Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporing Information:

Ligand modification on UiO-66 with unusual visible-light photocatalytic behavior for RhB degradation

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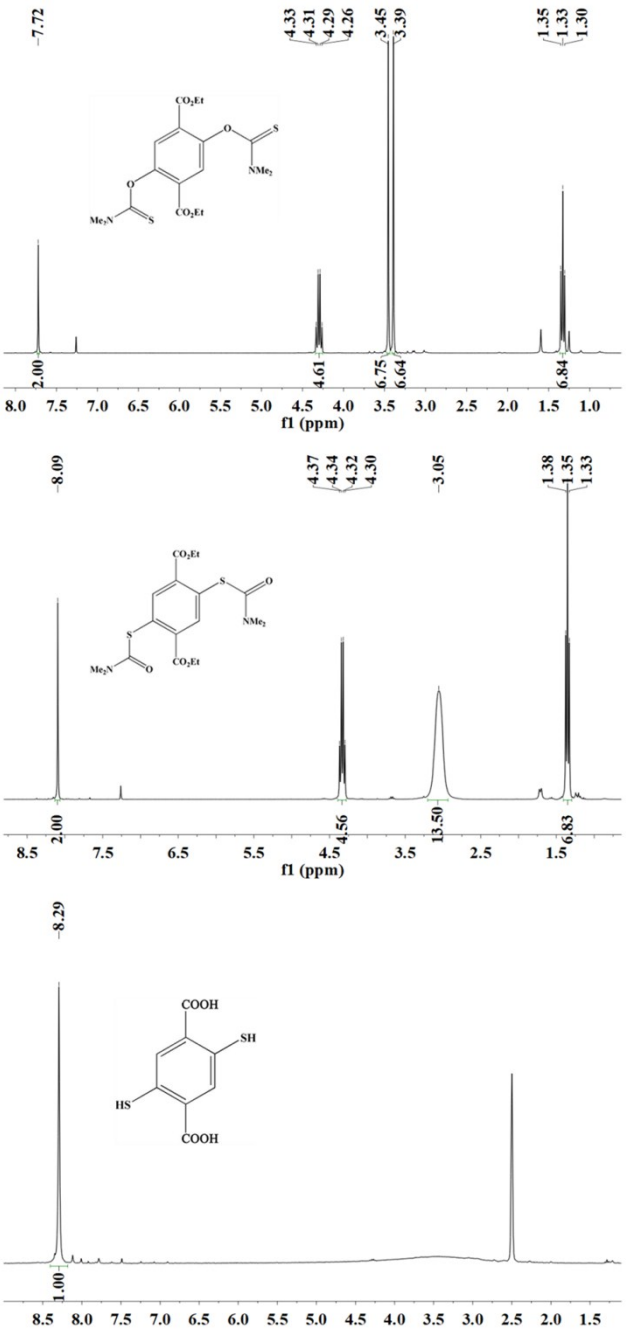

Figure S1. ^{1}H NMR spectrums of synthesized H_2BDC-2,5SH and two intermediates.

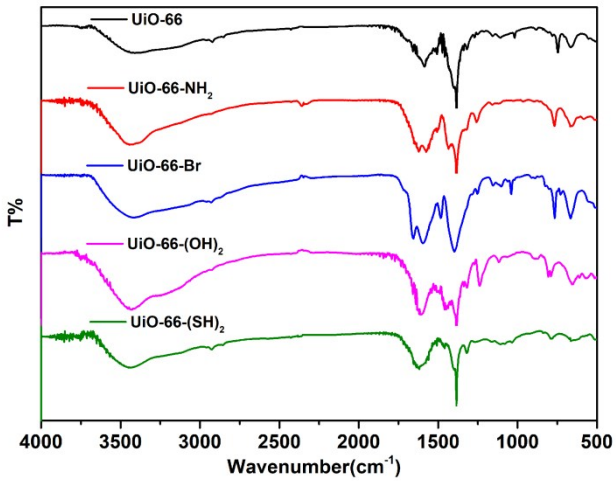

Figure S2. IR spectra of the UiO-66-X (X = H, NH_2, Br, $(OH)_2$, $(SH)_2$)

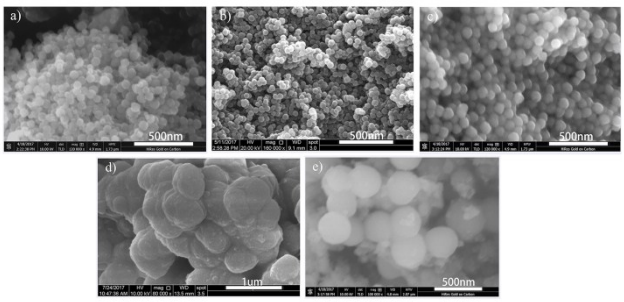

Figure S3. SEM images of the a) UiO-66, b) UiO-66-NH_2, c) UiO-66-Br, d) UiO-66-$(OH)_2$, e) UiO-66-$(SH)_2$

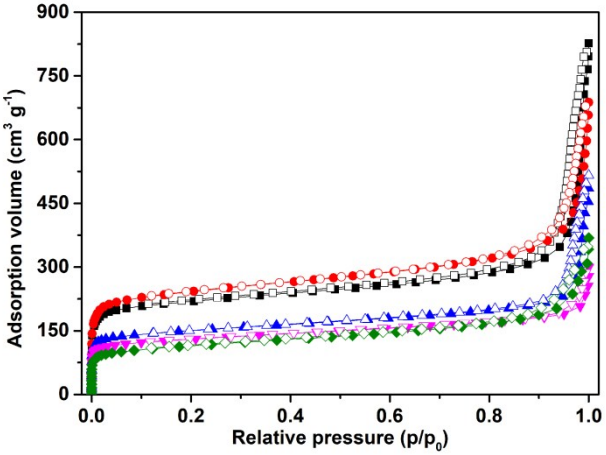

Figure S4. The N_2 adsorptions isotherms of UiO-66 (black), UiO-66-NH_2 (red), UiO-66-Br (blue), UiO-66-$(OH)_2$ (magenta), UiO-66-$(SH)_2$ (olive); Solid and hollow data correspond to the adsorption and desorption branches, respectively.

Table S1. Porosity properties of the UiO-66-X (X = H, NH_2, Br, $(OH)_2$, $(SH)_2$).

	UiO-66	UiO-66-NH_2	UiO-66-Br	UiO-66-$(OH)_2$	UiO-66-$(SH)_2$
BET surface area (m^2g^{-1})	835	917	563	482	418
Pore volume ($cm^3\ g^{-1}$)	0.56	0.60	0.36	0.29	0.33

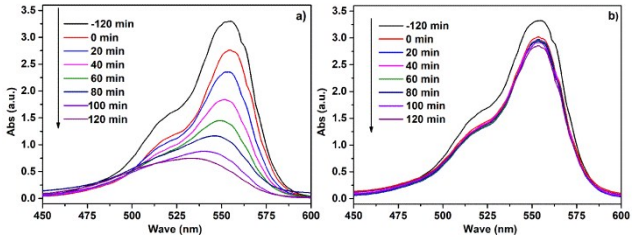

Figure S5. Absorption spectra of RhB solution in different irradiation time under visible light (400-780nm). a)15mg UiO-66 in 100 mL 20 mg L^{-1} RhB aqueous solution. b)15mg UiO-66-NH_2 in 100 mL 20 mg L-1 RhB aqueous solution.

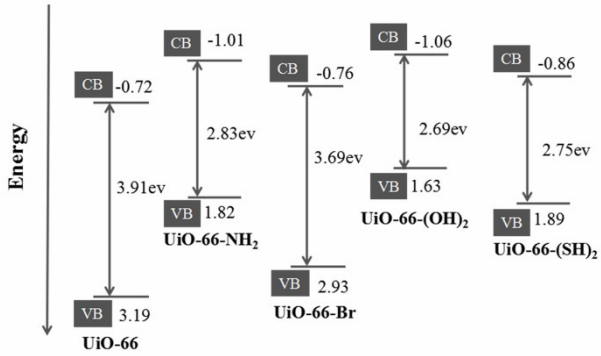

Figure S6. Diagram for the potential of UiO-66-X (X = H, NH_2, Br, $(OH)_2$, $(SH)_2$).

Table S2. The potential (V_{fb}, V_{CB} and V_{VB}) of the UiO-66-X (X = H, NH_2, Br, $(OH)_2$, $(SH)_2$).

Potential (V) \ Sample	UiO-66	UiO-66-NH_2	UiO-66-Br	UiO-66-$(OH)_2$	UiO-66-$(SH)_2$
Flat band (V_{fb})	-0.83	-1.12	-0.87	-1.17	-0.97
Conduction band (V_{CB})	-0.72	-1.01	-0.76	-1.06	-0.86
Valence band (V_{VB})	3.19	1.82	2.93	1.63	1.89

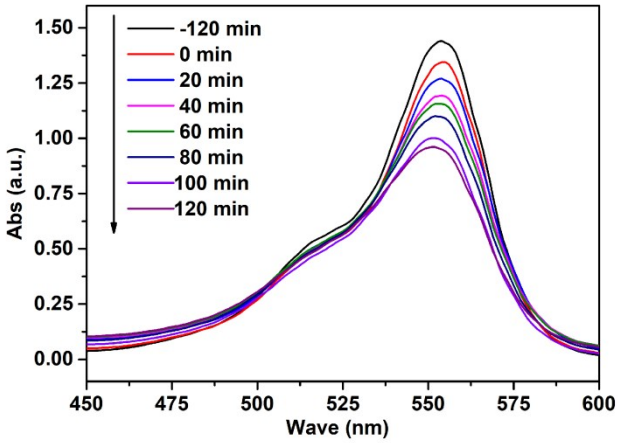

Figure S7. Absorption spectra of RhB in different irradiation time under visible light (400-780nm). Reaction solution: 20 mg UiO-66-NH_2 in 100 mL 10 mg L^{-1} RhB aqueous solution.

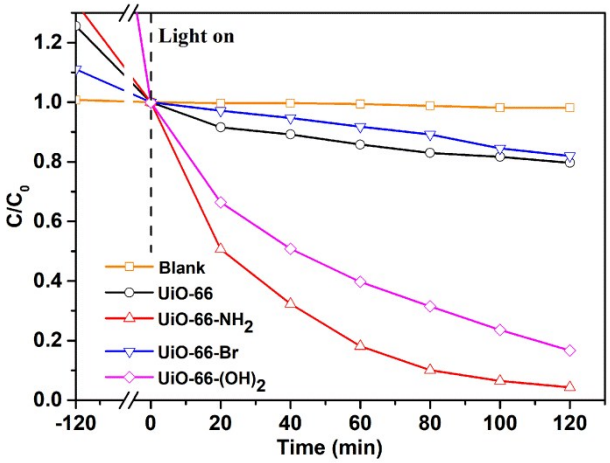

Figure S8. Photocatalytic reaction of Cr(VI) solution in the presence and absence (blank) of catalysts under visible-light irradiation (400-780 nm). Reaction condition: 15 mg catalyst in 100 mL 20 mg L^{-1} Cr(VI)solution, PH=2.