Table 1: Calculated surface areas (m2/g) for the 13 MOFs with GCMC isotherms. Cases where a software does not find a surface area are denoted by N/A. Zeo++ calculations are conducted with the same CIF files used to generate GCMC isotherms, and a 1.67 Å radius probe N2 molecule, the high accuracy flag, and 2,000 Monte Carlo samples per atom are used. All other software take as input the GCMC isotherms.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | SESAMI 1 (BET) | SESAMI 1 (BET+ESW) | SESAMI 2 (LASSO) | BETSI | pyGAPS | BEaTmap | Zeo++ |
| HKUST-1 | 2001 | 1933 | 2089 | 1962 | 1902 | 1980 | 2397 |
| IRMOF-1 | 3502 | 3543 | 3123 | 3519 | 3504 | N/A | 3722 |
| MIL-100 (Cr) | 2107 | 1853 | 2111 | 1799 | 1852 | 2094 | 1957 |
| MIL-100 (Fe) | 2386 | 2438 | 2203 | 2426 | 82 | 2423 | 1933 |
| MIL-101 | 3828 | 2862 | 2944 | 2879 | 2939 | 3331 | 3164 |
| MIL-53 (Al) | 1221 | 1168 | 1405 | 1164 | 1183 | 1212 | 1510 |
| MOF-74 (Mg) | 1828 | 1834 | 1902 | 1815 | 1839 | 1791 | 1796 |
| MOF-808 | 44 | N/A | 1275 | 1172 | N/A | 1147 | 1690 |
| NU-1000 | 2439 | 2181 | 2633 | 2082 | 2144 | 2672 | 3050 |
| NU-1200 | 2711 | 934 | 2601 | 1077 | 1073 | 2930 | 3192 |
| NU-1500 (Fe) | 3543 | 3594 | 3111 | 3756 | 3758 | 3492 | 3944 |
| UiO-66 | 1239 | 1239 | 1443 | 1201 | 1242 | 1304 | 1289 |
| ZIF-8 | 1429 | 1386 | 1575 | 1381 | 1390 | 1414 | 1588 |

Table 2: Comparison between calculated surface areas from software for isotherm to surface area calculation and from Zeo++, over the 13 MOFs with GCMC isotherms. The mean absolute percent error and Pearson correlation coefficient are taken with respect to Zeo++ calculations for each software, over all successful surface area calculations for that software.

|  |  |  |  |
| --- | --- | --- | --- |
| Surface area calculation software | Mean absolute percent error (MAPE) | Pearson correlation coefficient | Successful calculations (out of 13) |
| SESAMI 1 (BET) | 19.4 | 0.85 | 13 |
| SESAMI 1 (BET+ESW) | 17.9 | 0.72 | 12 |
| SESAMI 2 (LASSO) | 12.4 | 0.95 | 13 |
| BETSI | 18.7 | 0.77 | 13 |
| pyGAPS | 23.0 | 0.75 | 12 |
| BEaTmap | 12.6 | 0.93 | 12 |

Table 3: Calculated surface areas (m2/g) for the 9 MOFs with experimental isotherms. All software take as input the experimental isotherms.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | SESAMI 1 (BET) | SESAMI 1 (BET+ESW) | SESAMI 2 (LASSO) | BETSI | pyGAPS | BEaTmap |
| HKUST-1 | 1505 | 1466 | 1668 | 1500 | 1495 | 1498 |
| MOF-74 (Mg) | 1580 | 1467 | 1692 | 1575 | 1574 | 1565 |
| MOF-808 | 1998 | 900 | 1727 | 1021 | 2439 | 1752 |
| NU-1000 | 2154 | 2090 | 2385 | 2229 | 2654 | 2459 |
| NU-1200 | 2893 | 2718 | 2781 | 2758 | 3917 | 3069 |
| NU-1500 (Fe) | 3305 | 3409 | 2809 | 3328 | 3413 | 3227 |
| SIFSIX-3 (Ni) | 356 | 201 | 716 | 355 | 355 | 353 |
| UiO-66 | 1251 | 1228 | 1413 | 1250 | 1249 | 1246 |
| ZIF-8 | 1092 | 910 | 1214 | 1082 | 1082 | 1047 |