Supporting information

Porosity- and Content-Controlled Metal/Metal Oxide/Metal Carbide@Carbon (M/MO/MC@C) Composites Derived from MOFs: Mechanism Study and Application for Lithium-ion Batteries

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Note 1. Calculation of free energy changes in Figure 4.

To calculate free energy change of reaction, we use following gibbs free energy equation.

$$\Delta G = \Delta H - T\Delta S$$

Based on the following equation we can simply obtain enthalpy changes ($\Delta_f H°_{products}$, $\Delta_f H°_{reactants}$) and entropy changes ($S_{products}$, $S_{reactants}$) of the reaction.

Enthalpy change (ΔH) = $\sum \Delta_f H°_{products} - \sum \Delta_f H°°$

Entropy change (ΔS) = $\sum S_{products} - \sum S_{reactants}$

Eventually the ellinghem equation in figure 4 was plotted by temperature using free energy equation.

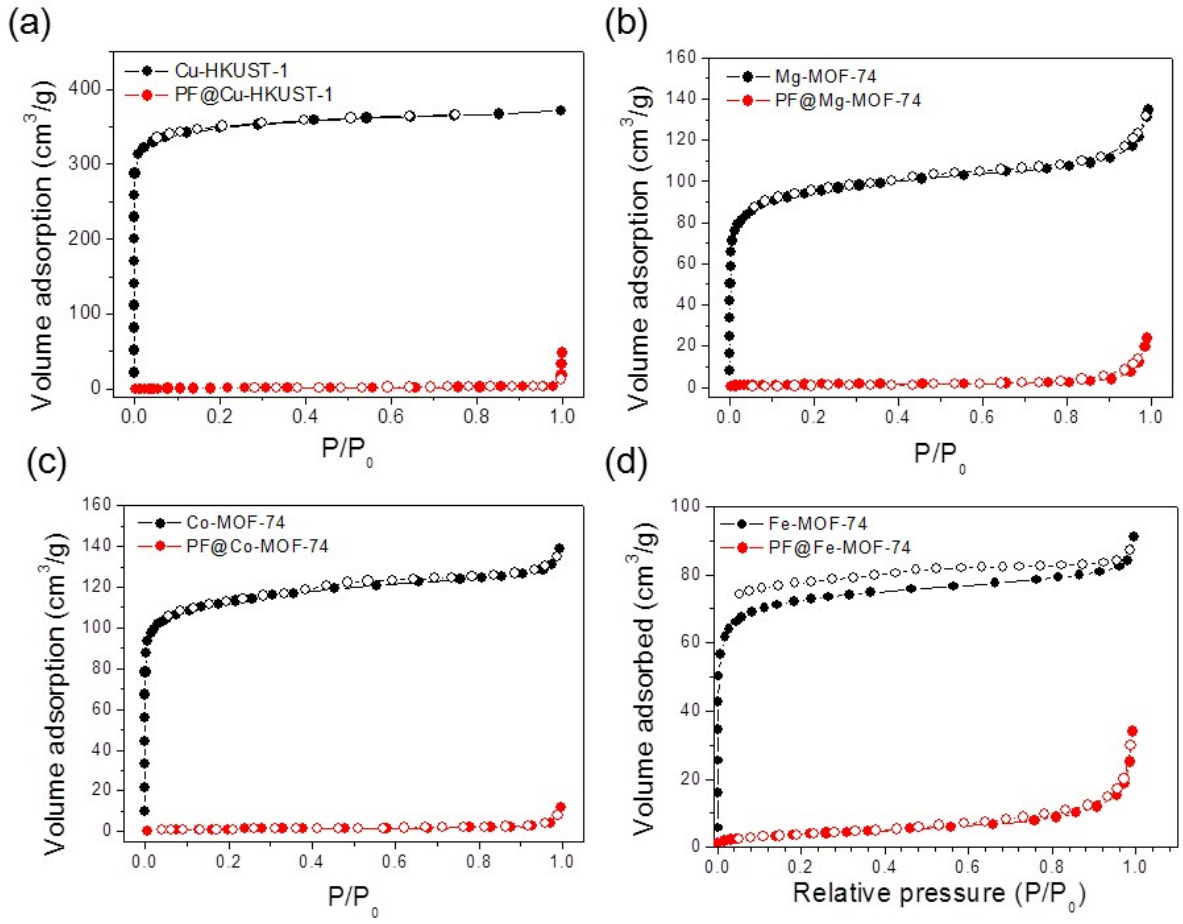

Figure S1. N_2 sorption isotherms for MOFs and PF@MOF samples: Cu-HKUST-1 and PF@Cu-HKUST-1 (a), Zn-HKUST-1 and PF@Zn-HKUST-1 (b), Co-MOF-74 and PF@Co-MOF-74 (c), and Fe-MOF-74 and PF@Fe-MOF-74.

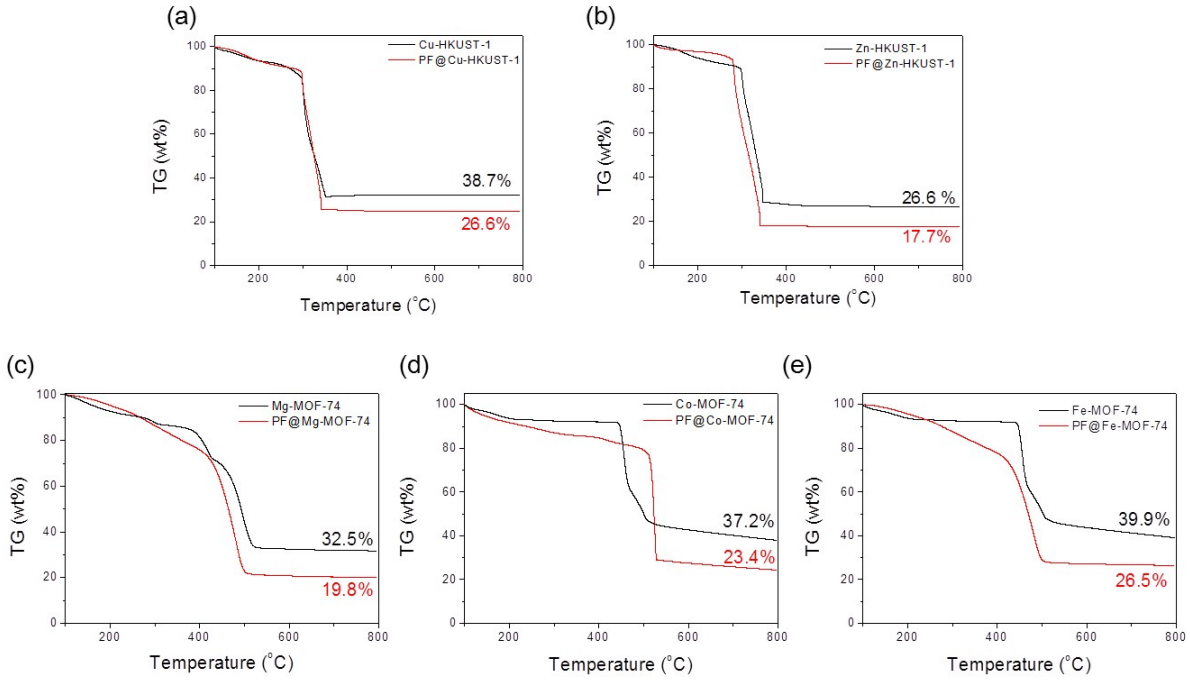

Figure S2. TGA results for MOFs and PF@MOF samples: Cu-HKUST-1 and PF@Cu-HKUST-1 (a), Zn-HKUST-1 and PF@Zn-HKUST-1 (b), Mg-MOF-74 and PF@Mg-MOF-74 (c), Co-MOF-74 and PF@Co-MOF-74 (d), and Fe-MOF-74 and PF@Fe-MOF-74 (e).

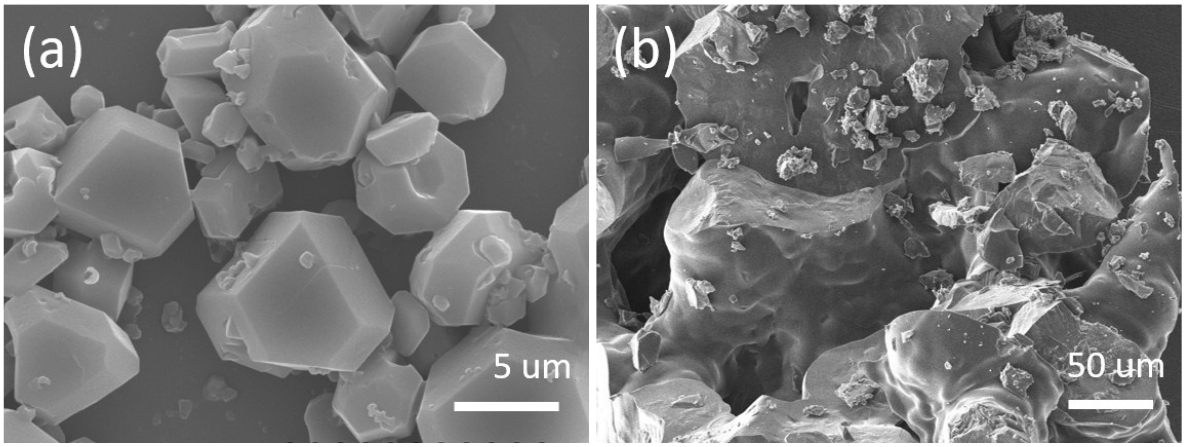

Figure S3. SEM images of ZIF-8 and PF@ZIF-8.

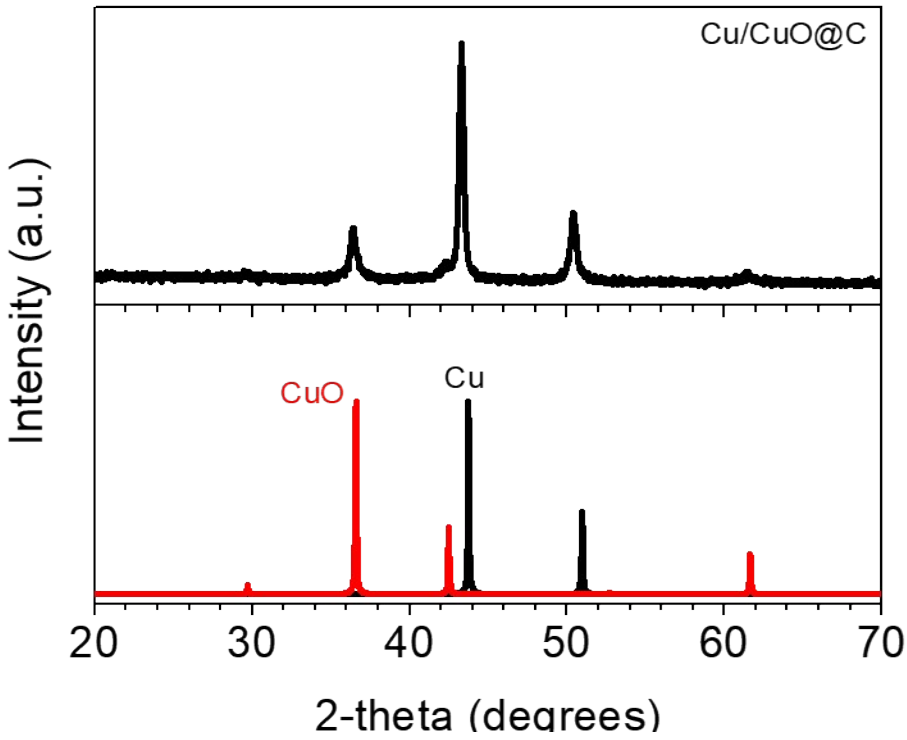

Figure S4. XRD pattern of Cu/CuO@C derived from PF@Cu-HKUST-1 thermolysis at 380 ^{o}C.

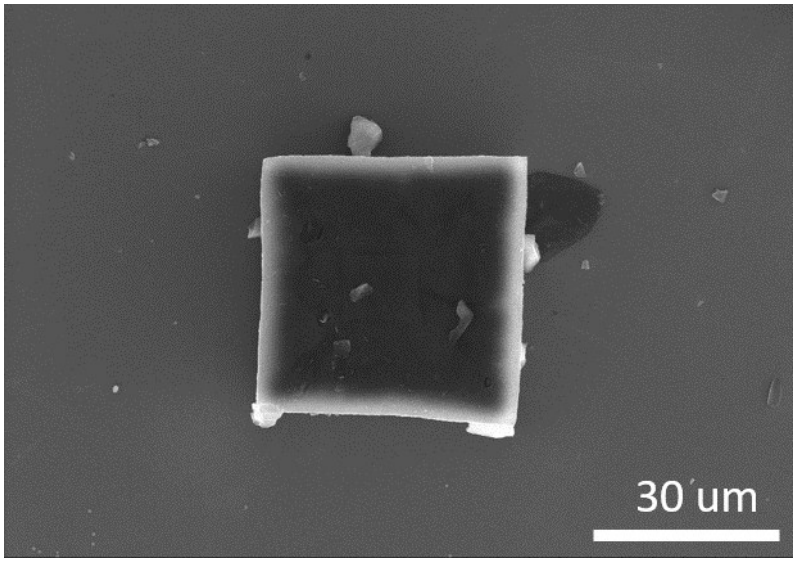

Figure S5. SEM image of cubic shaped carbon derived from PF@Zn-HKUST-1 at high temperature thermolysis (900 °C) condition.

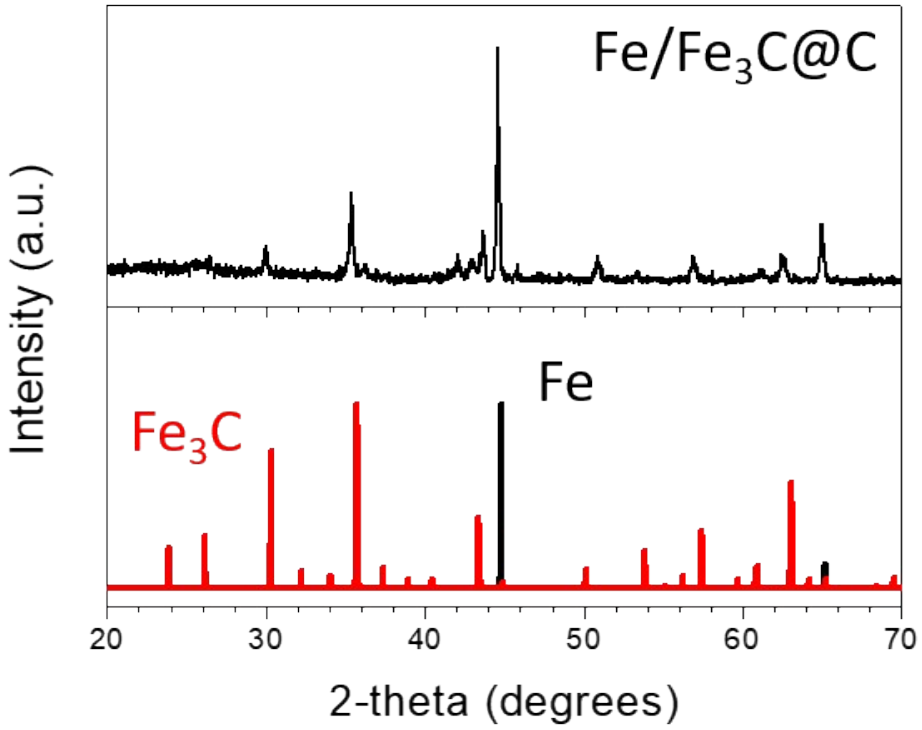

Figure S6. XRD pattern of $Fe/Fe_3C@C$ Heat treated at 1000 ^oC

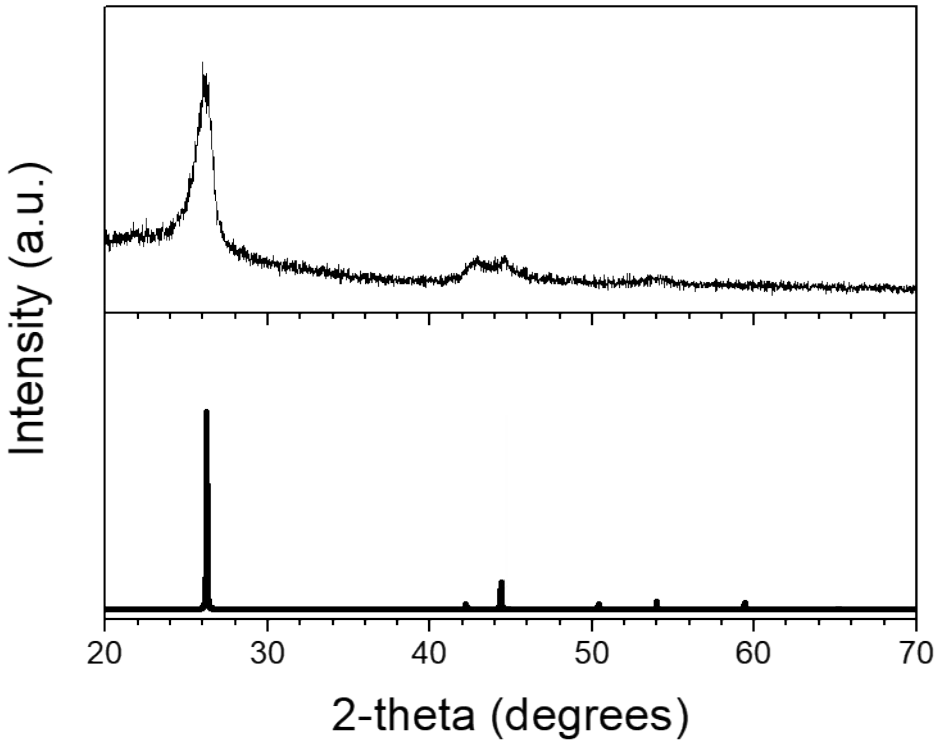

Figure S7. XRD pattern of Fe@C after acid treatment

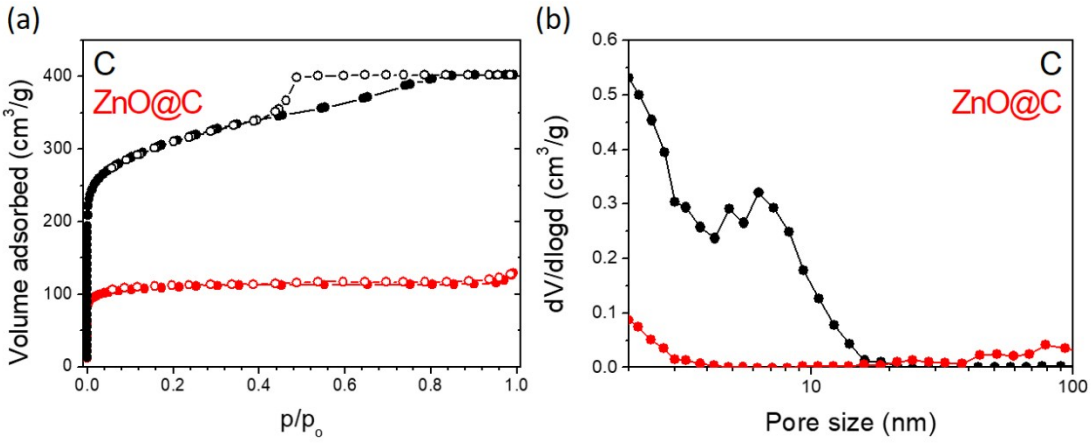

Figure S8. (a) N_2 isotherm at 77K and (b) BJH plot of ZnO@C and C.

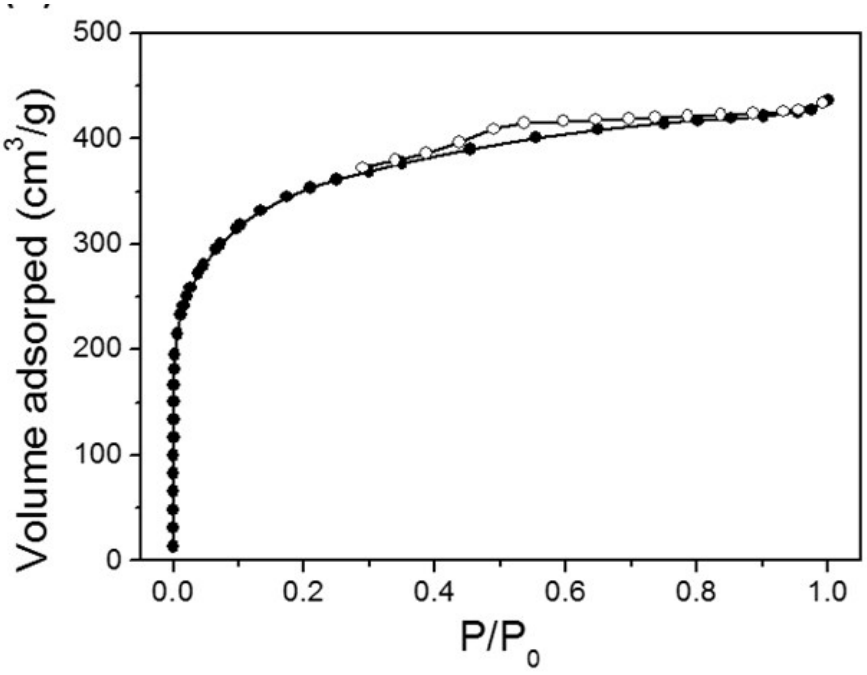

Figure S9. N_2 isotherm of MgO@C at 77K.

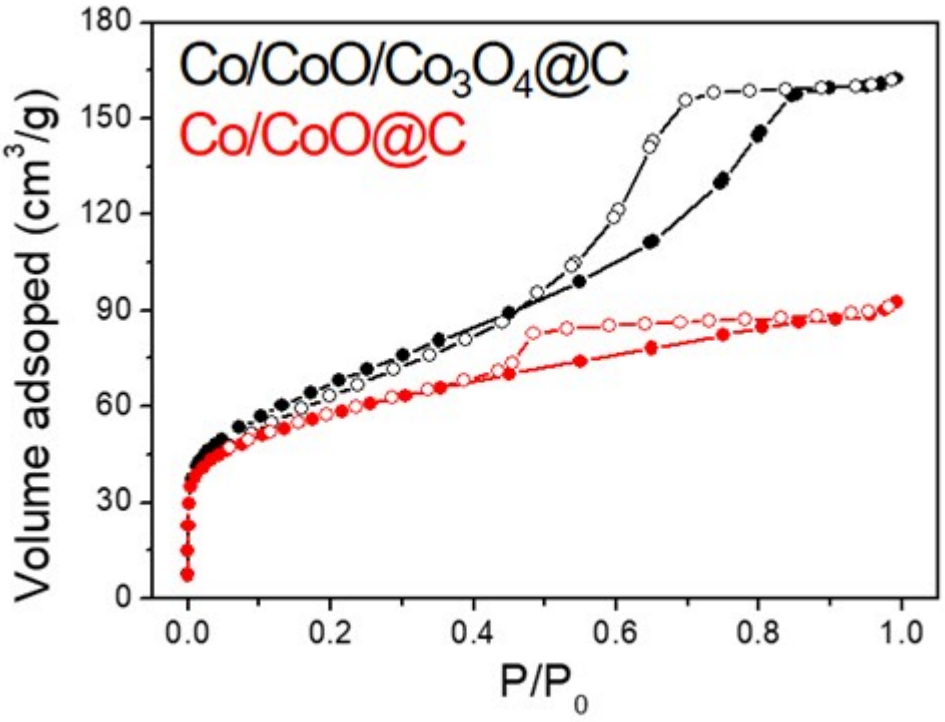

Figure S10. N_2 isotherms Co/CoO/Co_3O_4@C and Co/CoO@C at 77K.

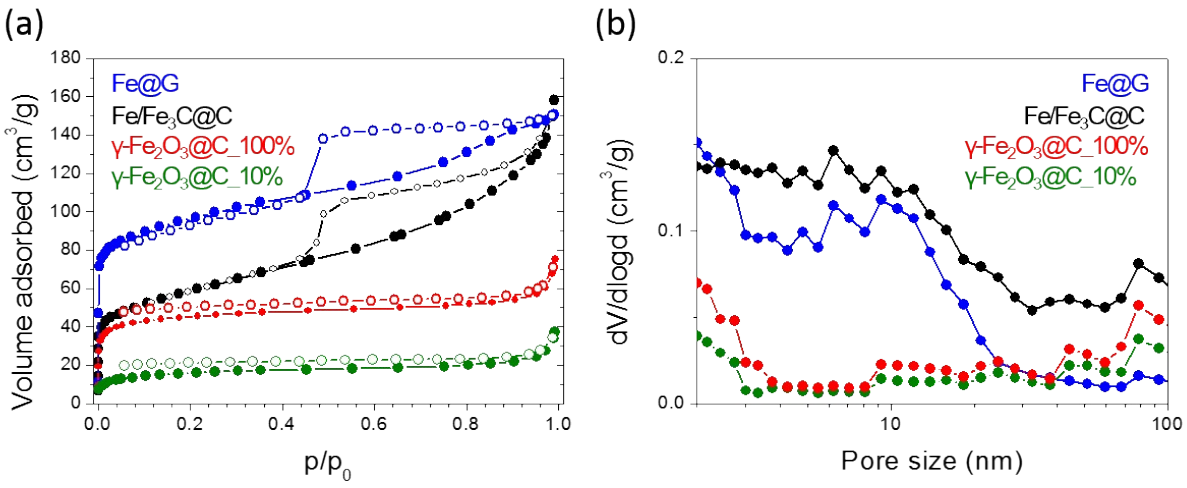

Figure S11. (a) N_2 isotherm at 77K and (b) BJH plot of Fe_2O_3@C_100 & 10%, Fe@G and Fe/Fe_3C@C

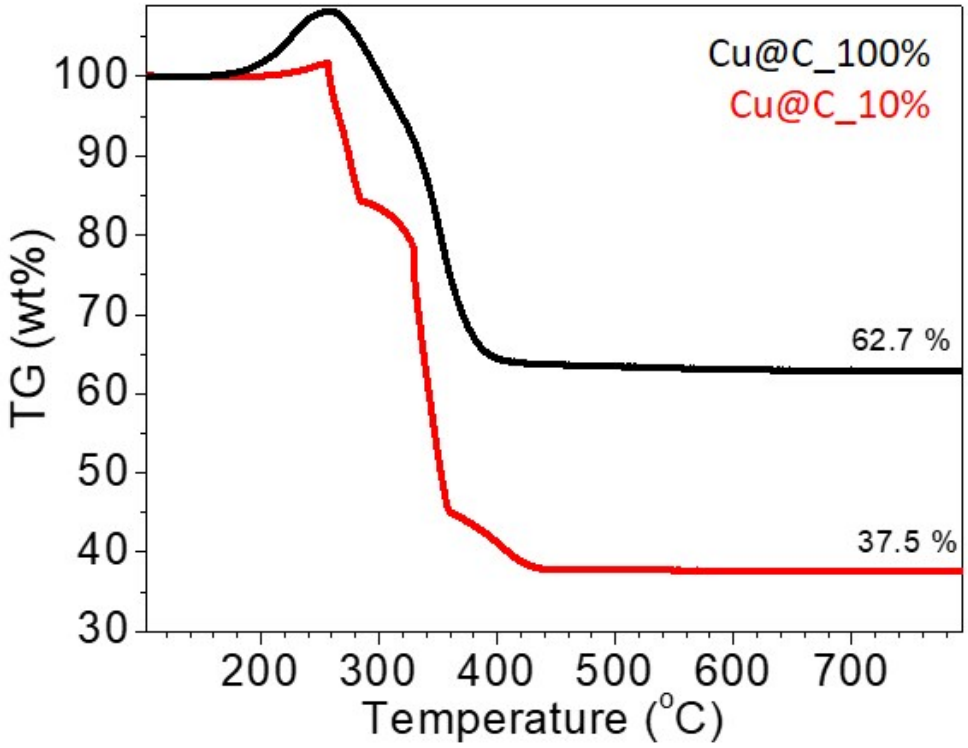

Figure S12. TGA data of Cu@C_100 & 10%.

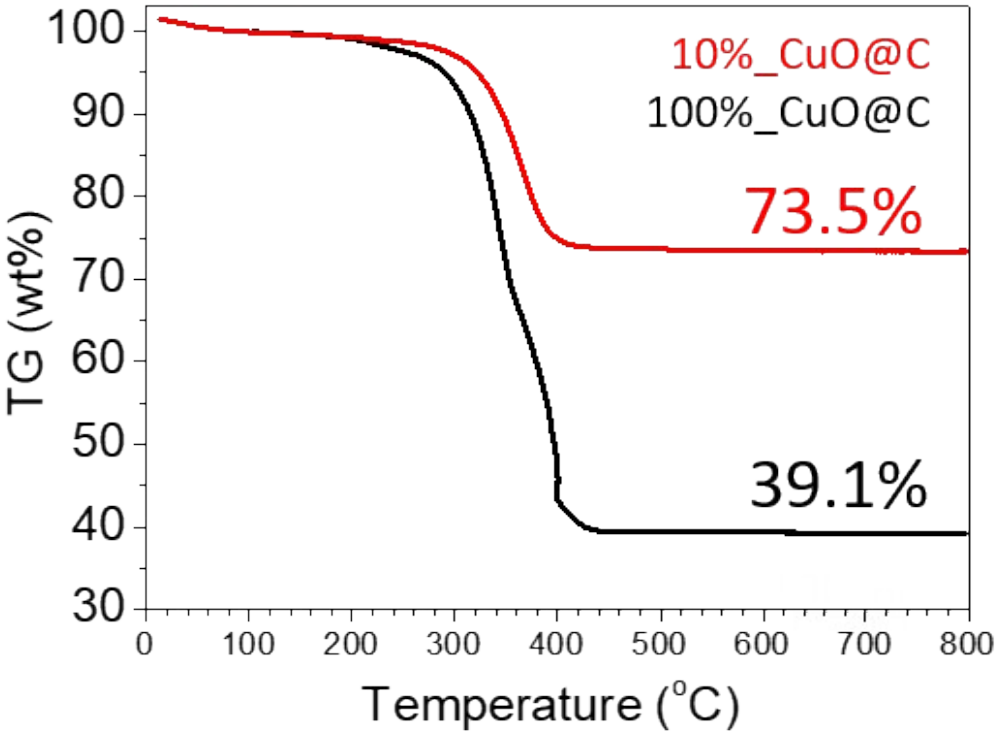

Figure S13. TGA data of CuO@C_100 & 10%.

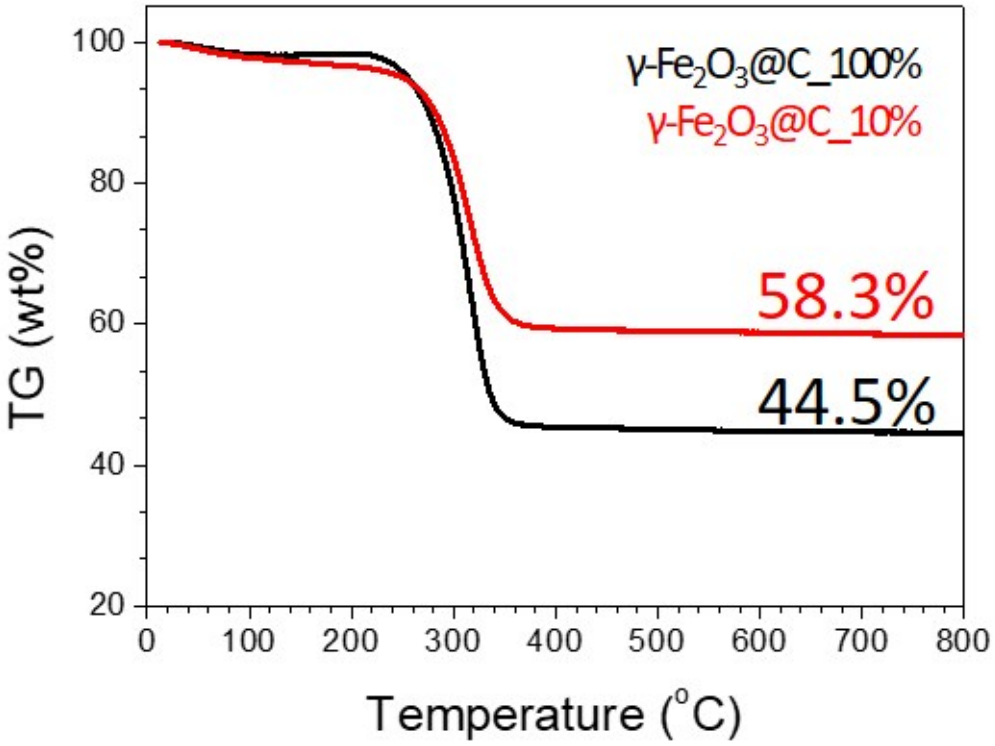

Figure S14. TGA data of γ-Fe_2O_3@C_100 & 10%.

Sample	S_{BET} (m^2/g)	V_{tot} (cm^3/g)	V_{micro} (cm^3/g)
Cu-HKUST-1	1377.4	0.57	0.54
PF@Cu-HKUST-1	4.1	0.02	-
Co-MOF-74	433	0.21	0.17
PF@Co-MOF-74	4.3	0.01	-
Fe-MOF-74	283	0.14	0.11
PF@Fe-MOF-74	3.9	0.01	-
Mg-MOF-74	364	0.2	0.14
PF@Mg-MOF-74	5.2	0.03	-

Table S1. Textural features for MOFs and PF@MOF samples.

Materials	S^o (KJ/mol·K)	H^o(KJ/mol)
CuO(s)	-157.3	42.6
γ-Fe_2O_3(s)	87.4	-808.1
Fe_3C(s)	220.1	25.1
Mg(g)	148.648	147.1
MgO(s)	26.95	-601.6
Zn(g)	160.9	130.4
ZnO(s)	-43.6	-350.4
CoO(s)	53.0	-237.7
Co_3O_4(s)	102.5	-891

Table S2. Thermodynamic data of Metal and Metal oxides