Supplementary Information

An atomically dispersed Pt/γ-$Mo_2N(O_{0.3})$ catalyst for hydrogen production via aqueous-phase reforming of methanol

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1 Supplementary Tables

TableS S1. Pt L_3-Edge EXAFS fitting results of the 1wt%Pt/γ-Mo_2N catalyst

Path	N	R	ΔE	σ^2 *10^{-3}	R-factor
Pt-N	1.1	1.84		1.5	
Pt-O	4.4	1.90	10.8	4.1	0.019
Pt-Pt	4.3	2.76		3.6	

Table S2. Surface fractions of the various species calculated from XPS of catalyst

Sample	Pt/%	Mo/%	N/%	O/%
γ-Mo_2N	-	10.1	67.3	22.6
0.2% Pt/γ-Mo_2N	0.17	9.5	70.1	20.2
1% Pt/γ-Mo_2N	1.3	13.1	72.1	14.2

Table S3. Catalytic performance of Pt/γ-$Mo_2N(O_{0.3})$ catalysts and conventional platinum catalysts in the APR of methanol

Catalyst	Pt loading (wt%)	Temperature /°C	ATOF (mol_{H2}/mol_{Pt}/h)	H_2 production rate (μmol_{H2}/g_{cat}/min)	Selectivity (%)		
					CO	CH_4	CO_2
1% Pt/γ-Mo_2N*	1.1	210	4968	4242	0.9	1.4	97.7
0.2% Pt/γ-Mo_2N*	0.19	210	14813	2532	0.7	0.9	98.4
1% Pt/γ-Mo_2N**	1.2	210	4898	4200	0.6	1.1	98.3
0.2%Pt/γ-Mo_2N**	0.22	210	14810	2529	0.6	0.9	98.5
γ-Mo_2N	-	210	-	-	-	-	-
2% Pt/α-MoC	2.2	190	13810	7776	-	-	-
1% Pt/MoO_3	1.1	210	115	98	0.8	2.1	97.1
1% Pt/Al_2O_3	1.0	210	294	252	0.5	3.3	96.2
1% Pt/$NiAl_2O_4$	1.4	210	512	438	0.5	25.4	74.1

Reaction conditions: n(CH_3OH) : n(H_2O) = 1:1, 20 ml total volume of liquid, 50 mg catalysts, 210 °C; reaction for 1 hour; initial pressure 3 MPa N_2. Pt loadings were measured by inductively coupled plasma atomic emission spectrometry (ICP-AES).

* Precursor is H_2PtCl_6

** Precursor is $Pt(NO_3)_2$

Table S4. Catalytic performance of Pt/γ-$Mo_2N(O_{0.3})$ under different temperatures

Catalyst	Temperature (°C)	H_2 production rate ($\mu mol_{H2}/ g_{cat}/min$)	Selectivity (%)		
			CO	CH_4	CO_2
0.2%Pt/γ-Mo_2N	180	976	0.9	0.1	99.0
	190	1372	0.7	0.9	98.4
	200	2101	0.7	1.1	98.2
	210	2529	0.6	0.9	98.5
	220	3409	0.5	1.3	98.2
	230	4138	0.5	1.5	98.0

Reaction conditions: 20 ml total volume of liquid CH_3OH, 50 mg catalysts, reaction for 1 hour; initial pressure 3 MPa N_2.

Table S5. Methanol dehydrogenation test

Sample	Temperature / ℃	H_2 production rate ($\mu mol_{H2}/ g_{cat}/min$)
1% Pt/γ-Al_2O_3	180	243
	210	350
	240	420
0.2% Pt/γ-$Mo_2N(O_{0.3})$	180	3102
	210	3631
	240	3813
1% Pt/γ-$Mo_2N(O_{0.3})$	180	4891
	210	5031
	240	5981
γ-$Mo_2N(O_{0.3})$	180	-
	210	-
	240	-

Reaction conditions: 20 ml total volume of liquid CH_3OH, 50 mg catalysts, reaction for 1 hour; initial pressure 3 MPa N_2.

2 Supplementary Figures

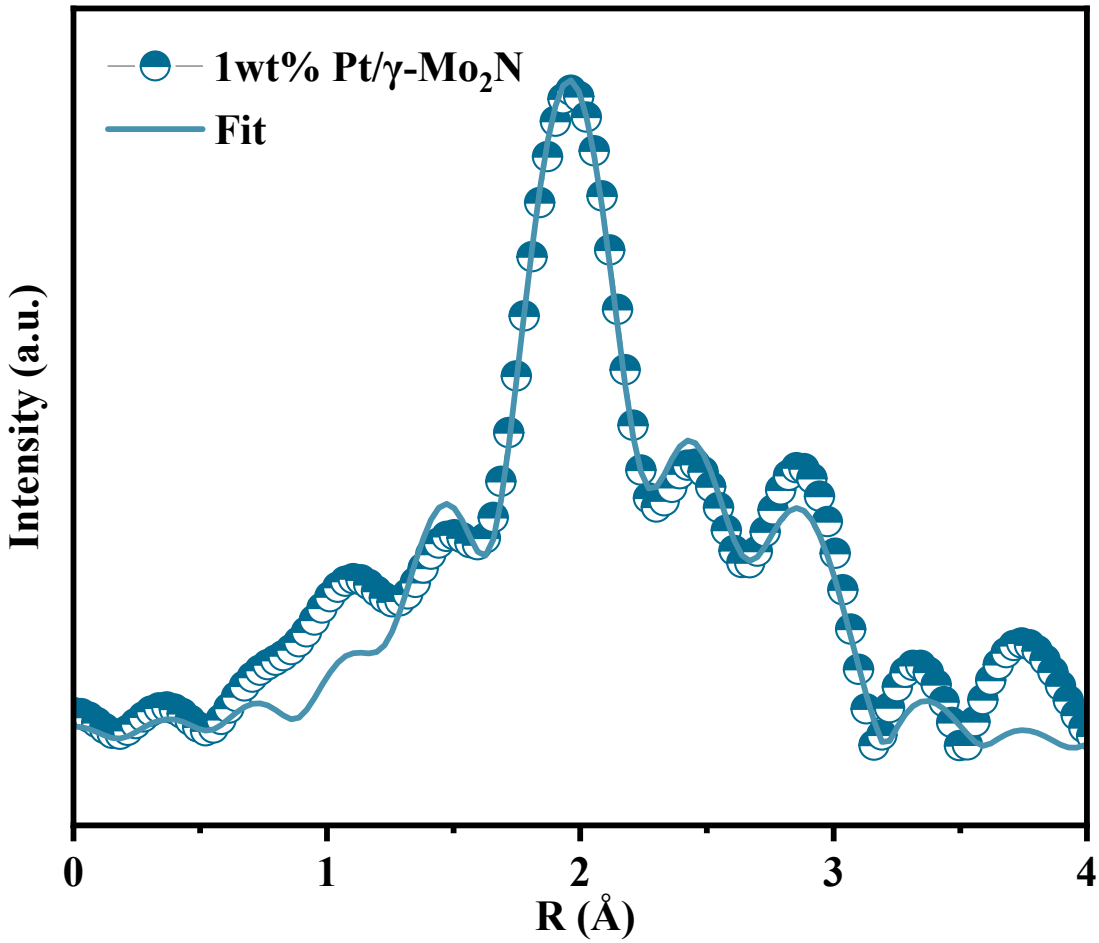

Figure S1. Fitting details for Pt L_3-edge EXAFS spectra obtained for the Pt/γ-$Mo_2N(O_{0.3})$ catalyst.

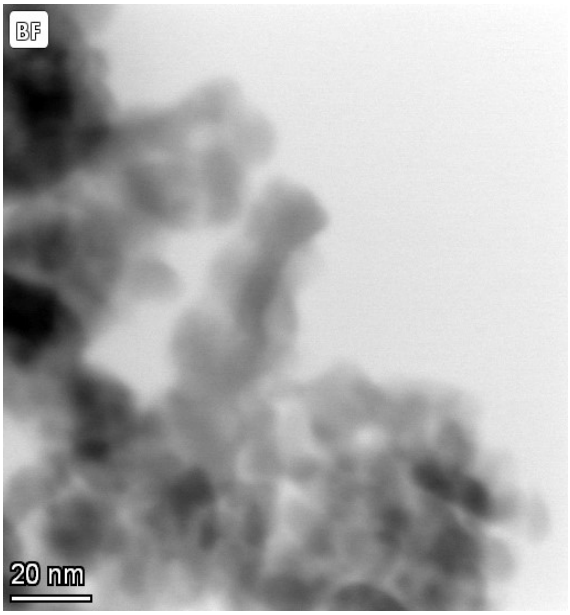

Figure S2. TEM image of 1%Pt/γ-$Mo_2N(O_{0.3})$.

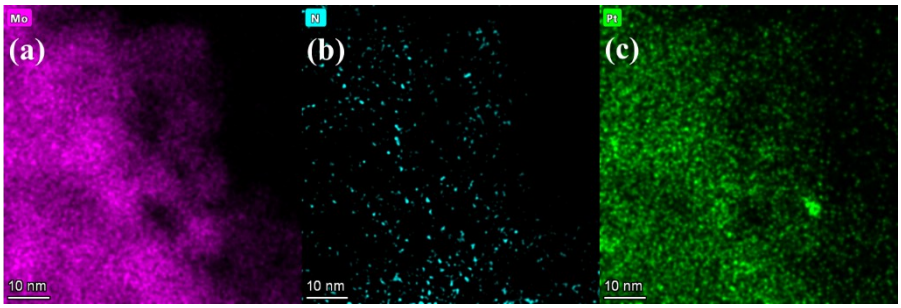

Figure S3. High-resolution STEM Z-contrast image of used 0.2% Pt/γ-$Mo_2N(O_{0.3})$ after 10 cycle stability.

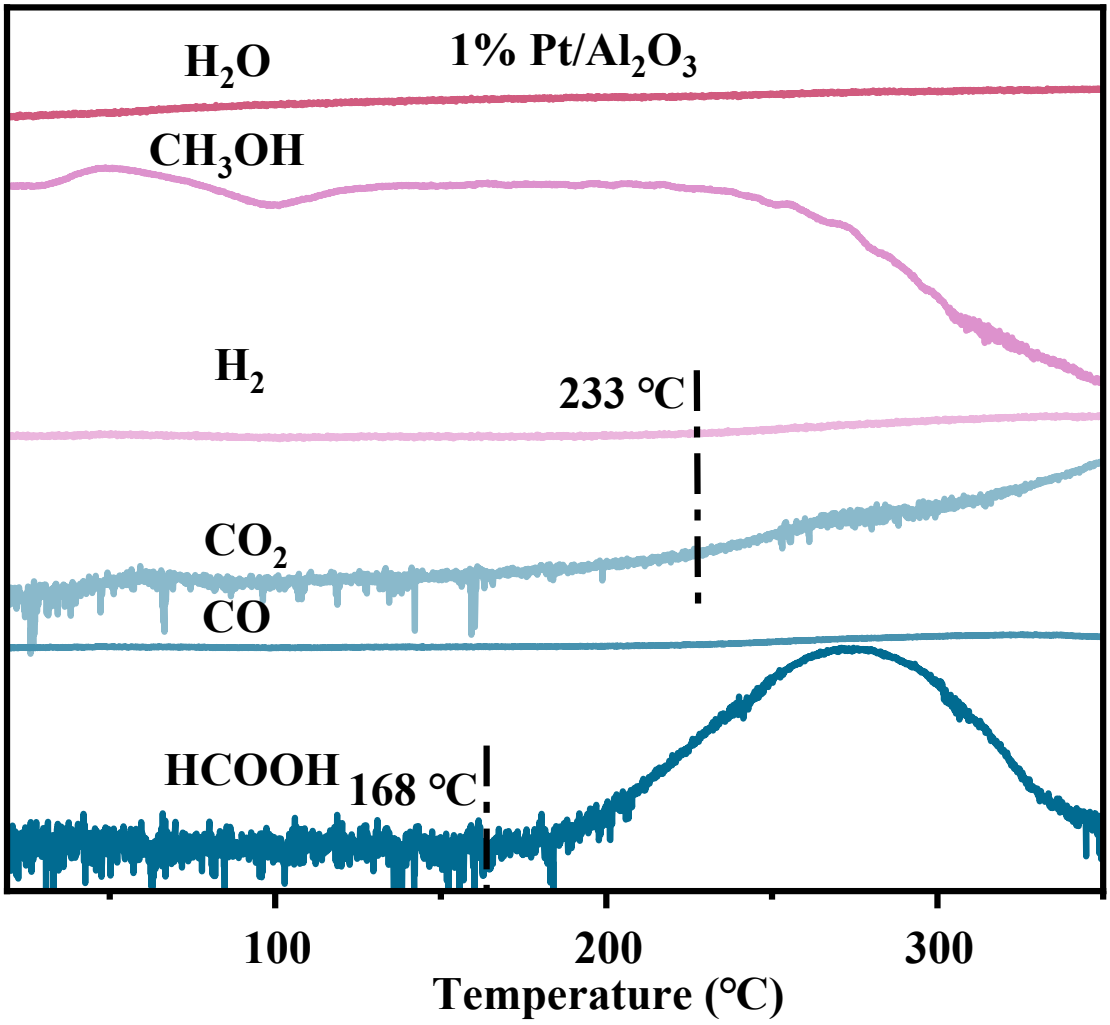

Figure S4. TPSR of methanol and water over 1% Pt/γ-Al_2O_3.

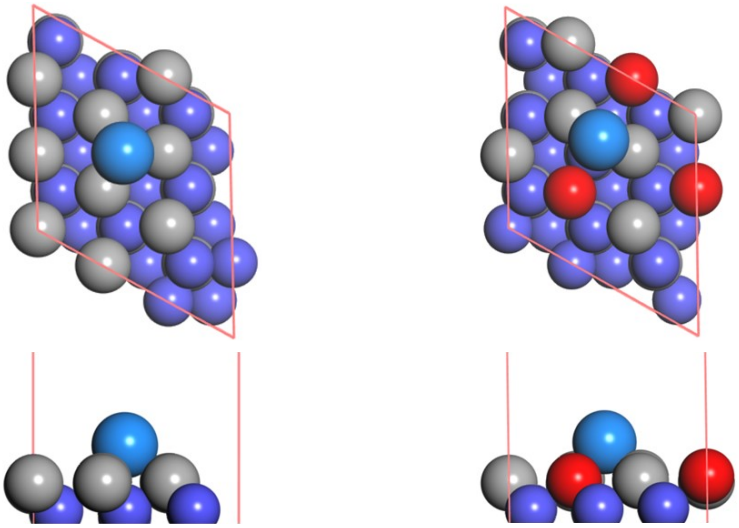

Figure S5. The top and side views for the structural models of Pt/γ-Mo_2N(111) and Pt/γ-$Mo_2N(O_{0.3})$(111). The Mo, Pt, N and O atoms are shown in purple, blue, gray, and red, respectively.

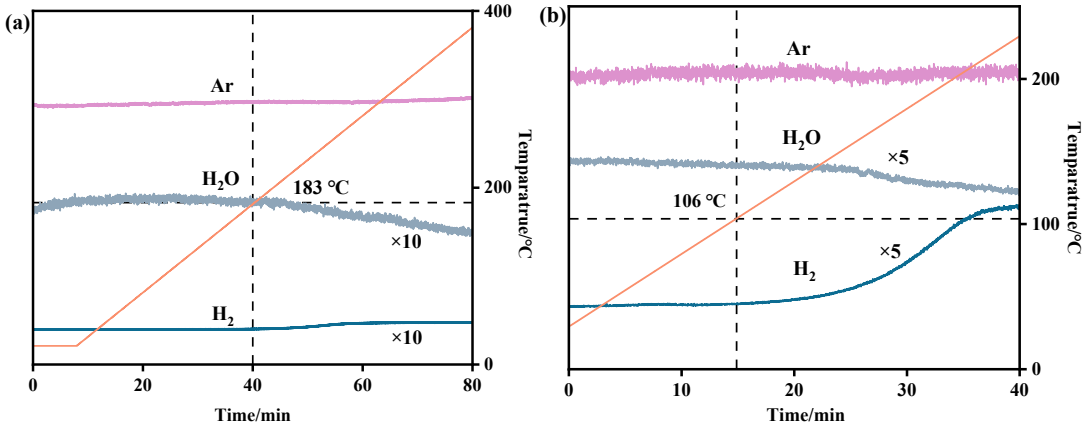

Figure S6. H_2O dissociation experiments for different catalysts: (a) γ-$Mo_2N(O_{0.3})$, (b) Pt/γ-$Mo_2N(O_{0.3})$.

3 Date sharing

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