Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Enhancing colorimetric detection of H_2O_2 and ascorbic acid on polypyrrole coating fluconazole functionalized POMOFs

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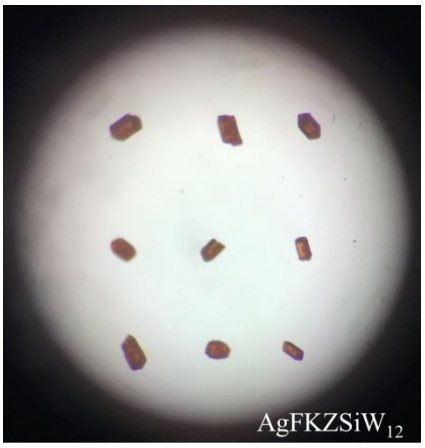


Fig. S1 Crystal photograph of $AgFKZSiW_{12}$ under optical microscope.

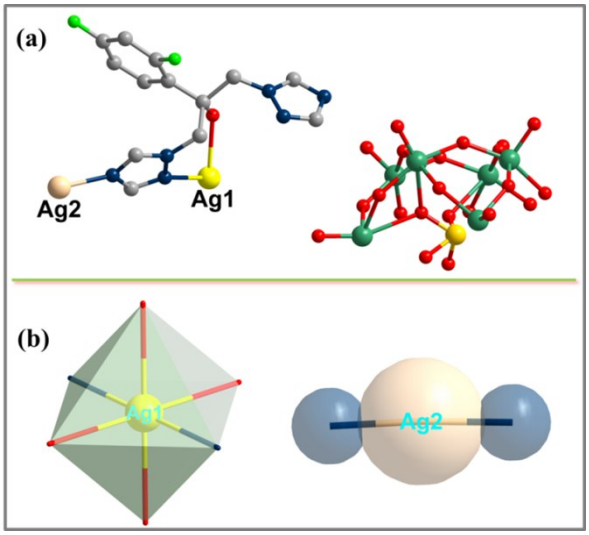


Fig. S2 (a) Combined ball/stick representation of the asymmetric unit of $AgFKZSiW_{12}$ (all the hydrogen atoms and water molecules have been omitted for clarity); (b) The coordination view of Ag ions.

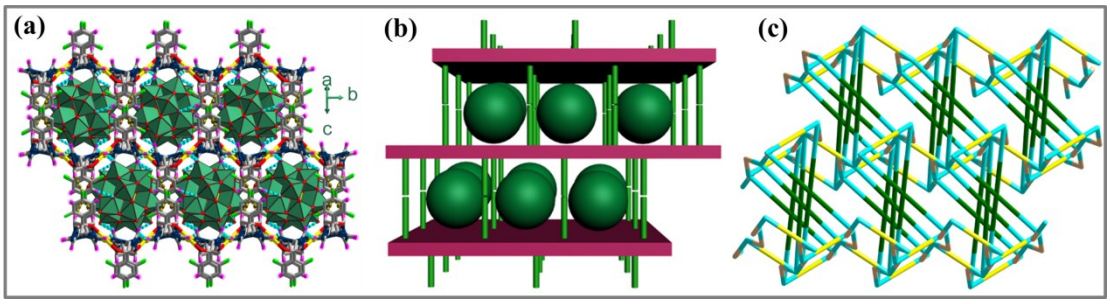


Fig. S3 Combined polyhedral/ball/stick (a), schematic (b), and topological representation (c) of the overall three-dimensional supramolecular hybrid framework along the *abc* plane in $AgFKZSiW_{12}$ (the turquoise nodes symbolize FKZ ligands).

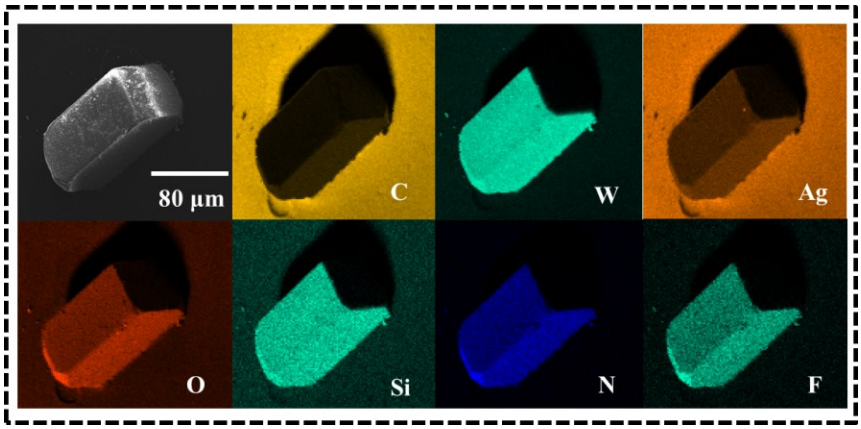
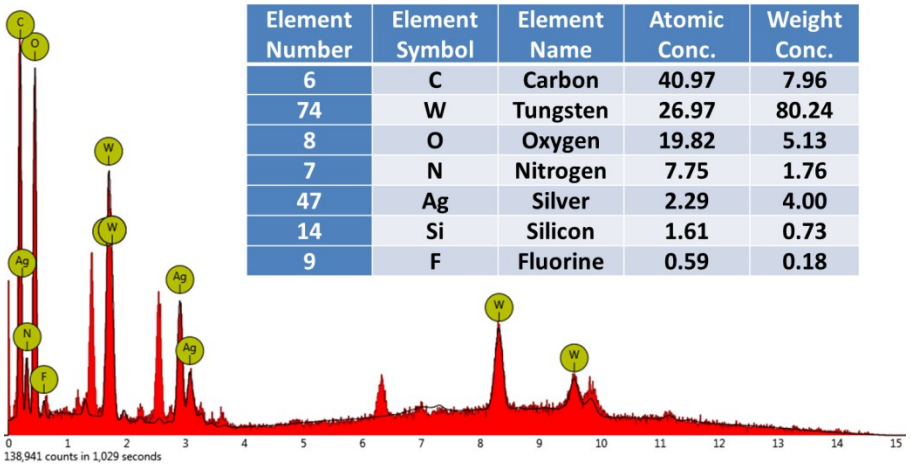


Fig. S4 The corresponding mapping images of C, W, Ag, O, Si, N, and F in $AgFKZSiW_{12}$.



Element Number	Element Symbol	Element Name	Atomic Conc.	Weight Conc.
6	C	Carbon	40.97	7.96
74	W	Tungsten	26.97	80.24
8	O	Oxygen	19.82	5.13
7	N	Nitrogen	7.75	1.76
47	Ag	Silver	2.29	4.00
14	Si	Silicon	1.61	0.73
9	F	Fluorine	0.59	0.18

Fig. S5 EDX spectrometry of AgFKZSiW_{12}@PPy.

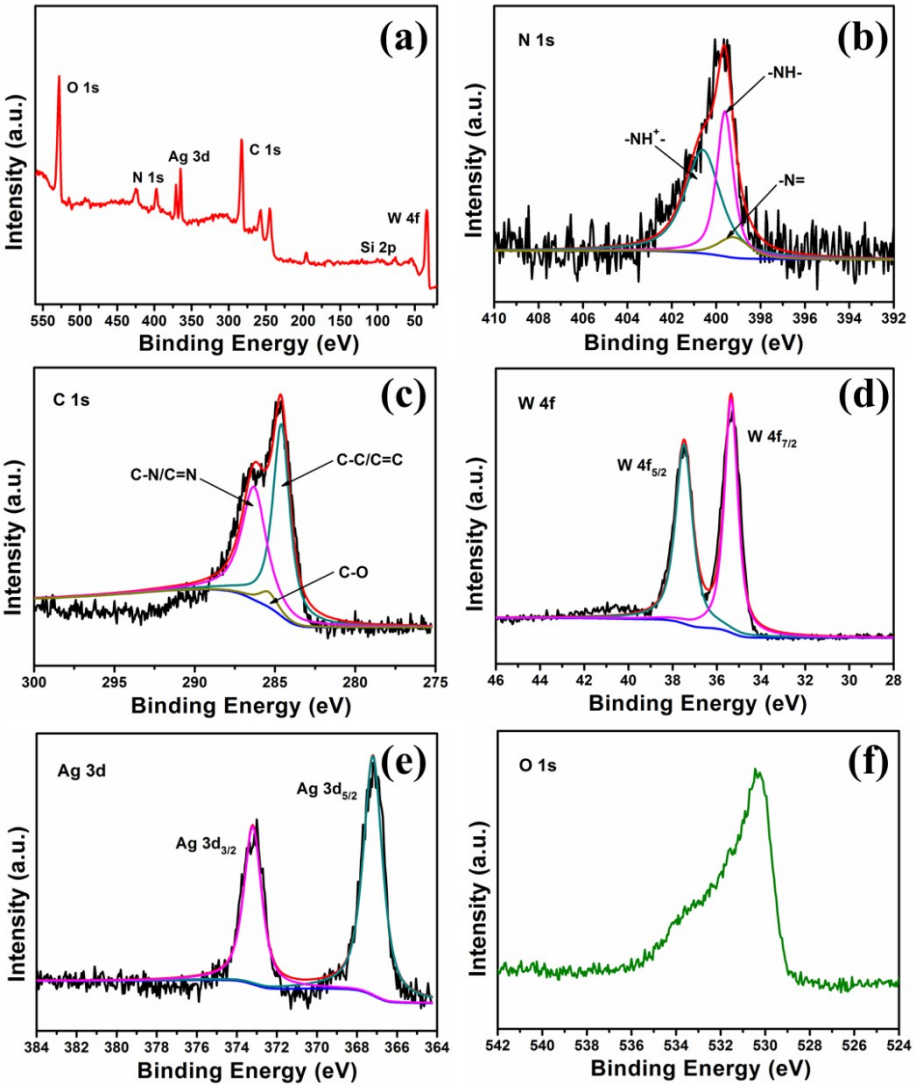


Fig. S6 (a) XPS spectra of AgFKZSiW_{12}@PPy; (b) N 1s; (c) C 1s; (d) W 4f; (e) Ag 3d; (f) O 1s.

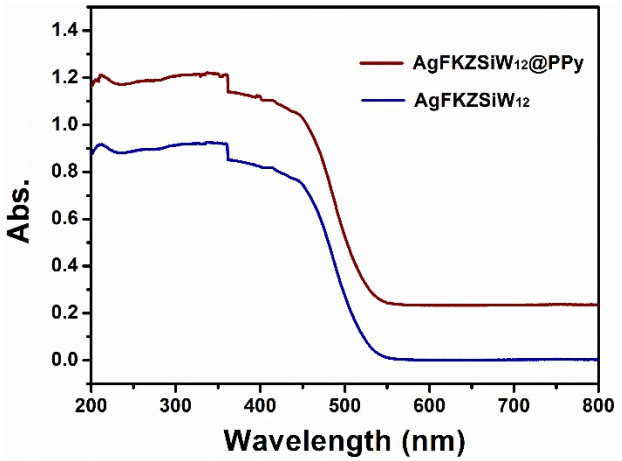


Fig. S7 DRS of $AgFKZSiW_{12}$ and $AgFKZSiW_{12}$@PPy.

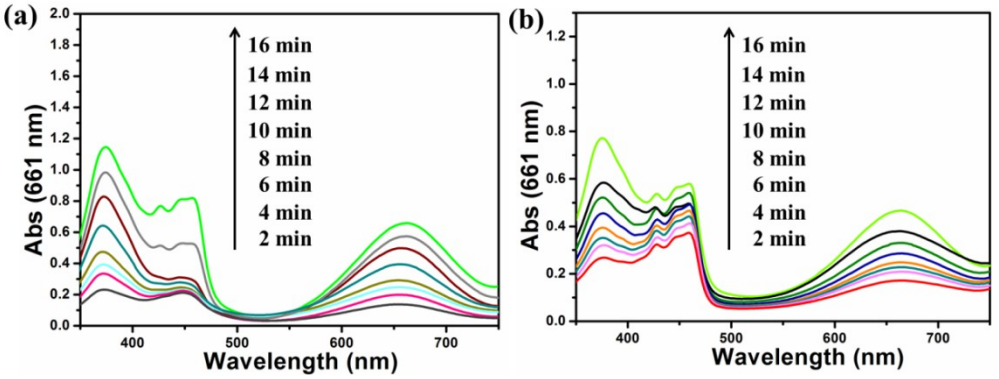


Fig. S8 UV-vis absorption spectra of $AgFKZSiW_{12}$ (a) and PPy (b) catalyzed TMB colorimetric system as a function of reaction time from 2 to 16 min.

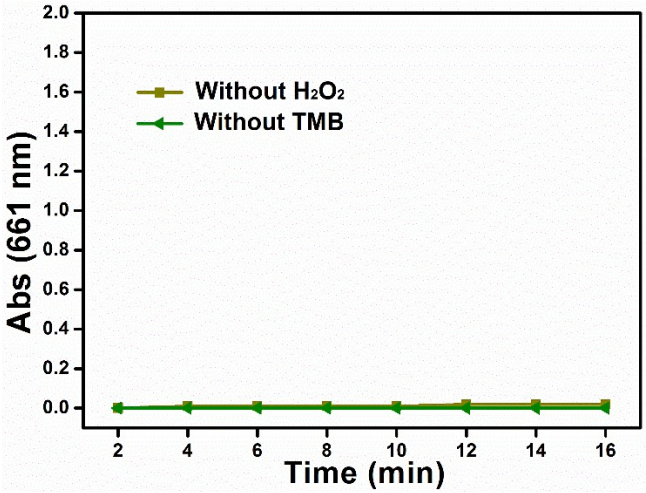


Fig. S9 Time-dependent absorbance of $AgFKZSiW_{12}$ in the absence of H_2O_2 or TMB. Typical reaction conditions: acetate buffer solution (pH=3.5), H_2O_2 83 μM and TMB 104 μM at 40 °C.

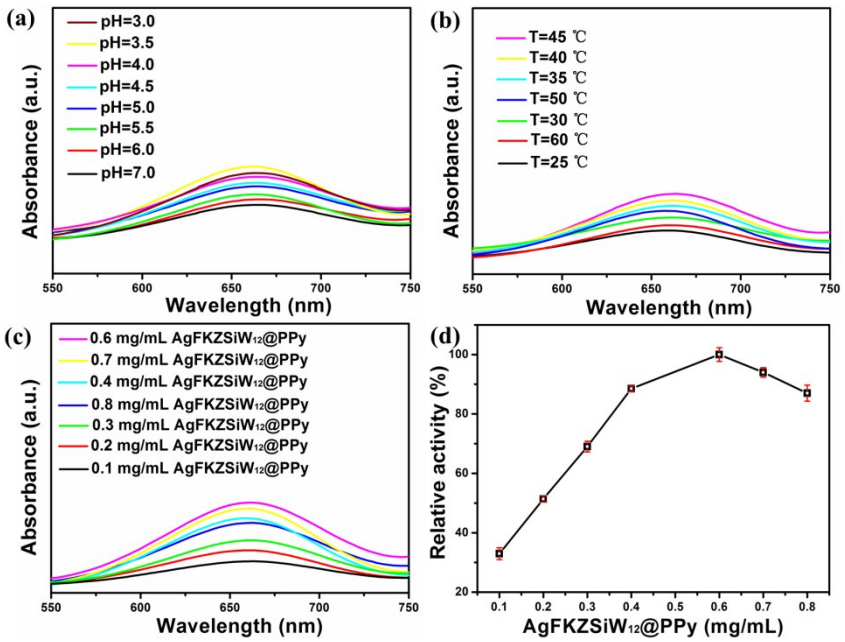


Fig. S10 UV-vis absorption spectra of AgFKZSiW$_{12}$@PPy catalyzed TMB colorimetric system as a function of reaction acidity (a), reaction temperature (b) and AgFKZSiW$_{12}$@PPy dosage (c). (d) Dependence of the peroxidase-like activity on AgFKZSiW$_{12}$@PPy dosage (dosage: 0.1, 0.2, 0.3, 0.4, 0.6, 0.7, 0.8 mg/mL).

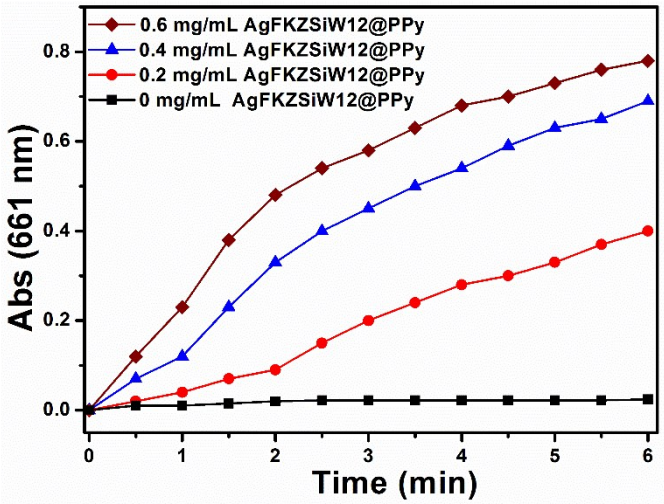


Fig. S11 Time-dependent absorbance changes at 661 nm in the presence of 0 mg/mL (black), 0.2 mg/mL (red), 0.4 mg/mL (blue), and 0.6 mg/mL (brown) AgFKZSiW$_{12}$@PPy in buffer solution (pH 3.5).

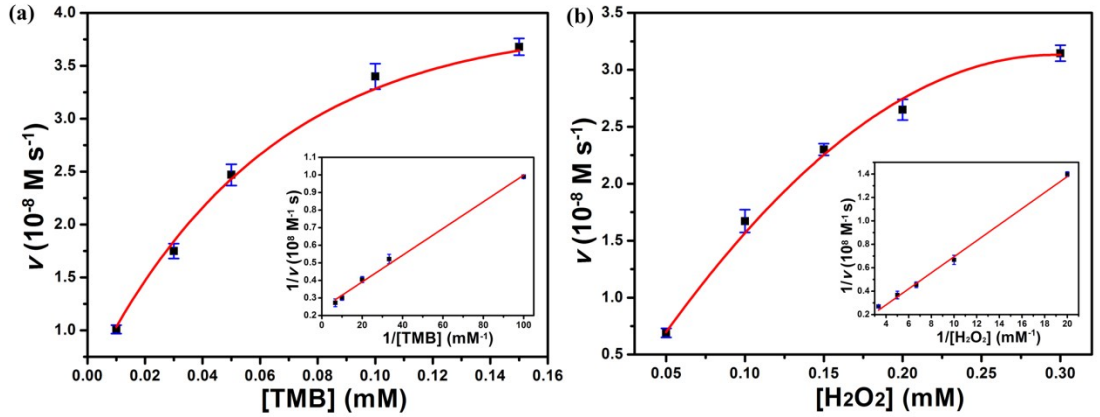


Fig. S12 Steady-state kinetic assays of $AgFKZSiW_{12}$: (a) 100 μM H_2O_2 with varying TMB concentration, (b) 40 μM TMB with varying H_2O_2 concentration. The reaction was performed in pH=3.5 buffer solution at 40 °C.

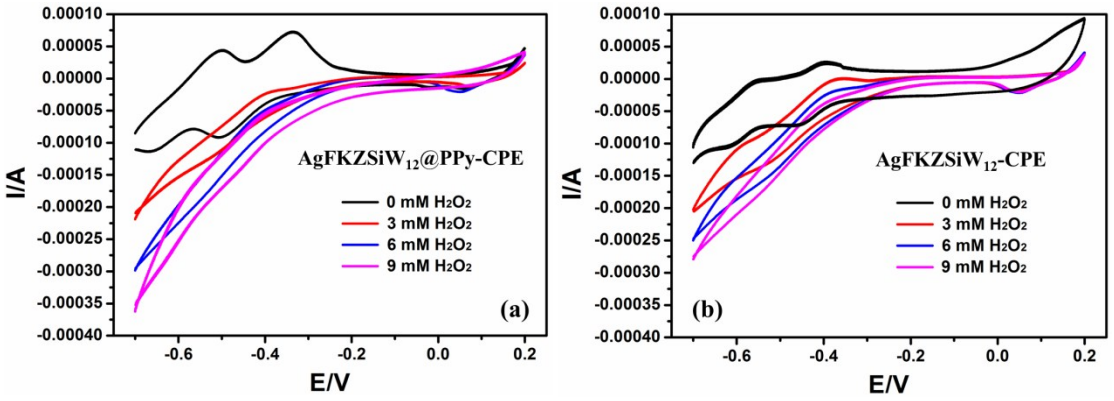


Fig. S13 CV curves of CPEs modified with $AgFKZSiW_{12}$@PPy (a) and $AgFKZSiW_{12}$ (b) in the presence of 0, 3, 6, and 9 mM H_2O_2.

Preparations of $AgFKZSiW_{12}$ and $AgFKZSiW_{12}$@PPy modified carbon paste electrode ($AgFKZSiW_{12}$-CPE and $AgFKZSiW_{12}$@PPy-CPE)

$AgFKZSiW_{12}$ modified carbon paste electrode ($AgFKZSiW_{12}$-CPE) was fabricated as follows: 96 mg of graphite powder and 8 mg of $AgFKZSiW_{12}$ were mixed and ground together by agate mortar and pestle to achieve a uniform mixture, and then 0.6 mL nujol was added with stirring. The homogenized mixture was packed into a glass tube with 1.2 mm inner diameter, and the tube surface was wiped with paper. Electrical contact was established with a copper rod through the back of the electrode. $AgFKZSiW_{12}$@PPy-CPE was made with $AgFKZSiW_{12}$@PPy in a similar manner.

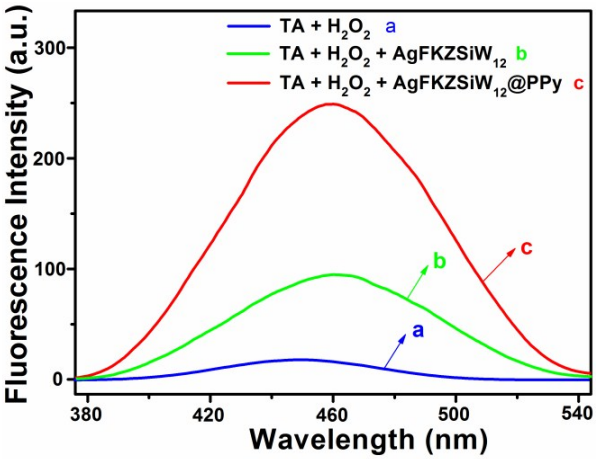


Fig. S14 Fluorescence spectra of TA solution (2×10^{-3} M) in the absence and presence of $AgFKZSiW_{12}$ and $AgFKZSiW_{12}$@PPy with H_2O_2 (100 mM). (a) 0 mg $AgFKZSiW_{12}$@PPy, (b) 3 mg $AgFKZSiW_{12}$, and (c) 3 mg $AgFKZSiW_{12}$@PPy during photoluminescence probing, respectively.

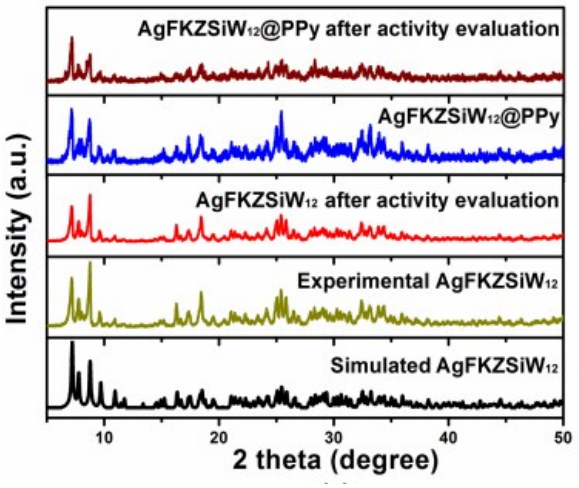


Fig. S15 PXRD patterns of $AgFKZSiW_{12}$ and $AgFKZSiW_{12}$@PPy before and after peroxidase-like activity evaluation.

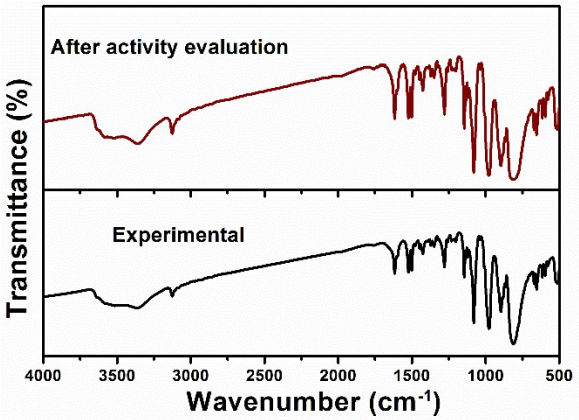


Fig. S16 FT-IR spectra of $AgFKZSiW_{12}$ before and after peroxidase-like activity evaluation.

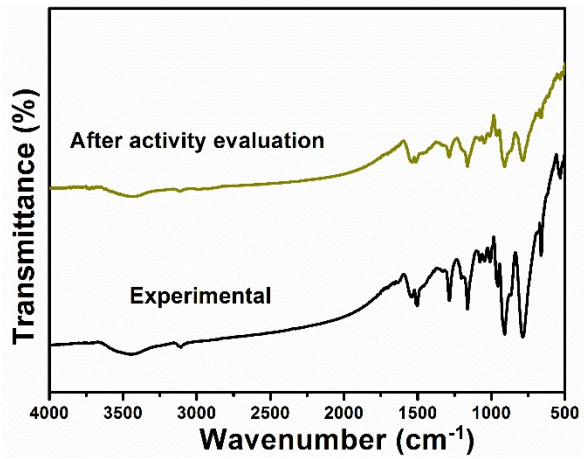
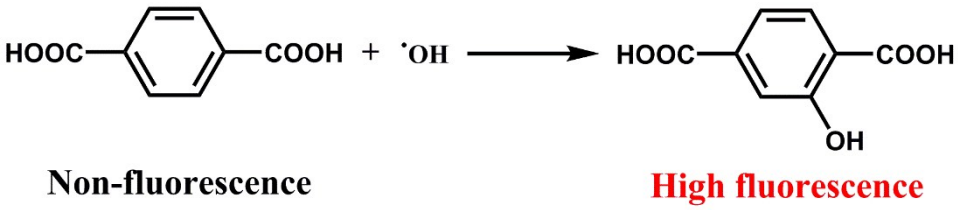


Fig. S17 FT-IR spectra of AgFKZSiW$_{12}$@PPy before and after peroxidase-like activity evaluation.

Fig. S18 Reusability of AgFKZSiW$_{12}$@PPy after repeated cycles.

Scheme S1. The oxidation reaction of TMB catalyzed by AgFKZSiW$_{12}$@PPy in the presence of H_2O_2.



Scheme S2. Hydroxyl radicals (·OH) induced the conversion of non-fluorescent terephthalic acid to highly fluorescent 2-hydroxyterephthalic acid.

Scheme S3. AA induced the conversion of oxTMB to TMB.

Table S1. Crystal data and structure refinements for $AgFKZSiW_{12}$.

Chemical formula	$C_{26}H_{29}Ag_3F_4N_{12}O_{42}SiW_{12}$
Formula weight	3847.33
CCDC	1850730
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	*C2/c*
a (Å)	31.006(2)
b (Å)	11.2468(7)
c (Å)	23.0508(16)
α (°)	90
β (°)	127.716(1)
γ (°)	90
V ($Å^3$)/Z	6358.7(7)/4
Density ($g·cm^{-3}$)	4.078
Abs coeff. (mm^{-1})	22.653
F(000)	6900.0
Data collect θ range	1.660 to 25.000°
Collected/ Independent Reflns	15481/5612
R_{int}	0.0600
Data/restraints/parameters	5612/6/481
Goodness-of-fit on F^2	1.076
Final R indices [I > 2δ(I)]	$R_1 = 0.0529$, $wR_2 = 0.1455$
R indices (all data)	$R_1 = 0.0616$, $wR_2 = 0.1521$
Largest diff. peak and hole ($e.Å^{-3}$)	2.333 and -4.412

$R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$, $wR_2 = \Sigma w(|F_0|^2-|F_c|^2)^2/\Sigma w(|F_0|^2)^2]^{1/2}$

Table S2. The BVS calculations of W and Ag atoms in $AgFKZSiW_{12}$ (BL= bond length, BV= bond valence).

BL for W1	**2.497 (O6)**	**1.917 (O11)**	**1.876 (O17)**	**1.922 (O18)**	**1.652 (O21)**	**1.922 (O23)**	
BL for W2	**1.667 (O2)**	**2.530 (O6)**	**1.863 (O9)**	**1.855 (O11)**	**1.870 (O12)**	**1.910 (O15)**	
BL for W3	**1.676 (O1)**	**1.906 (O5)**	**1.891 (O8)**	**1.903 (O14)**	**1.885 (O18)**	**2.518 (O20)**	
BL for W4	**1.920 (O12)**	**1.679 (O13)**	**1.870 (O14)**	**1.936 (O17)**	**1.895 (O19)**	**2.485 (O20)**	
BL for W5	**2.517 (O6)**	**1.874 (O8)**	**1.926 (O10)**	**1.883 (O15)**	**1.658 (O16)**	**1.894 (O23)**	
BL for W6	**1.678 (O3)**	**1.894 (O5)**	**2.490 (O7)**	**1.912 (O9)**	**1.877 (O10)**	**1.878 (O19)**	
BL for Ag1	**2.364 (N5)**	**2.364 (N5)**	**2.681 (O1W)**	**2.681 (O1W)**	**2.487 (O4)**	**2.487 (O4)**	
BL for Ag 2	**2.140 (N3)**	**2.135 (N6)**					
BV for W1	**0.1169**	**0.9277**	**1.0740**	**0.9113**	**2.3903**	**0.9113**	**6.3316 (total)**
BV for W2	**1.9653**	**0.1039**	**1.1250**	**1.1576**	**1.0973**	**0.9512**	**6.4005 (total)**
BV for W3	**2.1939**	**0.9649**	**1.0180**	**0.9753**	**1.0400**	**0.1084**	**6.3007 (total)**
BV for W4	**0.9178**	**2.1705**	**1.0973**	**0.8668**	**1.0035**	**0.1220**	**6.1782 (total)**
BV for W5	**0.1088**	**1.0817**	**0.8983**	**1.0475**	**2.0137**	**1.0641**	**6.2143 (total)**
BV for W6	**1.9077**	**1.0071**	**0.1198**	**0.9444**	**1.1141**	**1.1111**	**6.2046 (total)**
BV for Ag1	**0.2987**	**0.1879**	**0.0605**	**0.0605**	**0.2142**	**0.2142**	**1.0364 (total)**
BV for Ag2	**0.5473**	**0.4258**					**0.9732 (total)**

Table S3. Comparison of $AgFKZSiW_{12}$@PPy and other reported enzyme mimics for the detection of H_2O_2 and AA.

Enzyme mimics	Analyte	LOD (μM)	Range (μM)	Ref.
$H_4SiW_{12}O_{40}$ (HSiW)	H_2O_2	0.4	1-20	1
FF@PW_{12}@GO	H_2O_2	0.11	1-75	2
$Cu_6(Trz)_{10}(H_2O)_4[H_2SiW_{12}O_{40}]$	H_2O_2	1.37	10-50	3
$Na_4H_2[Cu_4(im)_{14}][Cu_3(H_2O)_3(BiW_9O_{33})_2]$	H_2O_2	0.12	1-50	4
$Na_4H_2[Cu_4(im)_{14}][Cu_3(H_2O)_3(SbW_9O_{33})_2]$	H_2O_2	0.12	1-50	4
$Na_4(NH_4)_{14}[Zr_4(\mu\text{-}O)_4(OAc)_2(P_2W_{16}O_{59})_2]$	H_2O_2	100	100-1000	5
MOF-808	H_2O_2	4.5	10-15000	6
$AgFKZSiW_{12}$@PPy	H_2O_2	0.12	1-100	**This work**
MOF-808	AA	15	30-1030	6

CuNPs@C	AA	1.41	10-1000	7
MIL-68/MIL-100	AA	6	30-485	8
$AgFKZSiW_{12}$@PPy	AA	2.7	1-80	**This work**

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Table S4. Determination of AA concentration in human serum samples using the proposed sensor.

Sample	Added (μM)	Measured (μM)	Recovery (%)	RSD (%, n=3)
Serum sample	0	5.337±0.104	–	1.9
	4	9.181±0.156	98.9	2.2
	8	13.453±0.216	101.7	2.0

Table S5. Selected bond lengths (Å) and bond angles (°) for $AgFKZSiW_{12}$.

Bond	**Lengths**	**Bond**	**Lengths**
O(20)-W(1)#2	2.397(17)	O(20)-W(4)#4	2.48(2)
C(2)-N(2)	1.27(2)	O(20)-W(3)	2.519(17)
C(2)-N(6)	1.37(2)	O(21)-W(1)	1.653(11)
C(3)-N(6)	1.32(2)	O(22)-Si(1)#7	1.53(2)
C(3)-N(1)	1.326(19)	C(4)-N(1)	1.423(19)
C(5)-N(5)	1.31(2)	O(22)-W(4)	2.512(18)
C(5)-N(3)	1.37(2)	O(22)-W(2)	2.420(16)
C(7)-F(1)	1.323(19)	O(22)-W(6)	2.489(19)
O(23)-W(5)#5	1.894(11)	O(23)-W(1)	1.922(12)
C(8)-N(4)	1.464(18)	Si(1)-O(6)#3	1.44(2)

Si(1)-O(22)#4	1.53(2)	Si(1)-O(7)#3	1.53(2)
C(11)-F(2)	1.305(18)	Si(1)-O(22)#2	1.53(2)
Ag(1)-N(5)#8	2.363(13)	Si(1)-O(20)#3	1.535(18)
C(13)-N(4)	1.315(19)	Ag(1)-O(4)#8	2.487(10)
C(13)-N(3)	1.28(2)	Ag(2)-N(6)#9	2.134(13)
N(3)-Ag(2)	2.140(12)	W(1)-O(18)#7	1.922(13)
N(4)-N(5)	1.332(19)	W(1)-O(20)#7	2.397(17)
N(5)-Ag(1)	2.363(13)	W(1)-O(6)#5	2.498(19)
N(6)-Ag(2)#1	2.134(13)	W(4)-O(14)#5	1.870(11)
O(1)-W(3)	1.678(10)	W(4)-O(17)#6	1.935(13)
O(2)-W(2)	1.667(11)	W(4)-O(20)#5	2.48(2)
O(3)-W(6)	1.678(11)	W(5)-O(15)#4	1.882(12)
O(4)-Ag(1)	2.487(10)	W(5)-O(23)#4	1.894(11)
O(5)-W(6)#2	1.895(12)	W(6)-O(10)#7	1.877(14)
O(5)-W(3)	1.905(13)	W(6)-O(5)#7	1.895(12)
O(6)-Si(1)	1.44(2)	W(6)-O(7)#7	2.490(17)
O(18)-W(1)#2	1.922(13)	O(17)-W(4)#6	1.935(13)
O(6)-W(1)#4	2.498(18)	O(18)-W(3)	1.884(14)
O(6)-W(5)	2.52(2)	O(19)-W(6)	1.877(11)
O(7)-Si(1)	1.53(2)	O(19)-W(4)	1.896(12)
O(7)-W(5)	2.439(19)	O(20)-Si(1)	1.535(18)
O(7)-W(6)#2	2.490(17)	O(14)-W(3)	1.903(12)
O(7)-W(3)	2.499(17)	O(15)-W(5)#5	1.882(12)
O(8)-W(5)	1.875(12)	O(15)-W(2)	1.911(11)
O(8)-W(3)	1.890(14)	O(16)-W(5)	1.658(13)
O(9)-W(2)	1.863(12)	O(17)-W(1)	1.877(13)
O(9)-W(6)	1.911(13)	O(11)-W(1)	1.916(12)
O(10)-W(6)#2	1.877(14)	O(12)-W(2)	1.869(10)
O(10)-W(5)	1.927(14)	O(12)-W(4)	1.921(12)
O(11)-W(2)	1.856(11)	O(13)-W(4)	1.679(12)
O(14)-W(4)#4	1.870(11)		

Bond	**Angles**	**Bond**	**Angles**
W(6)#2-O(5)-W(3)	140.1(8)	W(1)#4-O(6)-W(5)	90.3(7)
W(5)-O(7)-W(6)#2	92.8(7)	Si(1)-O(7)-W(6)#2	123.2(10)
C(5)-N(3)-Ag(2)	129.7(12)	W(5)-O(7)-W(3)	91.8(7)
W(2)-O(9)-W(6)	139.3(8)	W(6)#2-O(7)-W(3)	91.5(6)
W(6)#2-O(10)-W(5)	139.6(11)	W(5)-O(8)-W(3)	140.7(10)
C(5)-N(5)-Ag(1)	132.3(13)	W(2)-O(11)-W(1)	140.7(7)

N(4)-N(5)-Ag(1)	122.8(9)	W(2)-O(12)-W(4)	139.0(8)
C(13)-N(3)-Ag(2)	126.5(11)	W(4)#4-O(14)-W(3)	140.9(9)
C(3)-N(6)-Ag(2)#1	127.4(10)	W(5)#5-O(15)-W(2)	139.8(8)
C(2)-N(6)-Ag(2)#1	126.7(11)	W(1)-O(17)-W(4)#6	137.8(10)
Si(1)#7-O(22)-W(4)	122.5(8)	W(3)-O(18)-W(1)#2	137.6(10)
O(6)#5-O(22)-W(4)	132.3(11)	W(6)-O(19)-W(4)	141.1(8)
W(5)#5-O(23)-W(1)	137.3(8)	W(6)-O(22)-W(4)	90.7(7)
O(6)#3-Si(1)-O(6)	180.0(11)	W(2)-O(22)-W(4)	92.1(6)
O(6)#3-Si(1)-O(7)#3	68.4(9)	Si(1)-O(20)-W(4)#4	123.7(9)
O(6)-Si(1)-O(7)#3	111.6(9)	O(6)#3-Si(1)-O(7)	111.6(9)
O(6)-Si(1)-O(7)	68.4(9)	W(1)#2-O(20)-W(4)#4	93.5(7)
O(7)#3-Si(1)-O(7)	180.0	Si(1)-O(20)-W(3)	120.3(10)
O(6)#3-Si(1)-O(22)#4	110.5(9)	O(6)-Si(1)-O(22)#4	69.5(9)
O(7)#3-Si(1)-O(22)#4	71.5(9)	W(1)#2-O(20)-W(3)	92.4(5)
O(7)-Si(1)-O(22)#4	108.5(9)	W(4)#4-O(20)-W(3)	90.6(6)
O(6)#3-Si(1)-O(22)#2	69.5(9)	Si(1)#7-O(22)-O(6)#5	52.9(9)
O(6)-Si(1)-O(22)#2	110.5(9)	Si(1)#7-O(22)-O(7)#7	54.2(8)
O(7)#3-Si(1)-O(22)#2	108.5(9)	O(22)#4-Si(1)-O(22)#2	180.0
O(7)-Si(1)-O(22)#2	71.5(9)	O(6)#3-Si(1)-O(20)	67.8(9)
O(6)-Si(1)-O(20)	112.2(9)	Si(1)#7-O(22)-W(2)	126.4(10)
O(7)#3-Si(1)-O(20)	105.5(9)	O(22)#2-Si(1)-O(20)	108.3(9)
O(7)-Si(1)-O(20)	74.5(9)	O(6)#3-Si(1)-O(20)#3	112.2(10)
O(22)#4-Si(1)-O(20)	71.7(9)	O(6)-Si(1)-O(20)#3	67.7(9)
O(7)-Si(1)-O(20)#3	105.5(9)	W(2)-O(22)-W(6)	92.2(6)
O(22)#4-Si(1)-O(20)#3	108.3(9)	O(13)-W(4)-O(17)#6	101.2(7)
O(22)#2-Si(1)-O(20)#3	71.7(9)	O(14)#5-W(4)-O(17)#6	87.2(5)
O(20)-Si(1)-O(20)#3	179.999(10)	O(19)-W(4)-O(17)#6	86.2(6)
N(5)#8-Ag(1)-N(5)	180.0	O(12)-W(4)-O(17)#6	156.0(7)
N(5)#8-Ag(1)-O(4)#8	77.0(4)	O(13)-W(4)-O(20)#5	157.7(6)
N(5)-Ag(1)-O(4)#8	103.0(4)	O(14)#5-W(4)-O(20)#5	64.6(6)
N(5)#8-Ag(1)-O(4)	103.0(4)	O(19)-W(4)-O(20)#5	90.3(6)
O(7)#3-Si(1)-O(20)#3	74.5(9)	O(12)-W(4)-O(20)#5	94.1(6)
O(4)#8-Ag(1)-O(4)	180.0	O(17)#6-W(4)-O(20)#5	62.8(7)
N(6)#9-Ag(2)-N(3)	175.8(5)	O(13)-W(4)-O(22)	160.2(6)
O(21)-W(1)-O(17)	101.3(8)	O(14)#5-W(4)-O(22)	92.3(8)
O(21)-W(1)-O(11)	101.9(6)	O(19)-W(4)-O(22)	63.4(6)
O(17)-W(1)-O(11)	156.7(8)	O(12)-W(4)-O(22)	62.8(5)
O(21)-W(1)-O(23)	101.6(7)	O(17)#6-W(4)-O(22)	93.9(7)

O(17)-W(1)-O(23)	88.8(6)	O(20)#5-W(4)-O(22)	42.1(6)
O(11)-W(1)-O(23)	88.1(5)	O(16)-W(5)-O(8)	100.8(9)
O(21)-W(1)-O(18)#7	99.9(8)	O(16)-W(5)-O(15)#4	101.7(7)
O(17)-W(1)-O(18)#7	88.0(5)	O(8)-W(5)-O(15)#4	88.8(5)
O(11)-W(1)-O(18)#7	86.4(6)	O(16)-W(5)-O(23)#4	102.4(8)
O(23)-W(1)-O(18)#7	158.4(8)	O(8)-W(5)-O(23)#4	156.8(8)
O(21)-W(1)-O(20)#7	159.8(7)	O(15)#4-W(5)-O(23)#4	87.7(5)
O(17)-W(1)-O(20)#7	65.3(7)	O(16)-W(5)-O(10)	102.3(9)
O(11)-W(1)-O(20)#7	91.8(7)	O(8)-W(5)-O(10)	87.0(5)
O(23)-W(1)-O(20)#7	93.5(6)	O(15)#4-W(5)-O(10)	156.0(8)
O(18)#7-W(1)-O(20)#7	65.9(7)	O(23)#4-W(5)-O(10)	86.9(6)
O(21)-W(1)-O(6)#5	160.6(7)	O(16)-W(5)-O(7)	158.9(8)
O(17)-W(1)-O(6)#5	93.5(7)	O(8)-W(5)-O(7)	64.3(7)
O(11)-W(1)-O(6)#5	64.3(6)	O(15)#4-W(5)-O(7)	93.1(6)
O(23)-W(1)-O(6)#5	65.9(6)	O(23)#4-W(5)-O(7)	93.0(7)
O(18)#7-W(1)-O(6)#5	93.0(8)	O(10)-W(5)-O(7)	63.8(7)
O(20)#7-W(1)-O(6)#5	39.6(6)	O(16)-W(5)-O(6)	161.7(8)
O(2)-W(2)-O(11)	101.7(7)	O(8)-W(5)-O(6)	92.0(7)
O(2)-W(2)-O(9)	101.3(8)	O(15)#4-W(5)-O(6)	65.3(6)
O(11)-W(2)-O(9)	86.2(6)	O(23)#4-W(5)-O(6)	65.8(6)
O(2)-W(2)-O(12)	102.1(7)	O(10)-W(5)-O(6)	91.2(8)
O(11)-W(2)-O(12)	156.2(7)	O(7)-W(5)-O(6)	39.3(6)
O(9)-W(2)-O(12)	89.6(5)	O(3)-W(6)-O(10)#7	100.7(8)
O(2)-W(2)-O(15)	102.4(7)	O(3)-W(6)-O(19)	104.4(7)
O(11)-W(2)-O(15)	87.6(5)	O(10)#7-W(6)-O(19)	88.0(6)
O(9)-W(2)-O(15)	156.3(7)	O(3)-W(6)-O(5)#7	100.9(7)
O(12)-W(2)-O(15)	86.9(5)	O(10)#7-W(6)-O(5)#7	87.3(6)
O(2)-W(2)-O(22)	160.0(8)	O(19)-W(6)-O(5)#7	154.7(7)
O(11)-W(2)-O(22)	91.8(7)	O(3)-W(6)-O(9)	103.7(7)
O(9)-W(2)-O(22)	64.6(7)	O(10)#7-W(6)-O(9)	155.5(8)
O(12)-W(2)-O(22)	65.4(6)	O(19)-W(6)-O(9)	89.0(5)
O(15)-W(2)-O(22)	92.7(7)	O(5)#7-W(6)-O(9)	85.2(6)
O(1)-W(3)-O(18)	100.3(8)	O(3)-W(6)-O(22)	160.8(6)
O(1)-W(3)-O(8)	102.7(7)	O(10)#7-W(6)-O(22)	94.4(7)
O(18)-W(3)-O(8)	157.0(8)	O(19)-W(6)-O(22)	64.1(6)
O(1)-W(3)-O(14)	101.5(7)	O(5)#7-W(6)-O(22)	91.5(7)
O(18)-W(3)-O(14)	87.4(6)	O(9)-W(6)-O(22)	62.6(6)
O(8)-W(3)-O(14)	87.8(7)	O(3)-W(6)-O(7)#7	157.1(7)

O(1)-W(3)-O(5)	103.2(7)	O(10)#7-W(6)-O(7)#7	63.2(7)
O(18)-W(3)-O(5)	87.8(7)	O(19)-W(6)-O(7)#7	91.7(6)
O(8)-W(3)-O(5)	87.3(5)	O(5)#7-W(6)-O(7)#7	64.1(6)
O(14)-W(3)-O(5)	155.3(7)	O(9)-W(6)-O(7)#7	92.6(7)
O(1)-W(3)-O(7)	159.5(6)	O(22)-W(6)-O(7)#7	42.0(6)
O(18)-W(3)-O(7)	95.0(8)	O(14)-W(3)-O(7)	92.6(7)
O(8)-W(3)-O(7)	62.8(6)	O(5)-W(3)-O(7)	63.7(6)
O(18)-W(3)-O(20)	63.6(7)	O(1)-W(3)-O(20)	157.1(6)
O(8)-W(3)-O(20)	94.2(7)	O(13)-W(4)-O(12)	102.9(6)
O(14)-W(3)-O(20)	63.5(7)	O(14)#5-W(4)-O(12)	88.2(6)
O(5)-W(3)-O(20)	92.8(7)	O(19)-W(4)-O(12)	87.7(5)
O(7)-W(3)-O(20)	43.3(6)	O(13)-W(4)-O(19)	104.5(6)
O(13)-W(4)-O(14)#5	101.2(7)	O(14)#5-W(4)-O(19)	154.2(7)

Symmetry transformations used to generate equivalent atoms: #1 x+1/2, -y+1/2, z+1/2; #2 -x+3/2, y+1/2, -z+3/2; #3 -x+3/2, -y+1/2, -z+2; #4 x, -y, z+1/2; #5 x, -y, z-1/2; #6 -x+3/2, -y-1/2, -z+1; #7 -x+3/2, y-1/2, -z+3/2; #8 -x+1, -y, -z+1; #9 x-1/2, -y+1/2, z-1/2