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A 3D paddle-wheel type Cu(II)-based MOF with *pcu* topology as an efficient photocatalyst for antibiotics

Materials and Method

All the reagents to perform synthesis were obtained from commercial sources and were used without further purification. Powder X-ray diffraction (PXRD) data were collected using Bruker ADVANCE X-ray diffractometer with Cu-Kα radiation (λ=1.5418 Å) at 50 kV, 20 mA with a scanning rate of 6°/min and a step size of 0.02°. Fourier transform infrared (FT-IR) spectra for both the MOFs as KBr discs were recorded on Nicolet Impact 750 FTIR in the range of 400-4000 cm^{-1}. Scanning electron microscopy (SEM) was carried out on a FEI Quanta 400 FEG field emission scanning electron microscope. Nitrogen adsorption-desorption measurements were performed at 77 K in a liquid nitrogen bath on a Micromeritics ASAP 3020 analyzer. Samples were degassed at 150 ^oC for 10 h on degas vacuum system prior to analysis. The Brunauer-Emmett-Teller (BET) method was used to calculate the specific surface areas (S_{BET}). The UV–vis absorbance and diffuse-reflectance spectra (UV–vis DRS) were characterized by USA PE Lambda 750 S.

X-ray Crystallography

The single crystal X-ray diffraction data for the MOF **1** were collected on a Bruker SMART APEX diffractometer which was equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å) by using an ω-scan technique. The structures were solved by direct method (SHLEXS-2014) and refined using the full-matrix least-square procedure based on F^2 (Shelxl-2014). All the hydrogen atoms were generated geometrically and refined isotropically using a riding model. CCDC numbers: 2168426.

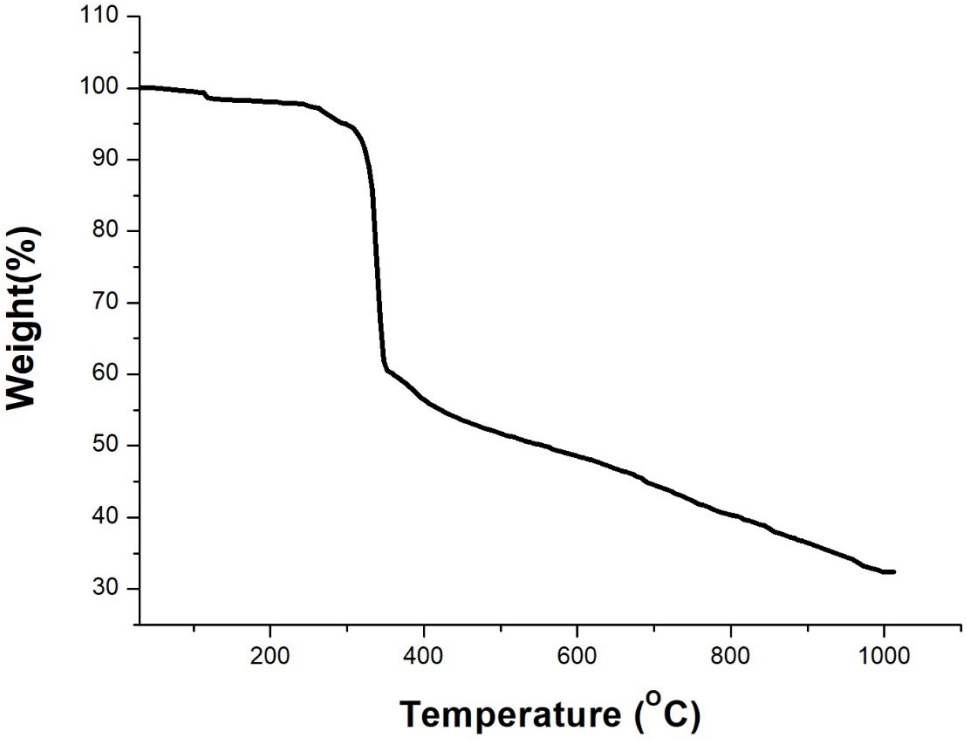

Fig. S1 The thermogravimetric plot for **1**

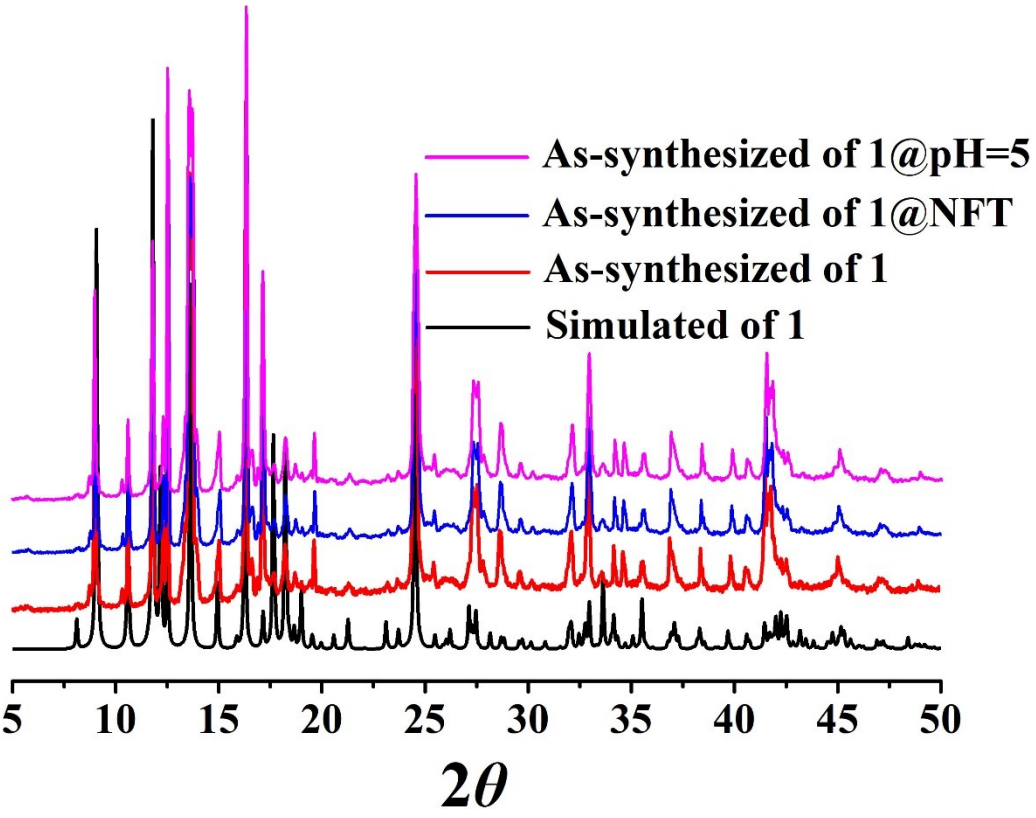

Fig. S2 Simulated, as-synthesized, **1**/NFT and **1**/pH =5 PXRD plots for **1**.

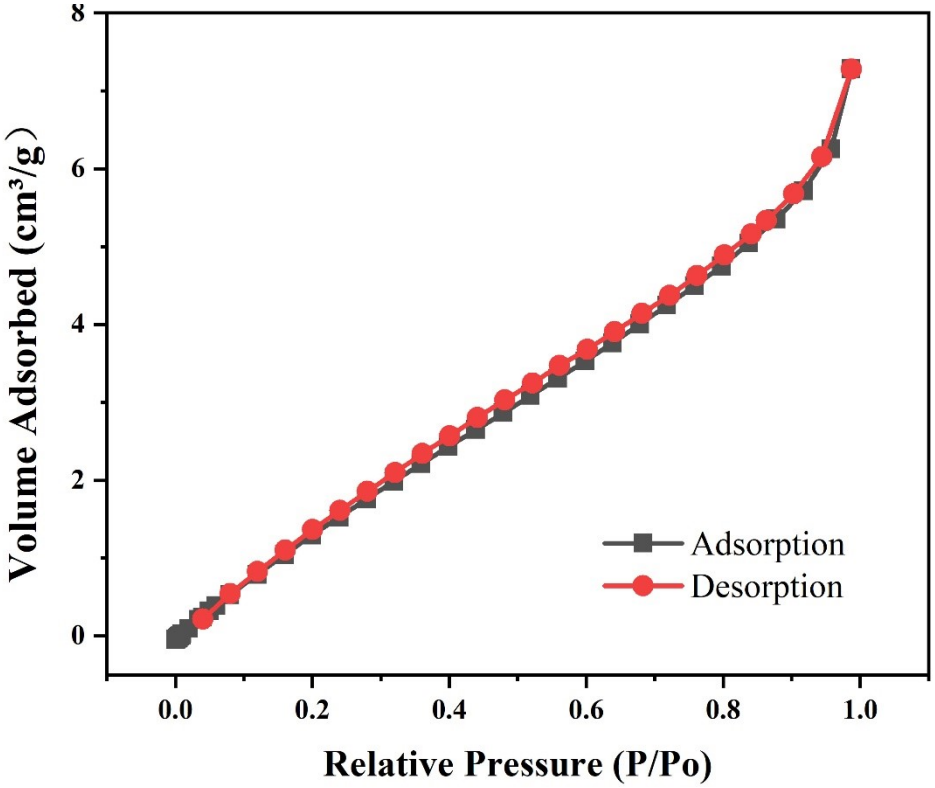

Fig. S3 sorption and desorption isotherms at 77 K for **1**.

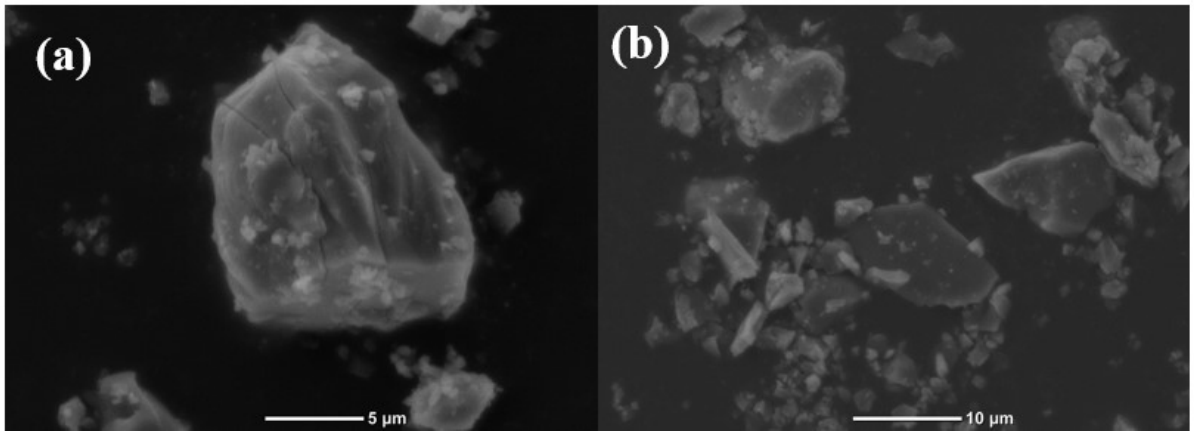

Fig. S4 view of the SEM before and after catalytic reaction.

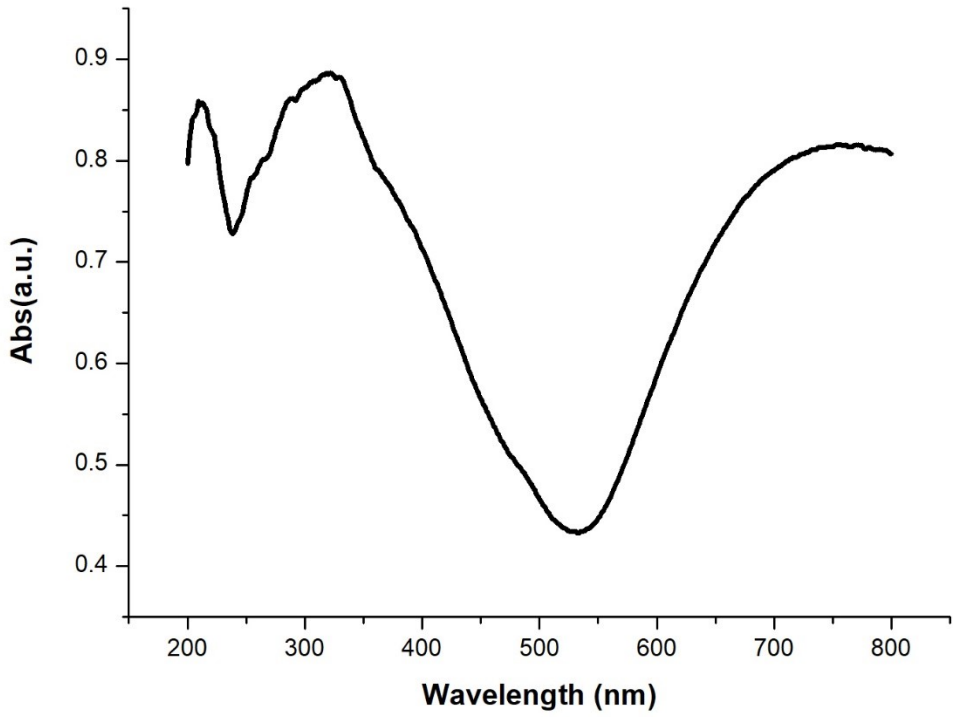

Fig. S5 UV-Vis spectrum for **1**.

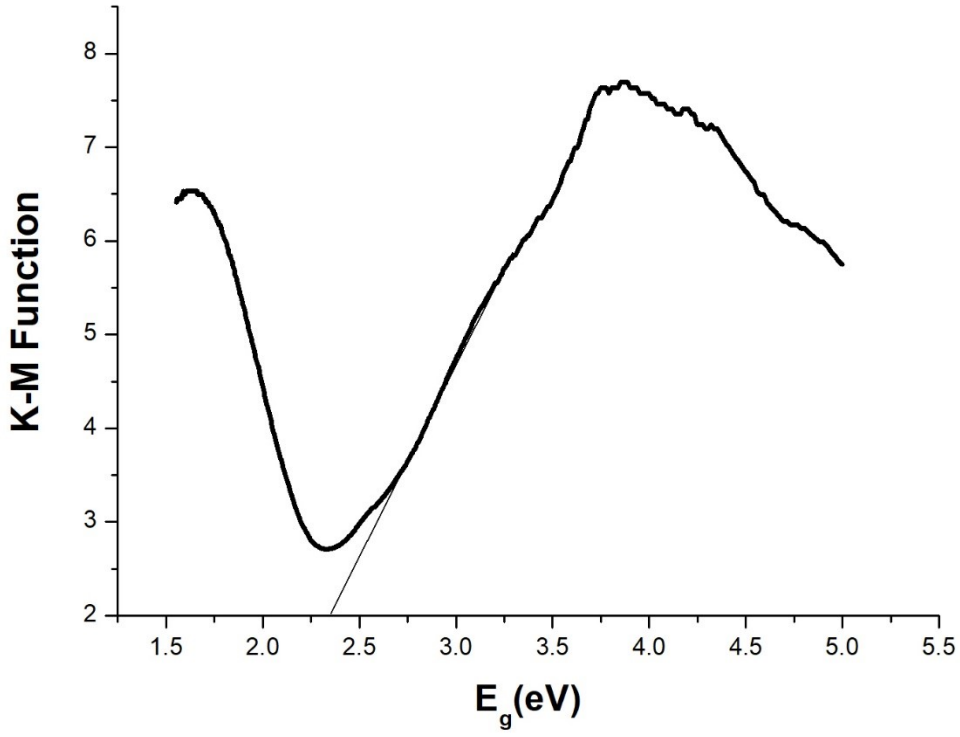

Fig. S6 K-M vs. E_g plot for **1**.

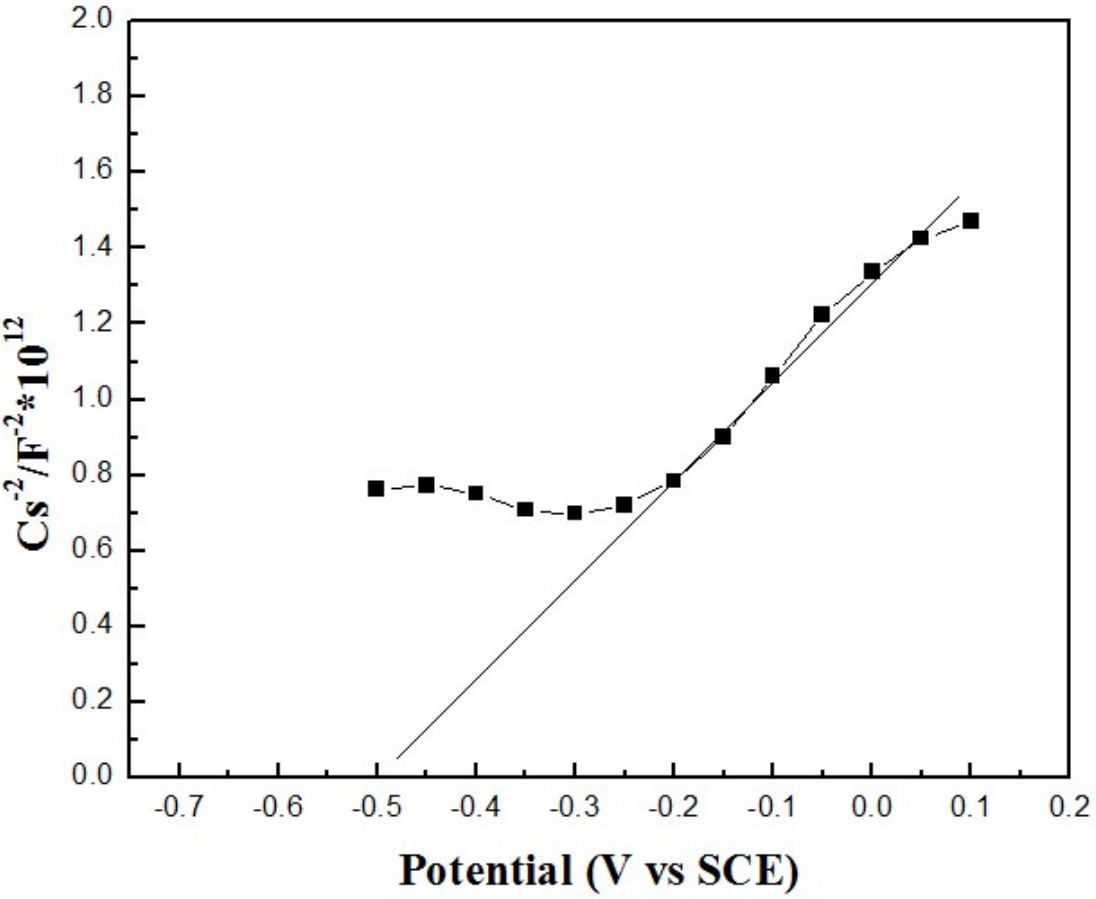

Fig. S7 typical Motte Schottky plot for **1**.

Table S1 Rate constants for the decomposition of antibiotics under different conditions

Antibiotics			K	R^2
CAP			0.00142	0.97655
NFT			0.03245	0.99488
MDZ			0.00276	0.97557
1	NFT	pH	*K*	R^2
Concentration of NFT				
50mg/100ml	10mg/L	pH=5	0.03245	0.99488
	20mg/L		0.02793	0.99848
	30mg/L		0.02779	0.97064
Dosage of sample				
40mg/100ml	10mg/L	pH=5	0.03021	0.99749
50mg/100ml			0.03245	0.99488
60mg/100ml			0.03002	0.99892
pH				
50mg/100ml	10mg/L	pH =4	0.00362	0.97773
		pH =5	0.03245	0.99488
		pH =6	0.02866	0.99282
Mechanism				
50mg/100ml	10mg/L	H_2O	0.03246	0.99488
		AO	0.02809	0.99773
		BQ	0.02588	0.98243
		TBA	0.0297	0.97923

Table S2. Crystallographic data and structure refinement details for **1**

Parameter	**1**
Formula	$C_{34}H_{22}N_4O_8Cu_2$
Formula weight	741.63
Crystal system	Monoclinic
Space group	*P2/n*
Crystal Color	Green
a, Å	10.9001(8)
b, Å	10.8846(8)
c, Å	13.6953(10)
α, °	90
β, °	108.552(1)
γ, °	90
V, Å ^{3}	1540.4(2)
Z	2
ρ_{calcd}, g/cm^3	1.599
μ, mm^{-1}	1.442
θ Range, deg	1.9-27.6
F(000)	752
Reflection Collected	9127
Independent reflections (R_{int})	0.027
Reflections with $I > 2\sigma(I)$	2827
R_1, wR_2 ($I > 2\sigma(I)$)*	0.0322, 0.0813
R_1, wR_2 (all data)**	0.0435, 0.0970

* $R = \sum(F_o - F_c)/\sum(F_o)$, ** $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum(F_o^2)^2\}^{1/2}$.

Table 3 Selected bond distances (Å) and angles (deg) for **1**

Bond	*d*, Å	Bond	*d*, Å
		1	
Cu(1)-O(1)	1.9820(19)	Cu(1)-O(3)	1.985(2)
Cu(1)-N(1)	2.126(2)	Cu(1)-O(2)#1	1.9762(19)
Cu(1)-O(4)#2	1.992(2)		
Angle	ω, deg	Angle	ω, deg

1			
O(1)-Cu(1)-O(3)	89.96(8)	O(1)-Cu(1)-N(1)	95.83(8)
O(1)-Cu(1)-O(2)#1	166.88(9)	O(1) -Cu(1)-O(4)#2	90.11(8)
O(3)-Cu(1)-N(1)	96.11(8)	O(2)#1-Cu(1)-O(3)	89.10(9)
O(3)-Cu(1)-O(4)#2	166.87(8)	O(2)#1-Cu(1)-N(1)	97.29(8)
O(4)#2-Cu(1)-N(1)	96.95(8)	O(2)#1-Cu(1)-O(4)#2	87.86(8)

Symmetry Codes: **For 1**: #1 = x, 1+y, z; #2 = 3/2-x, y, 3/2-z.