Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

BODIPY Functional Metal-Organic-Frameworks for Efficient Visible-Light-Driven Water Oxidation Without Additional Photosensitizers

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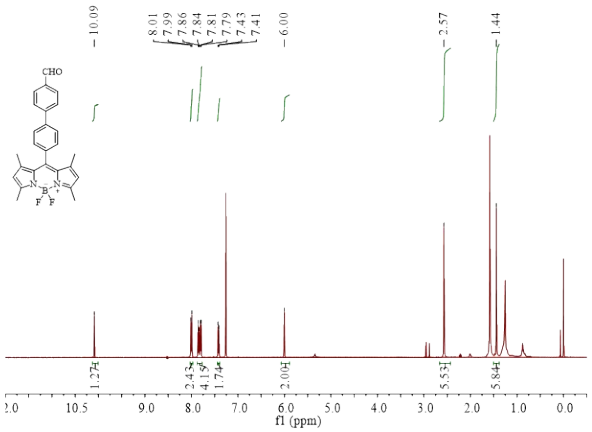

Fig. S1 The ^{1}HNMR spectrum of 5, 5-difluoro-10-(4'-formyl-[1, 1'-biphenyl]-4-yl)-1,3,7,9-tetramethyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide (CHO-BODIPY) in $CDCl_3$.

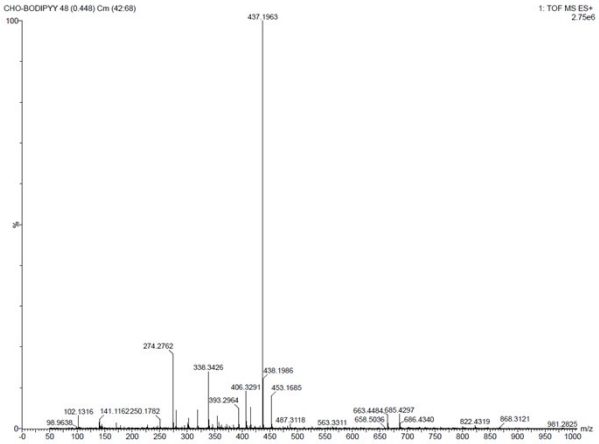

Fig. S2 The ESI-MS of CHO-BODIPY in CH_3OH ($[(M-H)+1/2H_2O]^+$=437.2).

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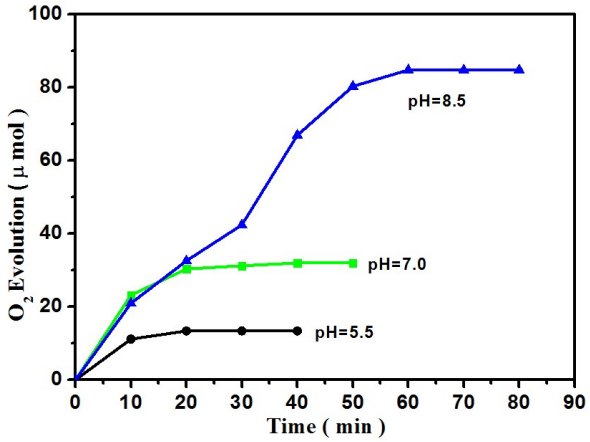

Fig. S3 O_2 evolution performance of 8 mg BODIPY-MIL-88B (Fe) in 2 mL phosphate buffer solution with 0.08 M $Na_2S_2O_8$ under various pH conditions.

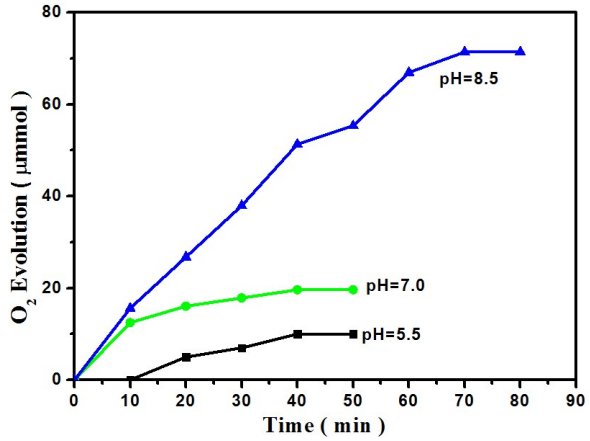

Fig. S4 O_2 evolution performance of 8 mg H-MIL-88B (Fe) in 2 mL phosphate buffer solution with 0.08 M $Na_2S_2O_8$ under various pH conditions.

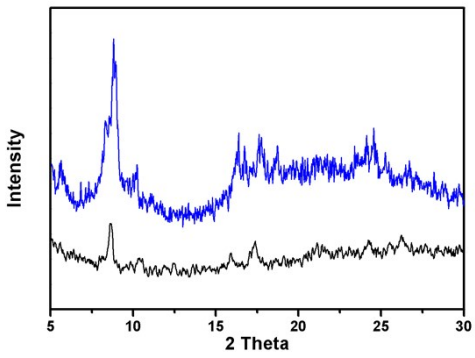

Fig. S5 XRD patterns of BODIPY-MIL-88B (Fe) before and after water oxidation (black line: after and blue line: before).

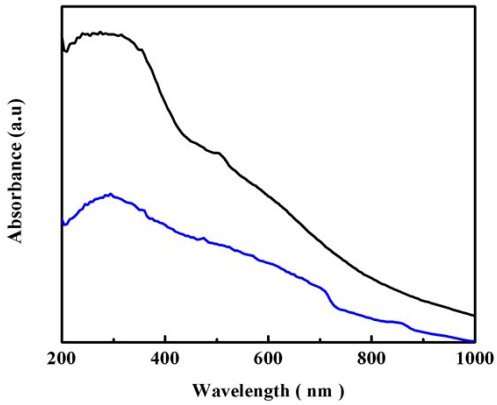

Fig. S6 UV-Vis diffuse reflectance spectra of BODIPY-MIL-88B (Fe) before and after water oxidation (black line: before and blue line: after).

Table S1 The water oxidation performance of different Iron-Carboxylate MOFs

MOFs	Photosensitizer	O_2 (μmol)	TON[a]	Reference
MIL-101 (Fe)[b]	$[Ru(bpy)_3]Cl_2$	36.5	27.3	[S1]
MIL-53 (Fe)[c]	$[Ru(bpy)_3]Cl_2$	49.6	35.4	[S2]
MIL-88(Fe)[d]	—	30	1.339	[S3]
H-MIL-88B(Fe)[c]	$[Ru(bpy)_3]Cl_2$	42.41	20.89	This work
H-MIL-88B(Fe)[c]	CHO-BODIPY	77.05	37.95	This work
BODIPY-MIL-88B(Fe)[c]	—	84.82	50.33	This work

[a] TON is defined as the total number of moles of O_2 per mole of catalyst
[b] Reaction conditions: 0.02 M $Na_2S_2O_8$ (electron acceptor), 80 mM sodium borate buffer (pH=10.0), 1 mg catalyst.
[c] Reaction conditions: 0.08 M $Na_2S_2O_8$ (electron acceptor), 20 mM sodium phosphate buffer (pH=8.5), 5 mg catalyst.
[d] Reaction conditions: 0.1 M $AgNO_3$(electron acceptor), 20 mg catalyst, 3 mL aqueous solution.

References

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