Supporting Information

Dispersion of Au Entities over Mo_2N and MoC for the Low-Temperature Water-Gas Shift Reaction

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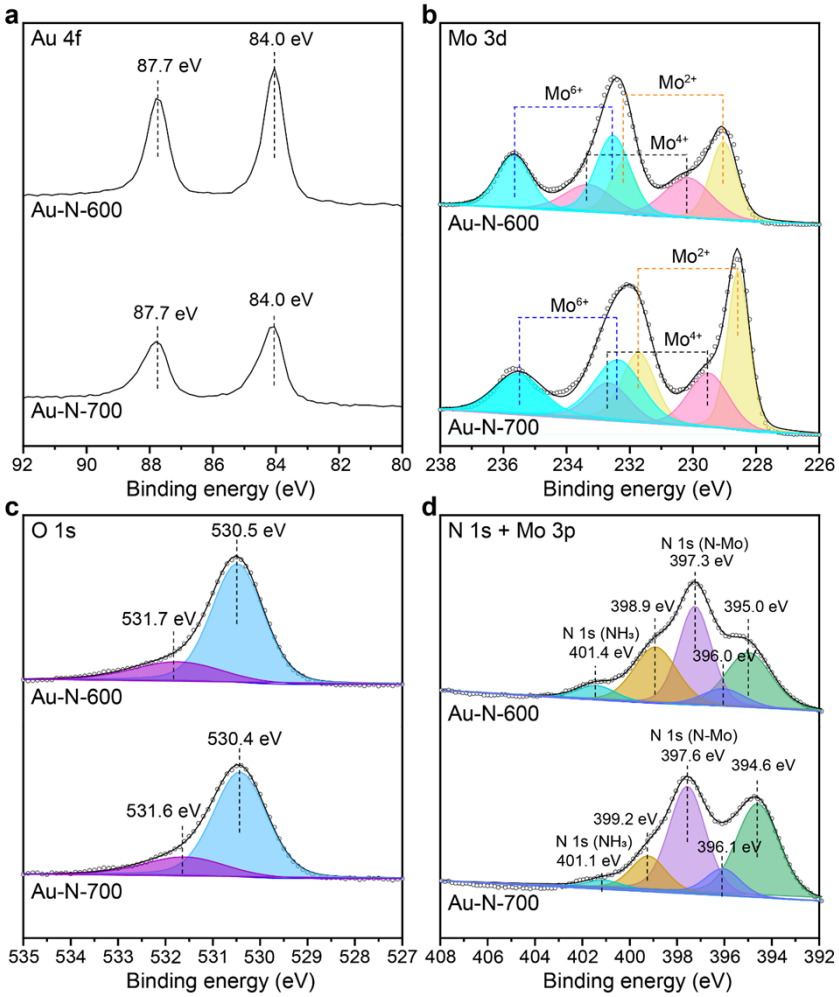

Fig. S1 XPS spectra of Au 4f (a), Mo 3d (b), O 1s (c) and N 1s and Mo 3p (d) in the Au/γ-Mo_2N samples. The binding energies at about 397.5 and 401 eV of N 1s peak are attributed to nitrogen of molybdenum nitride and chemisorbed NH_3, respectively. The binding energies at about 395.0, 396.0 and 399.0 eV of Mo 3p are assigned to Mo^{2+}, Mo^{4+} and Mo^{6+}, respectively.

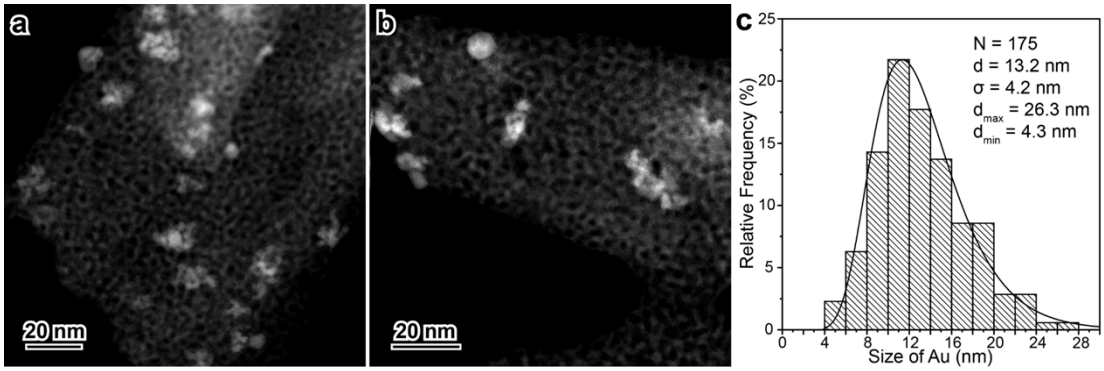

Fig. S2 STEM images (a, b) and size-distribution of Au entities (c) in the Au-N-600 sample.

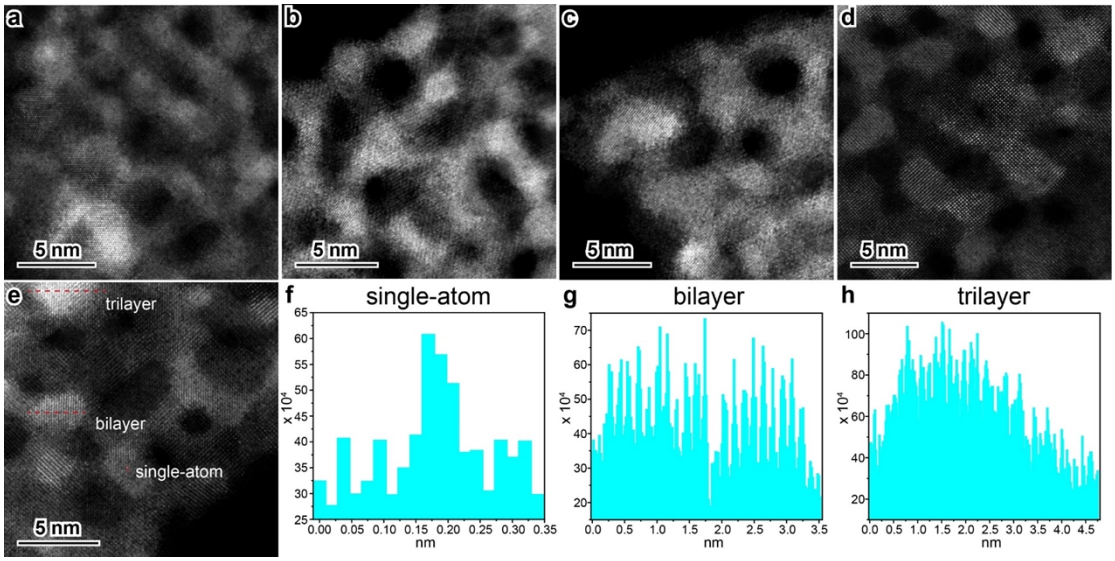

Fig. S3 STEM images and line-profile intensities of the Au-N-700 sample. Identification of Au bilayer and trilayer was done by comparing the profile intensities with that of the Au single-atoms.

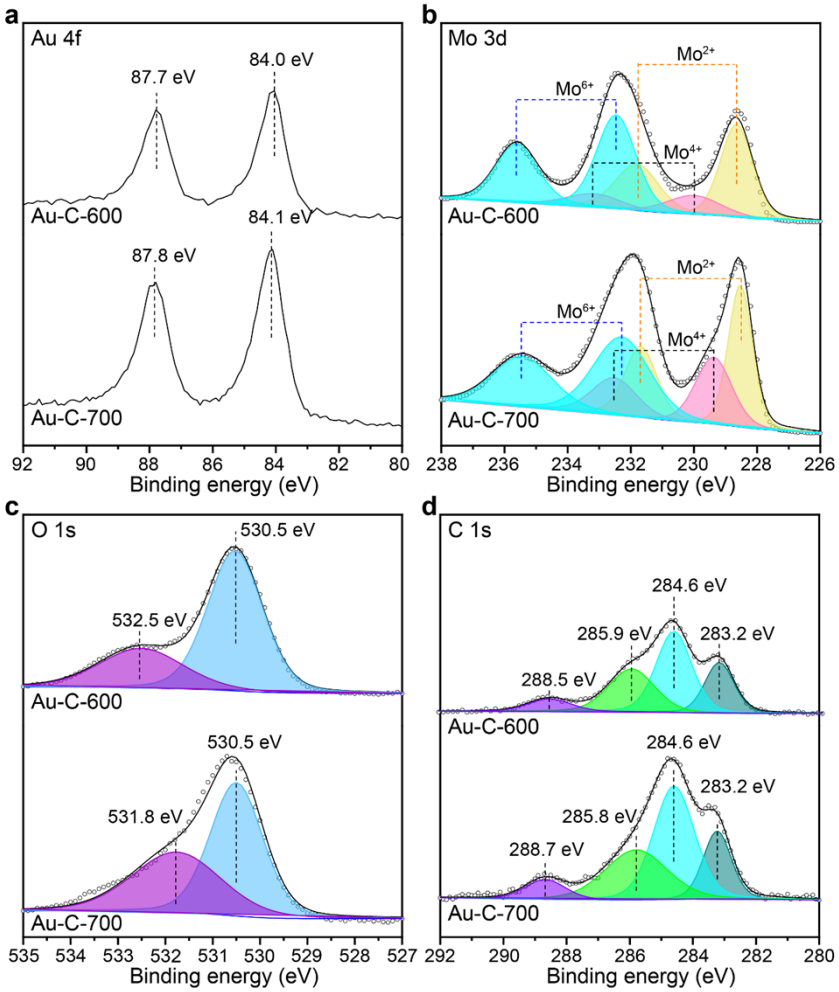

Fig. S4 XPS spectra of Au 4f (a), Mo 3d (b), O 1s (c) and C 1s (d) in the Au/α-MoC sample.

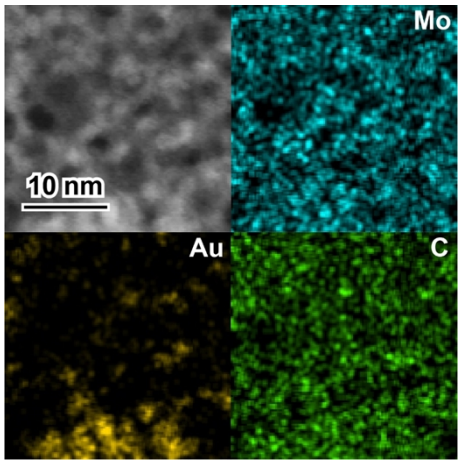

Fig. S5 STEM-EDS elemental mappings of the Au-C-600 sample.

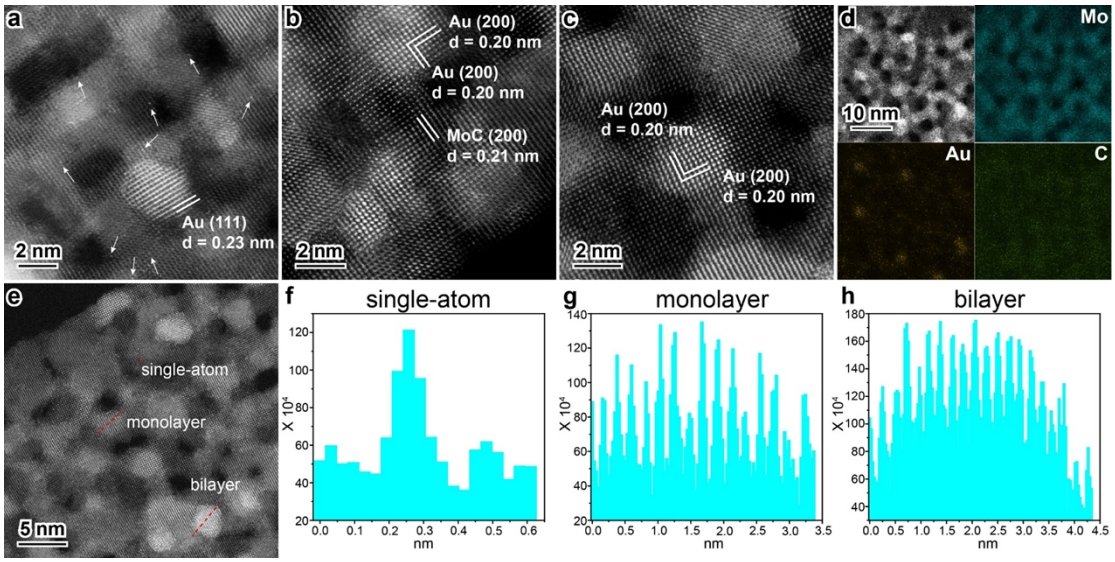

Fig. S6 STEM images and line-profile intensities of the Au-C-700 sample. Identification of Au monolayer and bilayer was done by comparing the profile intensities with that of the Au single-atoms. The arrows indicated single-atoms.

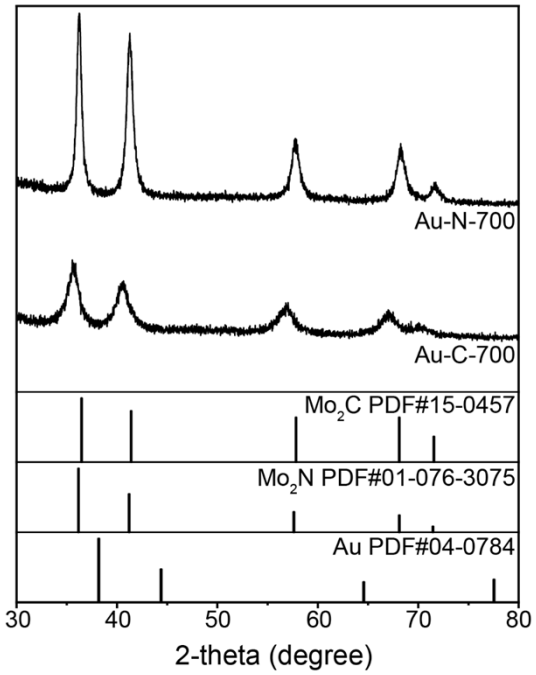

Fig. S7 XRD patterns of the spent catalysts after WGS reaction at 200 °C.

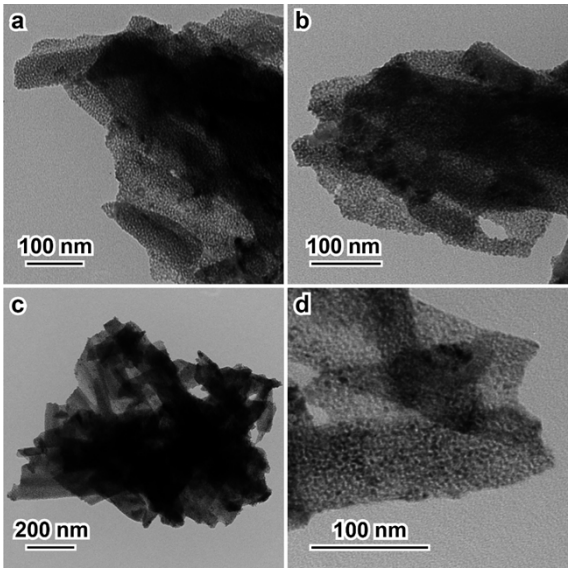

Fig. S8 TEM images of the spent Au-N-700 (a, b) and Au-C-700 (c, d) catalysts after WGS reaction at 200 °C.

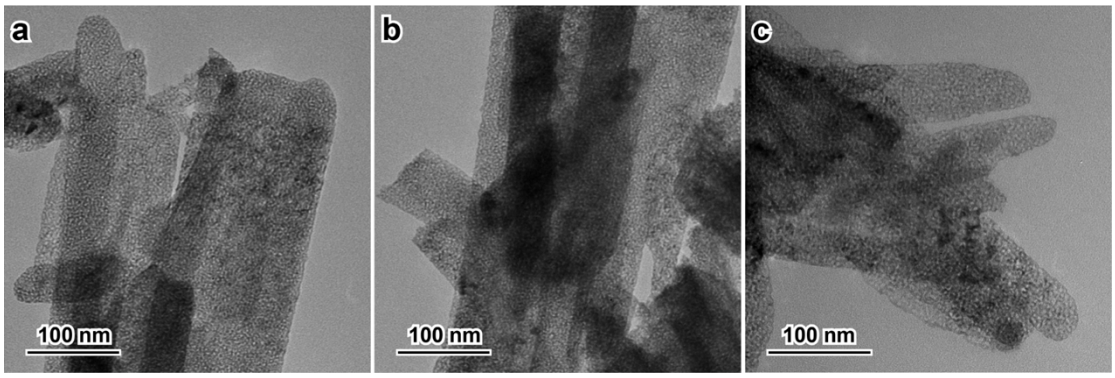

Fig. S9 TEM images of α-MoC.

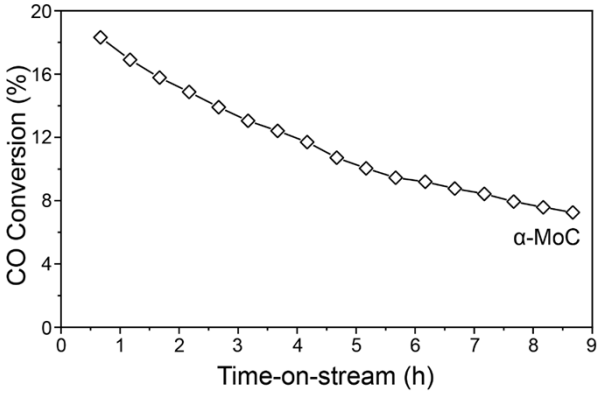

Fig. S10 Water gas shift reaction over α-MoC at 200 °C. Reaction condition: 5 mg α-MoC with 195 mg quartz sand, a feed stream of 3.0 vol.% CO/6.0 vol.% H_2O/He mixture at the flowrate of 66.7 mL min^{-1}.

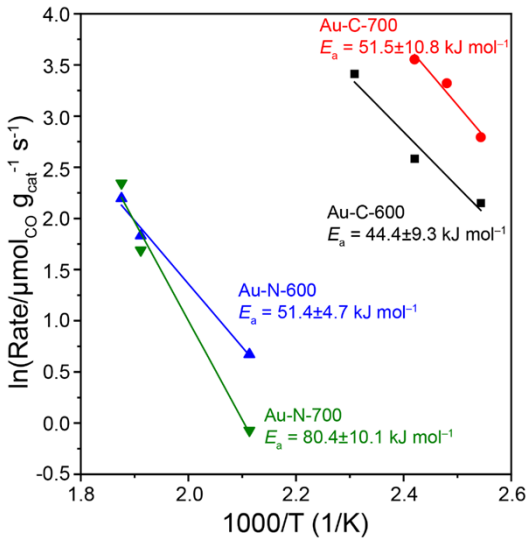

Fig. S11 Apparent activation energies (E_a) of the Au/γ-Mo_2N and Au/α-MoC catalysts.

Table S1. Cell parameters of γ-Mo_2N and α-MoC in the samples.

Sample	Phase	Cell parameters (nm)	Crystal size (nm)[a]
Au-N-600	γ-Mo_2N	0.419	6.6
Au-N-700	γ-Mo_2N	0.421	9.7
Au-C-600	α-MoC	0.419	6.8
Au-C-700	α-MoC	0.422	5.5

[a] The crystal size was calculated from the FWHM of the {200} diffraction line.

Table S2. Coordinating environments of Au from *R*-space fittings of Au L_3-edge EXAFS data.

Sample	Shell	R (Å)[a]	C.N.[b]	$\triangle E_0$ (eV)[c]	σ^2 (10^{-3} Å^2)[d]	R factor (%)
Au foil	Au–Au	2.86 ± 0.002	12.0 ± 0.04	5.6	8.0	0.3
Au-N-600	Au–Au	2.86 ± 0.03	8.7 ± 0.3	6.6	9.8	0.5
	Au–Mo	2.85 ± 0.09	0.4 ± 0.1		2.8	
Au-N-700	Au–Au	2.83 ± 0.004	7.5 ± 0.9	2.8	10.6	0.9
	Au–Mo	2.83 ± 0.11	0.2 ± 0.4		18.6	
Au-C-600	Au–Au	2.88 ± 0.02	7.7 ± 1.0	7.6	19.7	0.7
	Au–Mo	2.87 ± 0.01	1.5 ± 0.6		8.7	
	Au–C	2.13 ± 0.03	0.5 ± 0.5		11.6	
Au-C-700	Au–Au	2.86 ± 0.01	7.3 ± 0.6	4.6	9.0	1.0
	Au–Mo	2.82 ± 0.03	1.3 ± 0.3		9.0	
	Au–C	2.16 ± 0.04	0.6 ± 0.3		9.0	

[a] Atomic distance; [b] Coordination number; [c] Difference of potential between the sample and the standard; [d] Debye-Waller factor.