Supporting Information

Oxygen-assisted stabilization of single-atom Au during photocatalytic hydrogen evolution

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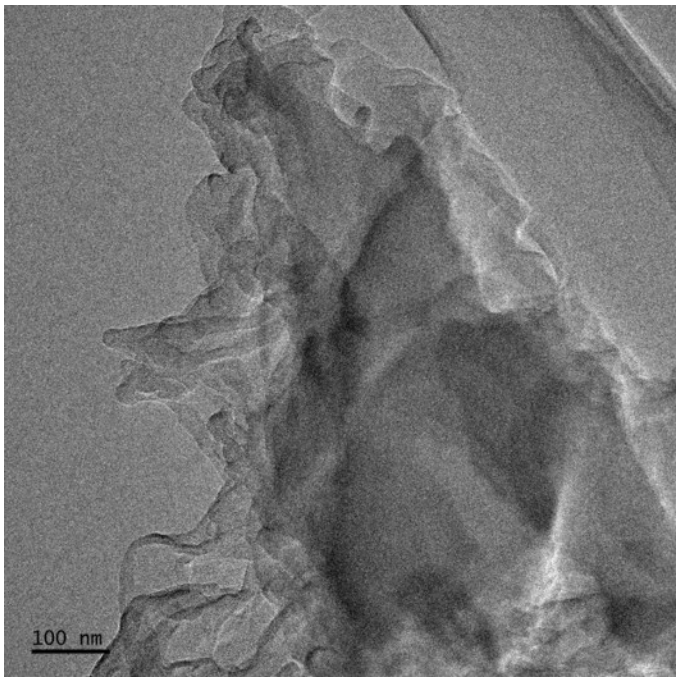

Figure S1. TEM image of CNUHAu

From the low magnification TEM image, it is obvious to see the morphology of graphitic carbon nitride(g-C_3N_4) is not affected by loading Au atoms. The wrinkled and disordered lamellar film remains. More importantly, there are no Au nanoparticles presented in CNUHAu.

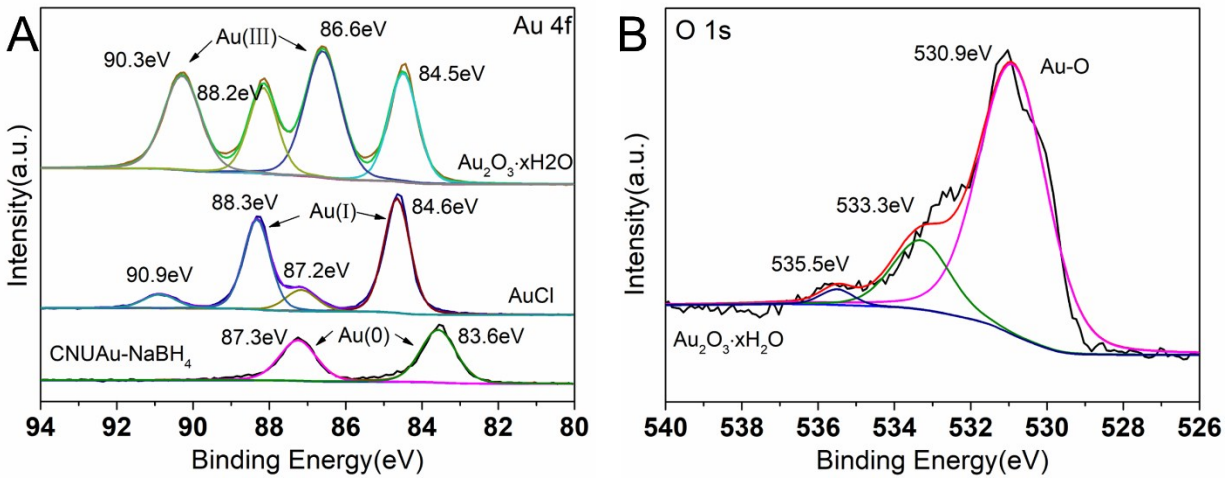

Figure S2. (A) Au 4f XPS spectra of CNUAu-$NaBH_4$, AuCl and $Au_2O_3 \cdot xH_2O$, (B) O 1s XPS spectra of $Au_2O_3 \cdot xH_2O$

As we known, there are three chemical valences for Au element. The Au with zero valence can be easily obtained by reduction of $HAuCl_4$ with $NaBH_4$. Hence, the references CNUAu-$NaBH_4$, AuCl and Au_2O_3 were also measured by XPS to determine the position of Au with different chemical valences. From Figure S2, it is easy to distinguish the binding energy of Au(Ⅰ) and Au(Ⅲ). More importantly, the position of Au-O bond can be found. It helps us to identify whether the Au-O bond forms or not in Au single atom combined g-C_3N_4 system.

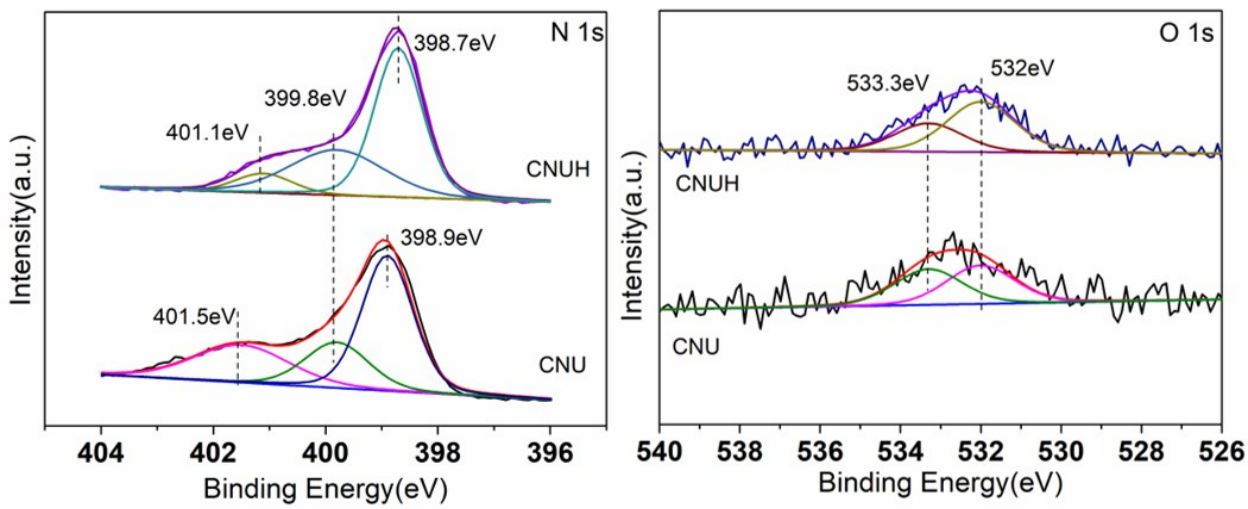

Figure S3. N 1s and O 1s XPS spectra for CNU and CNUH

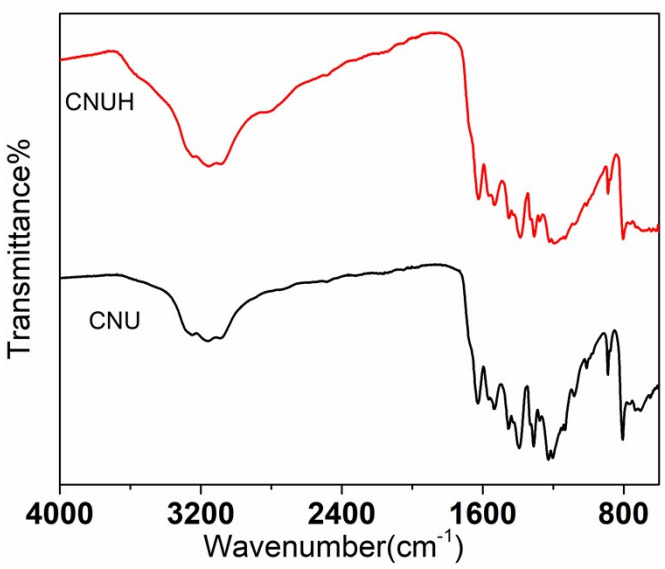

Figure S4. FTIR spectra of CNU and CNUH

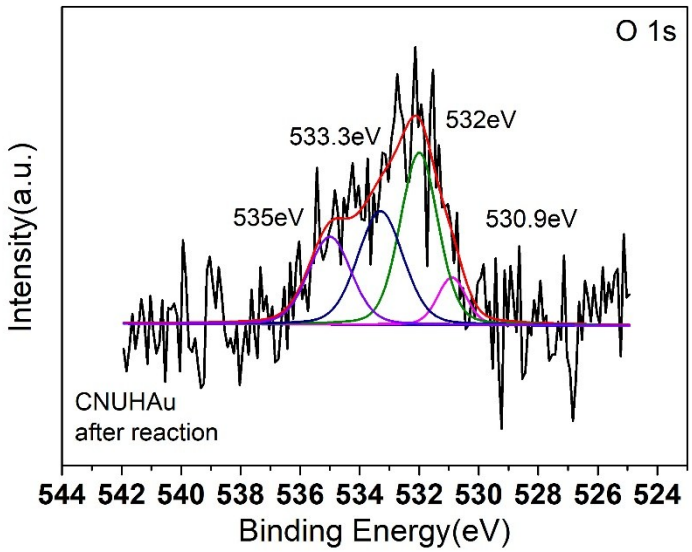

Figure S5. The O 1s XPS spectrum of CNUHAu after photocatalytic test

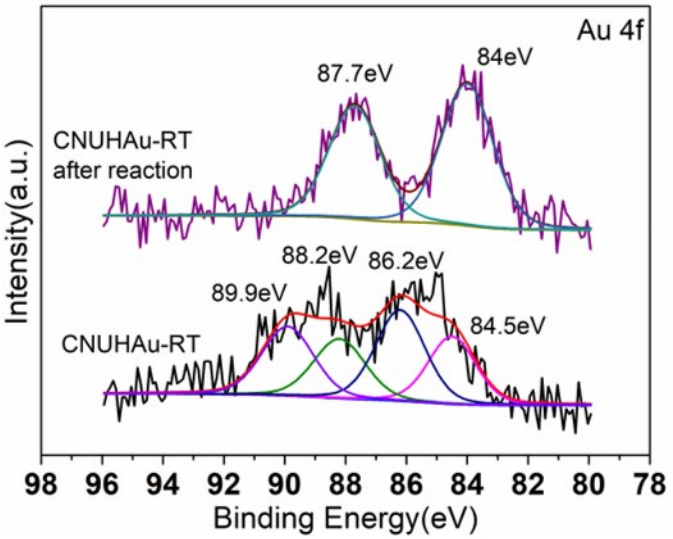

Figure S6. Au 4f XPS spectra for CNUHAu-RT sample before and after reaction

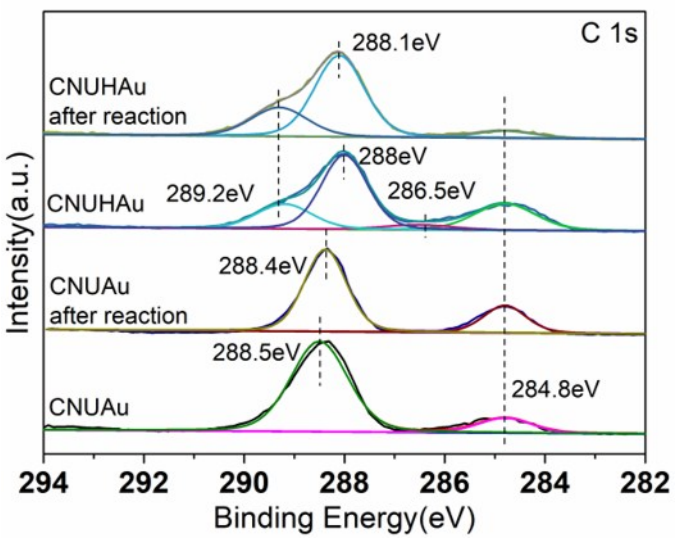

Figure S7. C 1s XPS spectra for CNUAu and CNUHAu before and after reaction

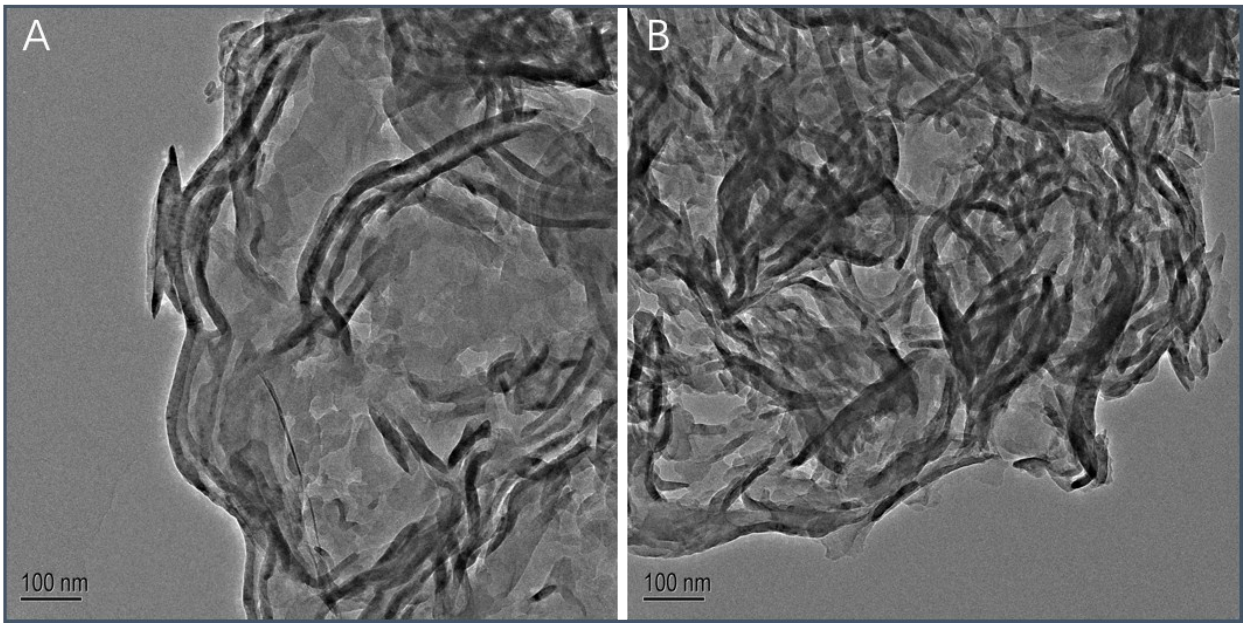

Figure S8. TEM image of CNU(A) and CNUH(B)

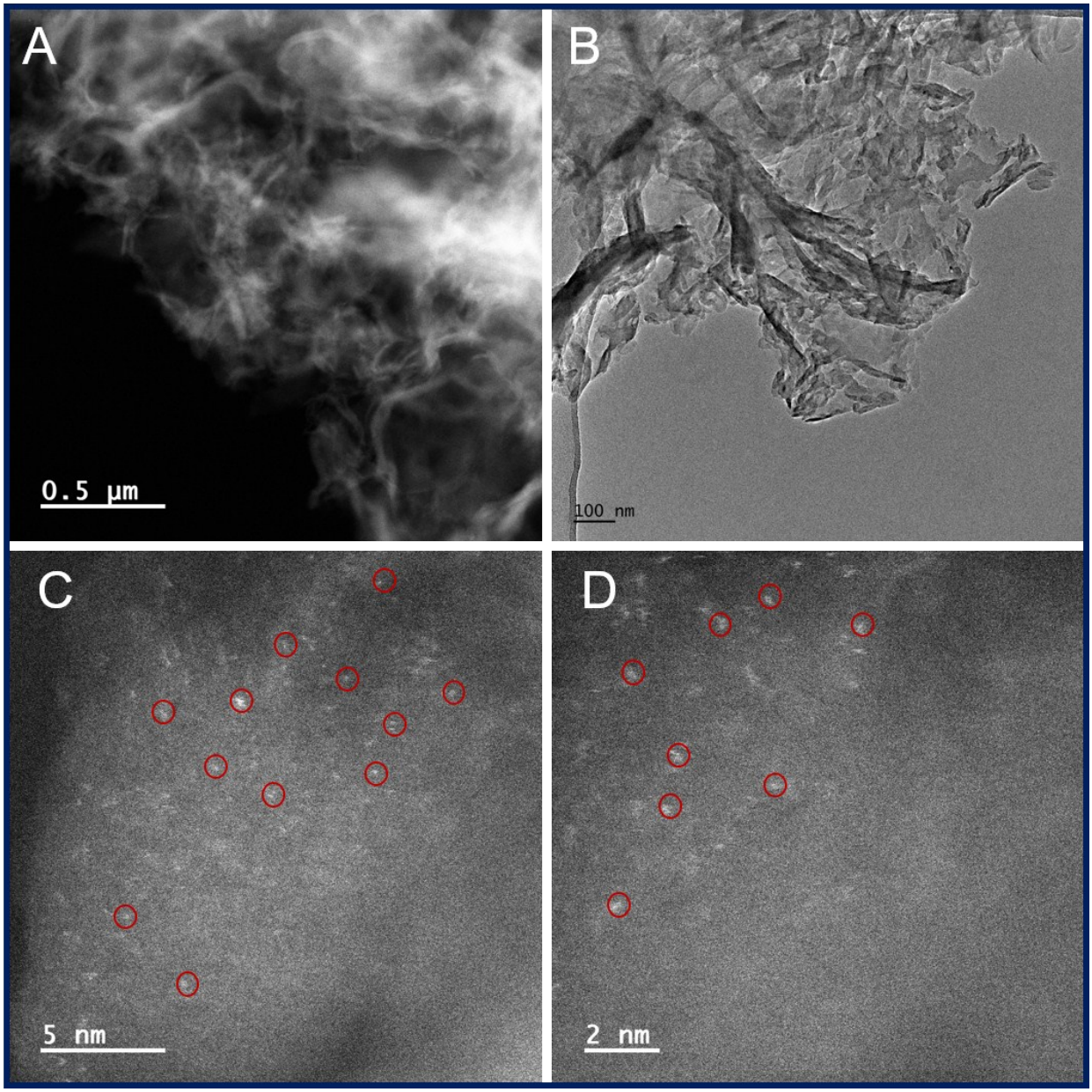

Figure S9. Aberration-corrected HAADF-STEM image(A,C,D) and TEM image(B) of the sample CNUAu

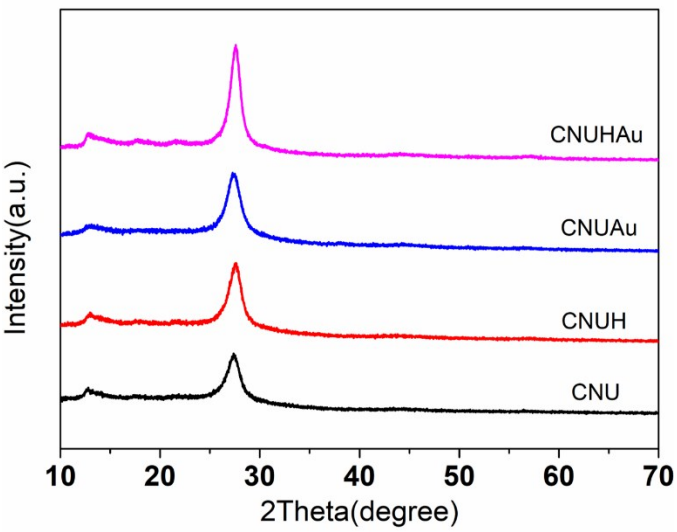

Figure S10. XRD pattern of CNU, CNUH, CNUAu and CNUHAu

Table S1. The content of element estimated from XPS spectra

ID	C at%	N at%	O at%
CNU	43.09	56.37	0.53
CNUH	38.02	58.71	3.27
CNUAu	43.48	53.00	3.09
CNUHAu	45.08	49.29	4.20