

## **Support Information for**

### **Study on gas adsorption and separation performance of alkyl functionalized MOF materials under wet conditions**

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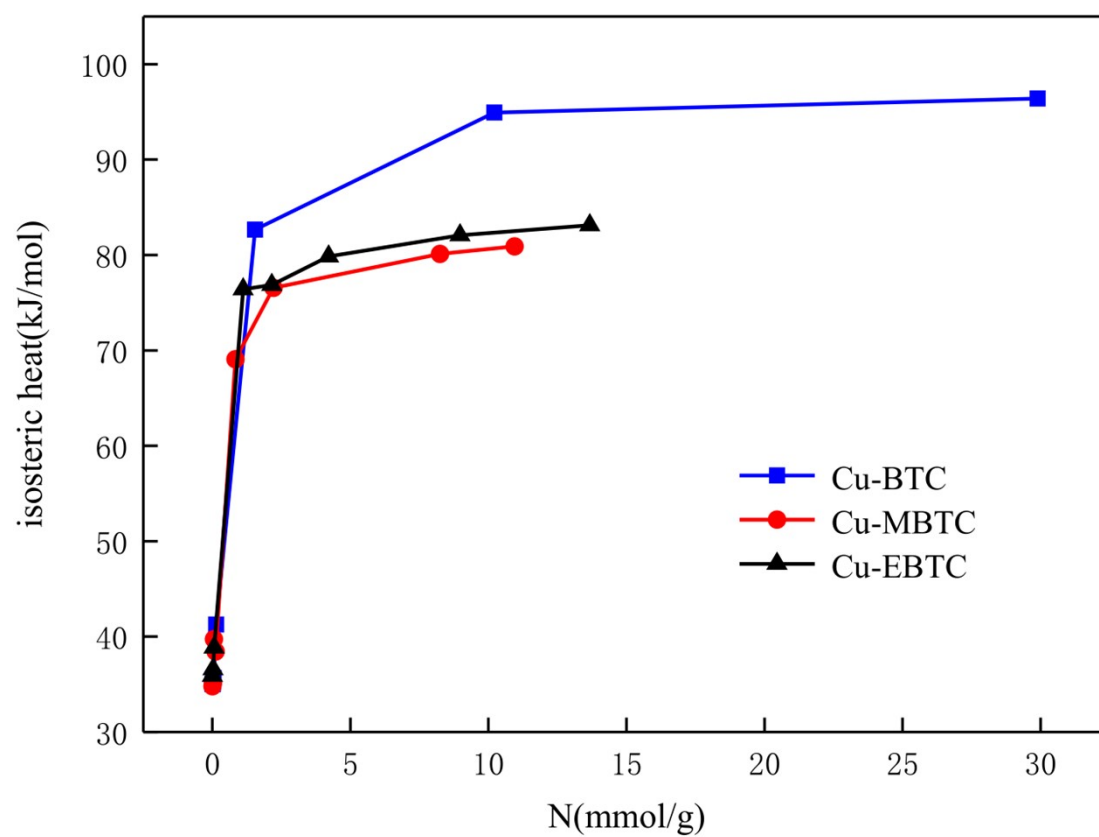
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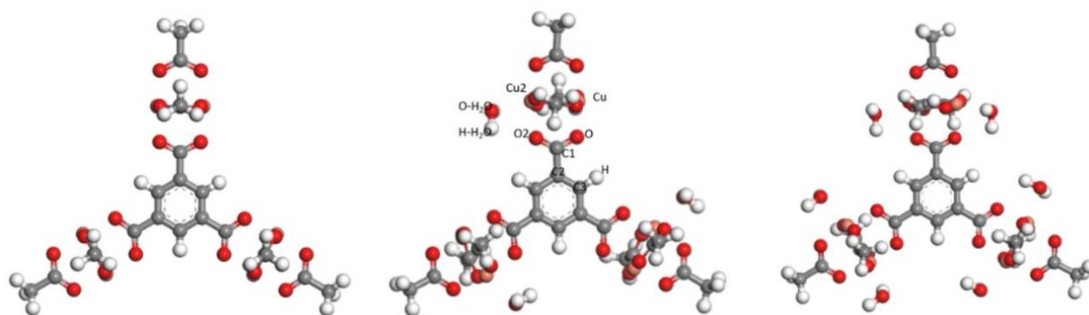
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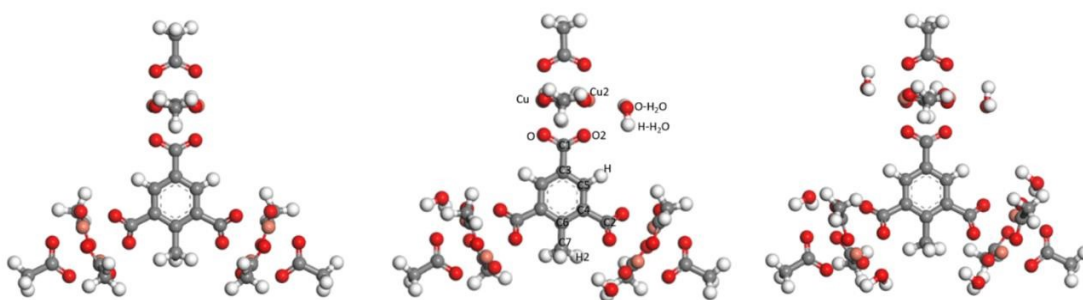


**Figure. S1** The heat of adsorption of Cu-BTC, Cu-MBTC and Cu-EBTC to water calculated by

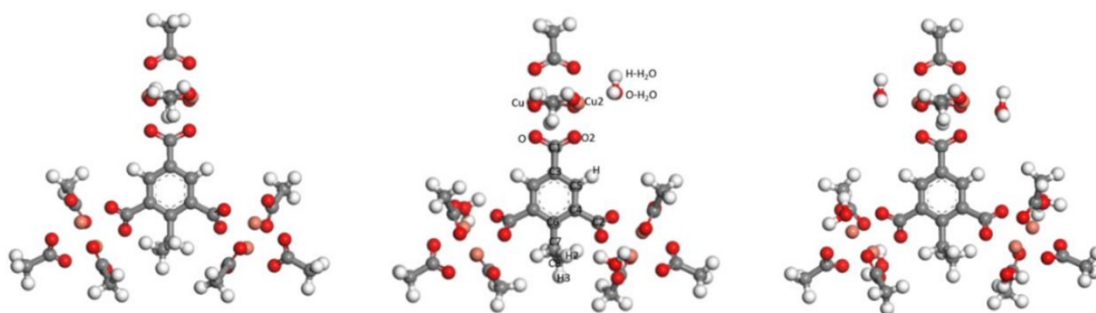
GCMC at 298 K



**Figure. S2** Schematic diagram of atomic distribution charge of Cu-BTC with different numbers of water molecules



**Figure. S3** Schematic diagram of atomic distribution charge of Cu-MBTC with different numbers of water molecules



**Figure. S4** Schematic diagram of atomic distribution charge of Cu-EBTC with different numbers of water molecules

**Table S1.** The atomic distribution charge of Cu-BTC with different numbers of water

| Atomic species                | molecules |                 |        |                |       |       |        |       |                    |                    |
|-------------------------------|-----------|-----------------|--------|----------------|-------|-------|--------|-------|--------------------|--------------------|
|                               | Cu        | Cu <sub>2</sub> | O      | O <sub>2</sub> | C1    | C2    | C3     | H     | O-H <sub>2</sub> O | H-H <sub>2</sub> O |
| Cu-BTC                        | 1.090     |                 | -0.632 |                | 0.677 | 0.037 | -0.135 | 0.140 |                    |                    |
| Cu-BTC containing 4 wt% water | 1.164     | 1.068           | -0.662 | -0.663         | 0.673 | 0.027 | -0.127 | 0.130 | -0.788             | 0.406              |
| Cu-BTC containing 8 wt% water | 1.116     |                 | -0.647 |                | 0.691 | 0.056 | -0.159 | 0.136 | -0.778             | 0.401              |

**Table S2.** The atomic distribution charge of Cu-MBTC with different numbers of water

| Atomic species                | molecules |                 |        |                |       |       |        |        |        |       |       |        |                |                    |                    |
|-------------------------------|-----------|-----------------|--------|----------------|-------|-------|--------|--------|--------|-------|-------|--------|----------------|--------------------|--------------------|
|                               | Cu        | Cu <sub>2</sub> | O      | O <sub>2</sub> | C1    | C2    | C3     | C4     | C5     | H     | C6    | C7     | H <sub>2</sub> | O-H <sub>2</sub> O | H-H <sub>2</sub> O |
| Cu-BTC                        | 1.078     |                 | -0.669 |                | 0.739 | 0.811 | -0.052 | -0.147 | -0.072 | 0.135 | 0.228 | -0.380 | 0.136          |                    |                    |
| Cu-BTC containing 4 wt% water | 1.164     | 1.074           | -0.700 | -0.640         | 0.699 | 0.821 | -0.012 | -0.128 | -0.099 | 0.137 | 0.219 | -0.382 | 0.111          | -0.790             | 0.410              |
| Cu-BTC containing 8 wt% water | 1.194     |                 | -0.700 |                | 0.714 | 0.808 | -0.007 | -0.124 | -0.108 | 0.143 | 0.232 | -0.382 | 0.123          | -0.790             | 0.410              |

**Table S3.** The atomic distribution charge of Cu-EBTC with different numbers of water

| Atomic species                | molecules |       |        |        |       |       |        |        |        |       |       |        |       |       |        |                    |
|-------------------------------|-----------|-------|--------|--------|-------|-------|--------|--------|--------|-------|-------|--------|-------|-------|--------|--------------------|
|                               | Cu        | Cu2   | O      | O2     | C1    | C2    | C3     | C4     | C5     | H     | C6    | C7     | H2    | C8    | H3     | O-H <sub>2</sub> O |
| Cu-BTC                        | 1.0744    |       | -0.675 |        | 0.726 | 0.844 | -0.038 | -0.058 | -0.132 | 0.126 | 0.059 | -0.023 | 0.044 | 0.003 | -0.004 |                    |
| Cu-BTC containing 4 wt% water | 1.150     | 1.079 | -0.720 | -0.673 | 0.717 | 0.898 | 0.039  | -0.122 | -0.135 | 0.132 | 0.152 | -0.202 | 0.097 | 0.134 | -0.034 | -0.765             |
| Cu-BTC containing 8 wt% water | 1.105     |       | -0.623 |        | 0.629 | 0.698 | 00.039 | -0.026 | -0.160 | 0.143 | 0.033 | -0.081 | 0.048 | 0.044 | -0.005 | -0.785             |

**Table S4.** The pore structure characterization parameters of Cu-BTC, Cu-MBTC, and Cu-EBTC

| under aqueous and anhydrous conditions |              |                              |                                  |                                  |
|----------------------------------------|--------------|------------------------------|----------------------------------|----------------------------------|
| Materials                              | Porosity (%) | Density (g/cm <sup>3</sup> ) | Pore volume (cm <sup>3</sup> /g) | Surface area (m <sup>2</sup> /g) |
| Cu-BTC                                 | 68.9         | 0.879                        | 0.78                             | 2195.1                           |
| Cu-MBTC                                | 59.8         | 0.945                        | 0.64                             | 1922.3                           |
| Cu-EBTC                                | 52.6         | 1.054                        | 0.50                             | 1646.7                           |
| Cu-BTC with 4wt% water                 | 64.6         | 0.918                        | 0.70                             | 2076.5                           |
| Cu-MBTC with 4wt% water                | 54.4         | 0.988                        | 0.55                             | 1662.4                           |
| Cu-EBTC with 4wt% water                | 46.3         | 1.097                        | 0.42                             | 1137.4                           |
| Cu-BTC with 8wt% water                 | 60.6         | 0.958                        | 0.63                             | 1701.2                           |
| Cu-MBTC with 8wt% water                | 47.8         | 1.028                        | 0.47                             | 1136                             |
| Cu-EBTC with 8wt% water                | 39.7         | 1.140                        | 0.35                             | 865.2                            |