Supporting Information

Single atom Cu anchored graphitic-C_3N_5 for photocatalytic selective oxidation of biomass-derived furfurals to maleic anhydride

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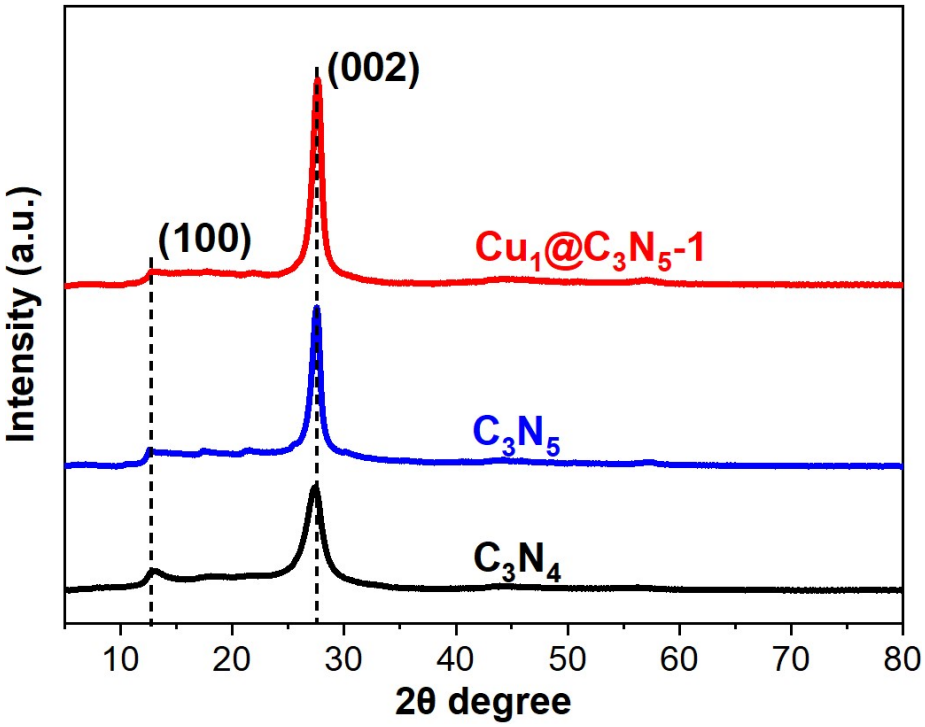

Figure S1 XRD patterns of C_3N_4, C_3N_5 and $Cu_1@C_3N_5$-1

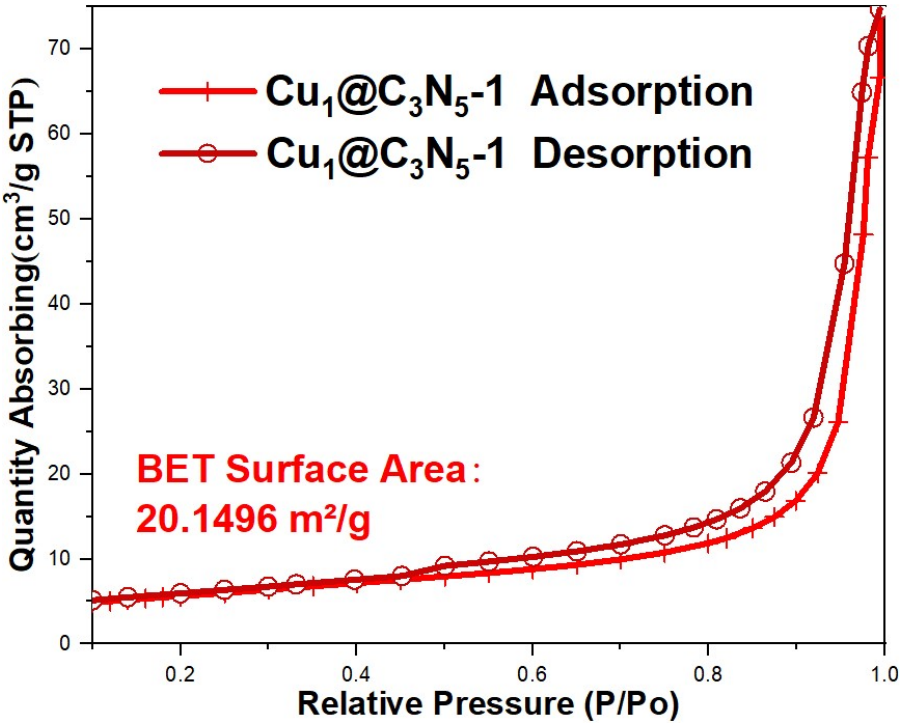

Figure S2 Isothermal adsorption-desorption curve of $Cu_1@C_3N_5$-1

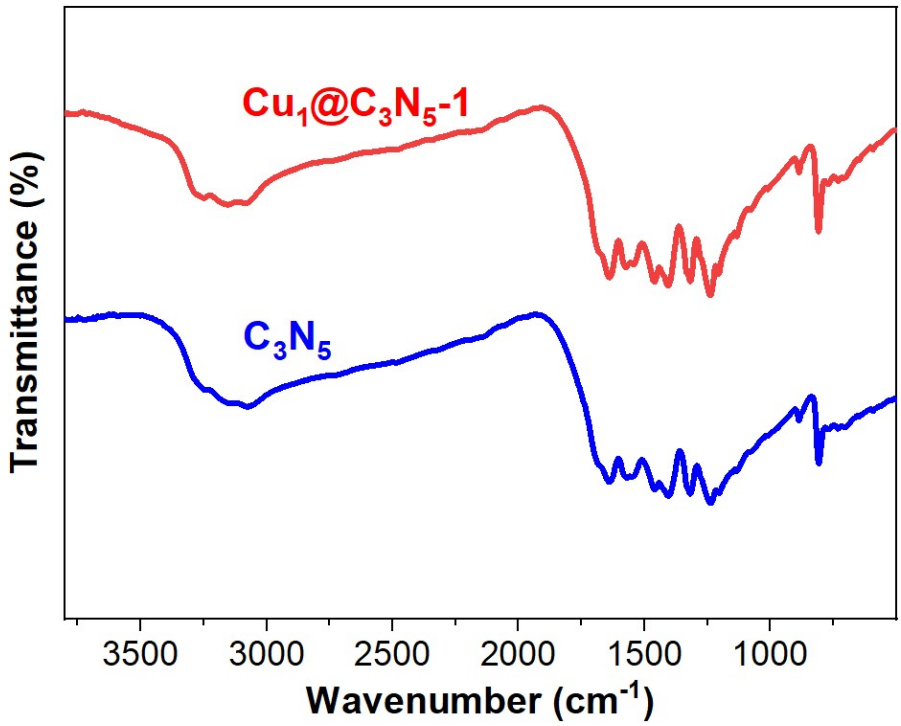

Figure S3 FT-IR spectra of C_3N_5 and $Cu_1@C_3N_5$-1

Table S1 The ICP results of $Cu_1@C_3N_5$-1

Catalyst	Mass content of Cu (mg/kg)
$Cu_1@C_3N_5$-1	18381.6
$Cu_1@C_3N_5$-1[a]	18114.8

[a] The recycled catalyst after 8 runs

Table S2 The elemental analysis results of $Cu_1@C_3N_5$-1

Quality (mg)	Name	N (%)	C (%)	H (%)	O (%)
2.001	$Cu_1@C_3N_5$-1	61.4	34.61	1.537	1.866

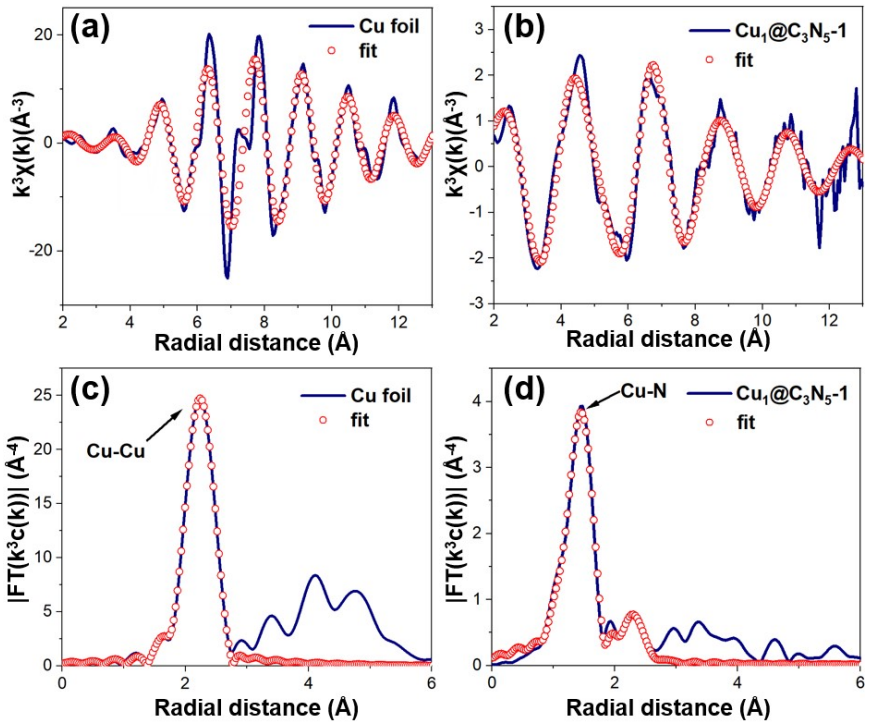

Figure S4 Comparison of experimentally obtained spectra and the corresponding best fit calculations of Cu foil (a, c) and $Cu_1@C_3N_5$-1 (b,d). EXAFS spectra (a, b), Fourier-transformed EXAFS spectra (c, d).

Table S3 EXAFS data fitting results of Samples.

Sample	Path	*CN*[a]	*R*(Å)[b]	σ^2 (Å^2)[c]	ΔE_0(eV)[d]	*R* factor
Cu K-edge (S_0^2=0.867)						
Cu foil-1	Cu-Cu	12*	2.542±0.003	0.0089	4.4	0.0031
Cu-1-tran	Cu-N	2.9±0.2	1.904±0.004	0.0070	3.4	0.0080

[a]*CN*, coordination number; [b]*R*, the distance between absorber and backscatter atoms; [c]σ^2, the Debye Waller factor value; [d]ΔE_0, inner potential correction to account for the difference in the inner potential between the sample and the reference compound; *R* factor indicates the goodness of the fit. $S0^2$ was fixed to 0.867, according to the experimental EXAFS fit of Cu foil by fixing *CN* as the known crystallographic value. * This value was fixed during EXAFS fitting, based on the known structure of Cu. Fitting conditions: *k* range：2.0 - 11.4; *R* range: 1.0-2.5; fitting space: R space; *k*-weight = 3. A reasonable range of EXAFS fitting parameters: $0.800 < S_0^2 < 1.000$; $CN > 0$; $\sigma^2 > 0$ Å^2; $|\Delta E_0| < 10$ eV; *R* factor < 0.02.

Table S4 The solvent effects on the oxidation of HMF[a]

Entry	Solvent	Yield of MA (%)
1	water	0
2	ethanol	0
3	methanol	0
3	acetone	11
4	ethyl acetate	24
5	**acetonitrile**	**98**
6	MeOH	0
7	acetonitrile[b]	18
8	acetonitrile[c]	40

[a] Reaction conditions: 126 mg HMF (1 mmol), 20 mg catalyst, 2 mL solvent, light source: 415 nm LED (12 W), 12 h, 40 °C. [b] The use of 1 equiv. MeOH. [c] The use of 0.5 equiv. MeOH.

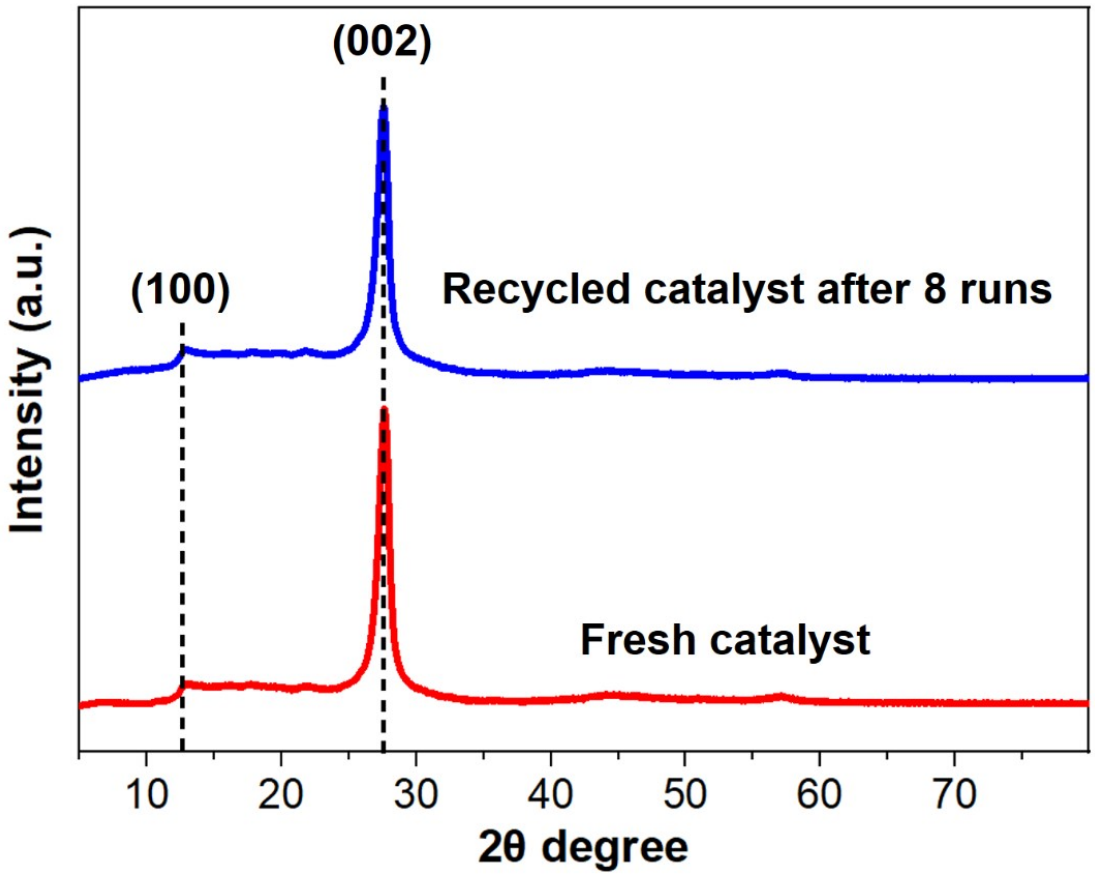

Figure S5 XRD patterns of $Cu_1@C_3N_5$-1 and its recycled sample after 8 runs

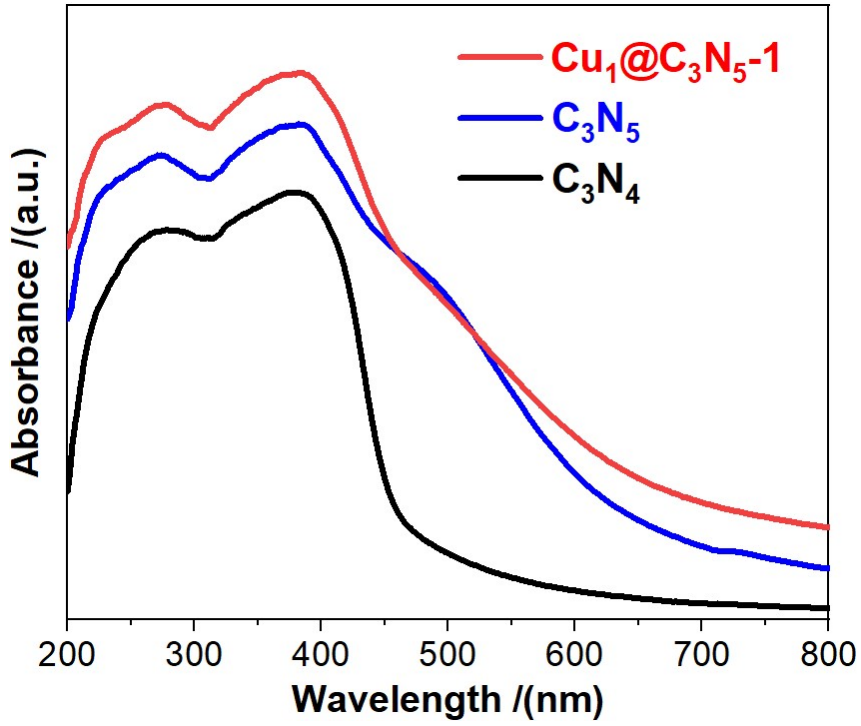

Figure S6 Diffuse-reflectance UV-vis spectra of C_3N_4, C_3N_5 and $Cu_1@C_3N_5$-1.

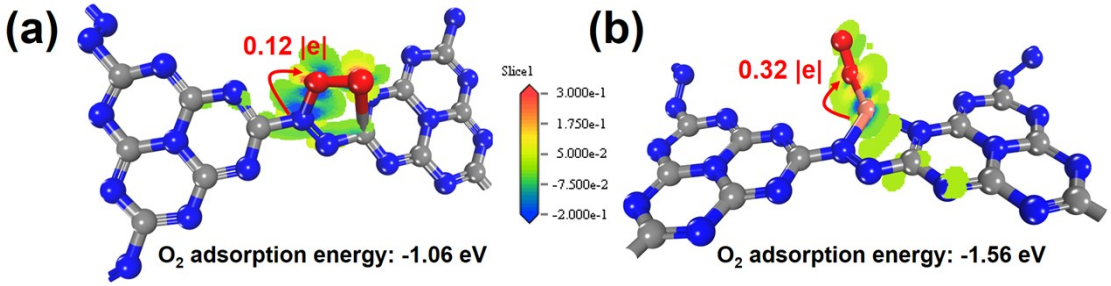

Figure S7 O_2 adsorption on (a) C_3N_5 and (b) $Cu_1@C_3N_5$-1. Grey, blue, red and pink balls represent carbon, nitrogen, oxygen and copper atoms, respectively