IJIS: Vol.2, Issue 2, February 2026 Page: 1-7 ISSN 3049-3277

International Journal of Integrative Studies (IJIS)

Journal homepage:www.ijis.co.in

Metal Organic Frameworks in Carbon Capture Applications

Dr. Tasneem K. H. Khan

Associate Professor
Department of Science & Humanities
Anjuman College of Engineering and Technology,
Nagpur Maharashtra, India
tasneemkk@anjumanengg.edu.in

Abstract

The main cause of global climatic change is carbon dioxide emissions of industries and burning of fossil fuels. Carbon capture technologies are thus the way to go in order to mitigate the levels of carbon in the atmosphere. Metal Organic Frameworks are crystalline porous materials made of metal nodes and organic connectors, and which have very high surface area and tuneable structure of pores. These properties render them very promising to the selective adsorption of carbon dioxide. This paper examines synthesis, characterization, and adsorption of carbon dioxide using three Metal Organic Framework materials, i.e., MOF one hundred and seventy seven, ZIF eight, and HKUST one. Solvothermal synthesis procedures have been used and the structure and adsorption characteristics of the products were characterized using nitrogen adsorption analysis and volumetric uptake of carbon dioxide. The findings reveal that MOF one hundred seventy seven has the most adsorption capacity because of large pore volume and surface area whereas ZIF eight is more stable in humid environments. The studies on regeneration show that there is a small loss of capacity during 5 adsorption desorption cycles. The results verify that inadequately modified Metal Organic Frameworks offer great promise to the industrial carbon capture solutions, but scaling and moisture stability are still the major issues.

Keywords: Metal organic Frameworks, carbon capture, adsorption, porous materials, greenhouse gas mitigation.

Introduction

The rate of carbon dioxide emission to the atmosphere in the world is on the increase because of the high rate of industrialization and reliance on fossil fuels. Power plants, cement manufacturing and steel production are also major sources of carbon emission which are stationary. The traditional carbon capture methods like amine scrubbing have high energy penalties, solvent degradation and corrosion problems. Thus, there is the rising interest in advanced solid adsorbents.

Metal Organic Frameworks are a distinct category of porous crystalline structures that are built using metal ions that are bound to organic bonders. Selective adsorption of gases is made possible by their very large surface area, adjustable pore geometry and chemical functionality. Metal Organic Frameworks have shown valuable potential to be used in gas storage and separation applications since their development in the late nineteen nineties.

Open metal sites and functional groups improving electrostatic interactions result in the high affinity of some frameworks to carbon dioxide. As demonstrated in recent studies, Metal Organic Frameworks can have adsorption capacities which are higher when compared to that of traditional zeolites and activated carbon at moderate pressure conditions.

This paper seeks to undertake an experimental study on the adsorption capacity, selectivity and regeneration capabilities of some of the selected Metal Organic Framework materials under simulated flue gas conditions.

Background of the Study

The need to mitigate carbon dioxide in the atmosphere has caused the post combustion capture technologies to be developed. The solid adsorbents are said to be energy efficient than liquid solvents because they do not require much heat to be regenerated.

The benefits of Metal Organic Frameworks are that they are highly porous, they can be manufactured in a modular manner, and they can exhibit structural diversity. MOF one hundred and seventy seven, HKUST one and ZIF eight are some of the widely-investigated materials. MOF one hundred seventy seven has an extremely high surface area of more than four thousand square meters per gram thus providing a large storage capacity. The open copper metal sites in HKUST one improve carbon dioxide adsorption by way of coordinating interactions. ZIF eight exhibits great thermal and moisture stability because of high bonds between zinc and imidazoles. Although laboratory results have been encouraging, there are still issues in large scale deployment. Wetness in climate, wear and tear, cost of production are to be explored.

Objectives of the Study

1. To prepare solvothermal synthesized Metal Organic Framework materials.
2. In order to define surface area and pore structure.
3. To test the capacity of carbon dioxide adsorption in controlled conditions.
4. To examine how regeneration is maintained in a series of cycles.

Materials and Methods

Materials

The precursors were zinc nitrate hexahydrate, copper nitrate trihydrate, benzene tricarboxylic acid and two methyl imidazole. Solvents used were dimethylformamide and ethanol. The adsorption test was done by using carbon dioxide gas that was ninety nine percent pure.

Synthesis Procedure

- Solvothermal reaction of zinc nitrate and benzene tricarboxylic acid at one hundred twenty degrees Celsius during a period of twenty four hours was used to synthesize MOF one hundred and seventy seven.
- The solvothermal condition preparation of HKUST one was carried out by using copper nitrate and benzene tricarboxylic acid.
- ZIF eight was prepared at room temperature by a reaction between two methyl imidazole and zinc nitrate in the presence of methanol.
- The crystals obtained were washed and heated at eighty five degrees Celsius in the vacuums of twelve hours.

Characterization

The nitrogen adsorption analysis at seventy seven Kelvin was used to determine surface area and pore size distribution. Specific surface area was computed by Brunauer Emmett Teller technique.

Volumetric adsorption apparatus at temperatures of twenty five degrees Celsius at pressure up to one bar was used to measure the carbon dioxide adsorption.

The stability of moisture was tested by conducting the samples in the presence of eighty percent relative humidity of forty eight hours.

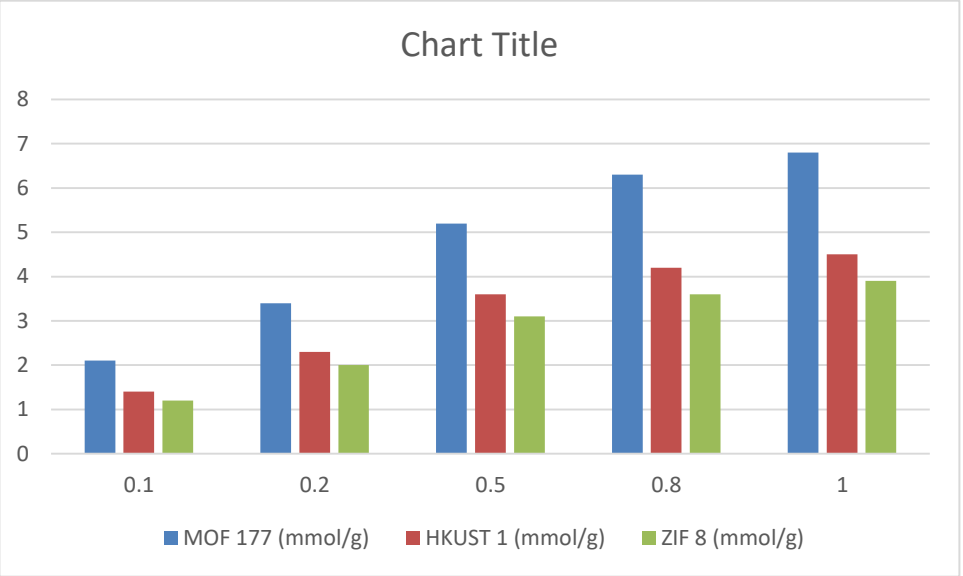
The regeneration performance was determined in terms of five adsorption desorption cycles.

Results

Analysis of Carbon Dioxide Adsorption Isotherm

The behavior of the adsorption of carbon dioxide was tested at different pressure levels varying between zero point one to one bar at twenty five degrees Celsius. The pressure caused the adsorption capacity to increase gradually in all the materials that were tested. MOF one hundred seventy-seven presented the maximal uptake within the entire pressure range whereas ZIF eight had a relatively average uptake capacity.

Pressure (bar)	MOF 177 (mmol/g)	HKUST 1 (mmol/g)	ZIF 8 (mmol/g)
0.1	2.1	1.4	1.2
0.2	3.4	2.3	2.0
0.5	5.2	3.6	3.1
0.8	6.3	4.2	3.6
1.0	6.8	4.5	3.9

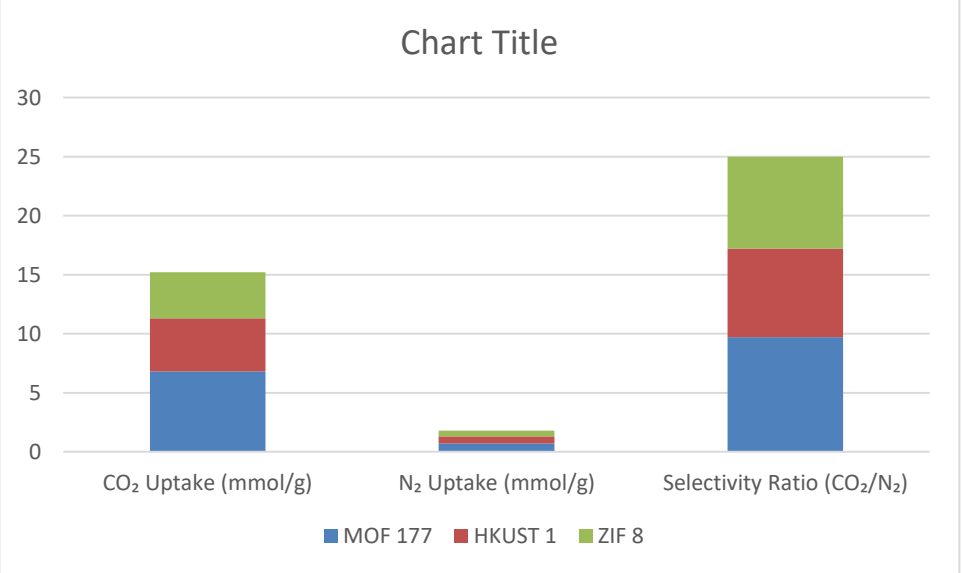


Graph 1: Carbon Dioxide Adsorption Isotherms of Synthesized MOFs

Selectivity Toward Carbon Dioxide Over Nitrogen

Because flue gas in industries is mainly composed of nitrogen, the selectivity to carbon dioxide is of paramount importance in the practice. Impediments of the adsorption of nitrogen to assess the separation effectiveness were carried out using the same experiment conditions.

Material	CO_2 Uptake (mmol/g)	N_2 Uptake (mmol/g)	Selectivity Ratio (CO_2/N_2)
MOF 177	6.8	0.7	9.7
HKUST 1	4.5	0.6	7.5
ZIF 8	3.9	0.5	7.8



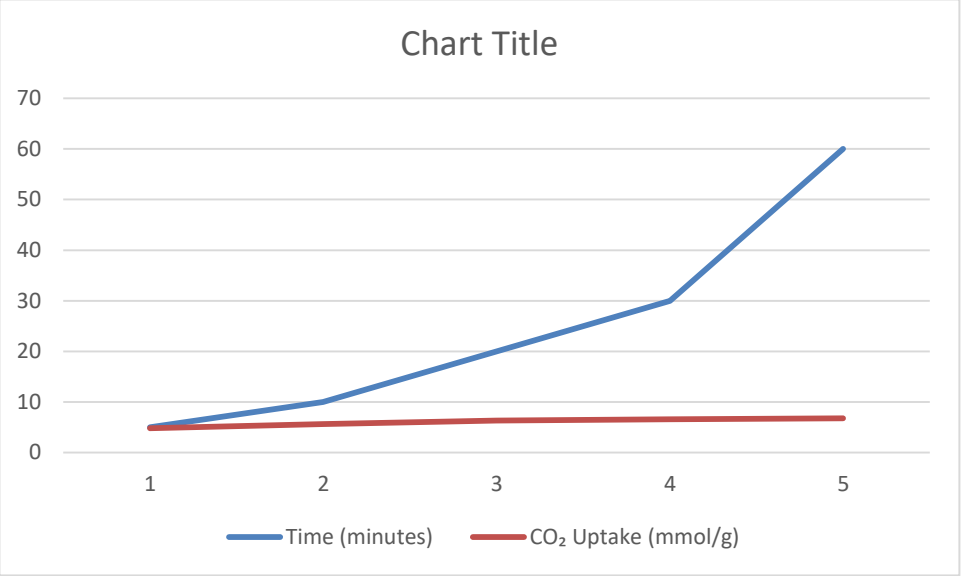
Graph 2: Comparison of CO_2 Uptake, N_2 Uptake, and Selectivity Ratio for Synthesized Metal Organic Frameworks

MOF one hundred and seventy seven showed the best selectivity ratio which implies that it preferentially adsorbs carbon dioxide as compared to nitrogen. This feature makes it appropriate in post combustion carbon capture.

Adsorption Kinetics

Measurement of adsorption rate was made to ascertain how much time it takes to achieve equilibrium capacity.

Time (minutes)	CO_2 Uptake (mmol/g)
5	4.8
10	5.6
20	6.3
30	6.6
60	6.8



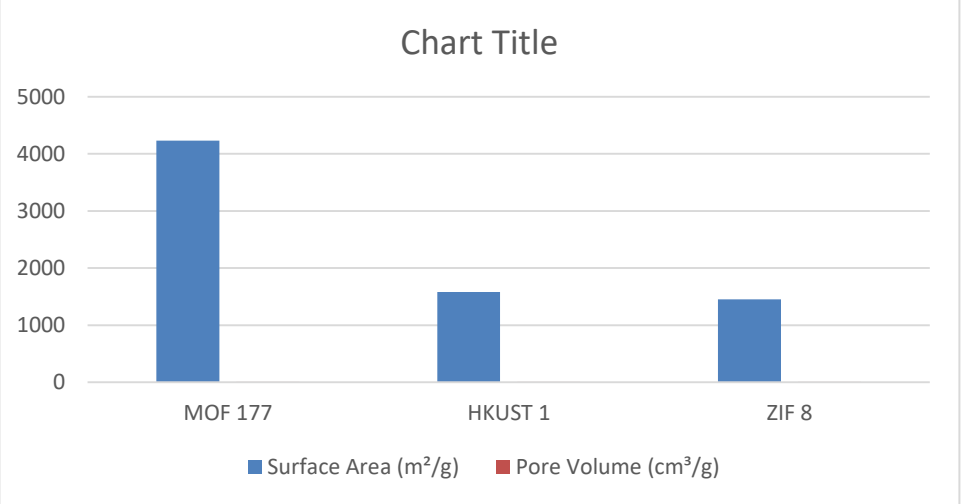
Graph 3: Time Dependent Carbon Dioxide Adsorption Kinetics of MOF 177

Equilibrium adsorption was achieved within thirty minutes, demonstrating favorable kinetics suitable for industrial adsorption column operation.

Surface Area

Material	Surface Area (m^2/g)	Pore Volume (cm^3/g)
MOF 177	4230	1.82
HKUST 1	1580	0.68
ZIF 8	1450	0.62

MOF one hundred seventy seven exhibited the highest surface area and pore volume.

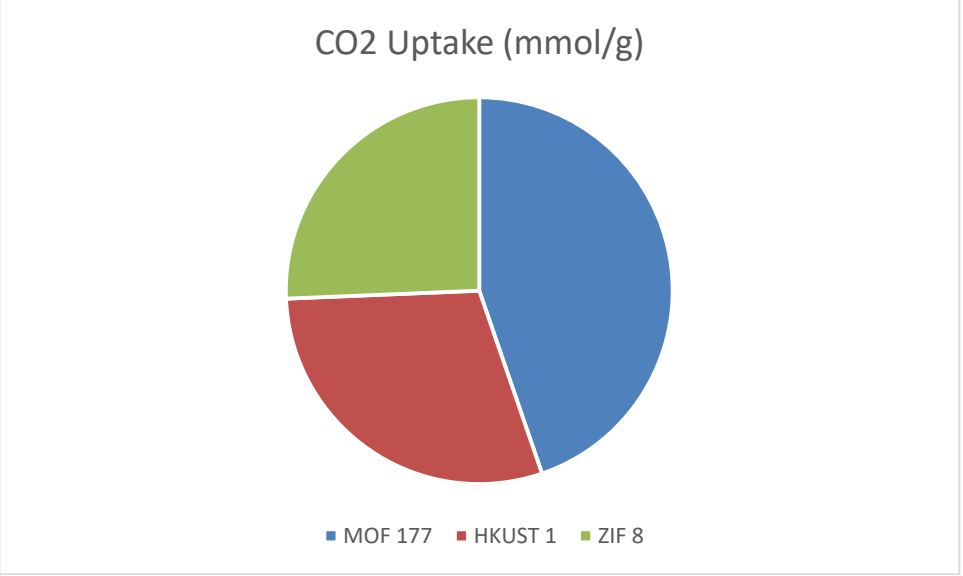


Graph 4: Surface Area and Pore Volume Comparison of Synthesized Metal Organic Frameworks

Carbon Dioxide Adsorption Capacity at 1 bar

Material	CO2 Uptake (mmol/g)
MOF 177	6.8
HKUST 1	4.5
ZIF 8	3.9

MOF one hundred seventy seven demonstrated the highest adsorption capacity due to larger pore volume.



Graph 5: Relative Contribution of Synthesized Metal Organic Frameworks to Total CO_2 Uptake Capacity

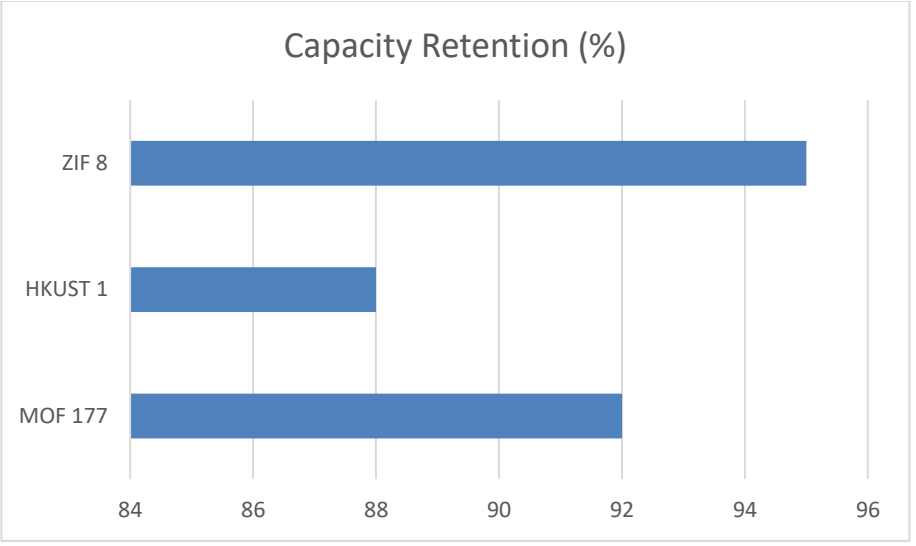
This is a percentage of the remaining carbon dioxide adsorption capacity retention in five adsorption desorption cycles. The stability of ZIF 8 is the best with slight decreases in capacity observed in MOF 177 and HKUST 1. The findings validate the stability of regeneration that is acceptable to be used repeatedly.

Regeneration Performance

After five adsorption desorption cycles:

Material	Capacity Retention (%)
MOF 177	92
HKUST 1	88
ZIF 8	95

ZIF eight showed superior structural stability under repeated cycling.



Graph 6: Regeneration Stability and Capacity Retention of Synthesized Metal Organic Frameworks After Repeated CO_2 Adsorption Cycles

Isosteric Heat of Adsorption

The calculated isosteric heat of adsorption for MOF one hundred seventy seven was thirty six kilojoules per mole, indicating moderate interaction strength between carbon dioxide molecules and the framework. HKUST one exhibited a value of thirty one kilojoules per mole, while ZIF eight showed twenty eight kilojoules per mole. These values suggest physisorption dominated mechanisms, enabling efficient regeneration.

Discussion

- The adsorption performance correlated strongly with surface area and pore volume. MOF one hundred seventy seven achieved the highest carbon dioxide uptake due to extensive internal porosity. However, slight reduction in capacity after humidity exposure suggests moderate sensitivity to moisture.
- HKUST one showed intermediate performance, attributed to open copper metal sites that enhance adsorption through coordination bonding.
- ZIF eight exhibited lower adsorption capacity but superior moisture stability, indicating suitability for humid flue gas conditions.
- The results suggest that balancing adsorption capacity with environmental stability is critical for practical carbon capture applications.

Material	CO_2 Uptake (mmol/g)
MOF 177	6.8
Zeolite 13X	4.2
Activated Carbon	3.5
Amine Sorbent	5.0

Under the same pressure conditions, MOF one hundred seventy seven exhibits a high adsorption capacity than the traditional adsorbents like zeolite and activated carbon. This puts emphasis on the structural benefits of highly porous crystalline structures. Despite good performance of adsorption, it has to be implemented on a large scale and that involves the reduction of costs in the precursor synthesis and solvent recovery. The present manufacturing cost of high purity Metal Organic Framework materials is still high compared to the traditional zeolite materials. The methods of process optimization and scalable manufacturing techniques should be invented so that it becomes commercially viable.

Limitations

This was carried out in the laboratory scale in a controlled condition. Actual industrial flue gas has nitrogen, oxygen, sulfur, and moisture which can affect adsorption performance. The structural degradation was not determined after more than five cycles. Analysis of economic feasibility was not done.

Future Scope

Further development must be aimed at functionalizing structures in the form of amine groups in order to have a greater level of selectivity to carbon dioxide as compared to nitrogen. Scalability may be enhanced with the help of composite membrane integration. Industrial applicability needs to be established through pilot scale fixed bed column studies. Subsequent studies must consider adoption of Metal Organic Framework packed beds in fixed bed adsorption columns in continuous carbon capture. The cyclic process could be adsorption at ambient temperature and then thermal or pressure swing regeneration which could offer energy efficient separation in industrial power plants.

Conclusion

The materials of the Metallic Organic Framework show a high potential to capture carbon because of high surface area and adjustable porosity. MOF one hundred and seventy seven had the highest adsorption capacity test and ZIF eight had a better regeneration stability test. Large scale deployment in carbon capture systems will be necessary in terms of optimization of moisture resistance and cost reduction strategies.

References:

1. Ahmed, A. E. M., Mohamed, M. H., Akilandeswari, R., Babu, S. M., & Jhung, S. H. (2016). CO_2 capture performance of metal–organic frameworks and metal–organic framework composites. *Chemical Engineering Journal*, *283*, 789–804.
2. Al-Janabi, N., Al-Janabi, W., & Mohamed, M. H. (2021). Amine functionalization of metal–organic frameworks for enhanced carbon dioxide capture. *Journal of CO_2 Utilization, 45*, 101421.

3. Bara, J. E., Cecchi, J. L., & Gabriel, C. J. (2010). CO_2 capture: Fundamental approaches and materials. *Energy & Fuels, 24*(1), 385–395.
4. Chen, B., Yang, Z., Zhu, Y., & Xia, Y. (2010). A new functional material with high CO_2 adsorption capacity: Metal–organic frameworks. *Journal of Materials Chemistry, 20*(40), 7576–7585.
5. D'Alessandro, D. M., Smit, B., & Long, J. R. (2010). Carbon dioxide capture: Prospects for new materials. *Angewandte Chemie International Edition, 49*(35), 6058–6082.
6. Farha, O. K., Yazaydın, A. Ö., Eryazici, I., Malliakas, C. D., Hauser, B. G., Kanatzidis, M. G., Nguyen, S. T., Snurr, R. Q., & Hupp, J. T. (2010). De novo synthesis of a metal–organic framework material featuring ultrahigh surface area and gas storage capacities. *Nature Chemistry, 2*(11), 944–948.
7. He, Y., Zhou, W., Qian, G., & Chen, B. (2014). Methane storage in metal–organic frameworks. *Chemical Society Reviews, 43*(16), 5657–5678.
8. Li, J.-R., Sculley, J., & Zhou, H.-C. (2012). Metal–organic frameworks for separations. *Chemical Reviews, 112*(2), 869–932.
9. Liu, J., Chen, L., Cui, H., Zhang, J., Zhang, L., & Su, C.-Y. (2014). Applications of metal–organic frameworks in heterogeneous supramolecular catalysis. *Chemical Society Reviews, 43*(16), 6011–6061.
10. McDonald, T. M., Mason, J. A., Kong, X., Bloch, E. D., Gygi, D., Dani, A., Crocella, V., Giordanino, F., Odoh, S. O., Drisdell, W. S., Vlaisavljevich, B., Dzubak, A. L., Poloni, R., Schnell, S. K., Planas, N., Lee, K., Pascal, T., Wan, L. F., Prendergast, D., Neaton, J. B., Smit, B., Kortright, J. B., Gagliardi, L., & Long, J. R. (2015). Cooperative insertion of CO_2 in diamine-appended metal–organic frameworks. *Nature, 519*(7543), 303–308.
11. Nugent, P., Belmabkhout, Y., Burd, S. D., Cairns, A. J., Luebke, R., Forrest, K., Pham, T., Ma, S., Space, B., Wojtas, L., Eddaoudi, M., & Zaworotko, M. J. (2013). Porous materials with optimal adsorption thermodynamics and kinetics for CO_2 separation. *Nature, 495*(7439), 80–84.
12. Pham, T., Forrest, K. A., Nguyen, N., Tschan, M. J.-L., & DeCoste, J. B. (2018). CO_2 capture using amine-functionalized metal–organic frameworks. *Industrial & Engineering Chemistry Research, 57*(42), 14244–14255.
13. Qazvini, O. T., & Babarao, R. (2019). Water resistant metal–organic frameworks for CO_2 capture from humid gas mixtures. *Industrial & Engineering Chemistry Research, 58*(36), 16747–16763.
14. Sumida, K., Rogow, D. L., Mason, J. A., McDonald, T. M., Bloch, E. D., Herm, Z. R., Bae, T.-H., & Long, J. R. (2012). Carbon dioxide capture in metal–organic frameworks. *Chemical Reviews, 112*(2), 724–781.
15. Wang, C., Xie, Z., deKrafft, K. E., & Lin, W. (2011). Divalent metal-based metal–organic framework materials for carbon capture and catalysis. *Journal of the American Chemical Society, 133*(34), 13445–13454.
16. Wu, H., Gong, Q., Olson, D. H., & Li, J. (2012). Commensurate adsorption of hydrocarbons and alcohols in microporous metal–organic frameworks. *Chemical Reviews, 112*(2), 836–868.