Electronic supplementary information

Application of a Ni mercaptopyrimidine MOF as a highly efficient catalyst for sunlight-driven hydrogen generation

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Figure S1. The amount of hydrogen photogenerated in the presence of $[Ni_2(PymS)_4]_n$ (15 µmol), Fl (2 mM) and TEA (15%) in water at pH = 10 (black); (b) the amount of hydrogen photogenerated by the filtrate of the aqueous solution containing $[Ni_2(PymS)_4]_n$ (15 µmol), TEA (15%) and Fl (2 mM) after stirring for 5 minutes.



Figure S2. FT-IR spectra (left) and powder PXRD patterns (right) of $[Ni_2(PymS)_4]_n$ before (black line) and after photocatalytic reactions (blue).



Figure S3. The amount of hydrogen photogenerated by $[Ni_2(PymS)_4]_n$ (10 µmol) with Fl (2 mM) and TEA (15%, v/v) in water with varied pH values from 7 to 10.



Figure S4. The amount of hydrogen photogenerated by $[Ni_2(PymS)_4]_n$ (10 µmol) with Fl (2 mM) in water when TEA changes from 5% to 15% (v/v).



Figure S5. The amount of hydrogen photogenerated by $[Ni_2(PymS)_4]_n$ (10 µmol) with TEA (15%) in water when Fl changes from 2 to 10 mM at pH = 10.



Figure S6. The amount of hydrogen photogenerated by $[Ni_2(PymS)_4]_n$ (5 µmol) with different particle sizes: (a) $20 \times 10 \times 20$ µm; (b) $11 \times 4 \times 10$ µm; (c) $4 \times 1 \times 4$ µm in the presence of Fl (2 mM) and TEA (15%) in an hour.



Figure S7. Emission quenching (left) and Stern-Volmer plot (right) of Fl (0.01 mM) by TEA in water at pH = 10.



Figure S8. UV-vis spectrum of Fl (0.002 mM) in aqueous NaOH solution (pH = 10).

Table S1 TON of the catalyst in different cycles

	Cycle 1	Cycle 2	Cycle 3	Cycle 4	
ТО	2.5	2.5	2.2	2.0	
Ν	2.5				

All data was calculated from the photocatalytic experiments in the presence of $[Ni_2(PymS)_4]_n$ (15 µmol) Fl (2 mM) and TEA (15%, v/v) at pH = 10.

Table S2 TOF of different amounts of catalyst for hydrogen production

m / ma	14	2.1	2.8	5.6	8.4	11.	
m _{cat} / mg	1.4					2	
TOF / h-	10.6	9.0	6.5	3.5	2.5	1.7	
1							

All data was calculated from the photocatalytic experiments in the presence of Fl (2 mM) and TEA (15%, v/v) at pH = 10.