

## **Electronic Supplementary Information**

### **Prussian blue nanoparticles encapsulated inside a metal-organic framework via in situ growth as promising peroxidase mimetics for enzyme-inhibitor screening**

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## **1. Determination of PB content in MIL-101(Cr)**

Determination of PB content in MIL-101(Cr) were prepared as follows<sup>[1]</sup>: First, 50 mg MIL-101(Cr)@PB was digested by HCl/HNO<sub>3</sub> solution and diluted to 25 mL. Then, 50 μL of digestion solution and 50 μL of 10% sulfosalicylic acid solution were added to 325 μL of pH2.0 HCl solution, then the absorbance at 502 nm was then measured. For the experiment of standard curve, detection procedure was the same as that of digestion solution but using standard iron(III) ion solution instead of digestion solution. Finally, indirect estimation the PB content in MIL-101(Cr) through the iron content.

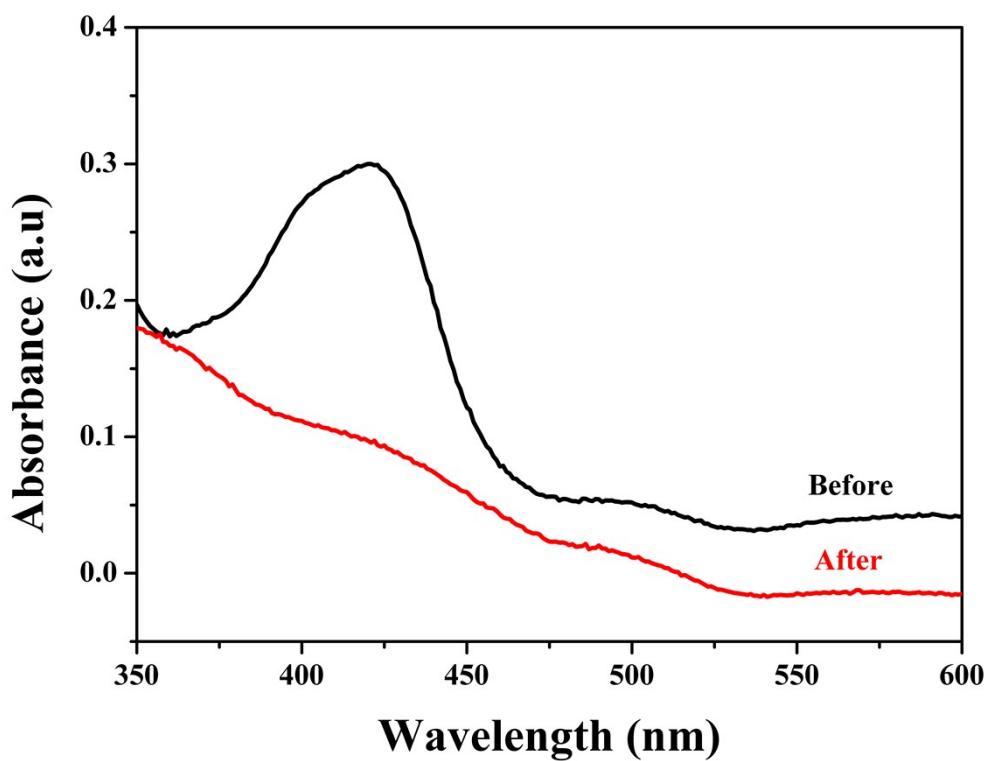


Fig.S1 UV–Vis spectra of 0.4 mM  $\text{Fe}(\text{CN})_6^{3-}$  aqueous solution before and after adsorption on  
MIL-101(Cr)@PB.

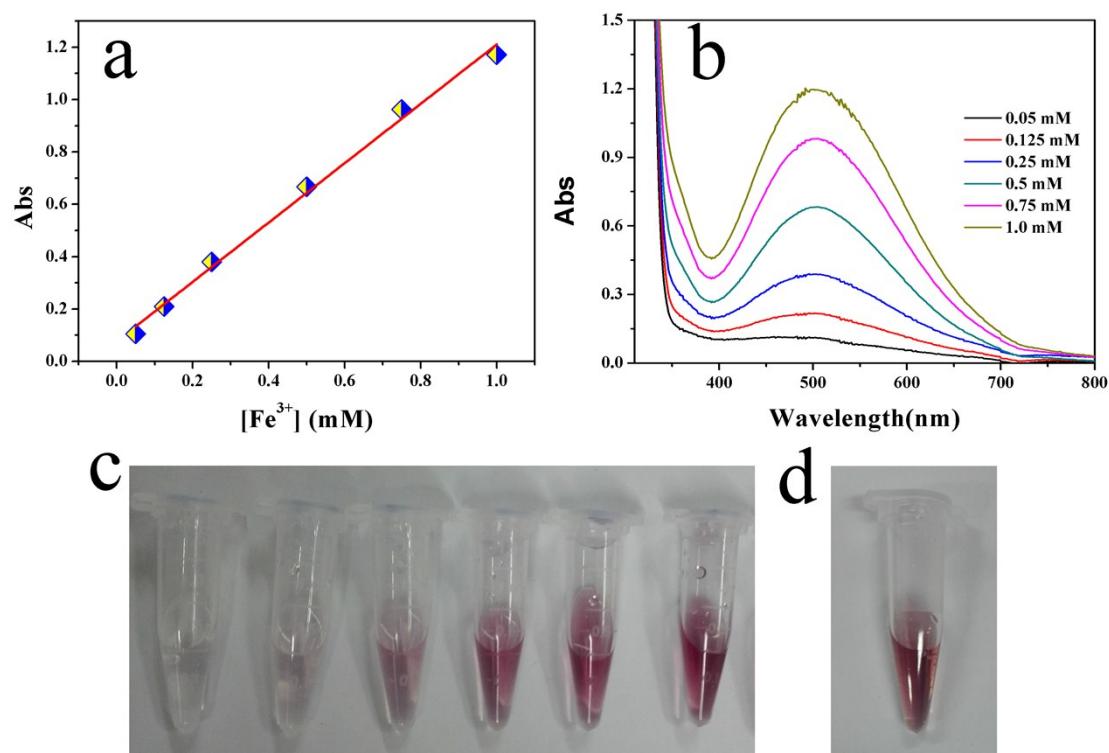


Fig.S2 Calibration plot for  $\text{Fe}^{3+}$  detection using sulfosalicylic acid as an analytical reagent (a) and its corresponding UV-Vis spectra (b), photographs (c); the photograph of digestive solution of MIL-101(Cr)@PB after adding sulfosalicylic acid (d).

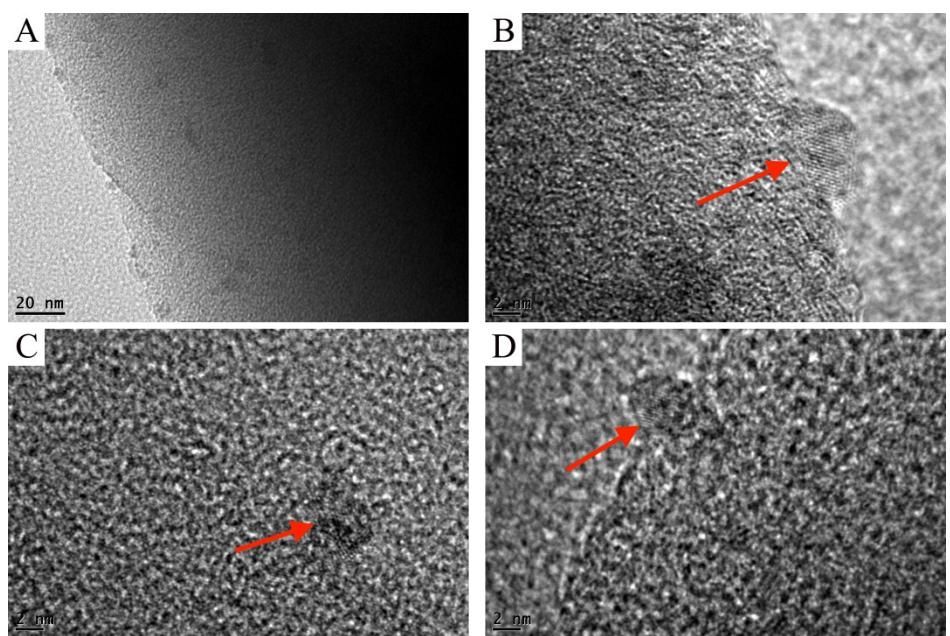


Fig. S3 HRTEM images of MIL-101(Cr)@PB.

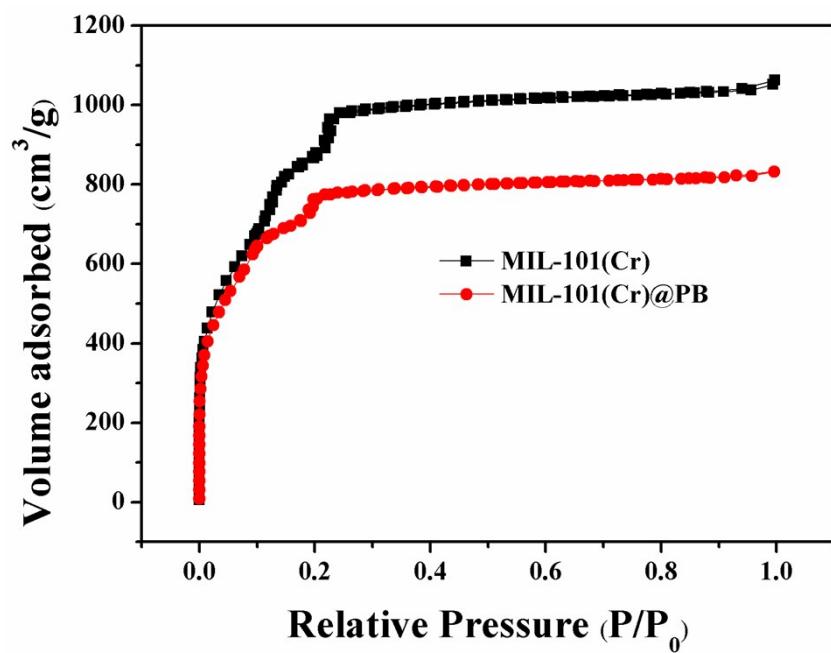


Fig. S4 Nitrogen adsorption and desorption isotherms of MIL-101(Cr) and MIL-101(Cr)@PB.

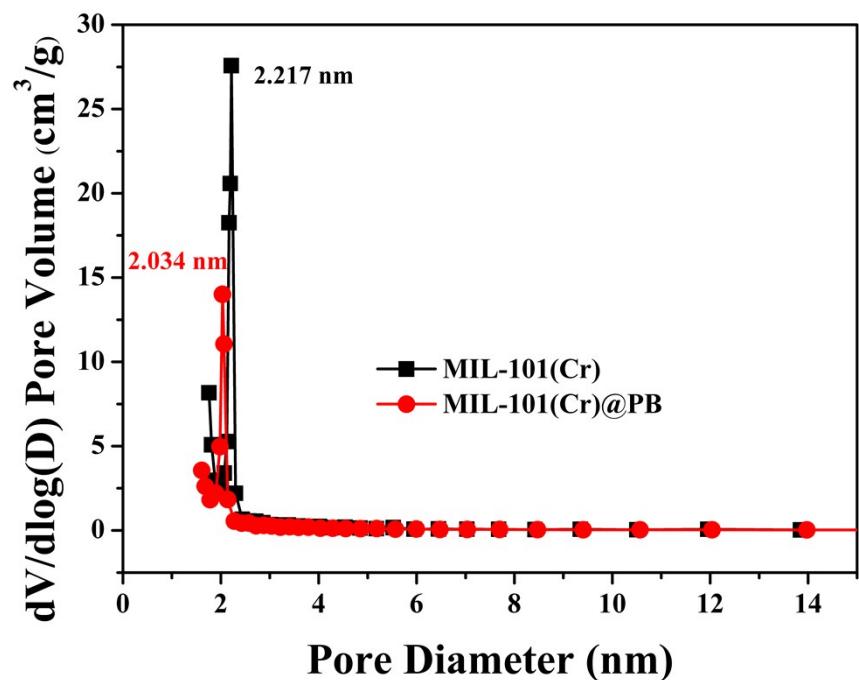


Fig. S5 BJH pore size distribution of MIL-101(Cr) and MIL-101(Cr)@PB.

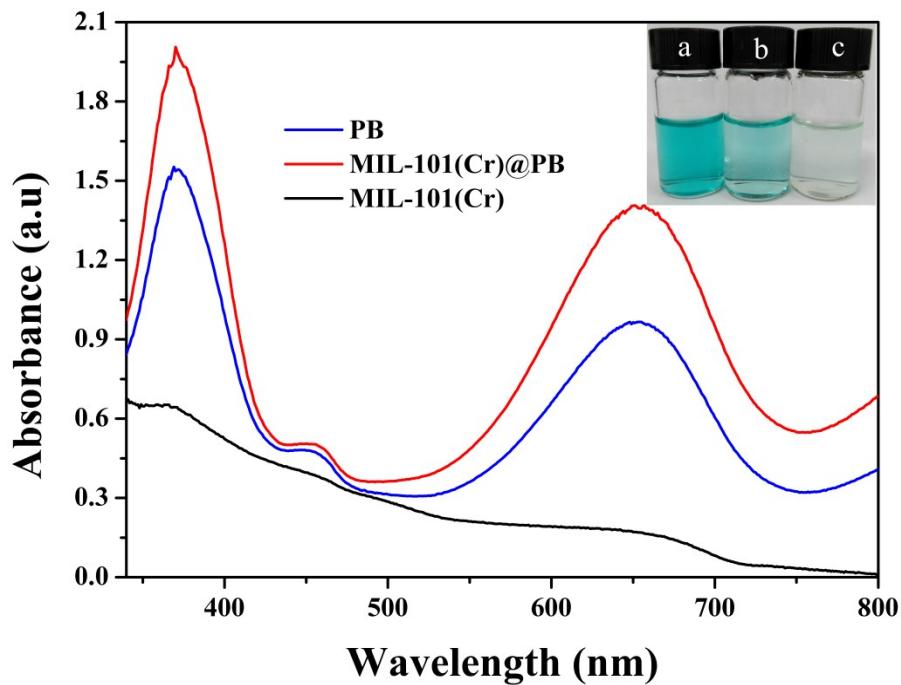


Fig. S6 UV–Vis absorption spectra of TMB–H<sub>2</sub>O<sub>2</sub> catalyzed by MIL-101(Cr)@PB, MIL-101(Cr) and PB. The inset shows photographs of TMB–H<sub>2</sub>O<sub>2</sub> catalyzed by MIL-101(Cr)@PB (a), PB (b) and MIL-101(Cr)(c).



Fig. S7 Images of oxidation color reaction of TMB (a), ABTS (b), OPD (c) and p-hydroxybenzoic acid /4-aminoantipyrine (d) by  $\text{H}_2\text{O}_2$  before (above) and after (below) by the catalysis of MIL-101(Cr)@PB.

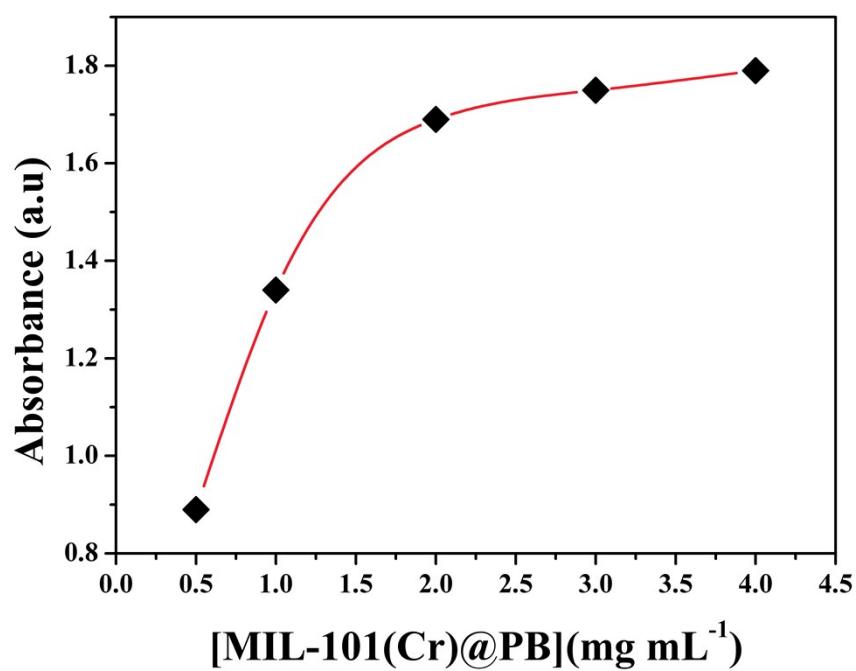


Fig. S8 Effect of catalyst amount on the peroxidase-like activity of MIL-101(Cr)@PB for the TMB oxidation.

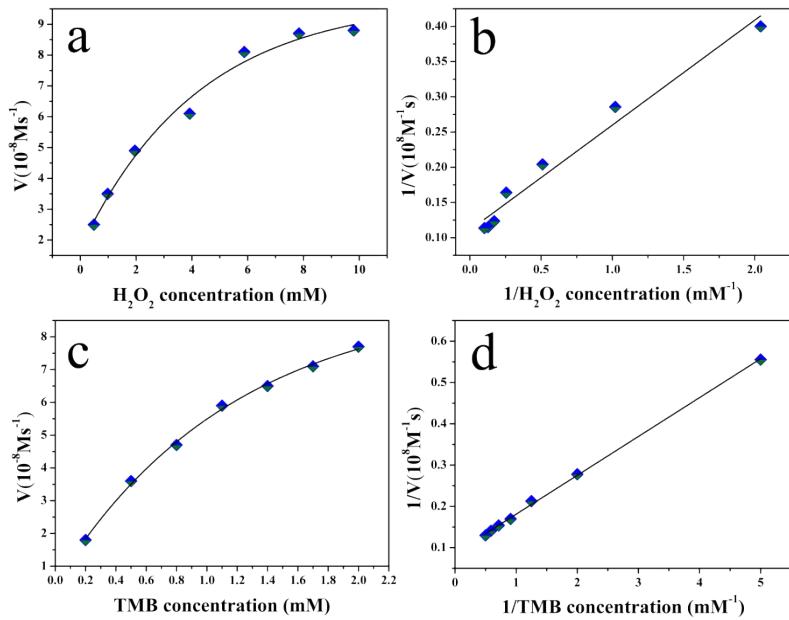


Fig. S9 Steady-state kinetic assay and catalytic mechanism of the MIL-101(Cr)@PB.

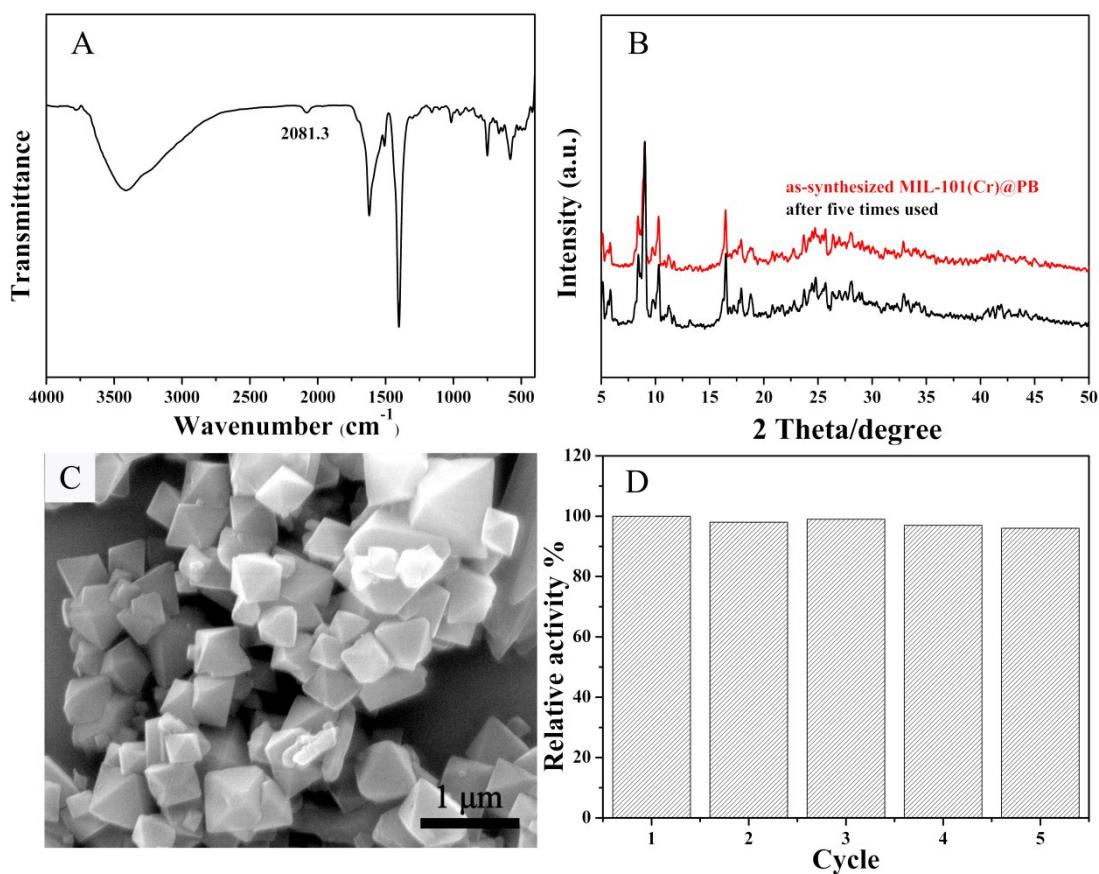


Fig. S10 Five consecutive catalysis cycles of MIL-101(Cr)@PB. FT-IR spectra (A), XRD patterns (B), SEM image (C) and relative activity (D).

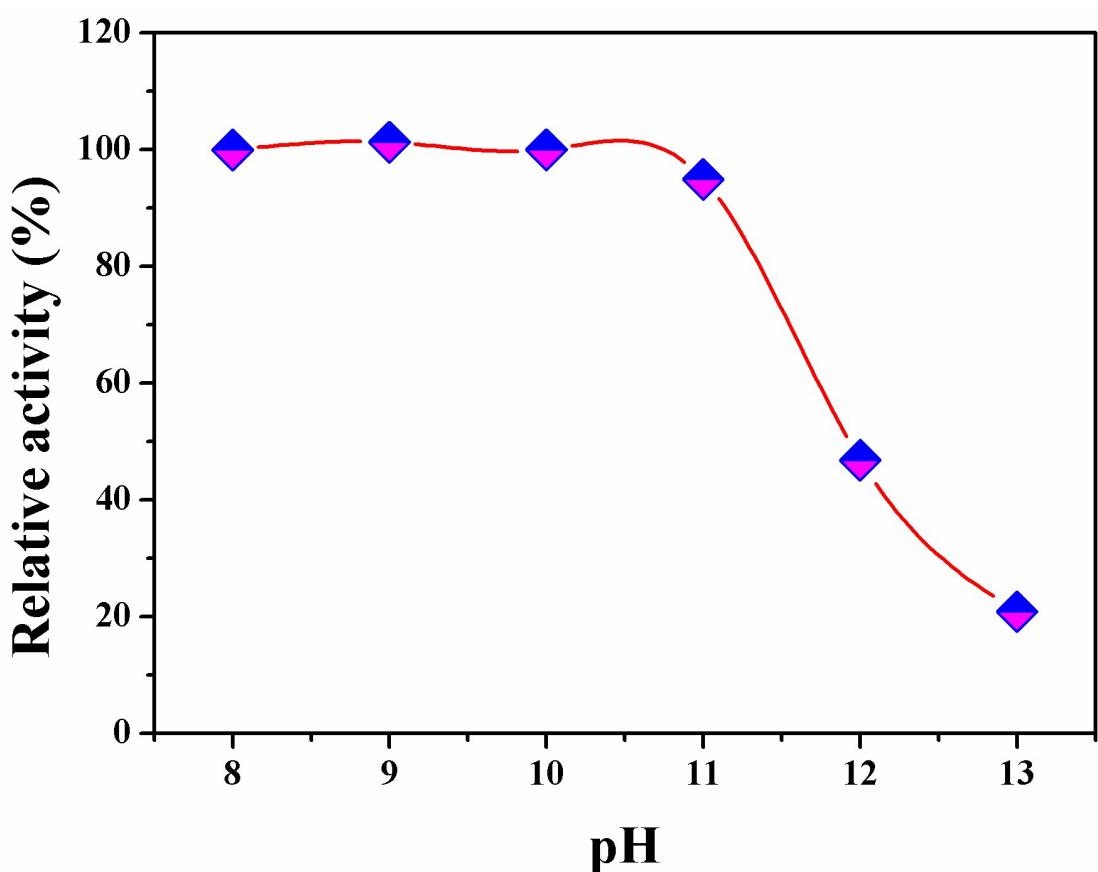


Fig. S11 The peroxidase-like activity of MIL-101(Cr)@PB after soaking in different pH solution for overnight.

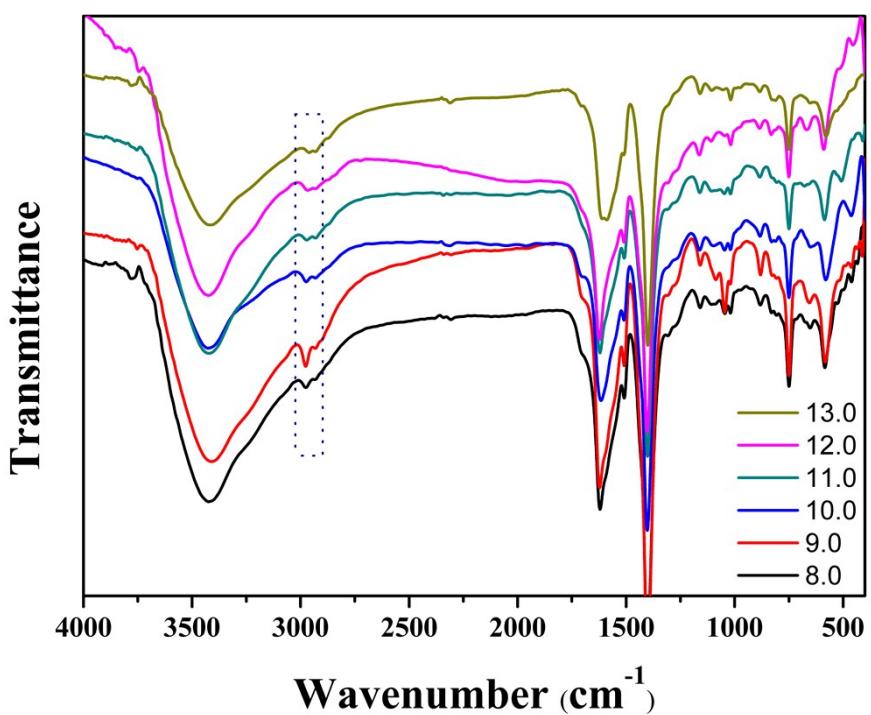


Fig. S12 FT-IR spectra of MIL-101(Cr)@PB after soaking in different pH solution for overnight.



Fig. S13 Images of oxidation color reaction of TMB before (A, B and C) and after (A', B' and C') treatment with 95°C for 40 min. MIL-101(Cr)@PB (A and A'), PB (B and B') and hemoglobin (C and C').

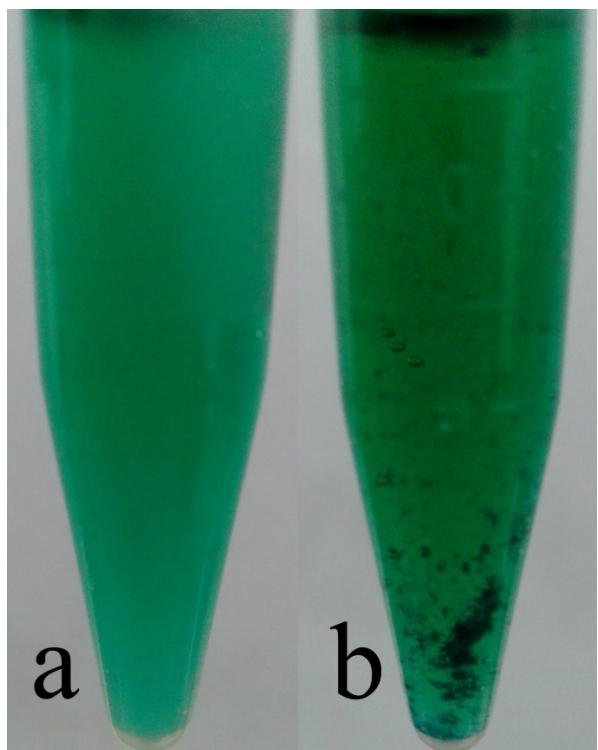


Fig. S14 Images of TMB solution oxidation catalyzed by MIL-101(Cr)@PB (a) and PB (b).

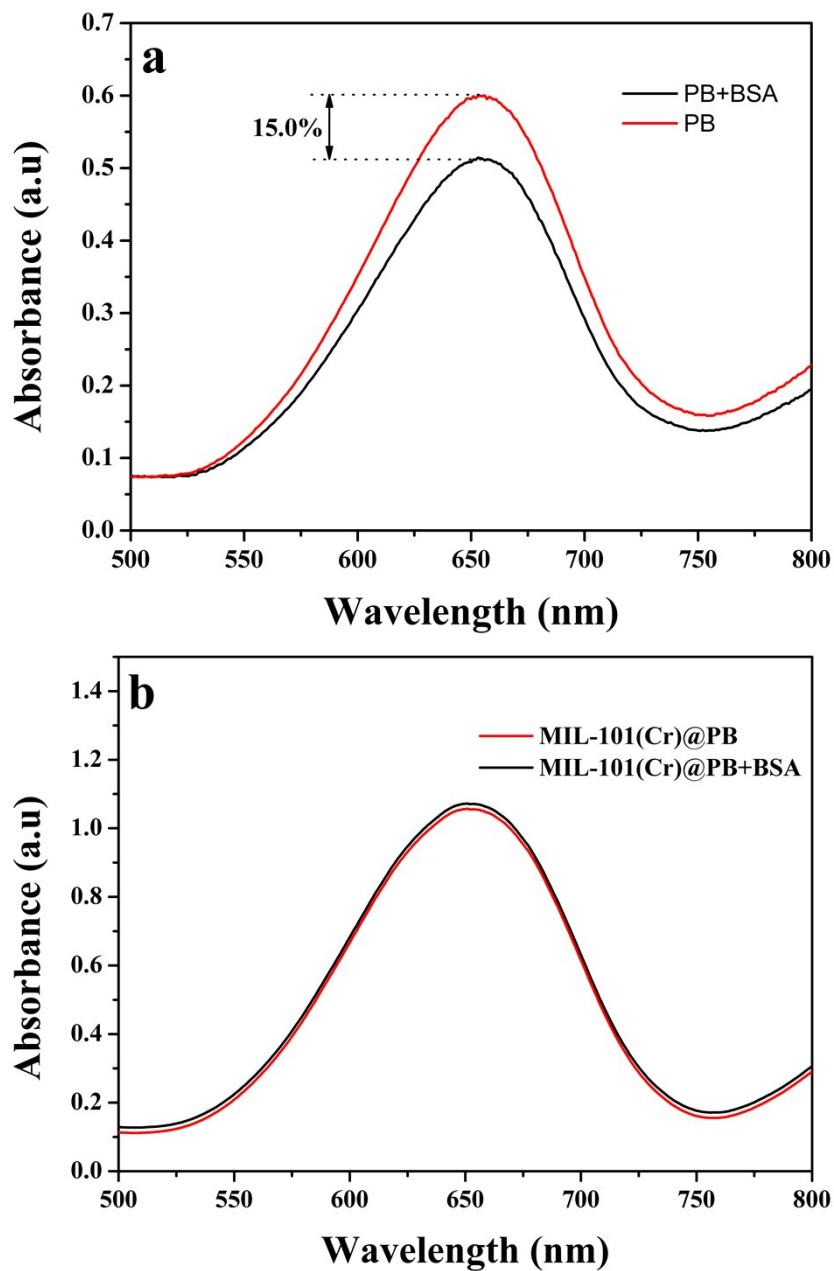


Fig. S15 Catalytic activity of PB (a) and MIL-101(Cr)@PB(b) in presence of protein.

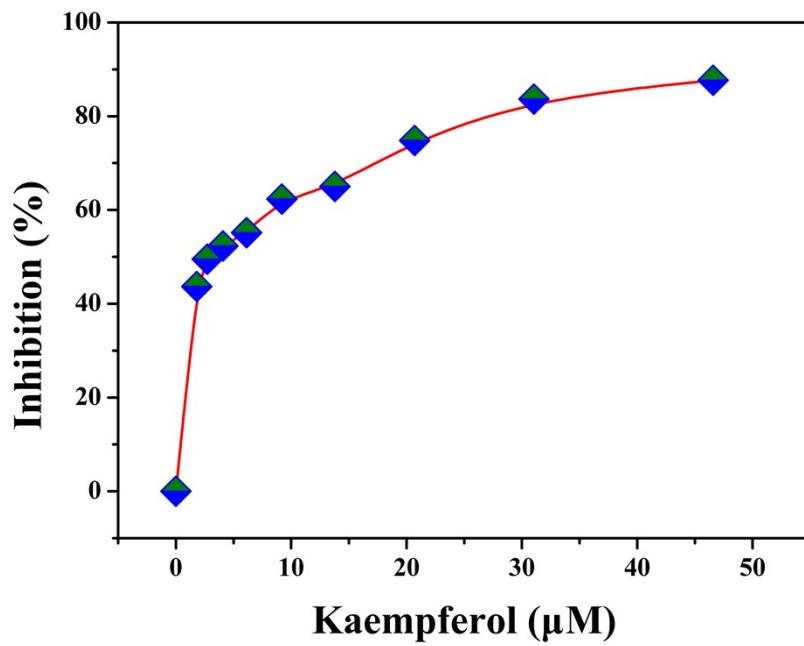


Fig. S16 Inhibition curves for XO inhibited by kaempferol.

Table S1. Comparison of the kinetic parameters of MIL-101(Cr)@PB and other nanomaterials.

Catalyst	Substance	$K_m/\text{mM}$	$V_{\max}/10^{-8}\text{M S}^{-1}$	Reference
$\text{ZnFe}_2\text{O}_4$	TMB	0.85	13.31	[2]
	$\text{H}_2\text{O}_2$	1.66	7.74	
$\text{Pt-MoO}_3$	TMB	0.106	4.3	[3]
	$\text{H}_2\text{O}_2$	3.2	3.8	
MWCNT@rGONR	TMB	0.12	9.28	[4]
	$\text{H}_2\text{O}_2$	1.68	3.15	
Hemin-GNs	TMB	5.1	5.55	[5]
	$\text{H}_2\text{O}_2$	2.2	5.06	
MWCNT-PB	TMB	0.09	14.2	[6]
	$\text{H}_2\text{O}_2$	1.33	11.1	
PBMNPs	TMB	0.307	106	[7]
	$\text{H}_2\text{O}_2$	323.6	117	
PB- $\text{Fe}_2\text{O}_3$	3,5-DTBC	1.22	4.31	[8]
	$\text{H}_2\text{O}_2$	91.54	8.3	
PB	ABTS	157.54	-	[9]
	$\text{H}_2\text{O}_2$	0.028	-	
MIL-53(Fe)	TMB	1.08	8.78	[10]
	$\text{H}_2\text{O}_2$	0.04	1.86	
Hemin@MOF	TMB	0.068	6.07	[11]
	$\text{H}_2\text{O}_2$	10.9	8.98	
CuNPs@C	TMB	1.65	12.05	[12]
	$\text{H}_2\text{O}_2$	1.89	5.3	
HRP	TMB	0.43	10	[13]
	$\text{H}_2\text{O}_2$	3.7	8.7	
MIL-101(Cr)@PB	TMB	0.88	11.5	This work
	$\text{H}_2\text{O}_2$	1.06	9.7	

## References

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