

**Table S1.** Flexible MOFs for gas adsorption and separation applications

| MOF                                                                                                                                            | Stimulus mode               | Gas storage/separation                                                     | Ref |
|------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|----------------------------------------------------------------------------|-----|
| MIL-53(Cr)                                                                                                                                     | pressure                    | CO <sub>2</sub> adsorption                                                 | 1   |
| [Zn <sub>2</sub> (TBIB) <sub>2</sub> (HTCPB) <sub>2</sub> ] $\cdot$ 9DMF $\cdot$ 19H <sub>2</sub> O                                            | temperature                 | CO <sub>2</sub> adsorption                                                 | 2   |
| MIL-53(Al)                                                                                                                                     | pressure, temperature       | D <sub>2</sub> /H <sub>2</sub> separation                                  | 3   |
| SHF-61                                                                                                                                         | guest molecule              | CO <sub>2</sub> /CH <sub>4</sub> separation                                | 4   |
| Cu(dhbc) <sub>2</sub> (4,4'-bipy)                                                                                                              | guest molecule              | C <sub>1</sub> /C <sub>2</sub> /C <sub>3</sub> -propyne separation         | 5   |
| LIFM-28                                                                                                                                        | guest molecule              | CO <sub>2</sub> /N <sub>2</sub> separation                                 | 6   |
| [Zn <sub>3</sub> (btca) <sub>2</sub> (OH) <sub>2</sub> ] $\cdot$ (guest) <sub>n</sub>                                                          | guest molecule              | CO <sub>2</sub> adsorption                                                 | 7   |
| Cu <sub>4</sub> (m <sub>4</sub> -O)(m <sub>2</sub> -OH) <sub>2</sub> (Me <sub>2</sub> trz-pba) <sub>4</sub>                                    | guest molecule,<br>pressure | C <sub>4</sub> -hydrocarbons adsorption                                    | 8   |
| NOTT-202a                                                                                                                                      | guest molecule              | CO <sub>2</sub> adsorption                                                 | 9   |
| MIL-53(Al)-NH <sub>2</sub>                                                                                                                     | guest molecule              | CH <sub>4</sub> adsorption                                                 | 10  |
| TIFSIX-14-Cu-I                                                                                                                                 | pressure                    | C <sub>3</sub> H <sub>6</sub> /C <sub>3</sub> H <sub>8</sub> separation    | 11  |
| ELM-12                                                                                                                                         | pressure                    | C <sub>2</sub> H <sub>2</sub> /C <sub>2</sub> H <sub>4</sub> separation    | 12  |
| MIL-53(Al)                                                                                                                                     | pressure, temperature       | CH <sub>4</sub> adsorption                                                 | 13  |
| Zn <sub>2</sub> (Atz) <sub>2</sub> Ox                                                                                                          | guest molecule              | C <sub>2</sub> H <sub>2</sub> /C <sub>2</sub> H <sub>4</sub> separation    | 14  |
| NJU-Bai8                                                                                                                                       | molecule                    | C <sub>3</sub> H <sub>6</sub> /C <sub>3</sub> H <sub>8</sub> separation    | 15  |
| Mn(in <sub>a</sub> ) <sub>2</sub>                                                                                                              | temperature                 | Xe/Kr separation                                                           | 16  |
| Cu <sub>4</sub> (m <sub>4</sub> -O)(m <sub>2</sub> -OH) <sub>2</sub> (Me <sub>2</sub> trzpb <sub>a</sub> ) <sub>4</sub>                        | temperature                 | C <sub>2</sub> /C <sub>3</sub> /C <sub>4</sub> -hydrocarbons<br>separation | 17  |
| NKU-FlexMOF-1                                                                                                                                  | temperature                 | C <sub>3</sub> H <sub>6</sub> /C <sub>3</sub> H <sub>8</sub> separation    | 18  |
| Co(bdp)                                                                                                                                        | guest molecule              | CO <sub>2</sub> /CH <sub>4</sub> separation                                | 19  |
| [Zn <sub>2</sub> (C <sub>20</sub> H <sub>12</sub> O <sub>4</sub> ) <sub>2</sub> (C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> )] <sub>n</sub> | guest molecule              | N <sub>2</sub> /CH <sub>4</sub> separation                                 | 20  |

**Reference :**

1. T. Devic, F. Salles, S. Bourrelly, B. Moulin, G. Maurin, P. Horcajada, C. Serre, A. Vimont, J.-C. Lavalley, H. Leclerc, G. Clet, M. Daturi, P. L. Llewellyn, Y. Filinchuk and G. Férey, *J. Mater. Chem. A*, 2012, **22**, 10266.
2. R. A. Agarwal, A. K. Gupta and D. De, *Cryst. Growth Des.*, 2019, **19**, 2010–2018.
3. J. Y. Kim, L. Zhang, R. Balderas-Xicohtencatl, J. Park, M. Hirscher, H. R. Moon and H. Oh, *J. Am. Chem. Soc.*, 2017, **139**, 17743–17746.
4. E. J. Carrington, C. A. McAnally, A. J. Fletcher, S. P. Thompson, M. Warren and L. Brammer, *Nat. Chem.*, 2017, **9**, 882–889.
5. L. Li, R. Krishna, Y. Wang, J. Yang, X. Wang and J. Li, *J. Mater. Chem. A*, 2016, **4**, 751–755.
6. C. X. Chen, Z. Wei, J. J. Jiang, Y. Z. Fan, S. P. Zheng, C. C. Cao, Y. H. Li, D. Fenske and C. Y. Su, *Angew. Chem.*, 2016, **55**, 9932–9936.
7. Y. Yue, J. A. Rabone, H. Liu, S. M. Mahurin, M.-R. Li, H. Wang, Z. Lu, B. Chen, J. Wang, Y. Fang and S. Dai, *J. Phys. Chem. C* 2015, **119**, 9442–9449.
8. M. Lange, M. Kobalz, J. Bergmann, D. Lässig, J. Lincke, J. Möllmer, A. Möller, J. Hofmann, H. Krautscheid, R. Staudt and R. Gläser, *J. Mater. Chem. A*, 2014, **2**, 8075–8085.
9. S. Yang, X. Lin, W. Lewis, M. Suyetin, E. Bichoutskaia, J. E. Parker, C. C. Tang, D. R. Allan, P. J. Rizkallah, P. Hubberstey, N. R. Champness, K. M. Thomas, A. J. Blake and M. Schroder, *Nat. Mater.*, 2012, **11**, 710–716.

10. T. Kundu, M. Wahiduzzaman, B. B. Shah, G. Maurin and D. Zhao, *Angew. Chem. Int. Ed.*, 2019, **58**, 8073–8077.
11. L. Yang, X. Cui, Y. Zhang, Q. Yang and H. Xing, *J. Mater. Chem. A*, 2018, **6**, 24452–24458.
12. L. Li, R.-B. Lin, R. Krishna, X. Wang, B. Li, H. Wu, J. Li, W. Zhou and B. Chen, *J. Mater. Chem. A*, 2017, **5**, 18984–18988.
13. T. Kundu, B. B. Shah, L. Bolinois and D. Zhao, *Chem. Mater.*, 2019, **31**, 2842–2847.
14. P.-D. Zhang, X.-Q. Wu, T. He, L.-H. Xie and J.-R. Li, *Chem. Commun.*, 2020, **56**, 5520–5523.
15. X. Wang, R. Krishna, L. Li, B. Wang, T. He, Y.-Z. Zhang, J.-R. Li and J. Li, *Chem. Eng. J.*, 2018, **346**, 489–496.
16. H. Wang, M. Warren, J. Jagiello, S. Jensen, S. K. Ghose, K. Tan, L. Yu, T. J. Emge, T. Thonhauser and J. Li, *J. Am. Chem. Soc.*, 2020, **142**, 20088–20097.
17. T. Hähnel, G. Kalies, R. Krishna, J. Möllmer, J. Hofmann, M. Kobalz and H. Krautscheid, *Microporous Mesoporous Mater.*, 2016, **224**, 392–399.
18. M.-H. Yu, B. Space, D. M. Franz, W. Zhou, C. He, L. Li, R. Krishna, Z. Chang, W. Li, T.-L. Hu and X.-H. Bu, *J. Am. Chem. Soc.*, 2019, **141**, 17703–17712.
19. M. K. Taylor, T. Runcevski, J. Oktawiec, J. E. Bachman, R. L. Siegelman, H. Jiang, J. A. Mason, J. D. Tarver and J. R. Long, *J. Am. Chem. Soc.*, 2018, **140**, 10324–10331.
20. E. R. Engel, A. Jouaiti, C. X. Bezuidenhout, M. W. Hosseini and L. J. Barbour, *Angew. Chem. Int. Ed.*, 2017, **56**, 8874–8878.