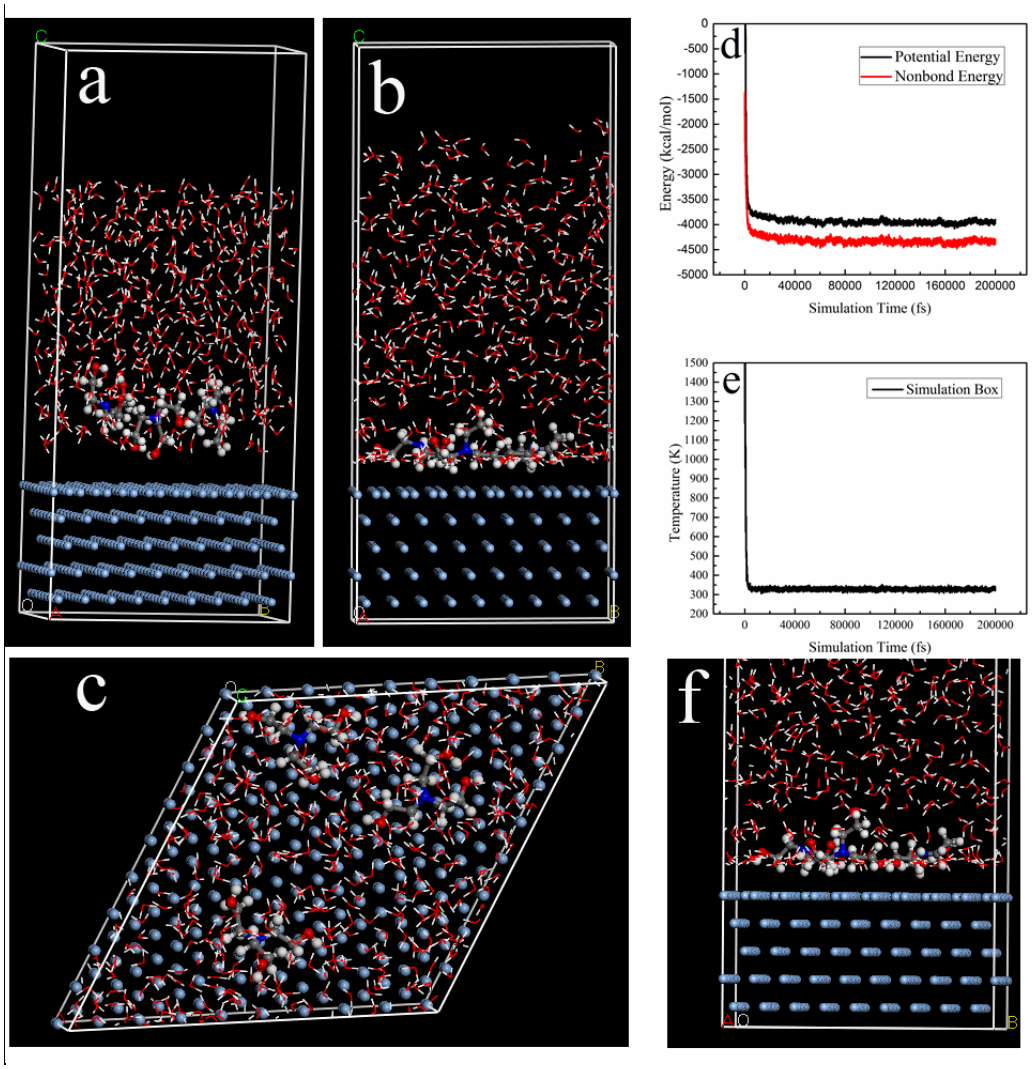

Fig. S20 (a) Initial configuration of the simulation box (Triethanolamine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Triethanolamine on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Triethanolamine on Ag surface.

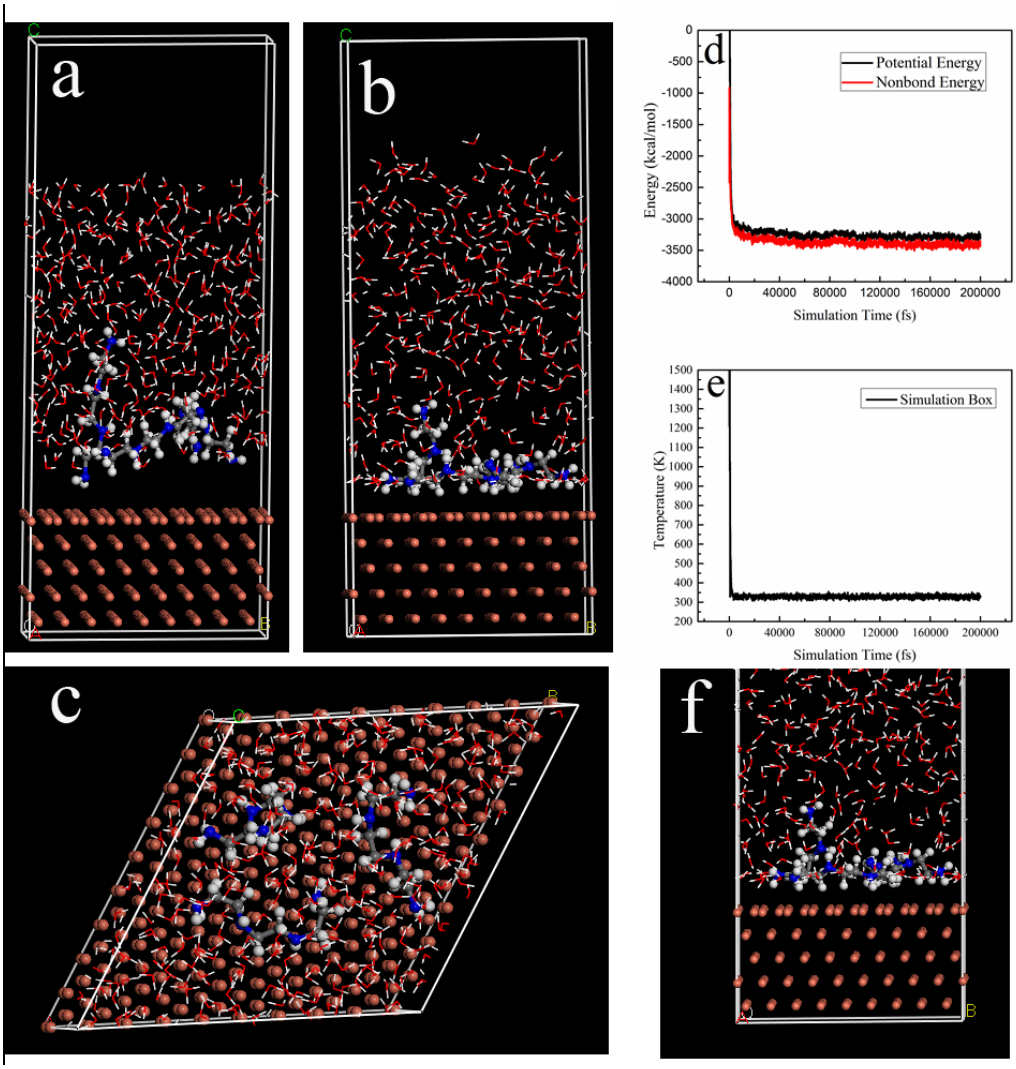

Fig. S21 (a) Initial configuration of the simulation box (Triethylenetetramine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Triethylenetetramine on the Cu surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Triethylenetetramine on Cu surface.

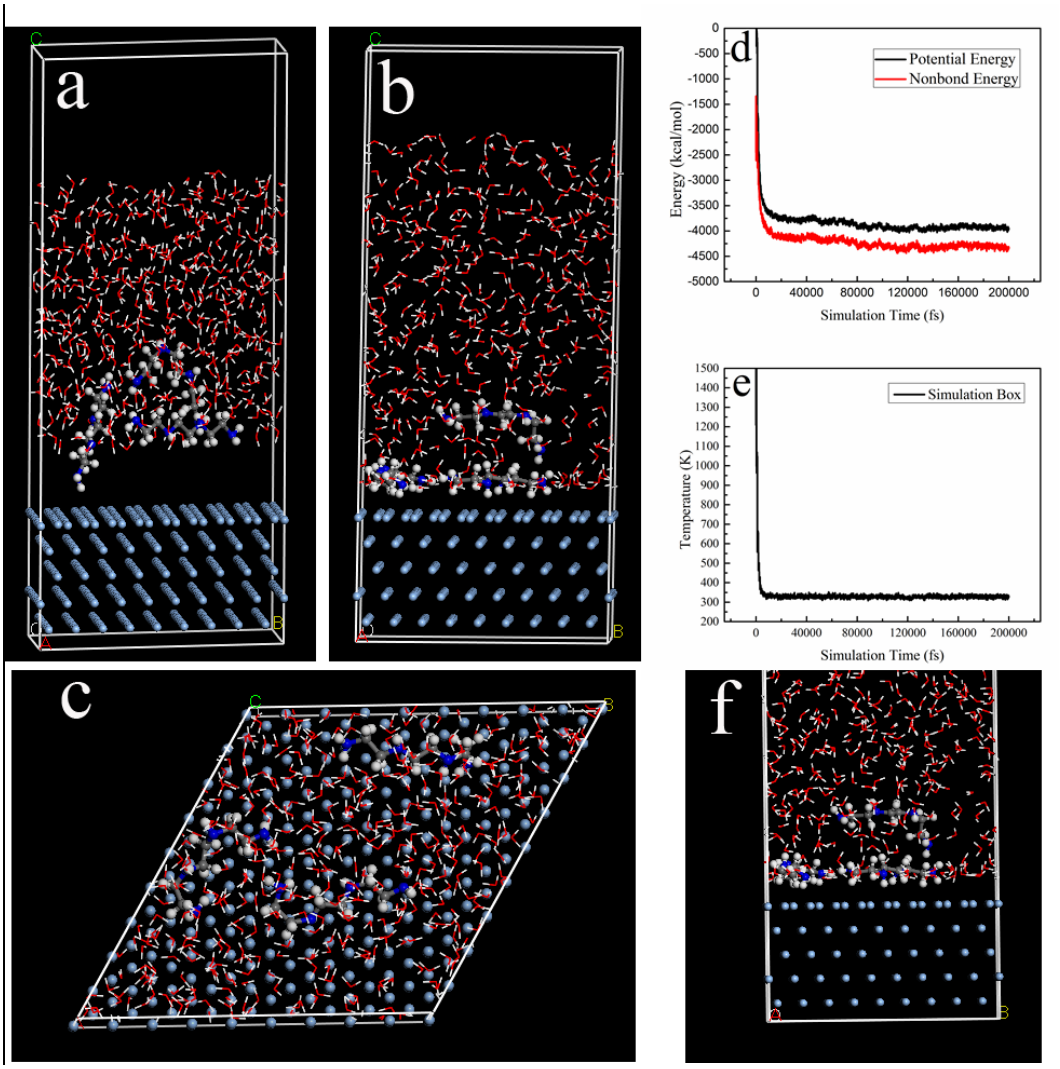

Fig. S22 (a) Initial configuration of the simulation box (Triethylenetetramine visualized by balls and sticks, water molecule visualized by lines). (b) Final equilibrium configuration of the MD simulation box (adsorption behaviors of Triethylenetetramine on the Ag surface). (c) Top view of the final equilibrium configuration of the simulation box. (d) Energy fluctuation curves of the MD simulation. (e) Temperature fluctuation curve of the MD simulation. (f) Interface adsorption structure of Triethylenetetramine on Ag surface.

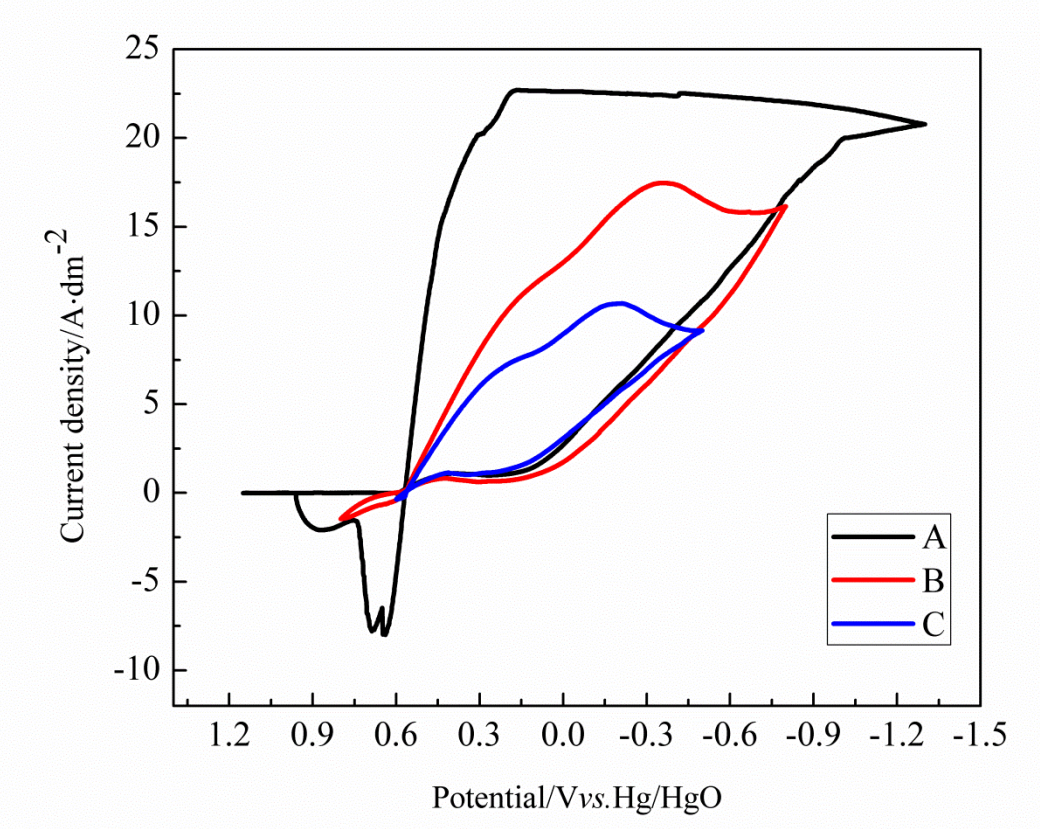

Fig. S23 Cyclic voltammograms of $AgNO_3$ solution initiated at open circuit potential with a sweep rate of 10 mV/s from: (A) -1.30 V to 1.15 V at 328K (B) -0.80 V to 0.80 V at 328K, (C) -0.60 V to 0.60 V at 328K.