**Towards Estimation of CO2 Adsorption on Highly Porous MOF-based Adsorbents Using Gaussian Process Regression Approach**

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**Table S1**. The details of the experimental data and the properties of the MOFs used in current study.

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | MOF | Vp (cm3/g) (Refs.) | Pressure range (bar) | Temperature range (K) | S (m2/g) | CO2 uptake (mmole/g) | No. Data | Refs. |
| 1 | MOF-2 | 0.227 1 | 0-42.2 | 298-298 | 345 | 0-3.2 | 39 | 2 |
| 2 | MOF-74 | 0.4 3 | 0-42.4 | 298-298 | 816 | 0-10.4 | 31 | 2 |
| 3 | MOF-505 | 1.83 4 | 0-42.5 | 298-298 | 1547 | 0-10.4 | 31 | 2 |
| 4 | Cu3(BTC)2 | 0.43 5 | 0-42.4 | 298-298 | 1781 | 0-10.7 | 30 | 2 |
| 5 | IRMOF-11 | 0.92 6 | 0-42.4 | 298-298 | 2096 | 0-14.8 | 32 | 2 |
| 6 | IRMOF-3 | 1.07 7 | 0-42.2 | 298-298 | 2160 | 0-18.9 | 37 | 2 |
| 7 | IRMOF-6 | 1.14 7 | 0-42.5 | 298-298 | 2516 | 0-19.7 | 37 | 2 |
| 8 | IRMOF-1 | 0.18 8 | 0-42.2 | 298-298 | 2833 | 0-22.0 | 35 | 2 |
| 9 | MOF-177 | 1.59 9 | 0-42.5 | 298-313 | 4508 | 0-33.9 | 69 | 2,9 |
| 10 | CuBTTri | 0.713 9 | 0.5460-39.866 | 313-313 | 1750 | 1.16-16.99 | 43 | 9 |
| 11 | MG2(dobdc) | 0.573 9 | 0.0005-35.317 | 313-313 | 1800 | 0.09-15.15 | 51 | 9 |
| 12 | CoBDP | 0.93 9 | 1.3102-38.288 | 313-313 | 2030 | 0.28-16.56 | 31 | 9 |
| 13 | BeBTB | 1.701 9 | 1.9600-38.834 | 313-313 | 4030 | 1.79-30.17 | 40 | 9 |

**Table S2.** The statistical parameters of previous correlations 10

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | PSO-ANFIS | DE-ANFIS | RBF | LSSVM |
| R2 | 0.958 | 0.930 | 0.997 | 0.997 |
| MSE | 2.571 | 4.362 | 0.204 | 0.167 |
| STD | 23.16 | 13.78 | 4.211 | 6.988 |

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