# Supplementary Information

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## Section 1. Crystallite size estimations by Scherrer method

$$Size = \frac{\lambda}{\beta \cos\theta}$$

**Equation 1.** Scherrer Equation

**Table 1.** Full width at half maximum and crystallite sizes estimated by Scherrer method

| MOF | Full Width at Half Maximum | Crystallite Size (Å) |
|---|---|---|
| Fe-BTC-110-1 | 1.325 | 67 |
| Fe-BTC-110-3 | 1.183 | 75 |
| Fe-BTC-110-5 | 0.959 | 93 |
| Fe-BTC-130-1 | 1.300 | 68 |
| Fe-BTC-130-3 | 1.044 | 85 |
| Fe-BTC-130-5 | 0.992 | 89 |
| Fe-BTC-150-1 | 1.079 | 82 |
| Fe-BTC-150-3 | 1.046 | 85 |
| Fe-BTC-150-5 | 0.778 | 114 |

## Section 2. SEM Images

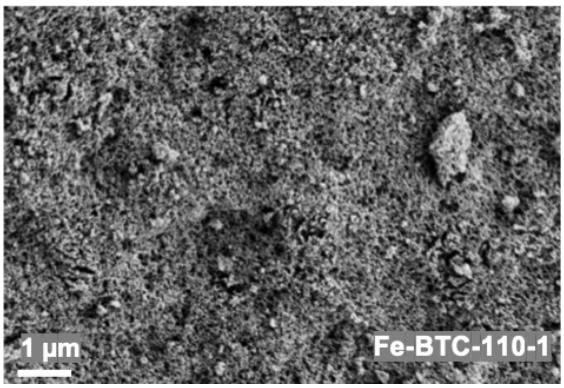


**Figure 1.** SEM image of Fe-BTC-110-1

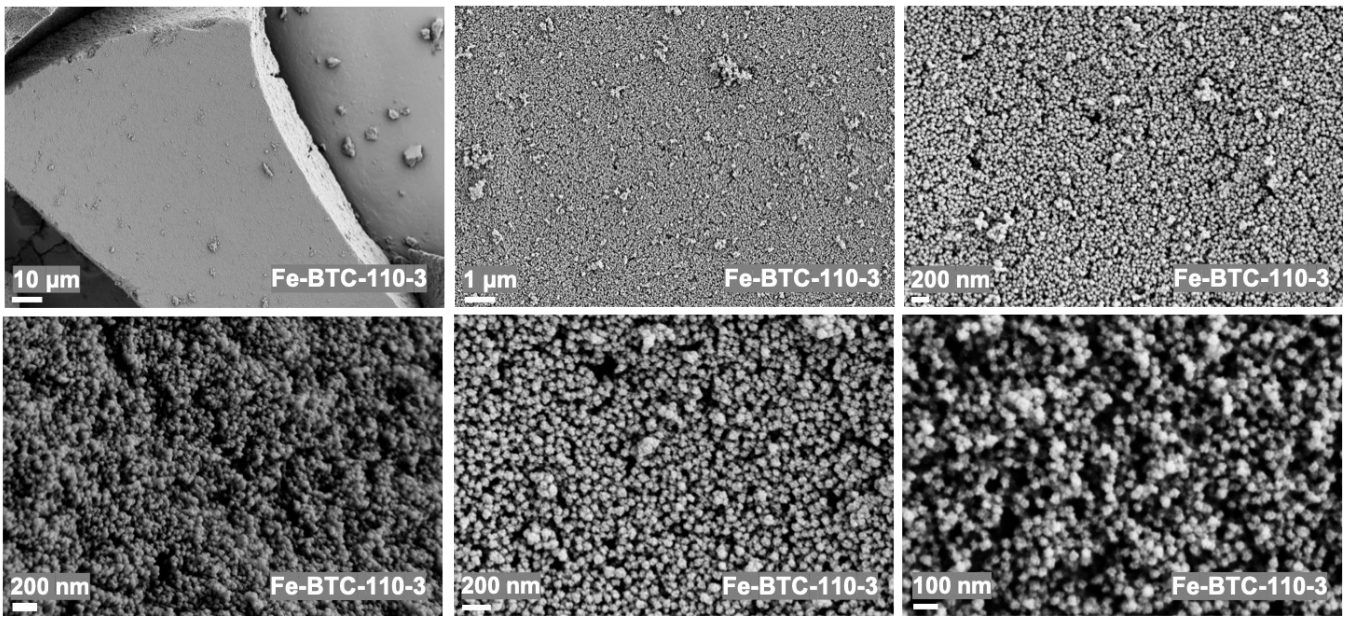


**Figure 2.** SEM images of Fe-BTC-110-3

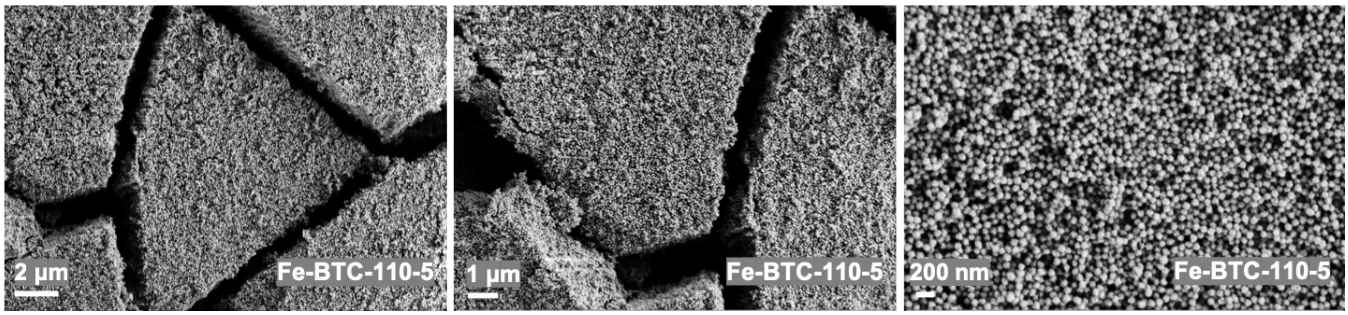


**Figure 3.** SEM images of Fe-BTC-110-5

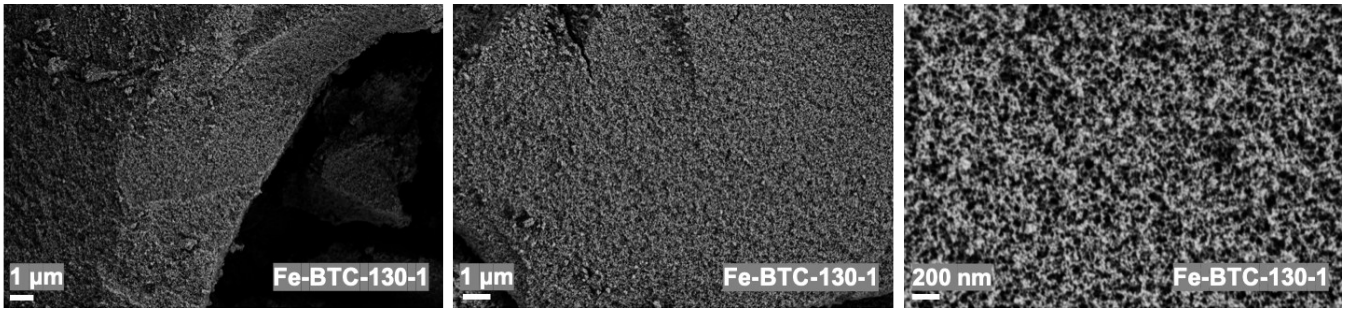


**Figure 4.** SEM images of Fe-BTC-130-1

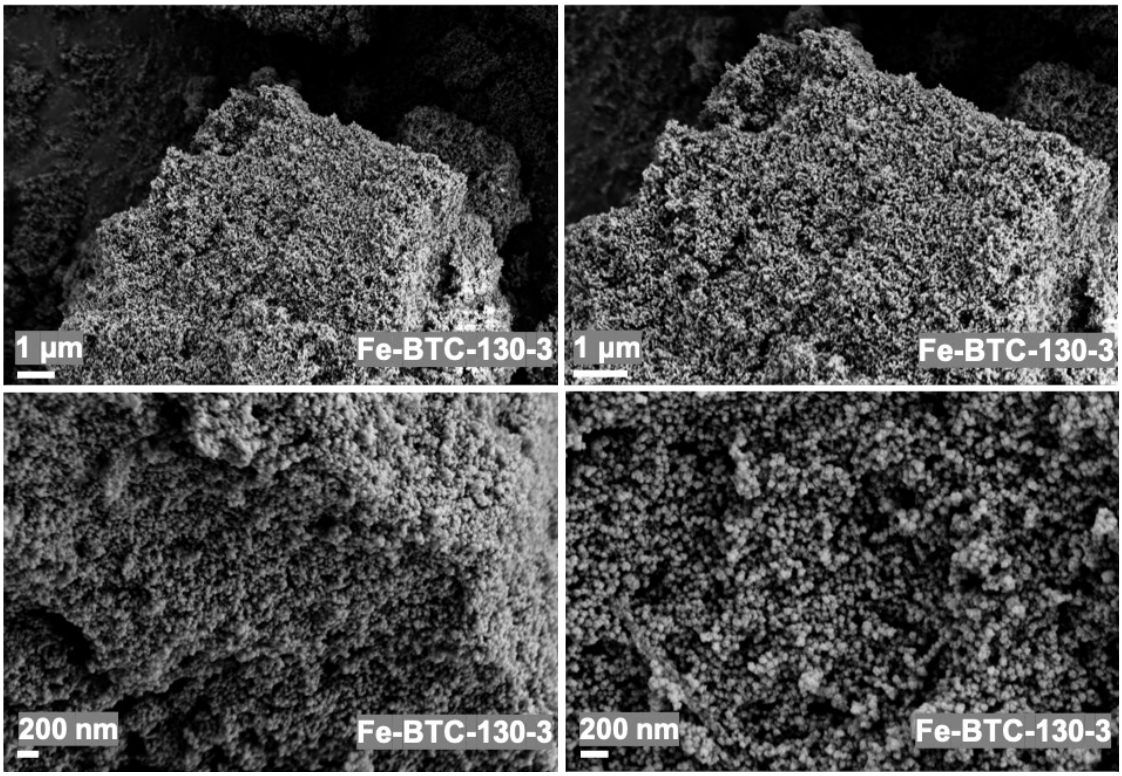


**Figure 5.** SEM images of Fe-BTC-130-3

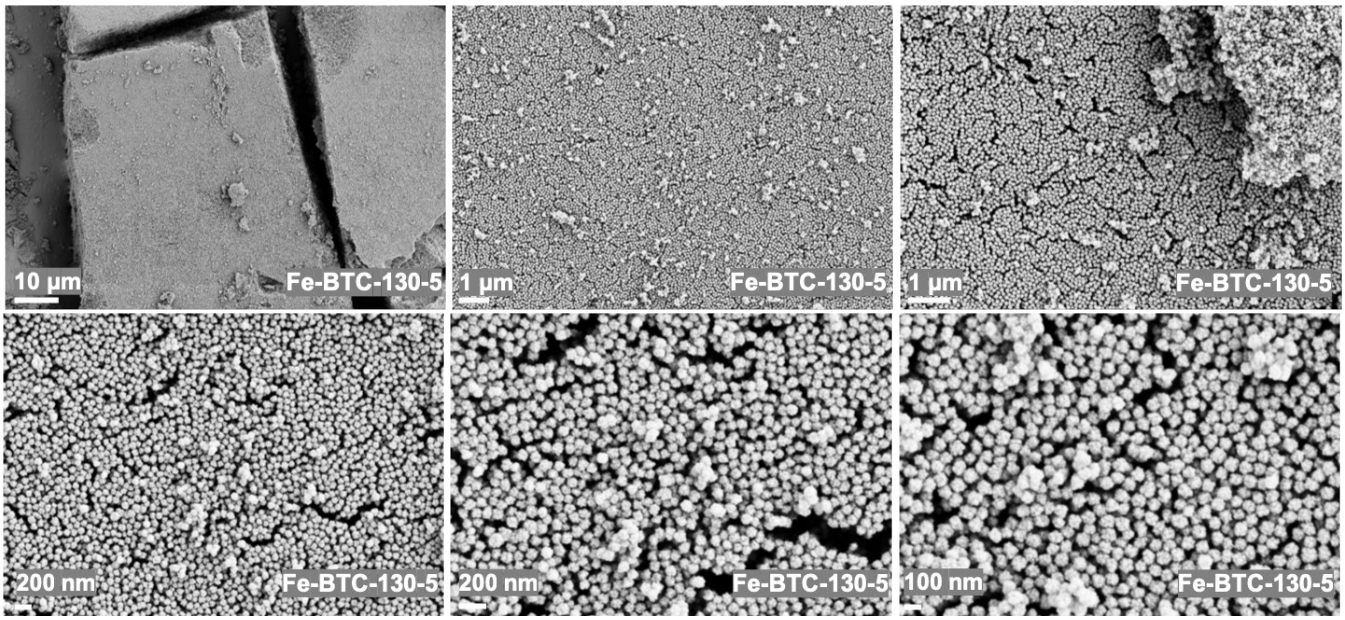


**Figure 6.** SEM images of Fe-BTC-130-5

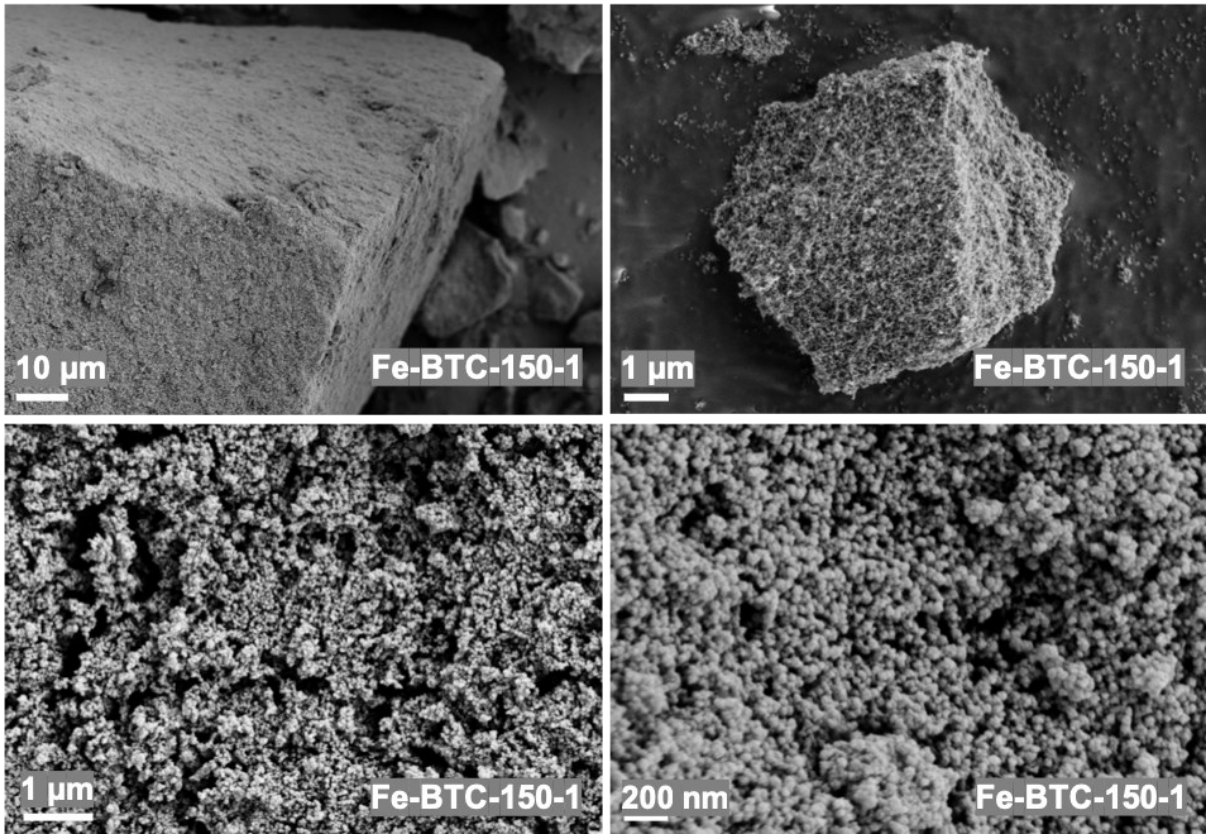


**Figure 7.** SEM images of Fe-BTC-150-1

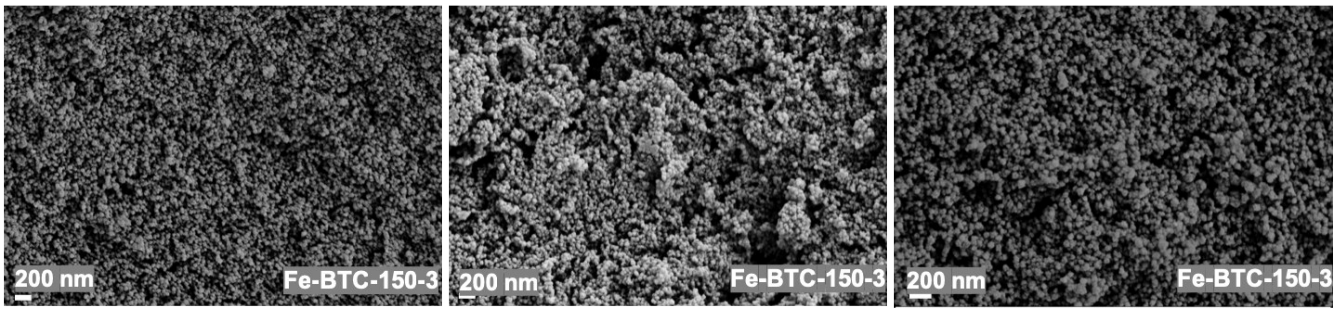


**Figure 8.** SEM images of Fe-BTC-150-3

## Section 3. $N_2$ sorption isotherms

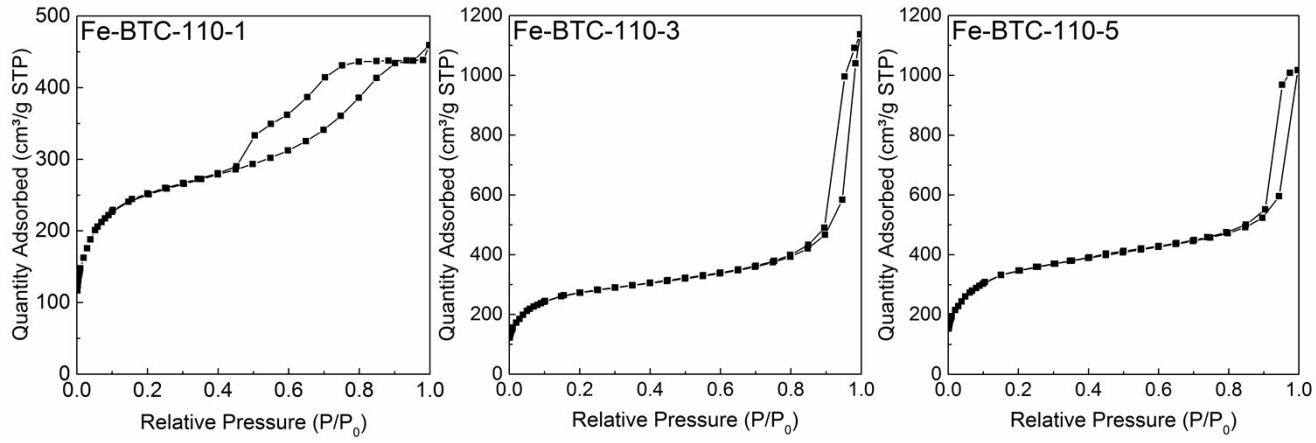


**Figure 9.** $N_2$ sorption isotherms of Fe-BTC-110-1, Fe-BTC-110-3, and Fe-BTC-110-5

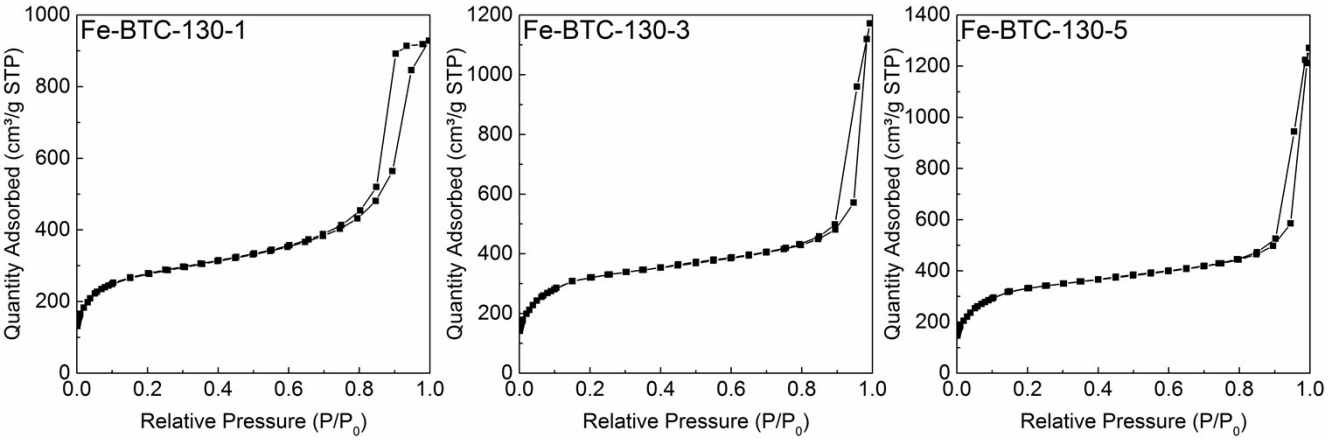


**Figure 10.** $N_2$ sorption isotherms of Fe-BTC-130-1, Fe-BTC-130-3, and Fe-BTC-130-5

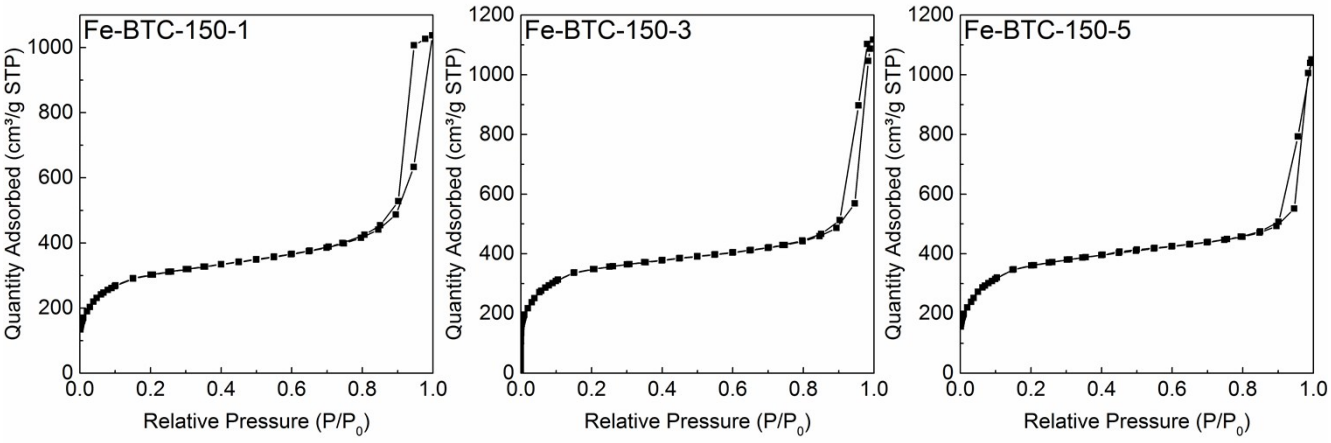


**Figure 11.** $N_2$ sorption isotherms of Fe-BTC-150-1, Fe-BTC-150-3, and Fe-BTC-150-5

## Section 4. NLDFT plots

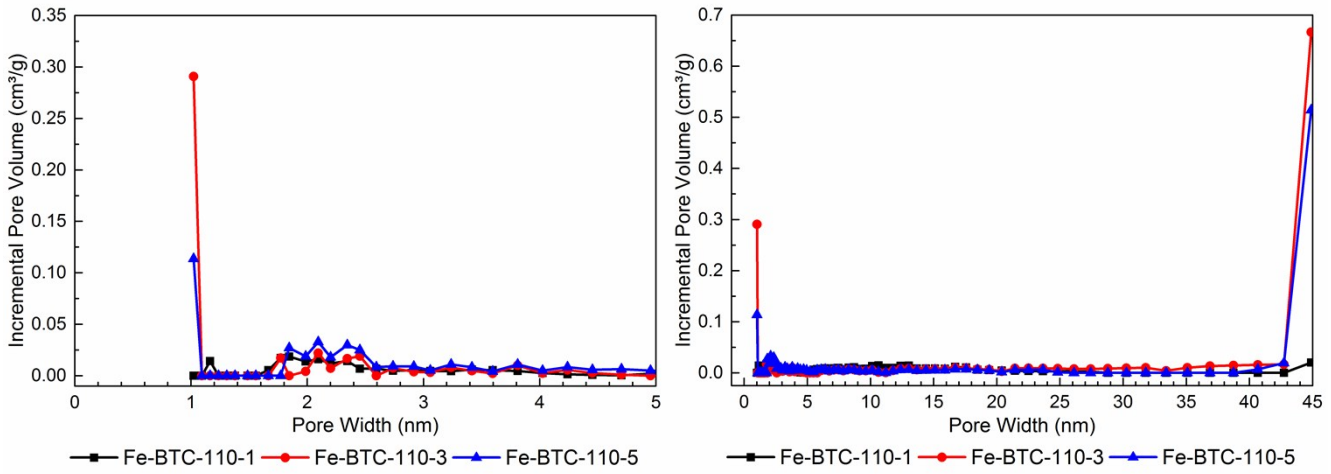


**Figure 12.** NLDFT plot of Fe-BTC-110-1, Fe-BTC-110-3, and Fe-BTC-110-5

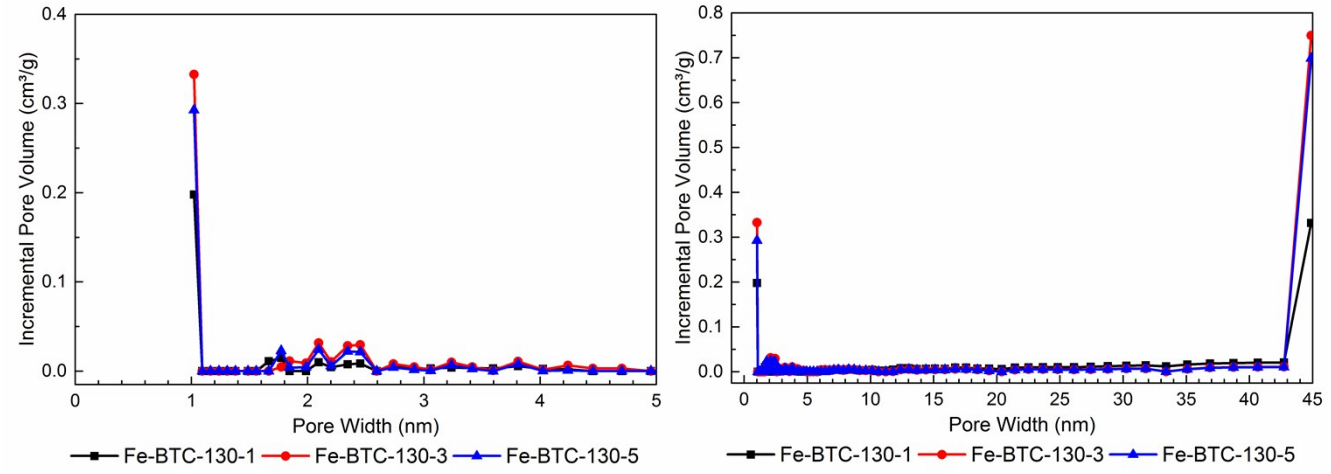


**Figure 13.** NLDFT plot of Fe-BTC-130-1, Fe-BTC-130-3, and Fe-BTC-130-5

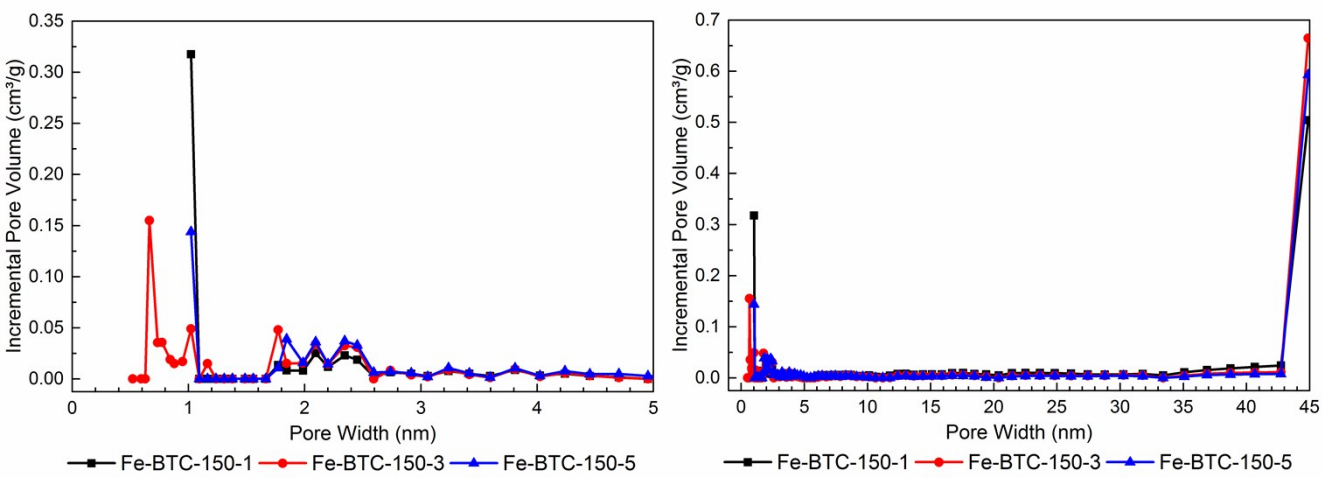


**Figure 14.** NLDFT plot of Fe-BTC-150-1, Fe-BTC-150-3, and Fe-BTC-150-5

## Section 5. TGA Results

**Table 2.** % mass loss during TGA analysis of Fe-BTC synthesized at 110 °C.

| Temperature Range (°C) | Fe:BTC 1 (%) | Temperature Range (°C) | Fe:BTC 3 (%) | Temperature Range (°C) | Fe:BTC 5 (%) |
|---|---|---|---|---|---|
| 25-189 | -10.0 | 25-178 | -16.8 | 25-195 | -18.7 |
| 189-342 | -11.5 | 178-373 | -12.4 | 195-371 | -10.1 |
| 342-423 | -7.8 | 373-577 | -24.9 | 371-599 | -26.5 |
| 423-570 | -24.9 | 577-781 | -12.2 | 599-829 | -11.3 |
| 570-717 | -11.1 | | | | |

**Table 3.** % mass loss during TGA analysis of Fe-BTC synthesized at 130 °C.

| Temperature Range (°C) | Fe-BTC 1 (%) | Temperature Range (°C) | Fe:BTC 3 (%) | Temperature Range (°C) | Fe:BTC 5 (%) |
|---|---|---|---|---|---|
| 25-182 | -7.2 | 25-191 | -7.6 | 25-177 | -26.4 |
| 182-347 | -12.2 | 191-359 | -11.2 | 177-325 | -6.1 |
| 347-564 | -32.3 | 359-554 | -30.3 | 325-415 | -8.6 |
| 564-781 | -12.0 | 554-623 | -2.2 | 415-518 | -18.0 |
| | | 623-752 | -11.3 | 518-694 | -12.7 |

**Table 4.** % mass loss during TGA analysis of Fe-BTC synthesized at 150 °C.

| Temperature Range (°C) | Fe:BTC 1 (%) | Temperature Range (°C) | Fe:BTC 3 (%) | Temperature Range (°C) | Fe:BTC 5 (%) |
|---|---|---|---|---|---|
| 25-179 | -8.3 | 25-168 | -7.4 | 25-178 | -8.2 |
| 179-334 | -9.2 | 168-342 | -11.4 | 178-374 | -11.7 |
| 334-556 | -34.5 | 342-547 | -30.6 | 374-570 | -24.4 |
| 556-776 | -13.0 | 547-754 | -13.2 | 570-766 | -17.0 |

**Table 5.** Percent residual mass at the end of TGA.

| Residual Mass (%) | 110 °C | 130 °C | 150 °C |
|---|---|---|---|
| **Fe:BTC 1** | 34.7 | 36.3 | 35 |
| **Fe:BTC 3** | 33.7 | 37.4 | 37.4 |
| **Fe:BTC 5** | 33.6 | 28.2 | 38.7 |

## Section 6. $CO_2$ sorption isotherms

### Langmuir Model:

$$\frac{C_e}{q_e} = \frac{1}{KQ^0} + \frac{C_e}{Q^0}$$

### Freundlich Model:

$$logq_e = logK_F + \frac{1}{n} logC_e$$

**Table 6.** Respective equations obtained from models

| MOF[a] | Langmuir Model | Freundlich Model |
|---|---|---|
| Fe-BTC-110-1 | *y = 0.1686x+669.57* <br> *$R^2$ = 0.9791* | *y = 0.639x-1.8419* <br> *$R^2$ = 0.9969* |
| Fe-BTC-110-3 | *y = 0.0821x+796.06* <br> *$R^2$ = 0.9944* | *y = 0.7741x-2.2584* <br> *$R^2$ = 0.9952* |
| Fe-BTC-110-5 | *y = 0.0828x+719.25* | *y = 0.7741x-2.2584* |

| | | |
|---|---|---|
| | *$R^2$ = 0.9876* | *$R^2$ = 0.9952* |

**Table 7.** Langmuir and Freundlich isotherm parameters

| MOF | Langmuir | Freundlich |
|---|---|---|
| Fe-BTC-110-1 | $Q_m$= 5.93 mg/g<br>$K_a$= 2.5E-04 $mg^{-1}$<br>$R^2$= 0.9791 | $K_F$=1.44E-02 mg/g<br>$\eta_F$= 1.56<br>$R^2$= 0.9969 |
| Fe-BTC-110-3 | $Q_m$= 12.2 mg/g<br>$K_a$= 1.03E-04 $mg^{-1}$<br>$R^2$= 0.9944 | $K_F$= 5.5E-03 mg/g<br>$\eta_F$= 1.29<br>$R^2$= 0.9952 |
| Fe-BTC-110-5 | $Q_m$= 12.1 mg/g<br>$K_a$= 1.25E-04 $mg^{-1}$<br>$R^2$= 0.9622 | $K_F$= 5.52E-03 mg/g<br>$\eta_F$= 1.29<br>$R^2$=0.9952 |

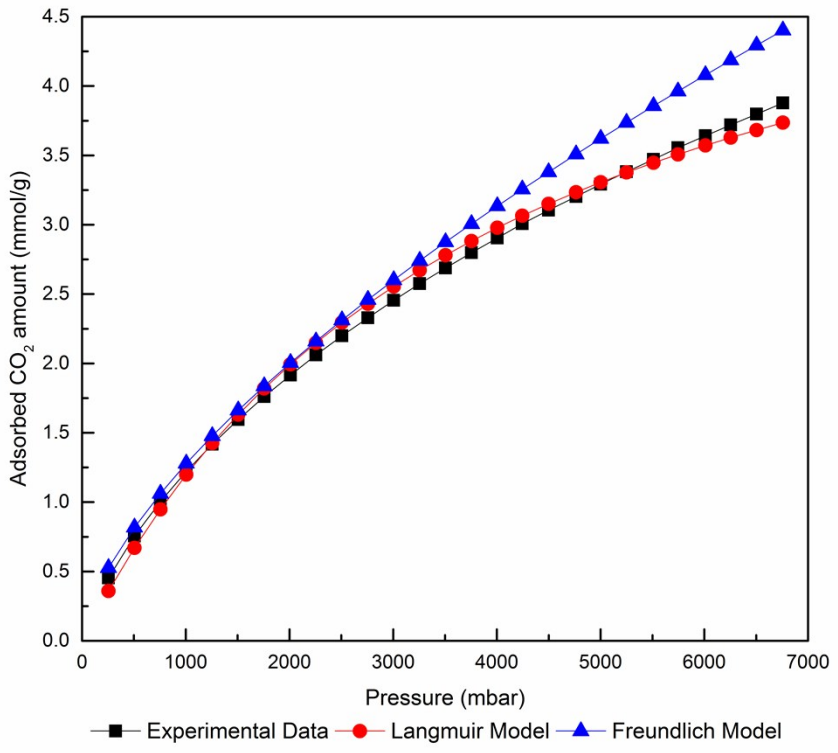


**Figure 15.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-110-1

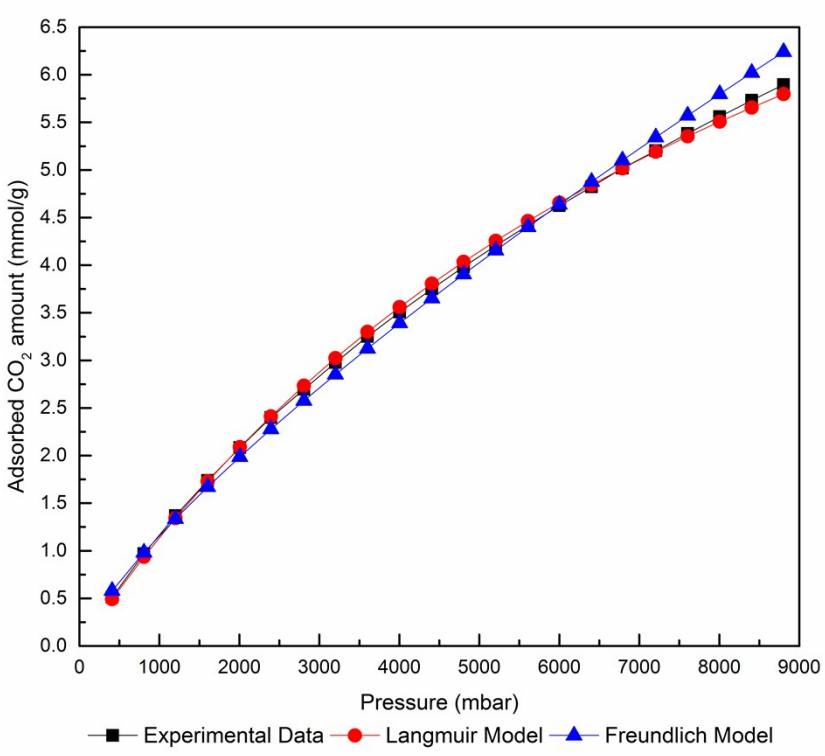


**Figure 16.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-110-3

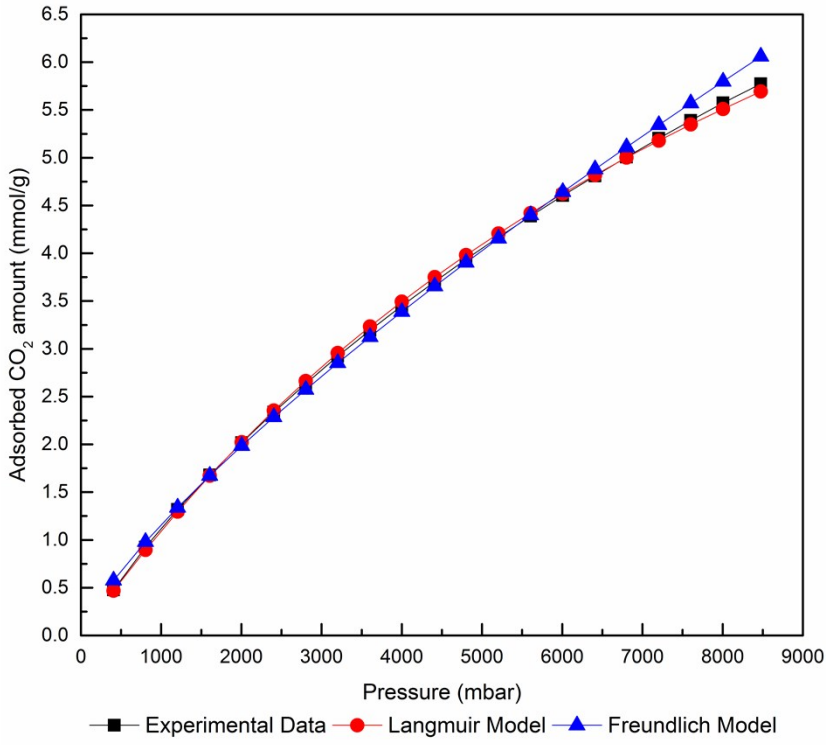


**Figure 17.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-110-5

**Table 8.** Respective equations obtained from models

| MOF[a] | Langmuir Model | Freundlich Model |
|---|---|---|
| Fe-BTC-130-1 | *y = 0.1153x+946.06*<br>*$R^2$ = 0.9921* | *y = 0.7736x-2.35*<br>*$R^2$ = 0.9931* |
| Fe-BTC-130-3 | *y = 0.1107x+656.9*<br>*$R^2$ = 0.9704* | *y = 0.7458x-2.1252*<br>*$R^2$ = 0.9995* |
| Fe-BTC-130-5 | *y = 0.0806x+855.78*<br>*$R^2$ = 0.9967* | *y = 0.8119x-2.4075*<br>*$R^2$ = 0.9951* |

**Table 9.** Langmuir and Freundlich isotherm parameters

| MOF | Langmuir | Freundlich |
|---|---|---|
| Fe-BTC-130-1 | $Q_m$= 8.67 mg/g<br>$K_a$= 1.2E-04 $mg^{-1}$<br>$R^2$= 0.9921 | $K_F$=4.45E-03 mg/g<br>$\eta_F$= 1.29<br>$R^2$= 0.9931 |
| Fe-BTC-130-3 | $Q_m$= 9.03 mg/g<br>$K_a$= 1.69E-04 $mg^{-1}$<br>$R^2$= 0.9704 | $K_F$= 7.5E-03 mg/g<br>$\eta_F$= 1.34<br>$R^2$= 0.9995 |
| Fe-BTC-130-5 | $Q_m$= 12.4 mg/g<br>$K_a$= 9.42E-05 $mg^{-1}$<br>$R^2$= 0.9967 | $K_F$= 3.91E-03 mg/g<br>$\eta_F$= 1.23<br>$R^2$=0.9951 |

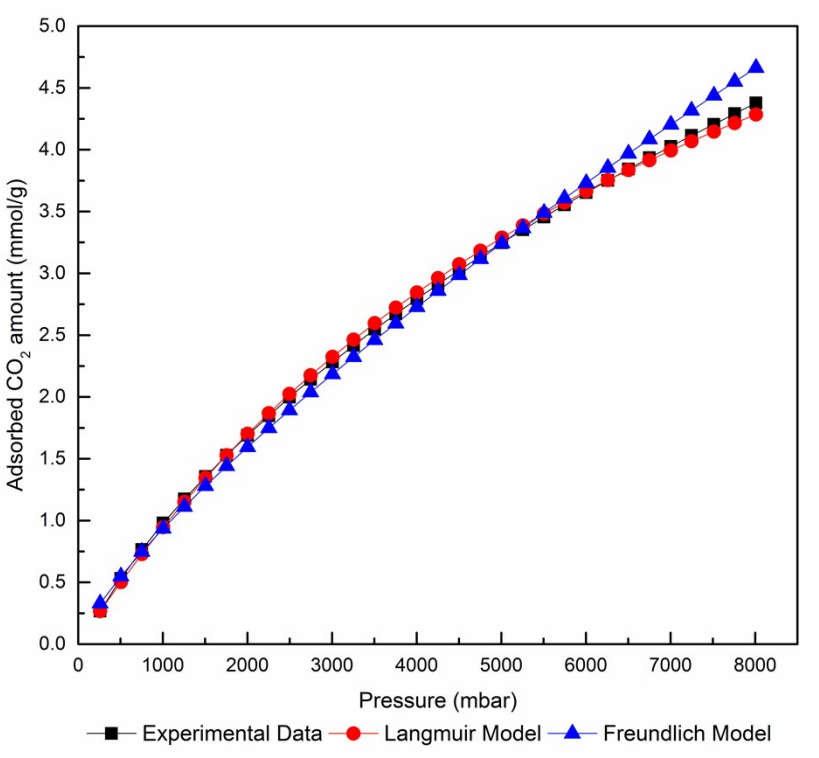


**Figure 18.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-130-1

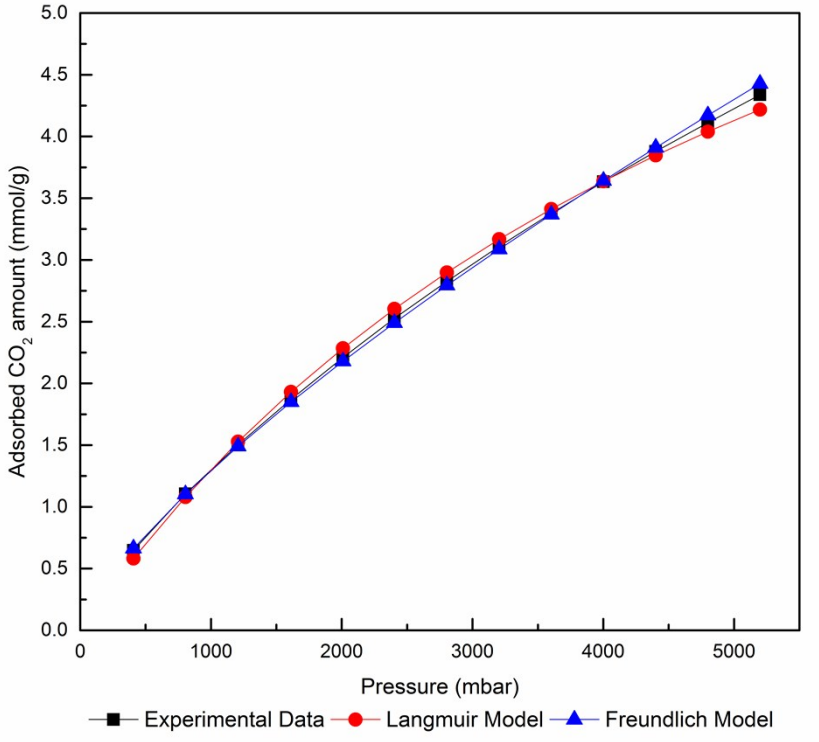


**Figure 19.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-130-3

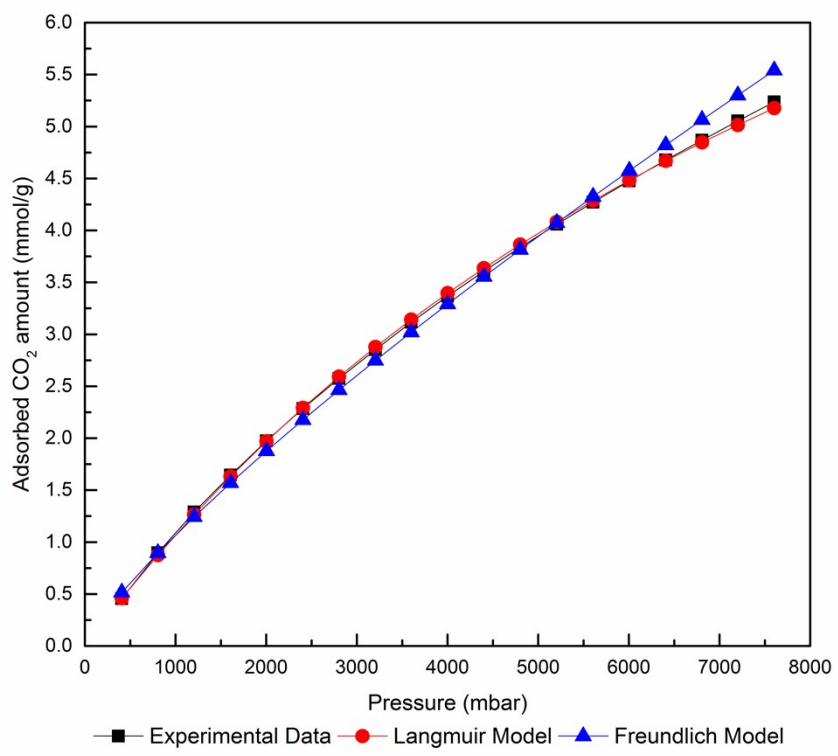


**Figure 20.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-130-5

**Table 10.** Respective equations obtained from models

| MOF[a] | Langmuir Model | Freundlich Model |
|---|---|---|
| Fe-BTC-150-1 | *y = 0.0846x+785.5*<br>*$R^2$ = 0.9931* | *y = 0.7708x-2.24*<br>*$R^2$ = 0.9965* |
| Fe-BTC-150-3 | *y = 0.0683x+797.35*<br>*$R^2$ = 0.9974* | *y = 0.8044x-2.3425*<br>*$R^2$ = 0.996* |
| Fe-BTC-150-5 | *y = 0.09x+972.86*<br>*$R^2$ = 0.982* | *y = 0.781x-2.3546*<br>*$R^2$ = 0.9984* |

**Table 11.** Langmuir and Freundlich isotherm parameters

| MOF | Langmuir | Freundlich |
|---|---|---|
| Fe-BTC-150-1 | $Q_m$= 11.82 mg/g<br>$K_a$= 1.08E-04 $mg^{-1}$<br>$R^2$= 0.9931 | $K_F$= 5.7E-03<br>$\eta_F$= 1.29<br>$R^2$= 0.9965 |
| Fe-BTC-150-3 | $Q_m$= 14.64 mg/g<br>$K_a$= 8.57E-05 $mg^{-1}$<br>$R^2$= 0.9974 | $K_F$= 4.5E-03<br>$\eta_F$= 1.24<br>$R^2$= 0.996 |

| | | |
|---|---|---|
| Fe-BTC-150-5 | $Q_m$= 11.1 mg/g<br>$K_a$= 9.25E-05 $mg^{-1}$<br>$R^2$= 0.982 | $K_F$= 4.42E-03<br>$\eta_F$= 1.28<br>$R^2$=0.9984 |

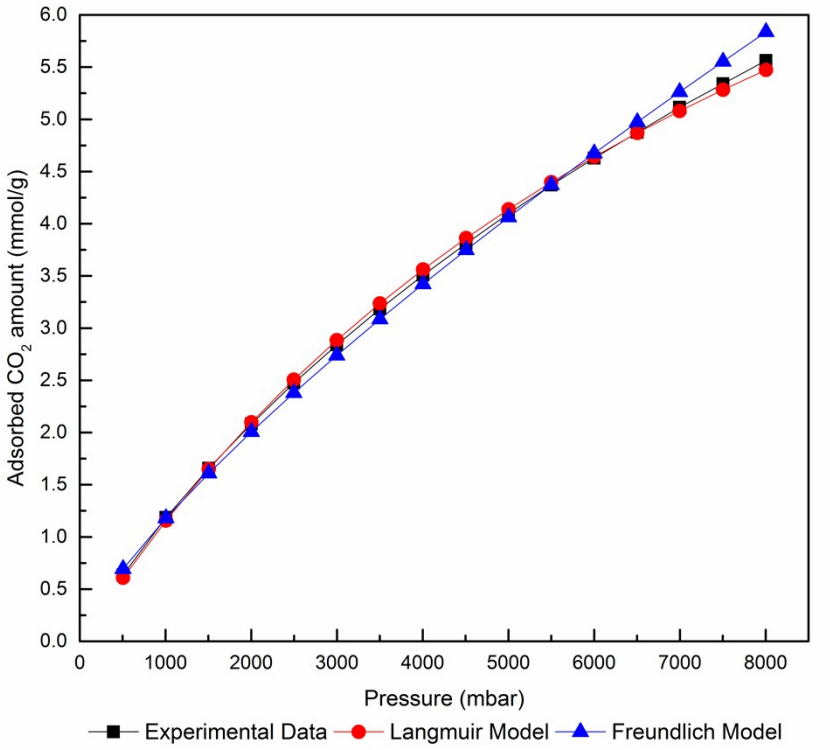


**Figure 21. Co**mparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-150-1

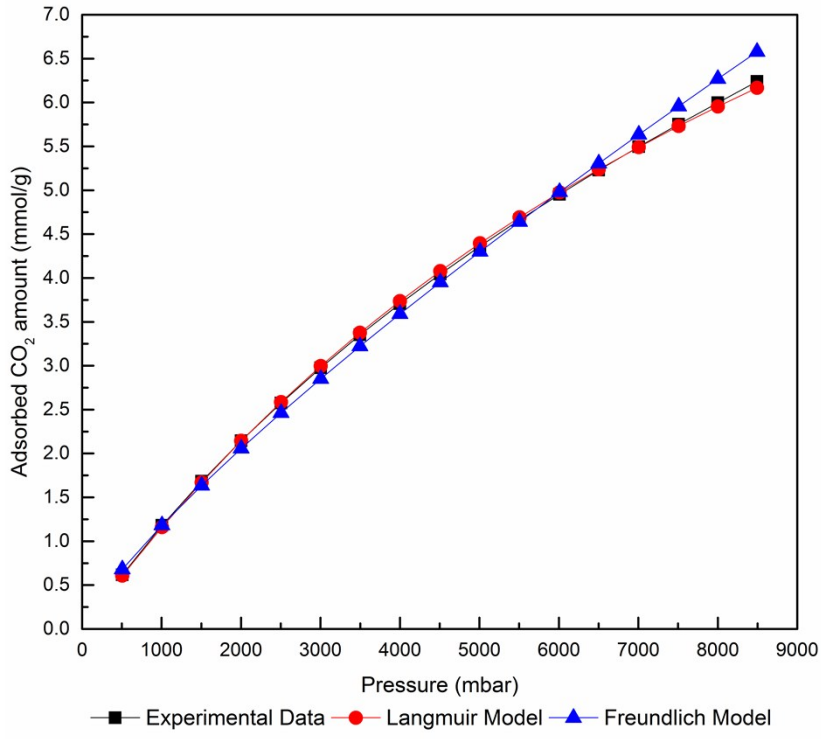


**Figure 22.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-150-3

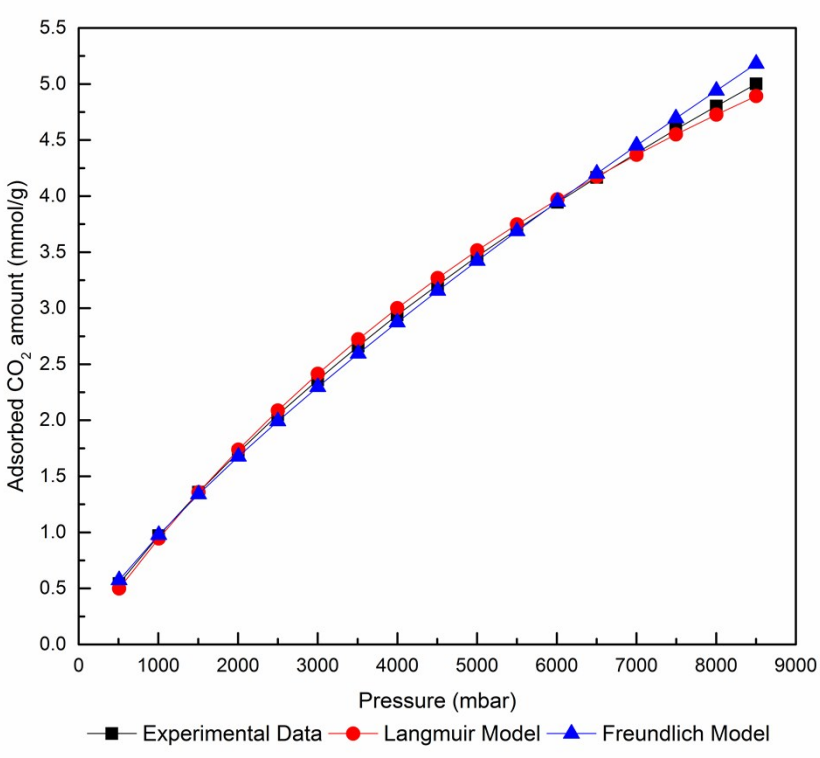


**Figure 23.** Comparison of experimental data and nonlinear fitting of Langmuir and Freundlich Model of Fe-BTC-150-5