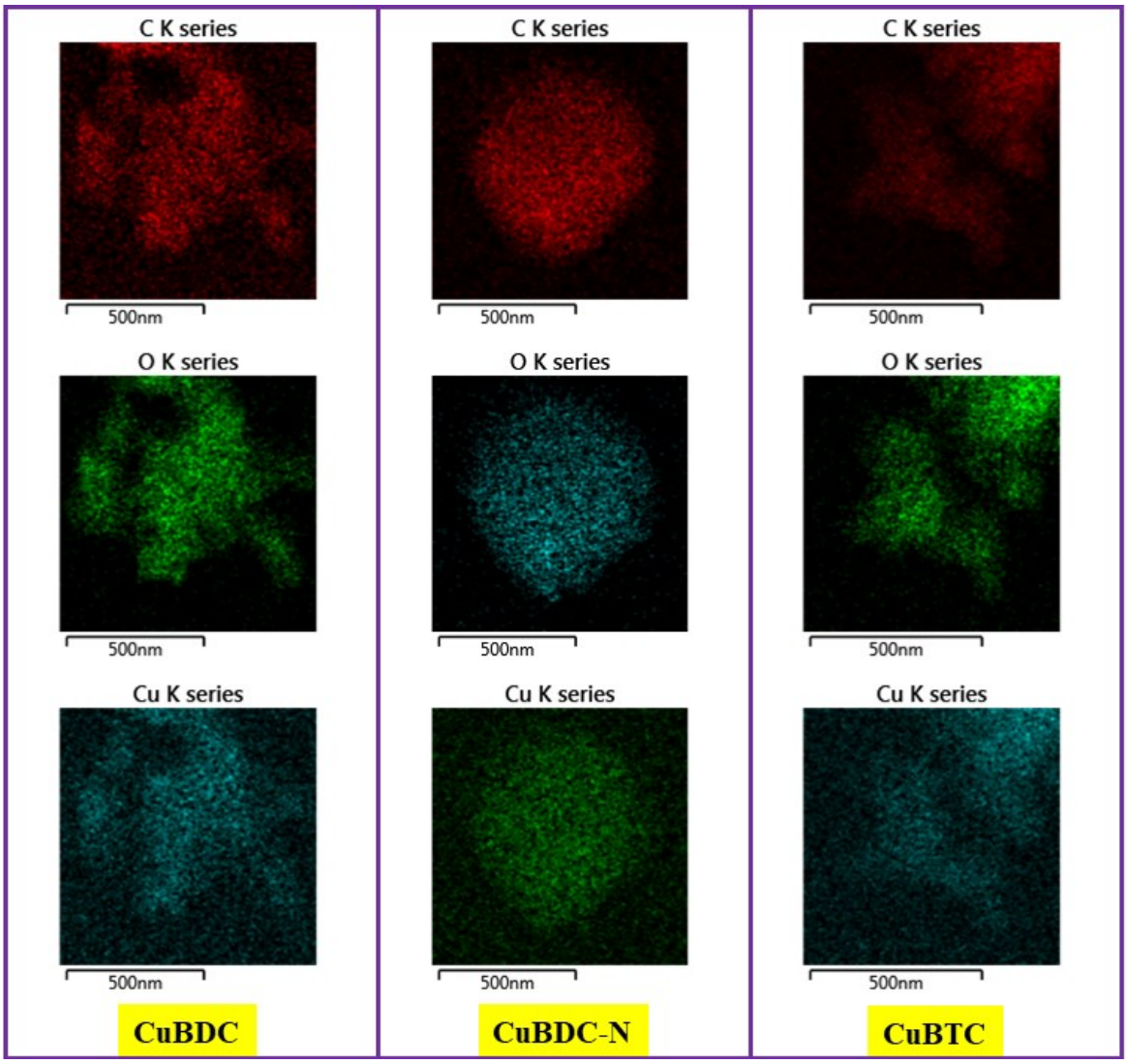
Electronic Supplementary Material (ESI) for RSC Advances.


# Chemisorption of hydrogen sulfide over copper-based metal-organic frameworks: Methanol and UV-assisted regeneration

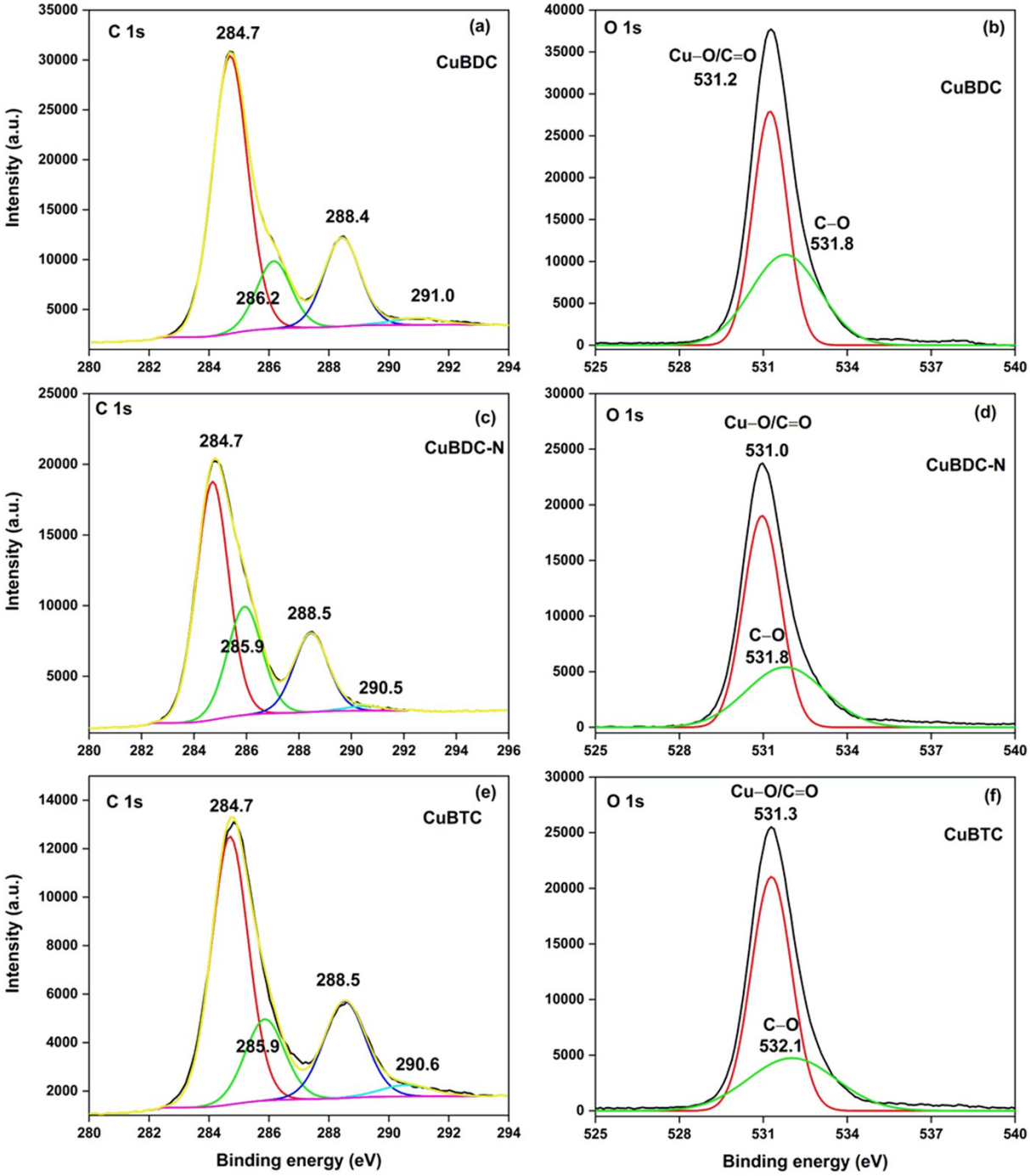
Nishesh Kumar Gupta[a,b], Suho Kim[a,b], Jiyeol Bae[b], Kwang Soo Kim[a,b*]

a. *University of Science and Technology (UST), Daejeon, Republic of Korea*

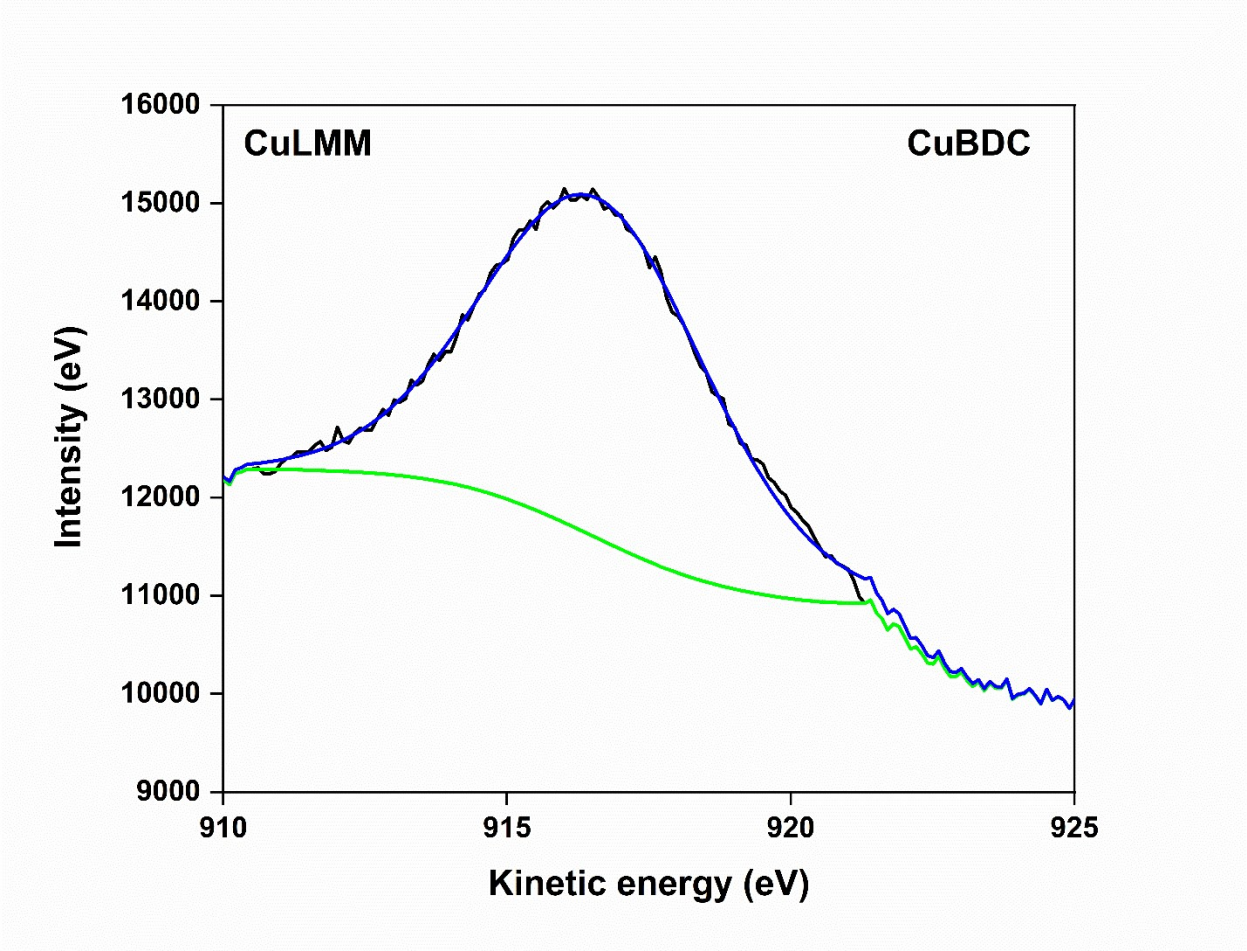
b. *Department of Land, Water, and Environment Research, Korea Institute of Civil Engineering and Building Technology (KICT), Goyang, Republic of Korea*



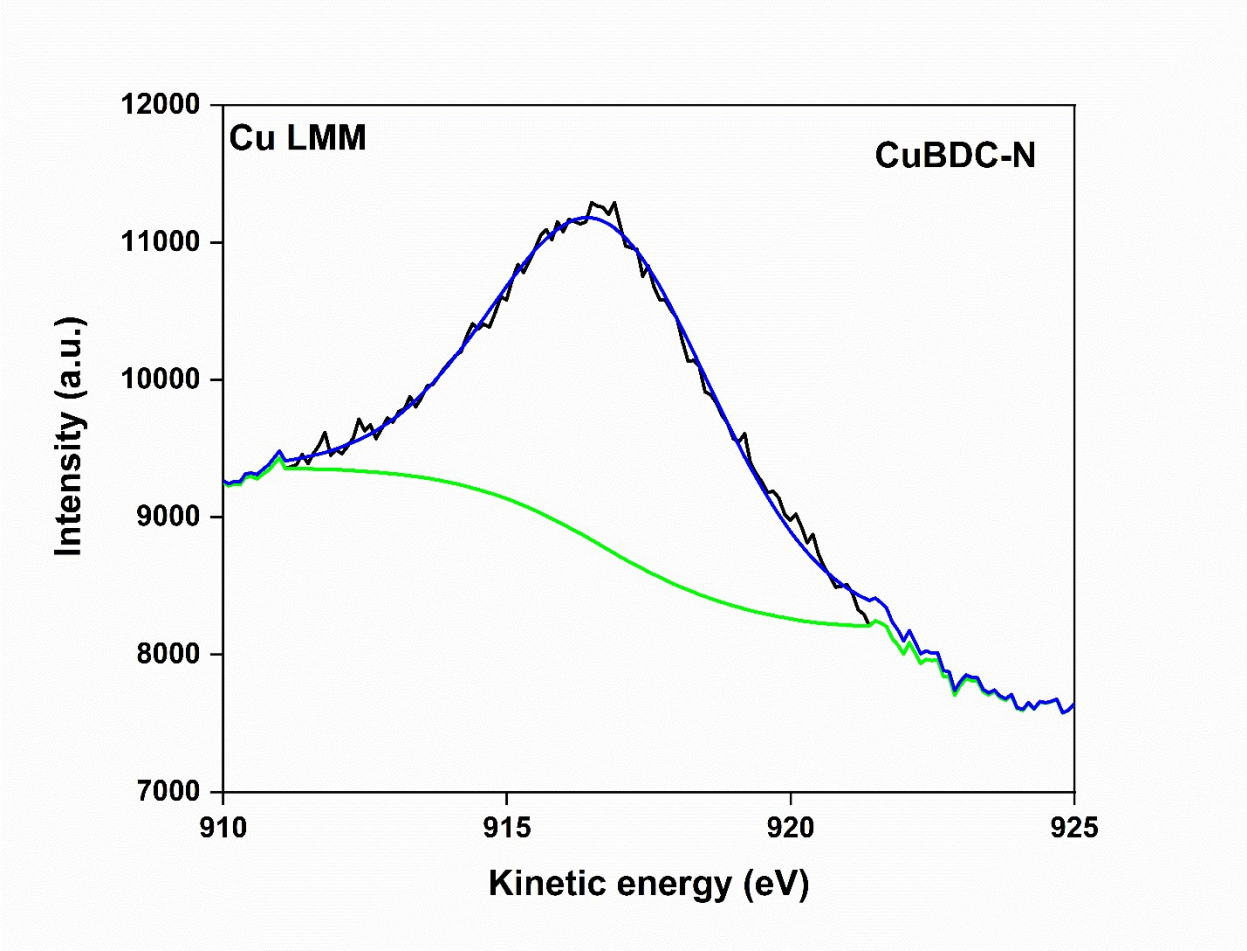

**S. Figure 1.** 2D elemental mapping of Cu-MOFs.



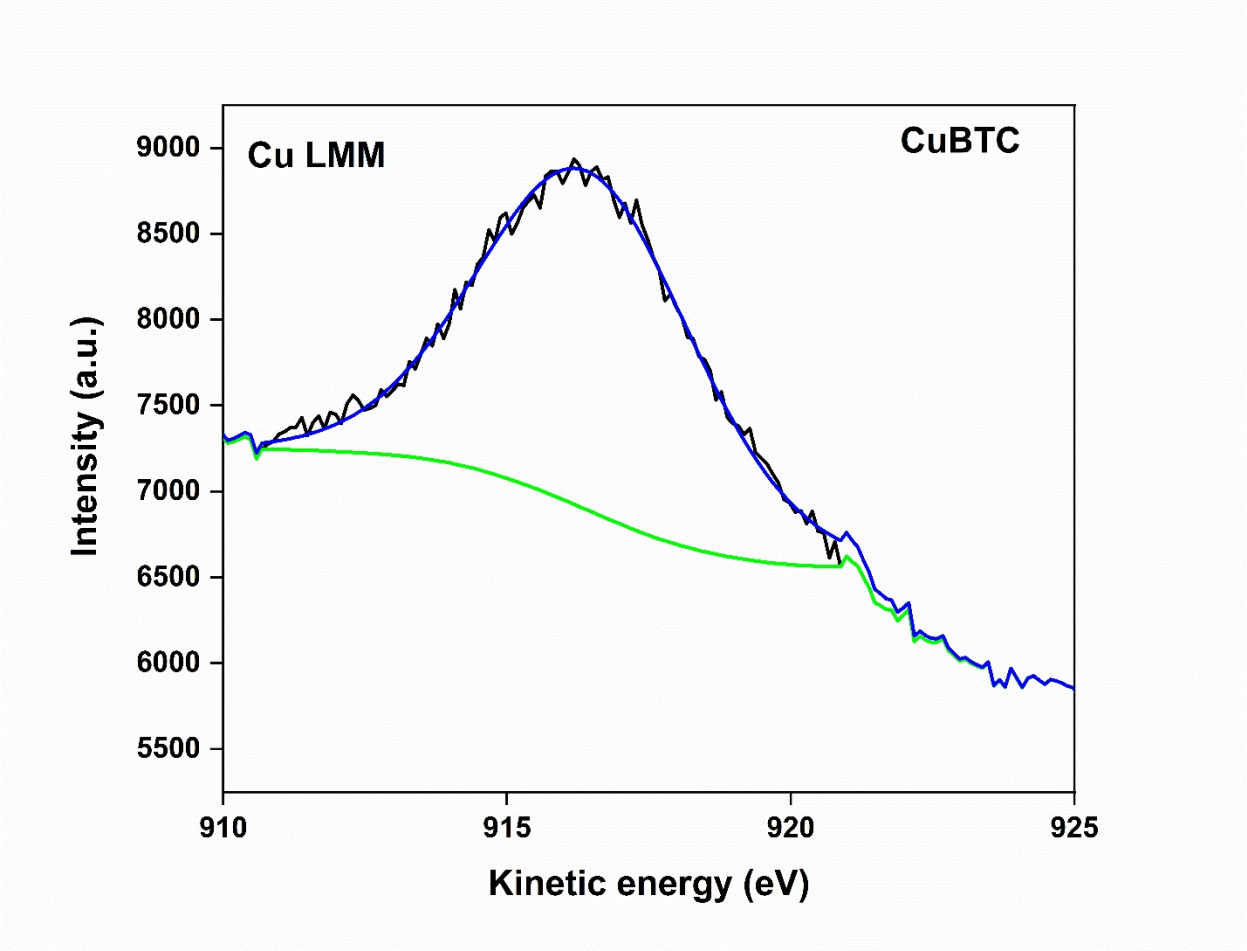

**S. Figure 2.** HRXPS C 1s spectra of (**a**) CuBDC; (**c**) CuBDC-N; (**e**) CuBTC; HRXPS O 1s spectra of (**b**) CuBDC; (**d**) CuBDC-N; (**f**) CuBTC.



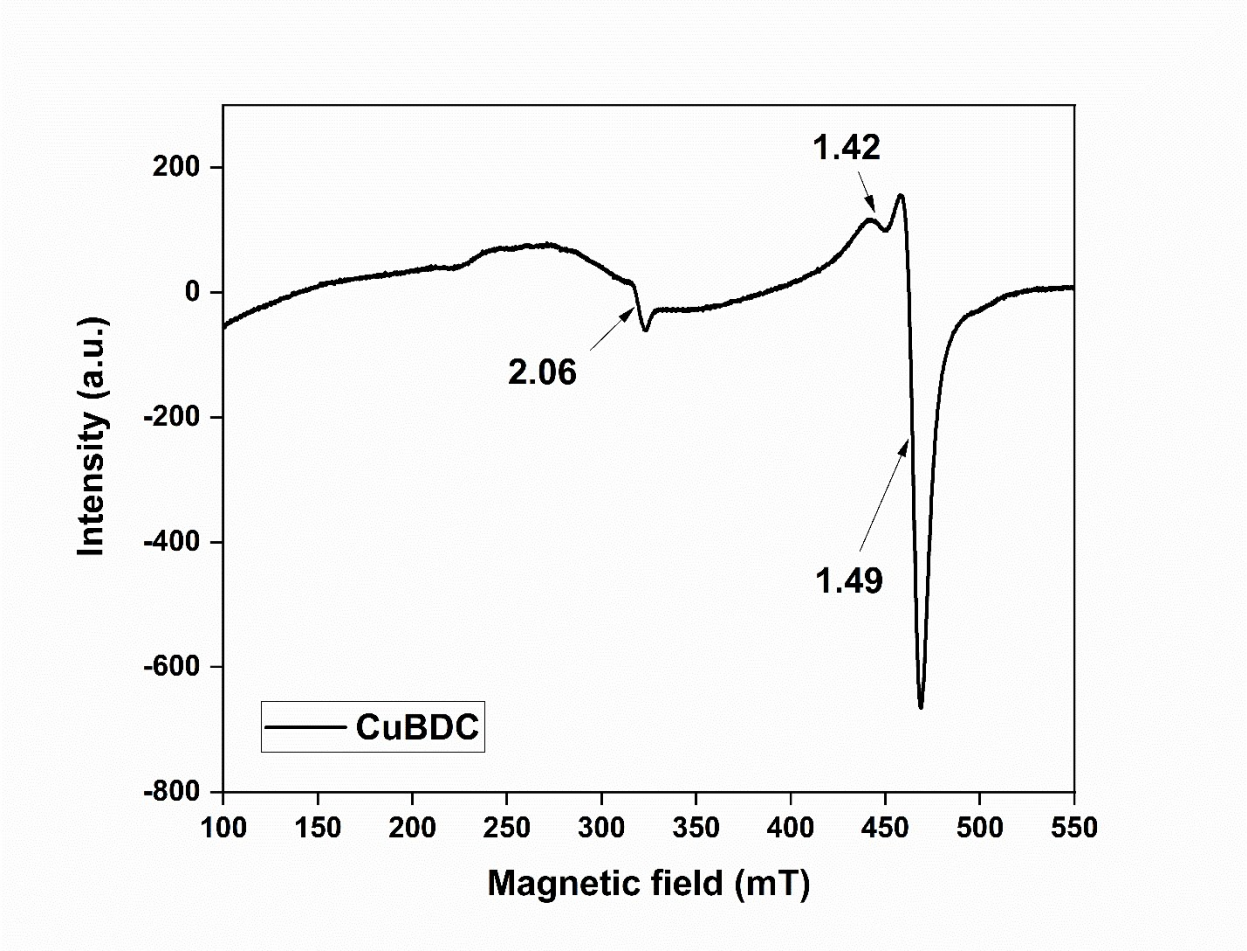

**S. Figure 3a.** HRXPS Cu LMM spectrum of CuBDC.



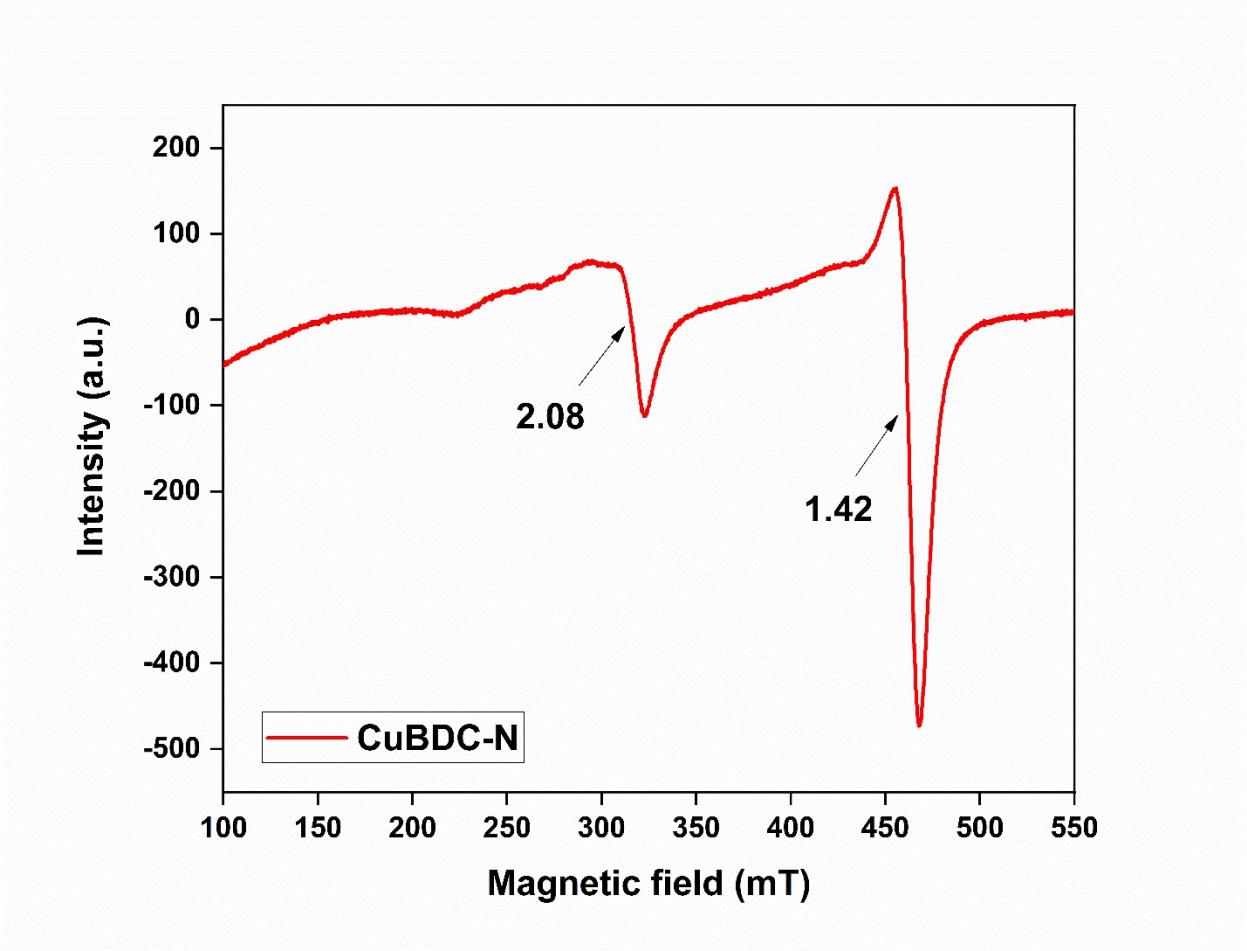

**S. Figure 3b.** HRXPS Cu LMM spectrum of CuBDC-N.



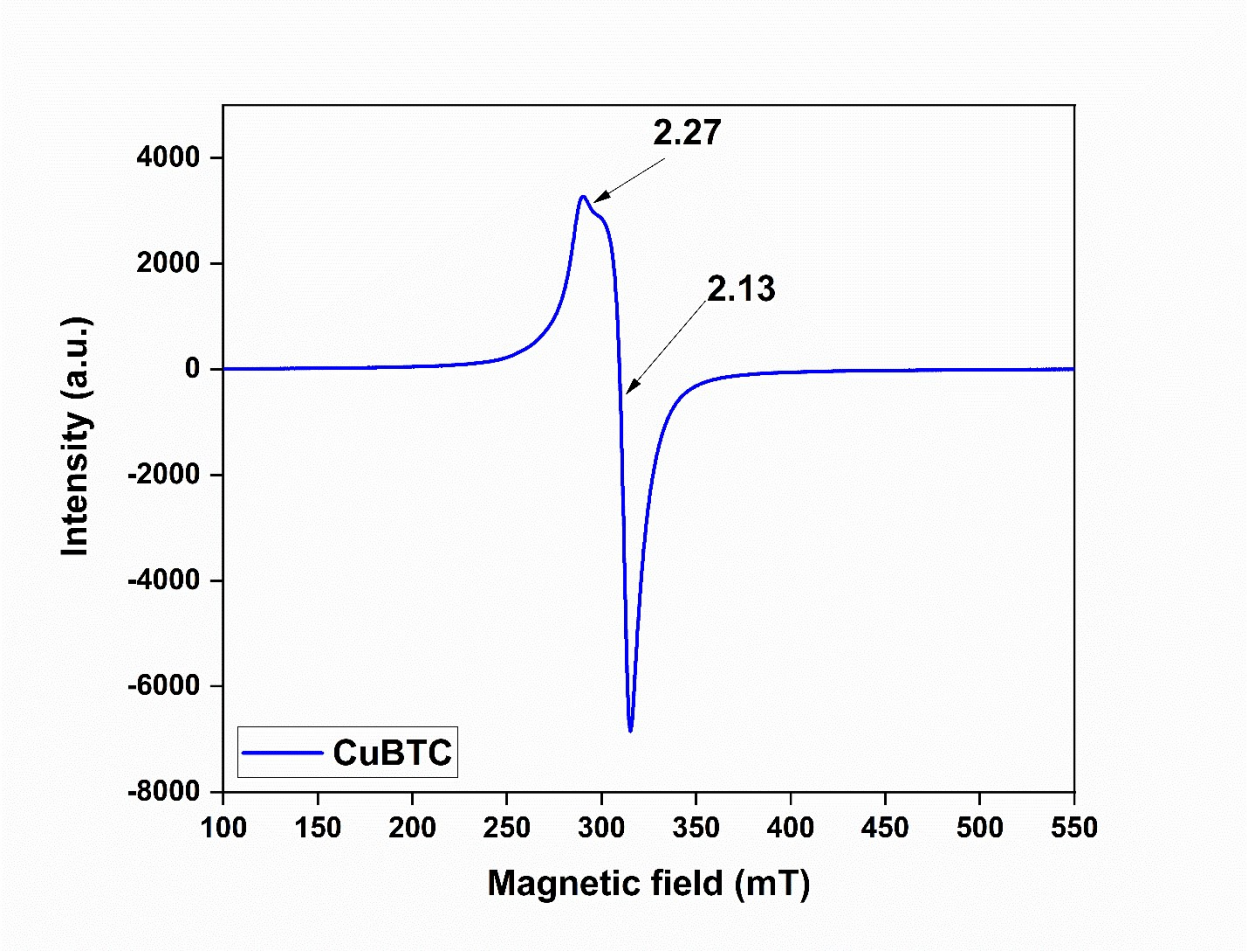

**S. Figure 3c.** HRXPS Cu LMM spectrum of CuBTC.




**S. Figure 4a.** ESR spectrum of CuBDC recorded at 25 ºC.




**S. Figure 4b.** ESR spectrum of CuBDC-N recorded at 25 ºC.




**S. Figure 4c.** ESR spectrum of CuBTC recorded at 25 ºC.

**S. Table 1.** Appearance and yield of synthesized Cu-MOFs

| MOF | Color | Yield (g) |
|---|---|---|
| **CuBDC** | Light blue | 14.07 |
| **CuBDC-N** | Dark green | 13.53 |
| **CuBTC** | Light blue | 11.61 |

**S. Table 2.** Miller indices and corresponding diffraction angle of CuBDC

| **2θ (degree)** | **hkl** | ***d* (Å)** | **Area%** | **FWHM** |
|---|---|---|---|---|
| 10.16 | 110 | 8.70 | 92.8 | 0.203 |
| 12.08 | 020 | 7.32 | 43.6 | 0.291 |
| 13.58 | 11-1 | 6.52 | 12.2 | 0.220 |
| 17.12 | -201 | 5.17 | 100.0 | 0.253 |
| 17.70 | 111 | 5.01 | 18.4 | 0.239 |
| 20.40 | 220 | 4.35 | 25.2 | 0.273 |
| 24.82 | 131 | 3.58 | 53.7 | 0.197 |

**S. Table 3.** Miller indices and corresponding diffraction angle of CuBDC-N

| **2θ (degree)** | **hkl** | ***d* (Å)** | **Area%** | **FWHM** |
|---|---|---|---|---|
| 10.28 | 110 | 8.60 | 74.1 | 0.139 |
| 11.82 | 001 | 7.48 | 46.0 | 0.180 |
| 13.14 | 11-1 | 6.73 | 14.4 | 0.148 |
| 16.80 | -201 | 5.27 | 100.0 | 0.149 |
| 18.02 | 111 | 4.92 | 23.3 | 0.182 |
| 20.70 | 220 | 4.29 | 20.6 | 0.138 |
| 24.71 | 131 | 3.60 | 46.1 | 0.121 |

**S. Table 4.** Miller indices and corresponding diffraction angle of CuBTC

| **2θ (degree)** | **hkl** | ***d* (Å)** | **Area%** | **FWHM** |
|---|---|---|---|---|
| 9.46 | 022 | 9.34 | 87.5 | 0.241 |
| 11.62 | 222 | 7.61 | 87.4 | 0.184 |
| 13.42 | 004 | 6.59 | 100.0 | 0.215 |
| 19.02 | 044 | 4.66 | 88.8 | 0.189 |
| 25.96 | 355 | 3.43 | 89.0 | 0.222 |

**S. Table 5.** Crystallite size and lattice parameters of Cu-MOFs

| Cu-MOF | *D* (nm) | Lattice parameters |
|---|---|---|
| **CuBDC** | 31.7 | Monoclinic, space group = C2/*m*; *a* = 11.37 Å, *b* = 14.62 Å, *c* = 7.72 Å, *β* = 108.49° |
| **CuBDC-N** | 46.6 | Monoclinic, space group = C2/*m*; *a* = 11.23 Å, *b* = 14.96 Å, *c* = 8.02 Å, *β* = 111.67° |
| **CuBTC** | 38.2 | Cubic, space group = F*m-3m*; *a* = 26.36 Å |

**S. Table 6.** The peak-fitting results of C 1s high resolution signals of CuBDC, CuBDC-N and CuBTC.

| Samples | Assignment | $E_B$ (eV) | FWHM (eV) | At. % |
|---|---|---|---|---|
| **CuBDC** | **C1s** $_{C=C}$ | 284.7 | 1.4 | 62.6 |
| | **C1s** $_{C-C,\ C-H}$ | 286.2 | 1.4 | 14.9 |
| | **C1s** $_{O-C=O}$ | 288.4 | 1.4 | 20.4 |
| | **C1s** $_{COOH}$ | 291.0 | 2.0 | 2.1 |
| **CuBDC-N** | **C1s** $_{C=C}$ | 284.7 | 1.4 | 55.0 |
| | **C1s** $_{C-C,\ C-H,C-N}$ | 285.9 | 1.5 | 26.5 |
| | **C1s** $_{O-C=O}$ | 288.5 | 1.5 | 18.5 |
| | **C1s** $_{COOH}$ | 290.5 | 1.6 | 1.2 |
| **CuBTC** | **C1s** $_{C=C}$ | 284.7 | 1.4 | 55.7 |

| | | | | |
|---|---|---|---|---|
| | **C1s** $_{C\text{-}C,\ C\text{-}H}$ | 285.9 | 1.5 | 18.1 |
| | **C1s** $_{O\text{-}C=O}$ | 288.5 | 1.6 | 22.9 |
| | **C1s** $_{COOH}$ | 290.6 | 2.0 | 3.3 |

**S. Table 7.** Curve fitting parameters from CuLMM Auger Signals for CuBDC, CuBDC-N and CuBTC samples.

| **Samples** | **BE (eV)** | **KE (eV)** | **α´(eV)** | **Assignment** |
|---|---|---|---|---|
| **CuBDC** | 570.6 | 916.6 | 1849.0 | $Cu^{+}$ |
| | | | 1850.6 | $Cu^{2+}$ |
| **CuBDC-N** | 570.0 | 916.8 | 1849.3 | $Cu^{+}$ |
| | | | 1851.0 | $Cu^{2+}$ |
| **CuBTC** | 570.6 | 916.4 | 1848.7 | $Cu^{+}$ |
| | | | 1850.7 | $Cu^{2+}$ |

**S. Table 8.** Elemental composition of Cu-MOFs using TEM-EDS analysis.

| **Element** | **CuBDC** | | **CuBDC-N** | | **CuBTC** | |
|---|---|---|---|---|---|---|
| | **Wt.%** | **At.%** | **Wt.%** | **At.%** | **Wt.%** | **At.%** |
| **C** | 46.99 | 67.50 | 58.64 | 76.67 | 56.94 | 77.55 |
| **O** | 22.44 | 24.20 | 17.85 | 17.52 | 14.86 | 15.20 |
| **Cu** | 30.58 | 8.30 | 23.51 | 5.81 | 28.20 | 7.26 |

**S. Table 9.** Surface elemental composition (atomic%) of Cu-MOFs using XPS analysis.

| Element | CuBDC | CuBDC-N | CuBTC |
|---|---|---|---|
| **C** | 65.66 | 63.14 | 60.48 |
| **Cu** | 5.93 | 4.98 | 6.60 |
| **O** | 28.41 | 24.46 | 32.92 |
| **N** | - | 7.42 | - |

**S. Table 10.** Surface elemental composition (atomic%) of fresh, spent, and regenerated CuBTC using XPS analysis.

| Element | CuBTC | Spent CuBTC | Reg. CuBTC |
|---|---|---|---|
| **C** | 60.48 | 50.67 | 55.05 |
| **O** | 32.92 | 38.08 | 34.92 |
| **Cu** | 6.60 | 7.33 | 8.53 |
| **S** | - | 3.91 | 1.49 |