Supporting Information

Atomically Dispersed Pt Inside MOF for Highly Efficient Photocatalytic Hydrogen Evolution

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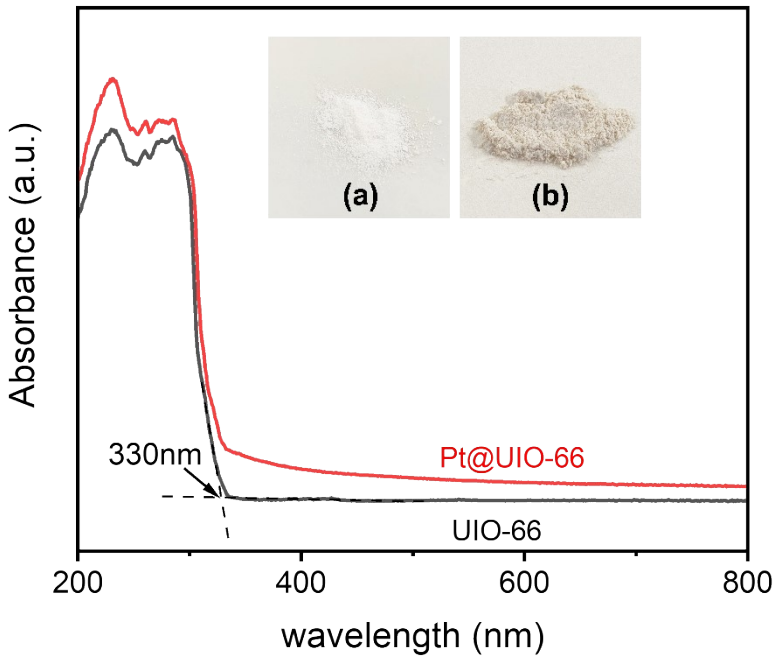

Figure S1. UV-vis diffraction spectra of UiO-66 and Pt@UiO-66, inset shows photographs of UiO-66 (a) and Pt@UiO-66 (b).

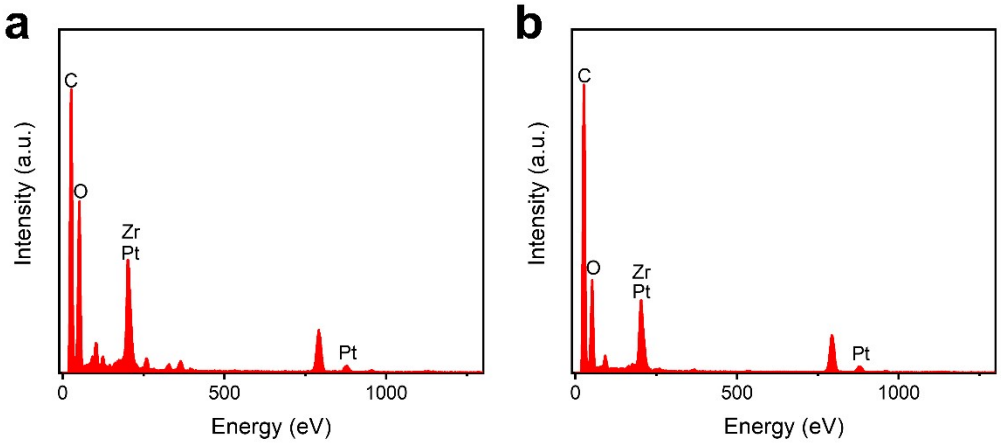

Figure S2. EDX spectrum of Pt@UiO-66(SC) (a) and Pt@UiO-66(b).

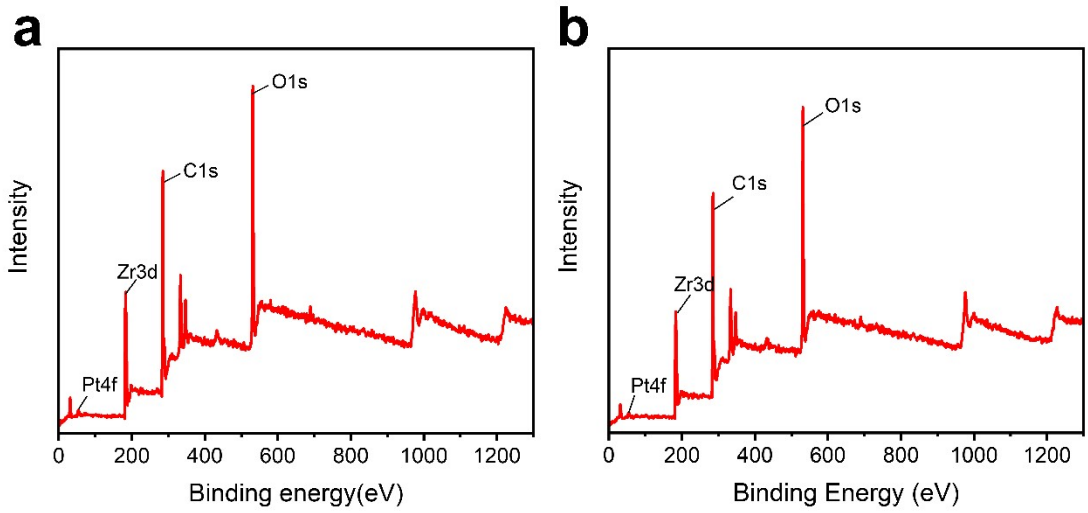

Figure S3. XPS survey scan of Pt@UiO-66(SC) (a) and Pt@UiO-66 (b).

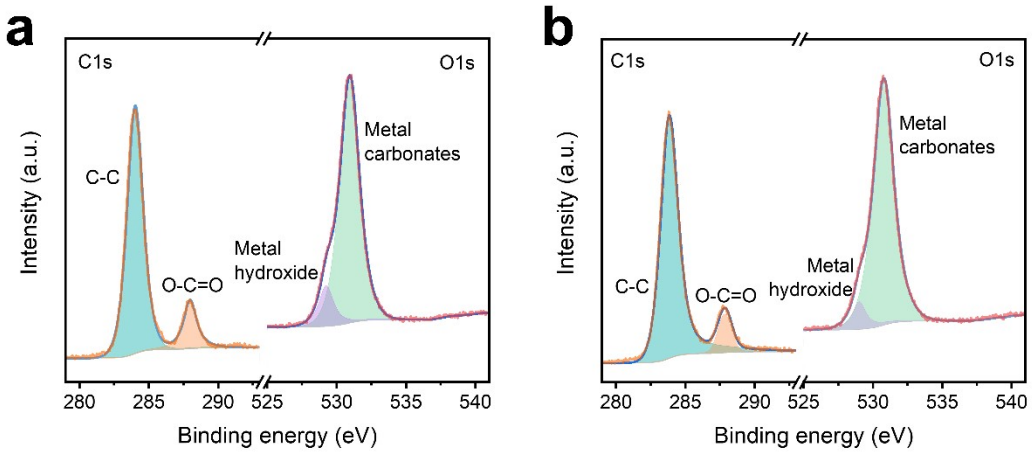

Figure S4. XPS scan of C 1s and O 1s, Pt@UiO-66(SC) (a), Pt@UiO-66(b).

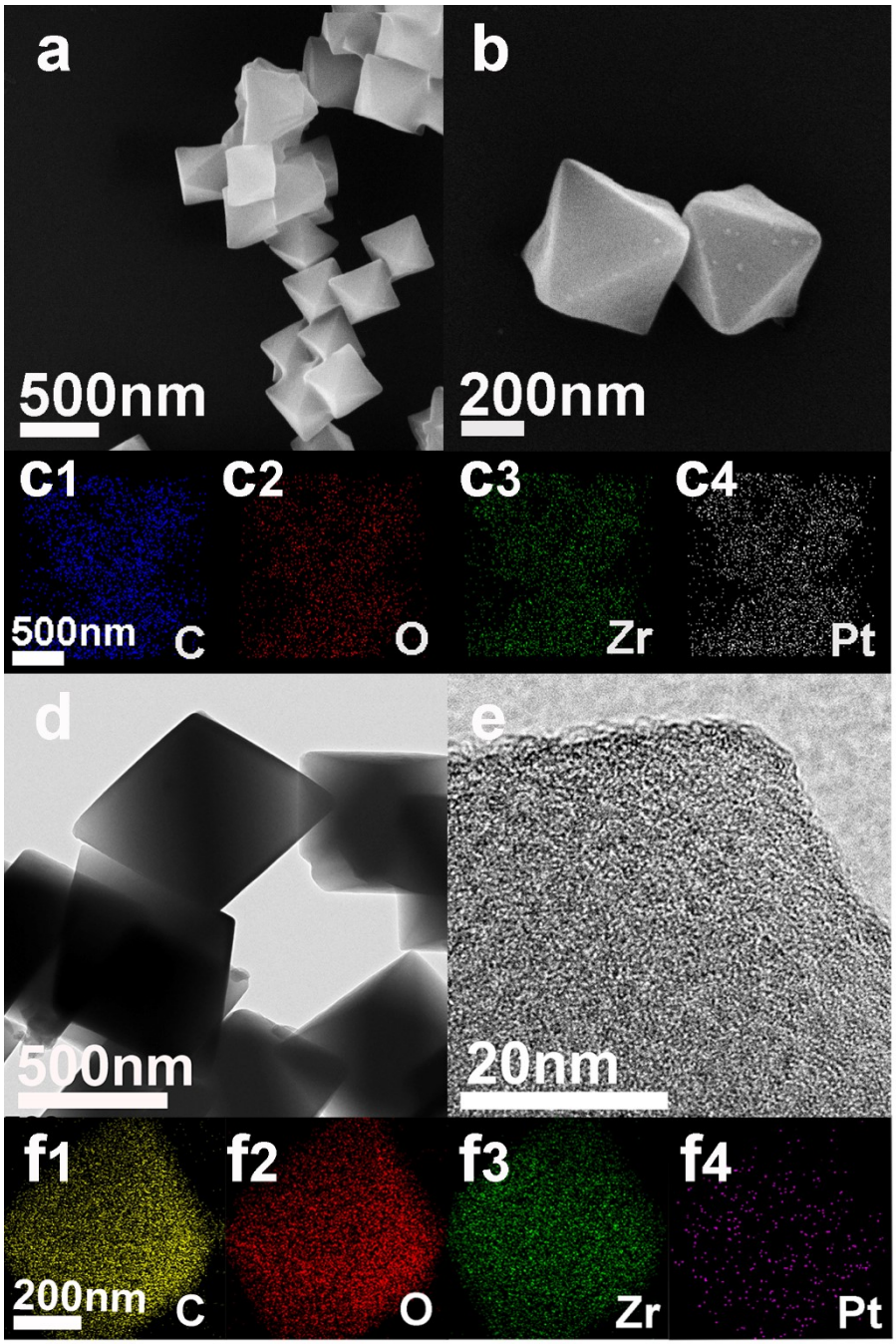

Figure S5. SEM images of Pt@UiO-66(SC) (a-c) and TEM images of Pt@UiO-66(SC) (d-f).

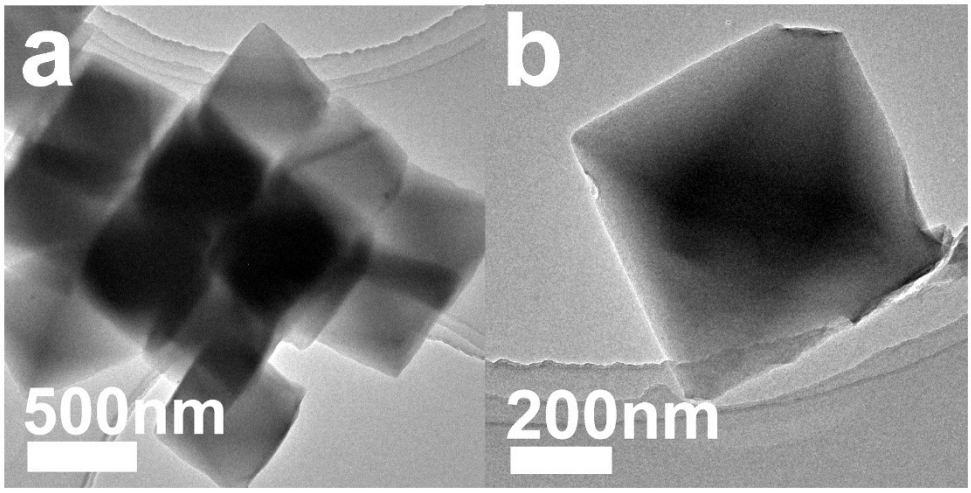

Figure S6. The TEM image of Pt@UiO-66 after three cycles of photocatalytic reactions

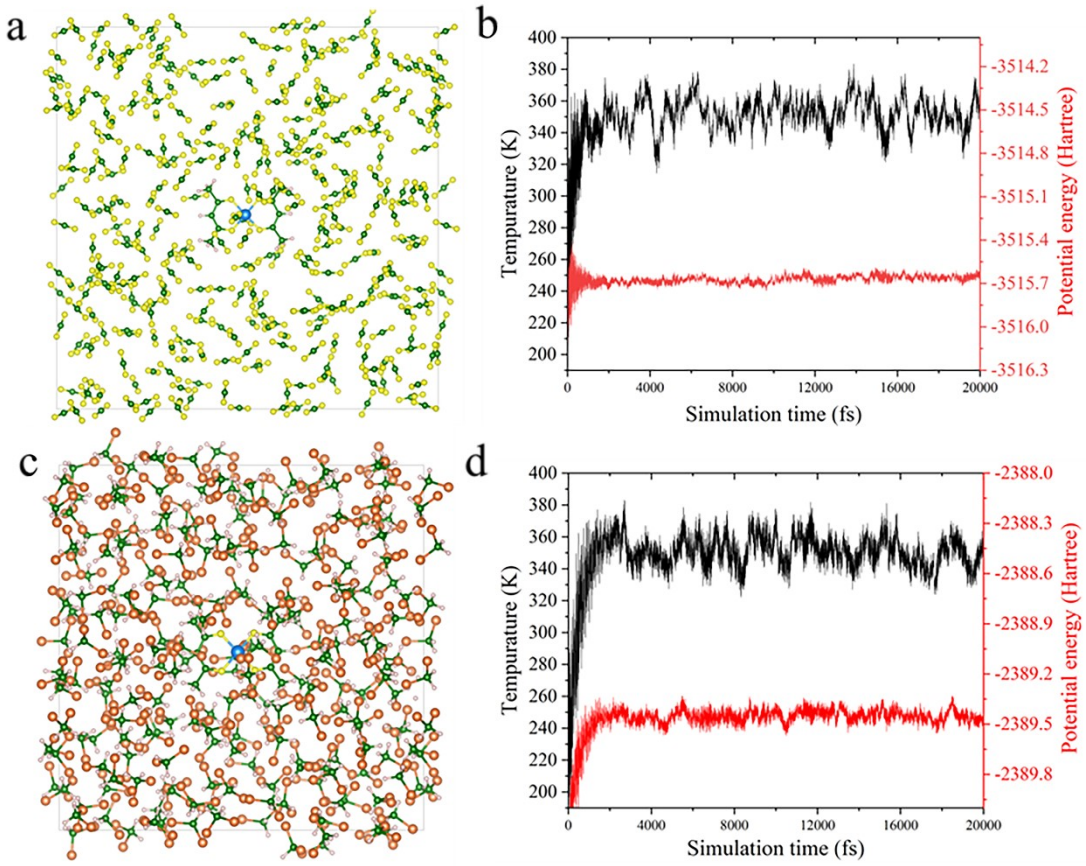

Figure S7. The molecular dynamic simulation of platinum acetylacetonate diffusing in CH_2Cl_2 and SC CO_2. the initial structure of SC CO_2 solvent, containing 300 CO_2 molecules and one platinum acetylacetonate molecule(a). Potential energy and temperature evolution in molecular dynamics simulations of SC CO_2 solvent(b). the initial structure of CH_2Cl_2 solvent, containing 200 CH_2Cl_2 molecules and one platinum acetylacetonate molecule(c). Potential energy and temperature evolution in molecular dynamics simulations of CH_2Cl_2 solvent. Green atom: C, yellow atom: O, blue atom: Pt, white atom: H, orange atom: Cl(d).

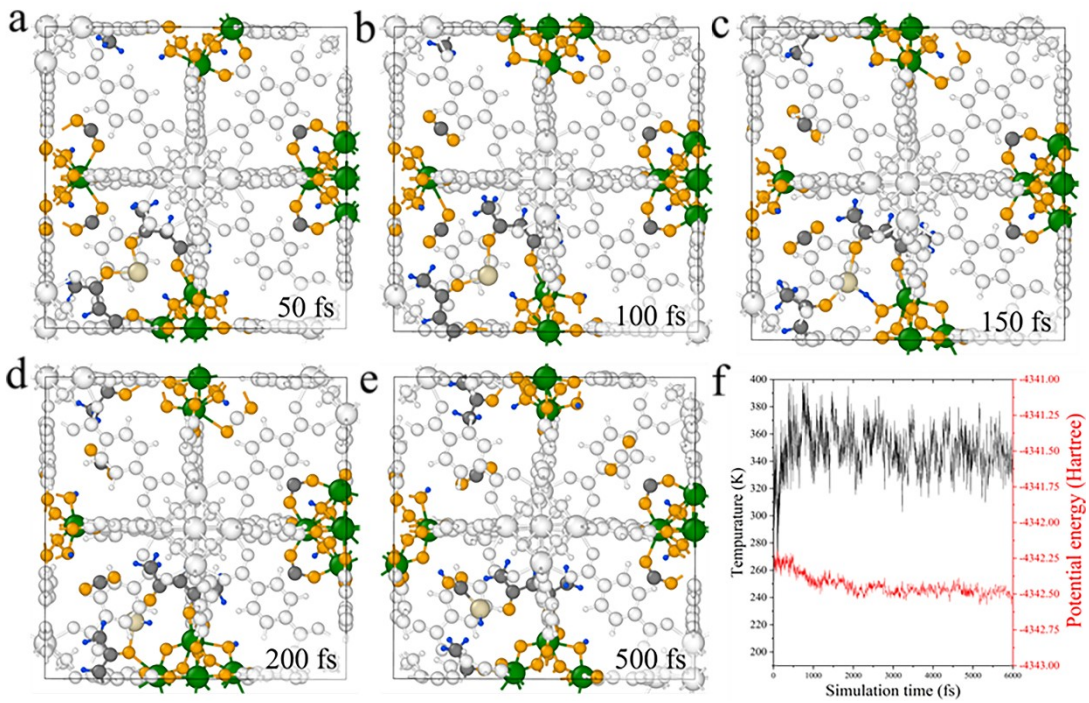

Figure S8. The molecular dynamics simulation used to explore the microscopic mechanism of platinum acetylacetonate destruction. The key frames(a-e). Potential energy and temperature evolution in molecular dynamics simulation (f).

Table S1. Inductively coupled plasma results for Pt contents in catalysts.

Mass of catalyst	Pt Wt%
Pt@UiO-66(SC)	0.03%
Pt@UiO-66	0.08%

Table S2. Summary of reported UiO-66 based photocatalysts.

Mass of catalyst	Dye	Light intensity	Concentration of sacrificial agent	Rate of H_2 evolution μmol/g/h	Ref.
Pt@UiO-66 5mg	RhB 10ppm	300W Xe lamp ≥420 nm	10%TEOA	3871	This work
Co-MoS/UiO-66/rGO 10 mg	EY 20 mg	300W Xe lamp ≥420 nm	15%TEOA	2233	[1]
NiO/UiO-66-NH_2 5 mg	EY 10 mg	300W Xe lamp ≥420 nm	3%TEOA	2550	[2]
MoS_2/UiO-66/Co_3O_4 10 mg	EY 20 mg	300W Xe lamp ≥420 nm	15%TEOA	2970	[3]
Pd/UiO-66 10 mg	EY 20 mg	5 W LED white light	15%TEOA	3600	[4]
MoS_2/UiO-66-NH_2/GO 30 mg	EY 28 mg	300W Xe lamp	10%TEOA	1069	[5]
Ni_4S_3/UiO-66/rGO 20 mg	EY 10 mg	N/A	15%TEOA	1866	[6]
NiS_2/UiO-66 10mg	ErB	300W Xe lamp ≥420 nm	10%TEOA	1840	[7]
Pt@UiO-66 50mg	RhB 10ppm	300W Xe lamp ≥420 nm	10%TEOA	116	[8]
Pt/TiO_2/UiO-66-NH_2/GO 10mg	RhB 4.8 ppm	300W Xe lamp ≥420 nm	2%TEOA	2700	[9]
Pt@UiO-66-NH_2 25mg	Calix [4] arene	300W Xe lamp ≥420 nm		1528	[10]
Ni_2P@UiO-66-NH_2 5mg		300W Xe lamp ≥380 nm	3%TEA	409.1	[11]
Pt(PTA)@UiO-66-NH_2 35mg		1.9 W white LED	EDTA	56	[12]
Pt/CD@NH_2-UiO-66/g-C_3N_4		300W Xe lamp	Sodium	2930	[13]

10mg	≥420 nm	ascorbate		
MoS_2/UiO-66/CdS 20mg	300W Xe lamp ≥420 nm	10%TA	1625	[14]
Pt@UiO-66-NH2 10mg	300W Xe lamp	8.3%TEOA	381.2	[15]

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