

Enhancing catalytic performance of PdAu catalysts by W-induced strong interaction for the direct synthesis of H₂O₂

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Figure and table captions

Figure S1. TEM, HAADF-STEM and particle size distribution images of (a~c) PdAu/TiO₂, (d~f) PdAu/WO₃-TiO₂, (g~i) WO₃-PdAu/TiO₂ and (j~l) PdAuWO₃/TiO₂.

Figure S2. (a) HRTEM, (b) HAADF-STEM and (c~f) corresponding EDS mapping of PdAu/TiO₂, (g~h) HAADF-STEM and corresponding EDS mapping of nanoparticle in PdAu/TiO₂.

Figure S3. (a) HAADF-STEM, (b~d) corresponding EDS mapping images of WO₃/TiO₂.

Figure S4. (a) HRTEM, (b) HAADF-STEM and (c~g) corresponding EDS mapping images of WO₃-PdAu/TiO₂, (h) HAADF-STEM and (i) corresponding line-scan of nanoparticle in WO₃-PdAu/TiO₂.

Figure S5. (a) HRTEM, (b) HAADF-STEM, (c~g) corresponding EDS mapping images of PdAuWO₃/TiO₂, (h) HAADF-STEM and (i) corresponding line-scan of nanoparticle in PdAuWO₃/TiO₂.

Figure S6. Point scan data of nanoparticles in the catalysts.

Figure S7. XRD patterns of the catalysts.

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Figure S9. (a) Pd 3d and (b) Au 4f XPS spectrums of PdAu/WO₃-TiO₂ catalysts with different W content.

Table S1. The actual amount of Pd, Au and W loaded on the catalysts.

Table S2. List of catalysts for the direct synthesis of H₂O₂ in previous literatures.

Table S3. The mass ratio of Pd, Au and W in the catalysts measured by XPS and ICP.

Table S4. Surface Pd⁰ and Pd²⁺ percent of PdAu/WO₃-TiO₂ catalysts with different W content.

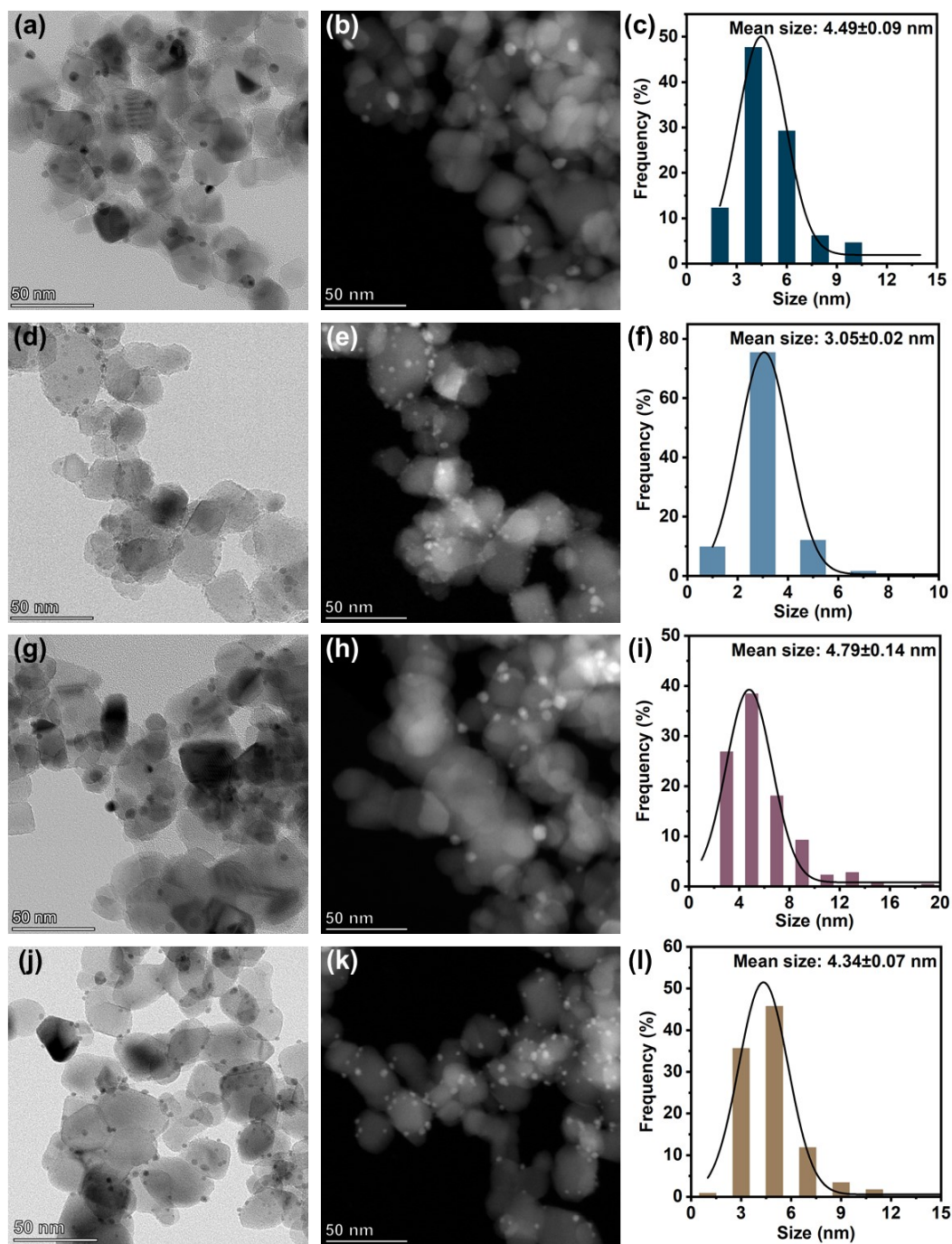


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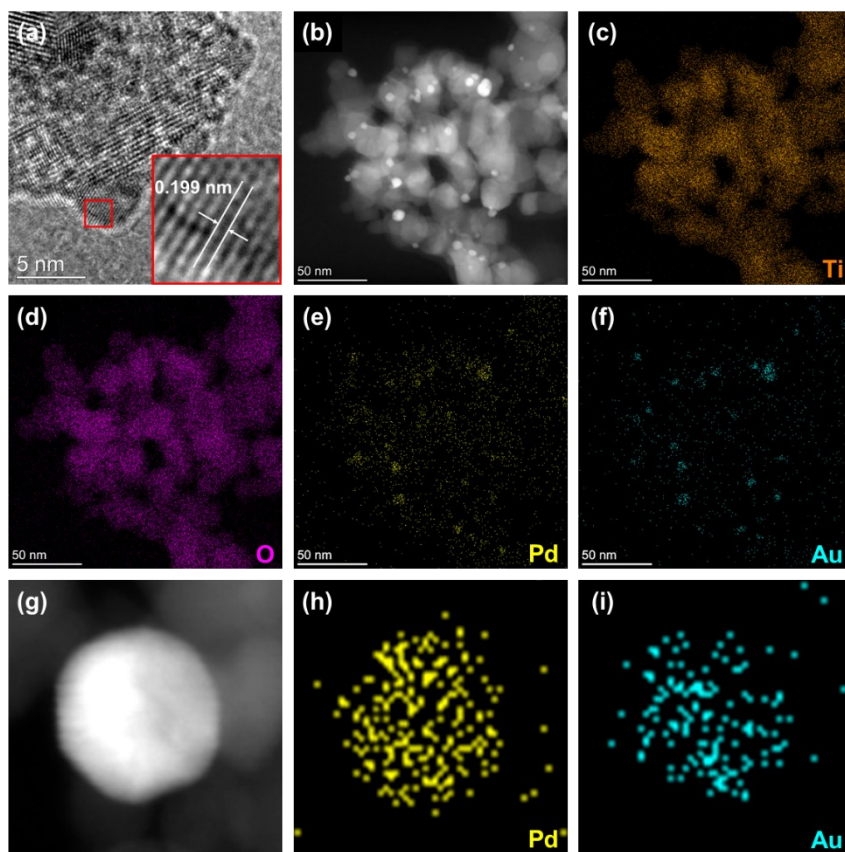


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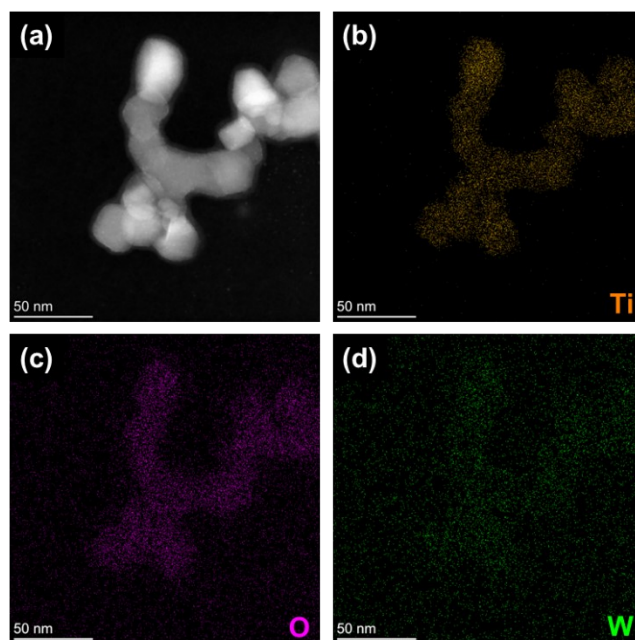


Figure S3. (a) HAADF-STEM, (b~d) corresponding EDS mapping images of WO_3/TiO_2 .

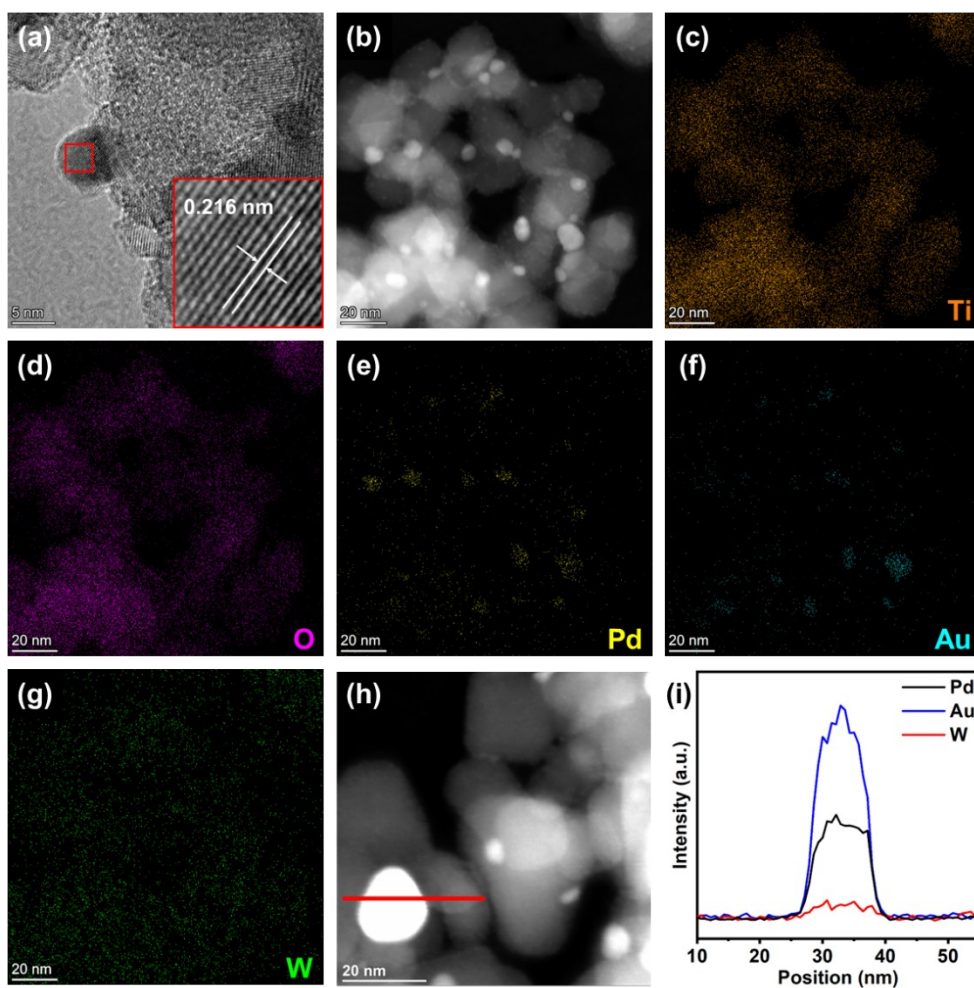


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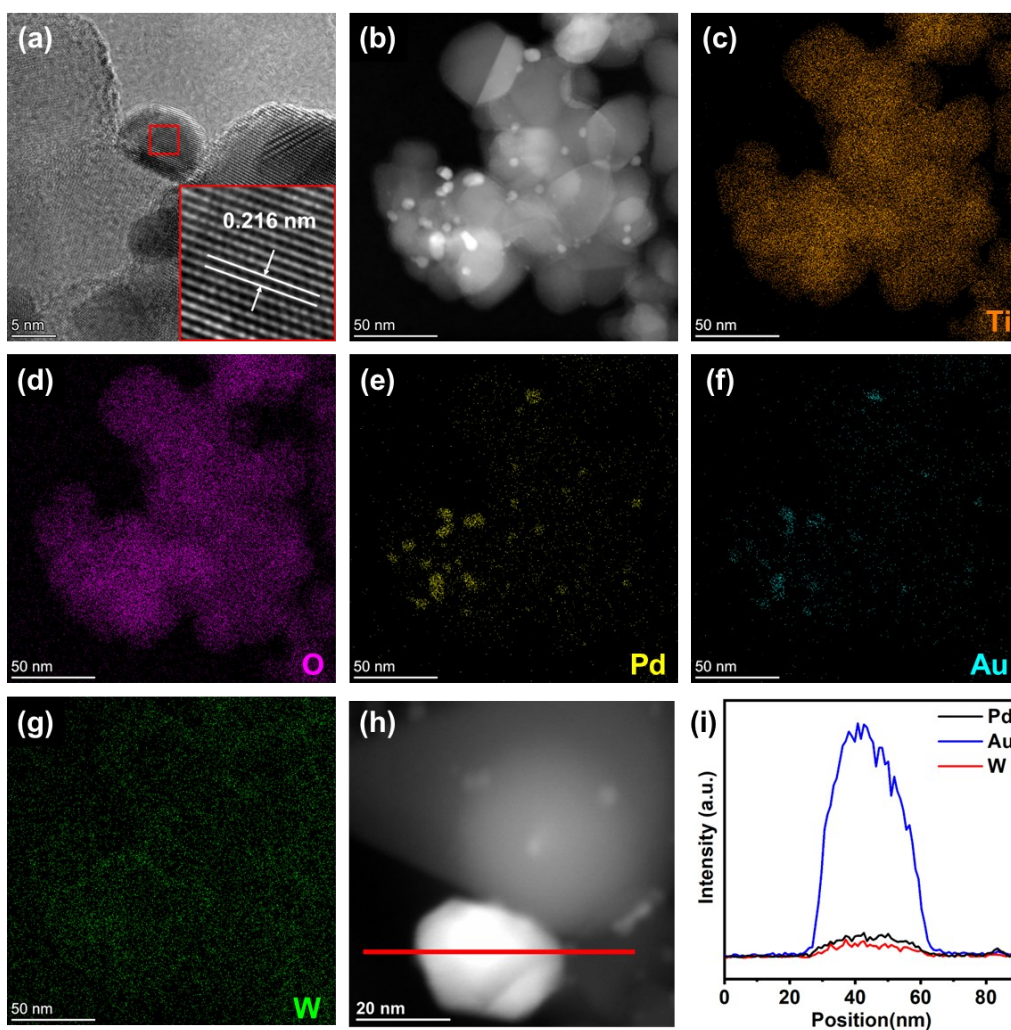


Figure S5. (a) HRTEM, (b) HAADF-STEM and (c~g) corresponding EDS mapping images of PdAuWO₃/TiO₂, (h) HAADF-STEM and (i) corresponding line-scan of nanoparticle in PdAuWO₃/TiO₂.

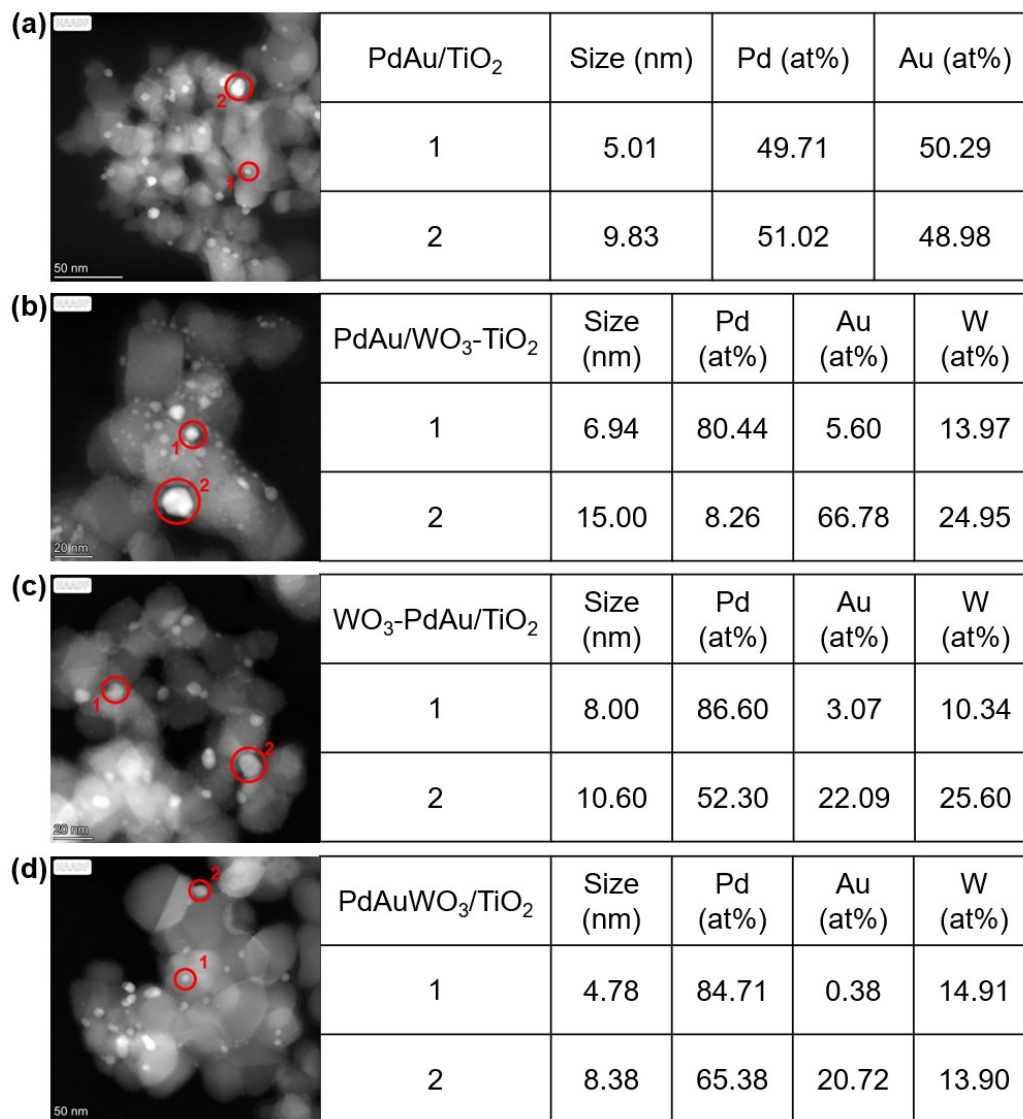


Figure S6. Point scan data of nanoparticles in the catalysts.

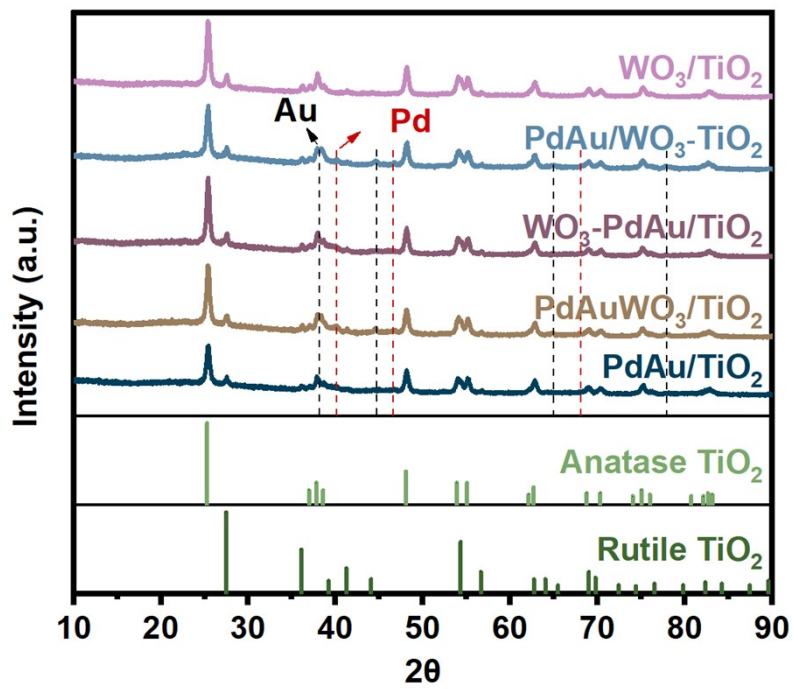


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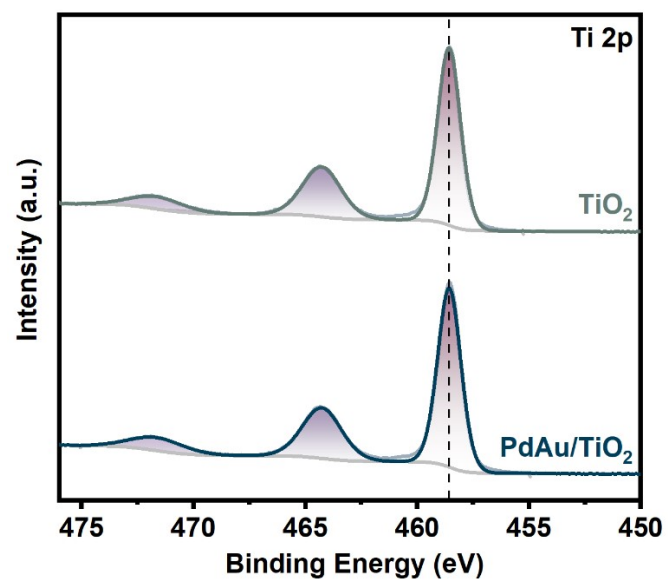


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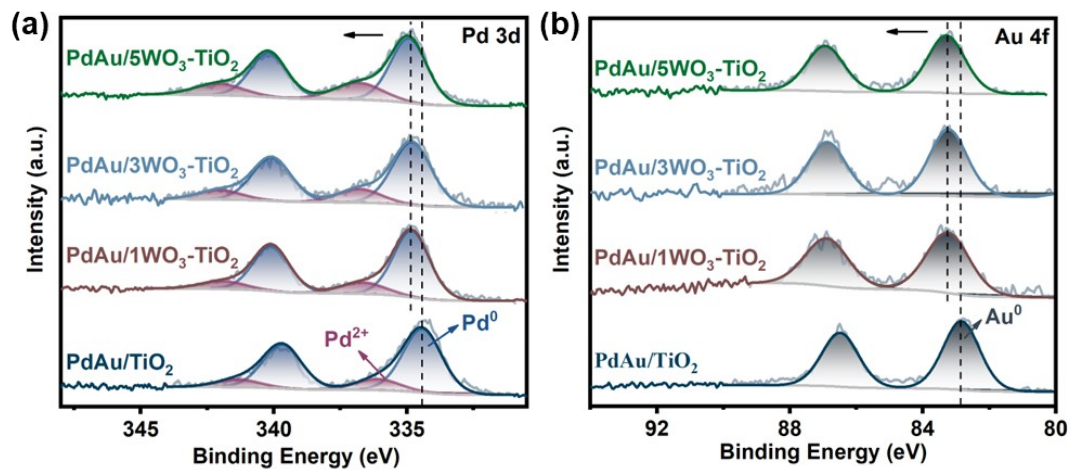


Figure S9. (a) Pd 3d and (b) Au 4f XPS spectra of PdAu/WO₃-TiO₂ catalysts with different W content.

Table S1. The actual amount of Pd, Au and W loaded on the catalysts.

Catalyst	Pd (wt%)	Au (wt%)	W (wt%)
PdAu/TiO ₂	2.7	2.8	—
PdAuWO ₃ /TiO ₂ (3W)	2.7	2.8	3.3
WO ₃ -PdAu/TiO ₂ (3W)	2.6	2.6	3.2
PdAu/WO ₃ -TiO ₂ (3W)	2.7	2.9	3.1
WO ₃ /TiO ₂	—	—	3.2
PdAu/1WO ₃ -TiO ₂	2.8	2.8	1.1
PdAu/2WO ₃ -TiO ₂	2.8	2.7	1.8
PdAu/4WO ₃ -TiO ₂	2.8	2.7	3.5
PdAu/5WO ₃ -TiO ₂	2.8	2.8	5.0
PdAu/SiO ₂	3.0	3.2	—
PdAu/WO ₃ -SiO ₂ (3W)	3.0	3.1	3.2

Table S2. List of catalysts for the direct synthesis of H₂O₂ in previous literatures.

Reaction Catalyst	Additive	Reaction		Reaction		Productivity (mol _{H₂O₂} kg _c at ⁻¹ h ⁻¹)	Selectivity (%)
		Temperatur e (°C)	Time (h)	Pressure (MPa)	Solvent		
PdAu/WO₃-TiO₂ (In this work)	H₂SO₄	2	0.25	4	CH₃OH+H₂O	662.6	85.5
W-Pd/Al ₂ O ₃ ¹	H ₂ SO ₄	2	0.25	4	CH ₃ OH+H ₂ O	125.3	59.1
Pd ₆ Pb/TiO ₂ ²	/	0	0.5	4	CH ₃ OH+H ₂ O	170.1	56.7
Pd ₃ Pb cubes/s-TiO ₂ ³	/	30	1	4	C ₂ H ₅ OH	222.4	53
R-PdNi/TiO ₂ -C ⁴	/	25	1.5	0.1	H ₂ O	83.3	96.15
PdAu@HZSM-5 ⁵		2	0.5	4	CH ₃ OH+H ₂ O	27.73	90
Au-Pd/TiO ₂ ⁶	CO ₂	2	0.5	4	CH ₃ OH+H ₂ O	93	44
Au-Pd-G6%T ⁷	H ₂ SO ₄	5	1	4	CH ₃ OH	55	64
PdTe/Al ₂ O ₃ ⁸	H ₂ SO ₄	10	1/6	0.1	C ₂ H ₅ OH	84.7	52.9
AuPdPt/TiO ₂ ⁹	/	2	0.5	4	CH ₃ OH+H ₂ O	112	37
Pd@NiO ₃ /TiO ₂ ¹⁰	/	2	0.5	4	CH ₃ OH+H ₂ O	89	81
Pd-Sb/TiO ₂ ¹¹	H ₂ SO ₄	10	1/6	0.1	C ₂ H ₅ OH	46.6	73
Pd-Zn/ Al ₂ O ₃ ¹²	H ₂ SO ₄	2	0.25	3	CH ₃ OH	216.2	78.5
Pd/HAp ¹³	H ₂ SO ₄	10	0.5		C ₂ H ₅ OH	37.1	43
AuPd/2LbL ¹⁴	NaBr+H ₂ SO ₄	42	3	2	C ₂ H ₃ N+H ₂ O	210	67
Pd-Te/TiO ₂ ¹⁵	H ₂ SO ₄	10	1/6	0.1	CH ₃ OH	29.3	~100
Pd-Ag/SiO ₂ ¹⁶	H ₂ SO ₄	2	0.25	3	CH ₃ OH	58.3	70.9
3 wt% Pd-2 wt% Sn/TiO ₂ ¹⁷	/	2	0.5	4	CH ₃ OH+H ₂ O	61	96
Pd/SiO ₂ ¹⁸	KBr+ H ₂ PO ₄	20	3	0.1	C ₂ H ₅ OH+H ₂ O	4.77	62
Pd/N-TiO ₂ ¹⁹	H ₂ SO ₄	10	2	0.1	C ₂ H ₅ OH	41	58.8
Pd/HNb ₃ O ₈ -NS ²⁰	/	20	4	0.2	CH ₃ OH	2.3	16
Pd/TiO ₂ ²¹	H ₂ SO ₄	10	0.5	0.1	CH ₃ OH	29.9	61
Pd/C ²²	HCl	10	4	/	C ₂ H ₅ OH+ H ₂ O	134.9	74

PdAu/TiO ₂ ²³	H ₂ SO ₄	10	1/6	0.1	C ₂ H ₅ OH	69.9	48.1
Pd/PAH-K2621 ²⁴	HBr	30	3	5	CH ₃ OH	12.7	73
Pd/C ²⁵	H ₂ SO ₄	20	4	2.1	H ₂ O	170	59.4
Au-Pd/C ²⁶	/	2	0.5	4	CH ₃ OH+H ₂ O	110	80
Pd-Au/ZrO ₂ ²⁷	H ₂ SO ₄	20	5	0.1	CH ₃ OH	16.7	52

Table S3. The mass ratio of Pd, Au and W in the catalysts measured by XPS and ICP.

Catalysts	Measurement method	Pd (wt%)	Au (wt%)	W (wt%)
PdAu/TiO ₂	XPS	44.72	55.28	—
	ICP	48.9	51.1	—
PdAuWO ₃ /TiO ₂ (3W)	XPS	5.97	4.43	89.6
	ICP	30.7	31.7	37.6
WO ₃ -PdAu/TiO ₂ (3W)	XPS	11.54	11.33	77.13
	ICP	30.4	31.3	38.3
PdAu/WO ₃ -TiO ₂ (3W)	XPS	7.82	6.54	85.63
	ICP	31.6	33.2	35.2
PdAu/SiO ₂	XPS	47.83	52.17	—
	ICP	49.0	51.0	—
PdAu/WO ₃ -SiO ₂ (3W)	XPS	30.72	32.16	37.13
	ICP	32.2	33.4	34.4

Table S4. Surface Pd⁰ and Pd²⁺ percent of PdAu/WO₃-TiO₂ catalysts with different W content.

Catalyst	Pd ⁰ (%)	Pd ²⁺ (%)
PdAu/1WO ₃ -TiO ₂	82.46	17.54
PdAu/3WO ₃ -TiO ₂	80.53	19.47
PdAu/5WO ₃ -TiO ₂	74.69	25.31

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