

Efficient propylene/ethylene separation in highly porous metal-organic frameworks

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Table S1. Crystal data and structure refinements for Fe2M-L.

	Fe₂Mn-L	Fe₂Co-L	Fe₂Ni-L
empirical formula	Fe ₂ MnC ₇₈ H ₁₁₂ O ₂₈	Fe ₂ CoC ₇₈ H ₁₁₂ O ₂₈	Fe ₂ NiC ₇₈ H ₁₁₂ O ₂₈
<i>M</i>	1832.43	1836.42	1836.20
Temperature/K	100(2)	100(2)	100(2)
crystal system	Trigonal	Trigonal	Trigonal
space group	<i>R</i> -3c	<i>R</i> -3c	<i>R</i> -3c
<i>a</i> /Å	27.4975(2)	27.6077(3)	27.5618(2)
<i>c</i> /Å	73.1343(7)	72.6748(11)	72.9933(6)
<i>V</i> /Å ³	47889.2(8)	47970.6(13)	48020.7(8)
<i>Z</i>	18	18	18
<i>D</i> _{calc} /g cm ⁻³	1.144	1.144	1.143
<i>μ</i> /mm ⁻¹	3.694	3.943	2.940
reflns collected	54790	55582	58594
Independent reflns	9061	9081	10223
<i>R</i> _{int}	0.0620	0.0686	0.0349
<i>θ</i> range (°)	3.546 to 65.080	3.559 to 65.082	3.549 to 71.075
Completeness	99.7 %	99.8 %	99.8 %
GOF	1.025	1.017	1.019
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)] ^a	0.0639	0.0675	0.0592
<i>wR</i> ₂ (all data) ^b	0.1569	0.1615	0.1497
<i>Δρ</i> _{max/min} (e/Å ³)	0.685/-0.651	0.999/-0.701	0.903/-0.445

^a *R*₁ = $\sum ||F_o| - |F_c|| / \sum |F_o|$, ^b *wR*₂ = $[\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$.

Table S2. ICP-AES analysis results for the bulk samples of Fe2M-L.

Sample	Percentage of Fe ion	Percentage of M ion	Molar ratio of Fe to M
Fe₂Mn-L	66.5	33.5	1.99
Fe₂Co-L	66.8	33.2	2.01
Fe₂Ni-L	66.2	33.8	1.96

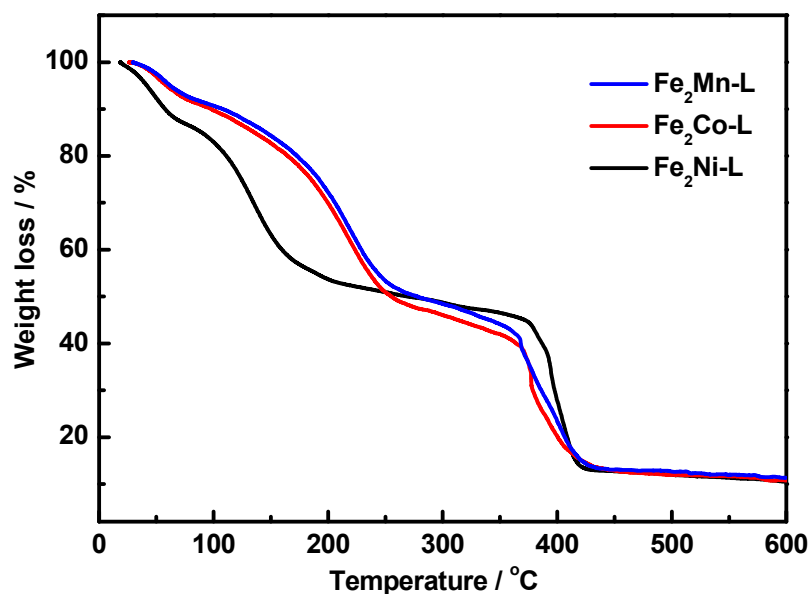


Figure S1. TGA curves of the as-synthesized Fe₂M-L samples, indicating the presence of about 12 DMF molecules per formula inside their pores.

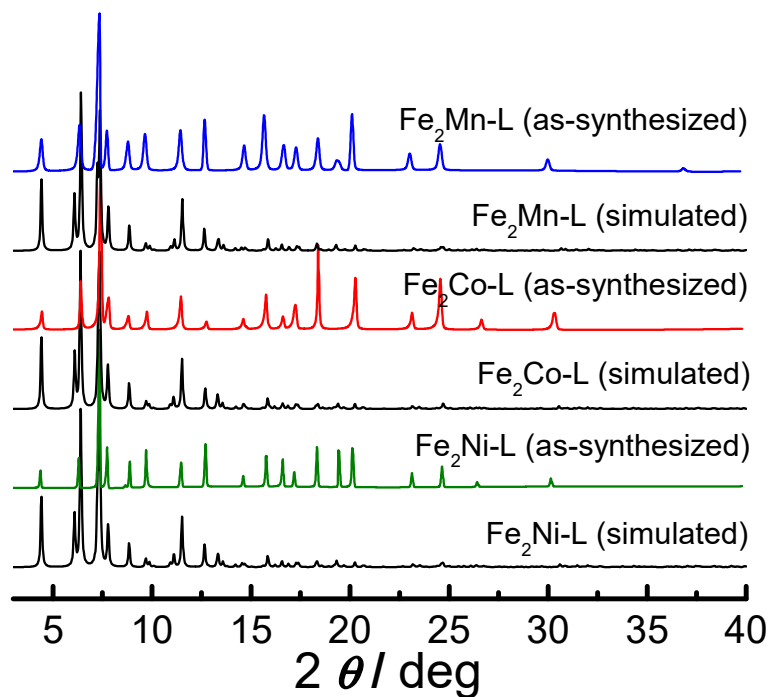


Figure S2. PXRD patterns of the as-synthesized Fe₂M-L samples in comparison with their simulated PXRD patterns.

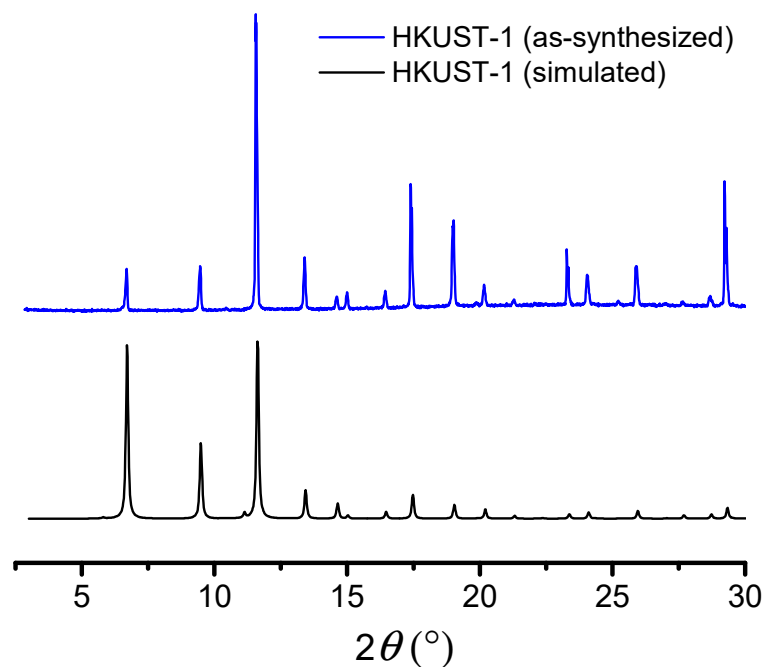


Figure S3. PXRD pattern of the as-synthesized HKUST-1 sample in comparison with its simulated PXRD pattern.

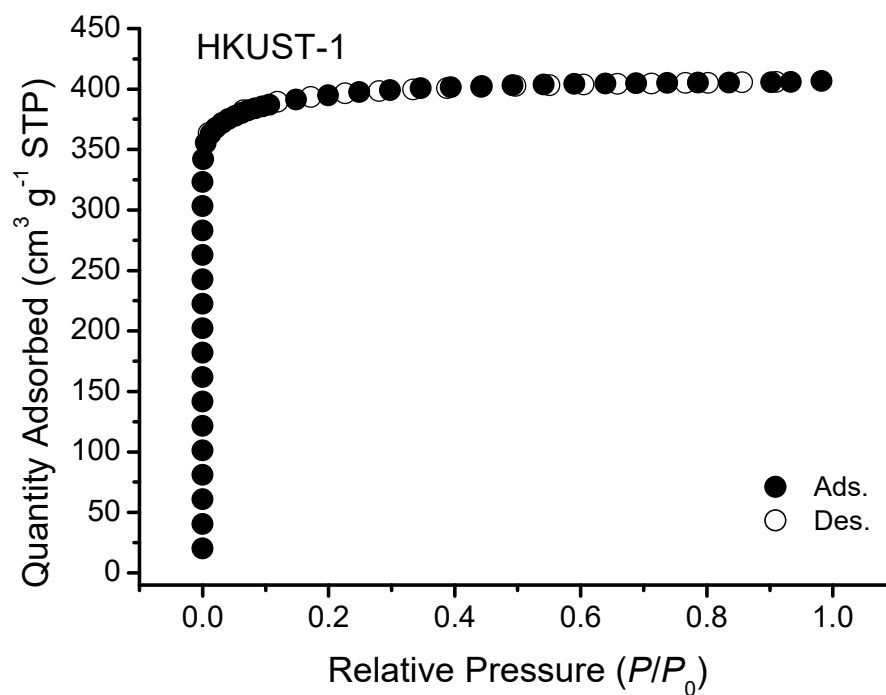


Figure S4. N₂ adsorption isotherm of the prepared HKUST-1 sample recorded at 77 K.

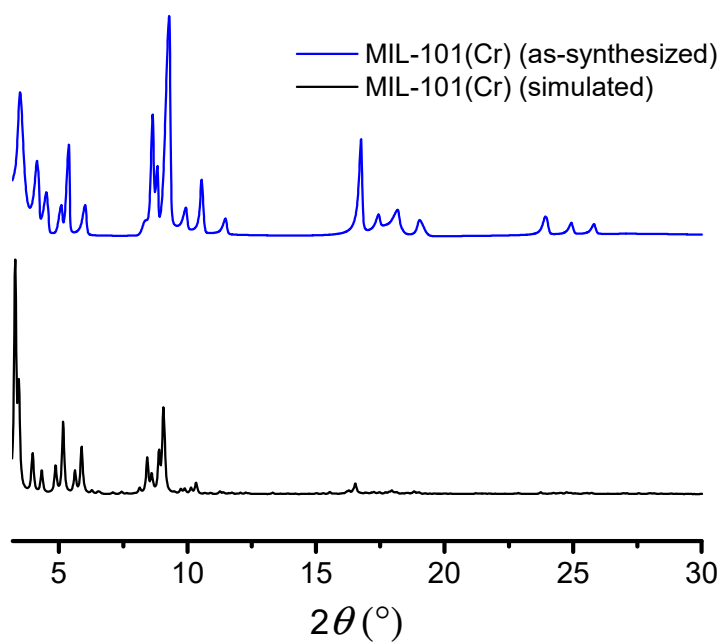


Figure S5. PXRD pattern of the as-synthesized MIL-101(Cr) sample in comparison with its simulated PXRD pattern.

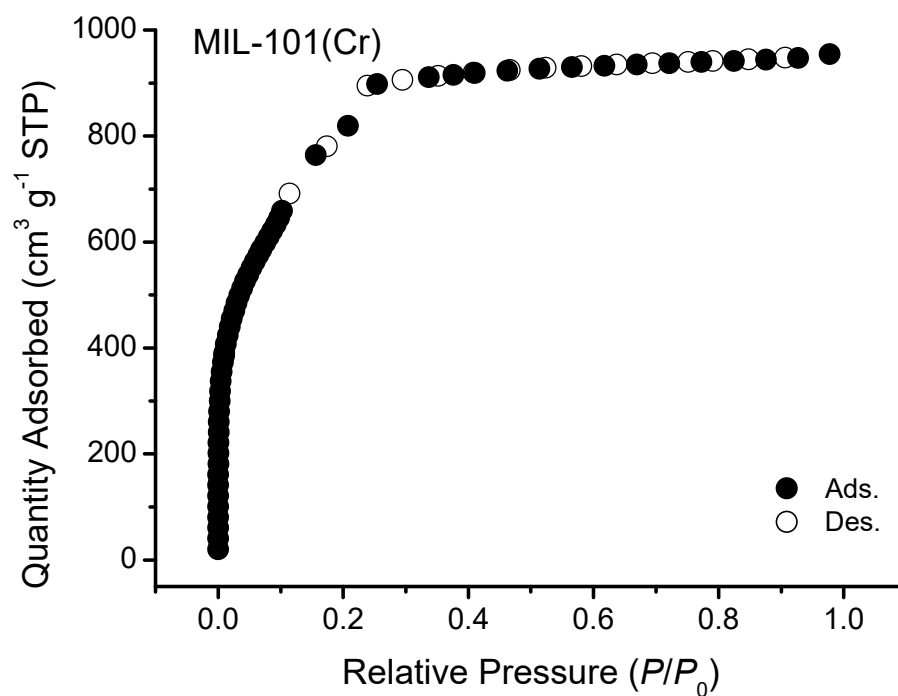


Figure S6. N₂ adsorption isotherm of the prepared MIL-101(Cr) sample recorded at 77 K.

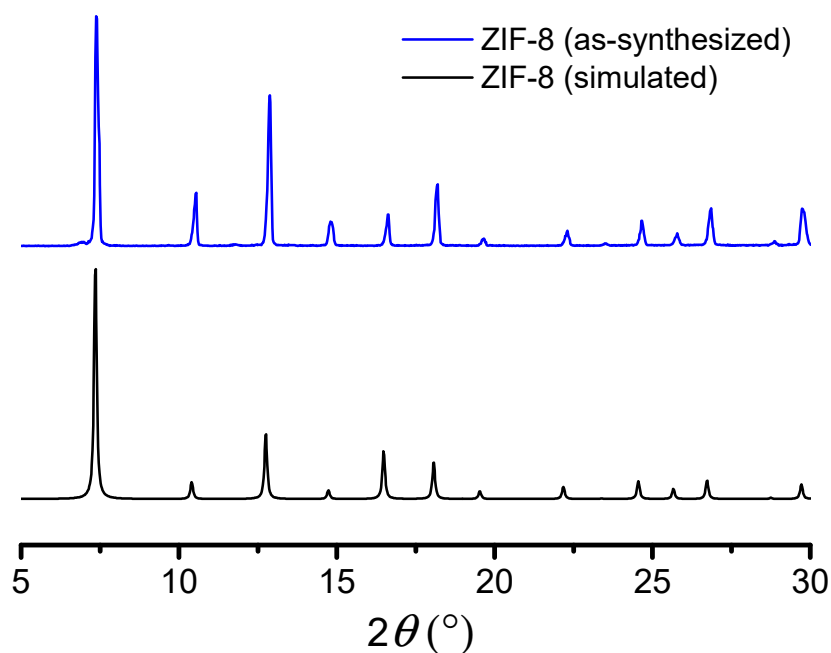


Figure S7. PXRD pattern of the as-synthesized ZIF-8 sample in comparison with its simulated PXRD pattern.

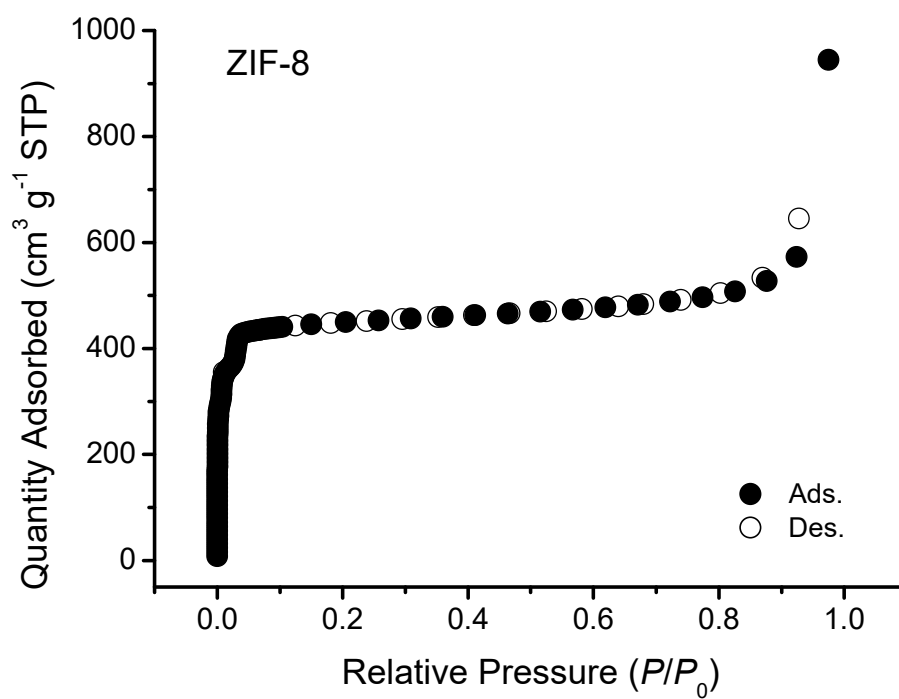


Figure S8. N₂ adsorption isotherm of the prepared ZIF-8 sample recorded at 77 K.

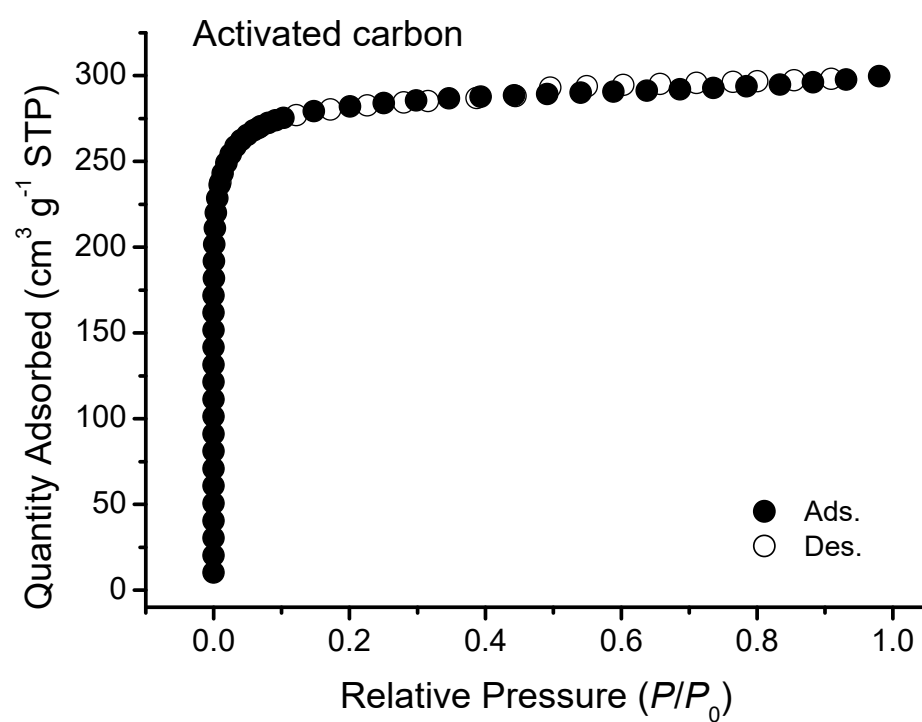


Figure S9. N₂ adsorption isotherm of the activated carbon sample recorded at 77 K.

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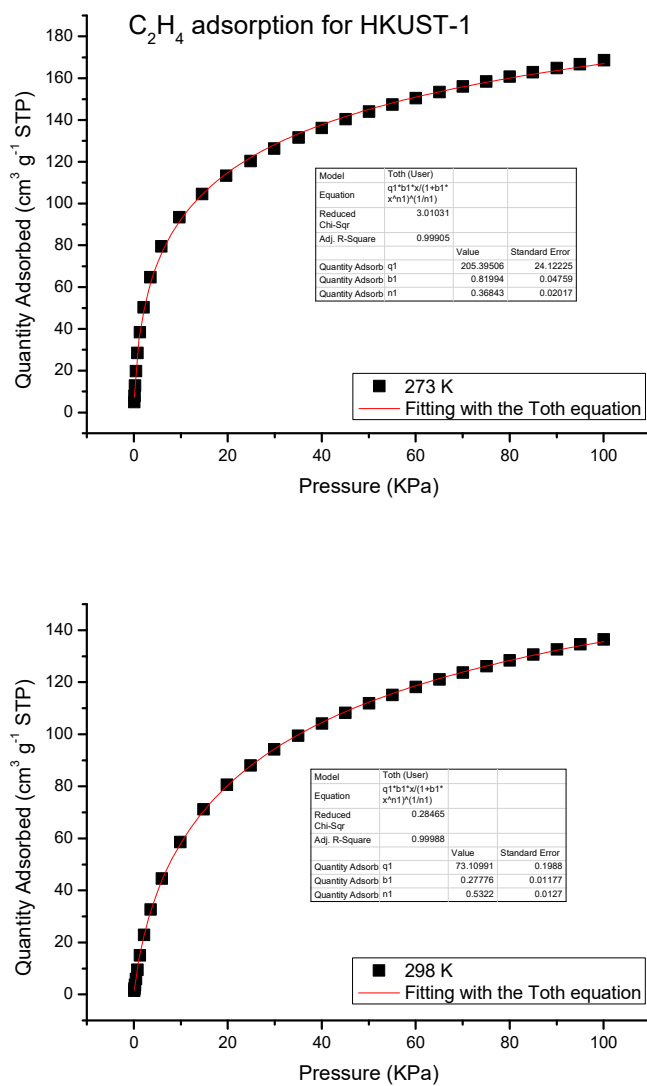


Figure S10. C_2H_4 adsorption isotherms of the prepared HKUST-1 sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

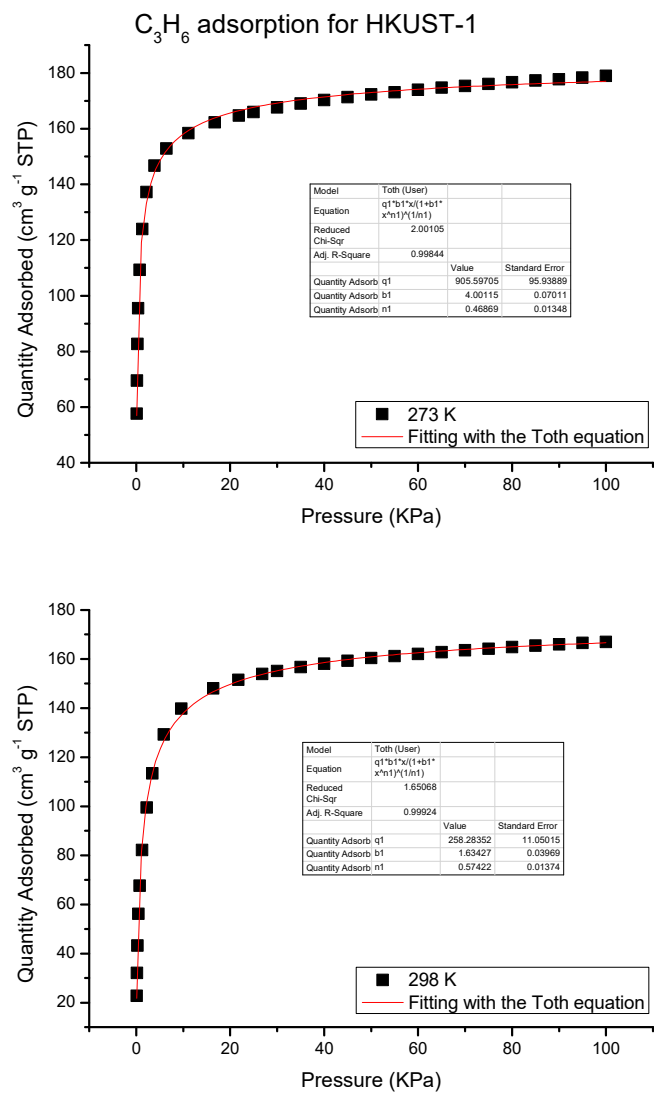


Figure S11. C₃H₆ adsorption isotherms of the prepared HKUST-1 sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

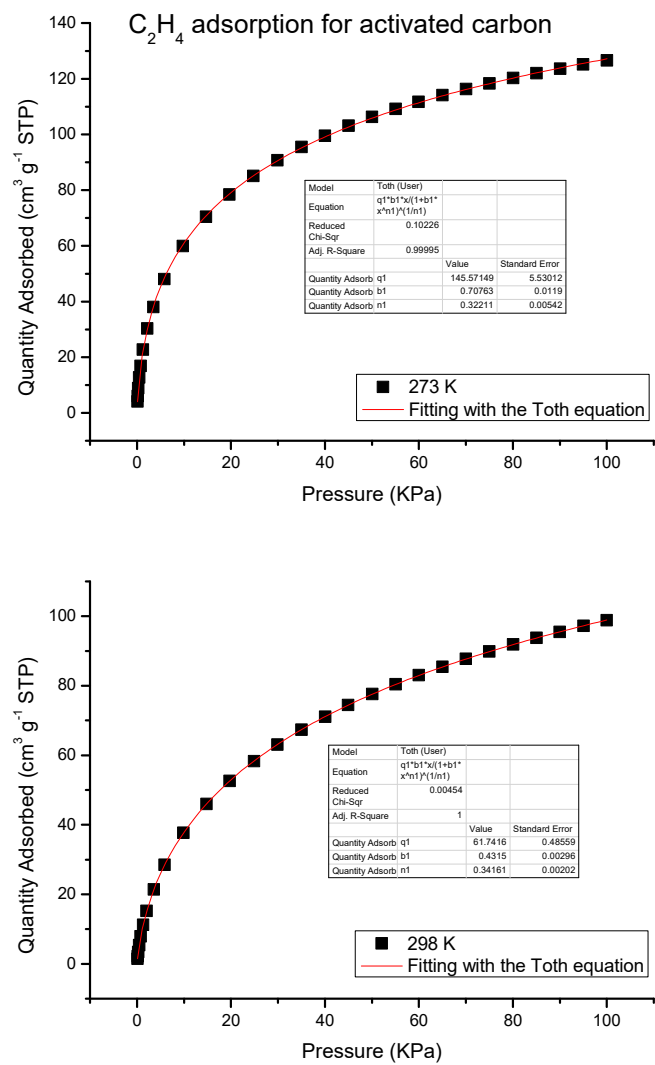


Figure S12. C₂H₄ adsorption isotherms of the activated carbon sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

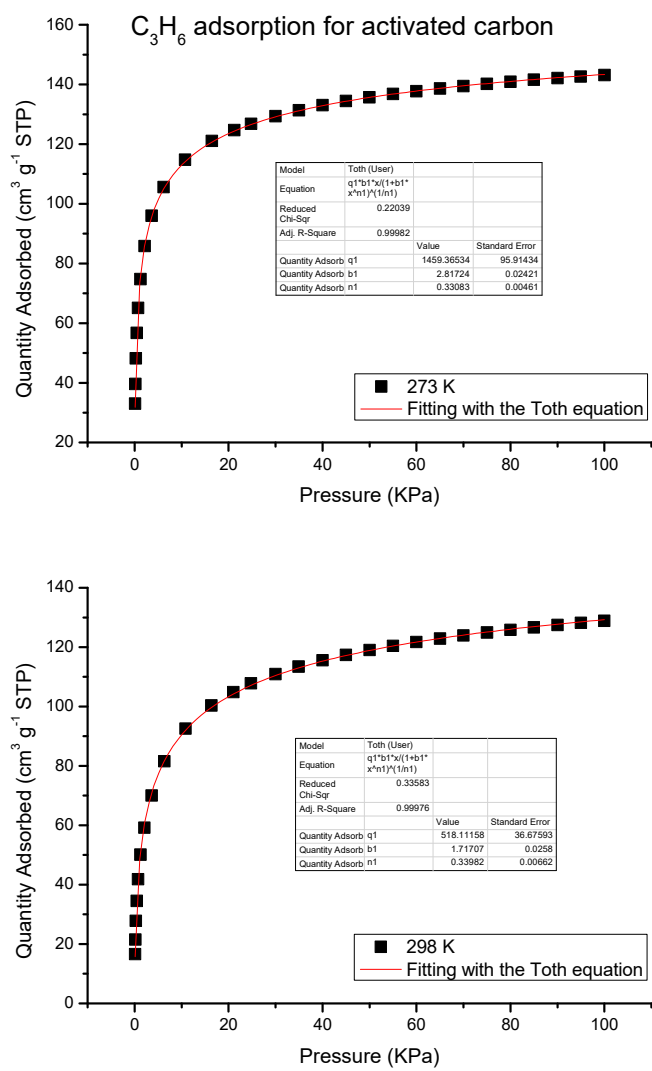


Figure S13. C₃H₆ adsorption isotherms of the activated carbon sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

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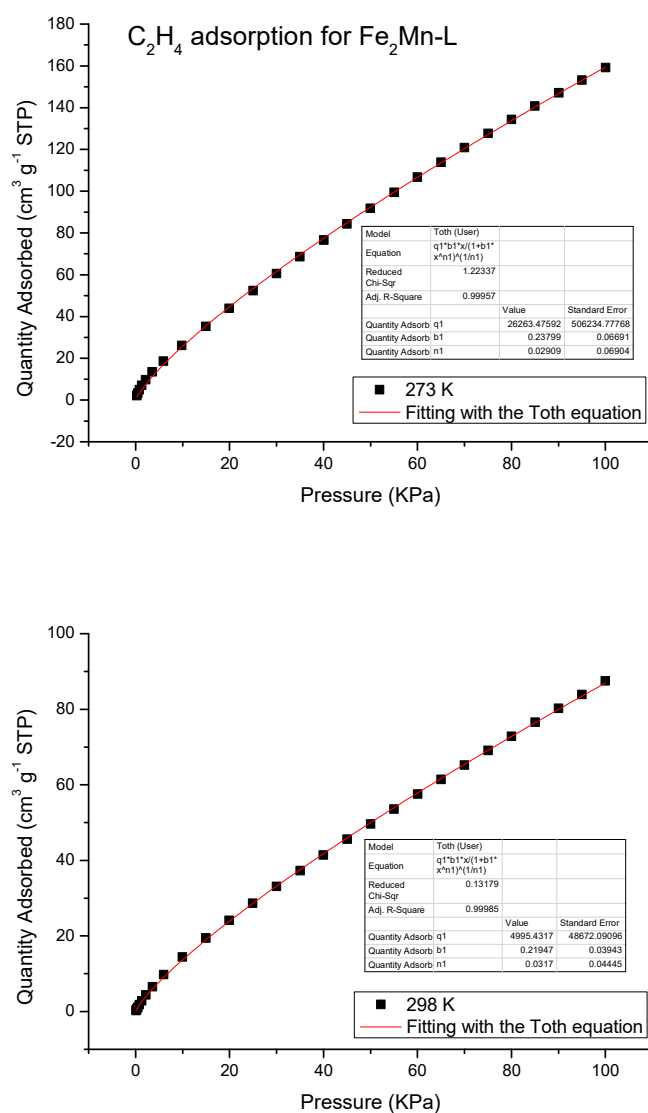


Figure S14. C_2H_4 adsorption isotherms of the Fe_2Mn-L sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

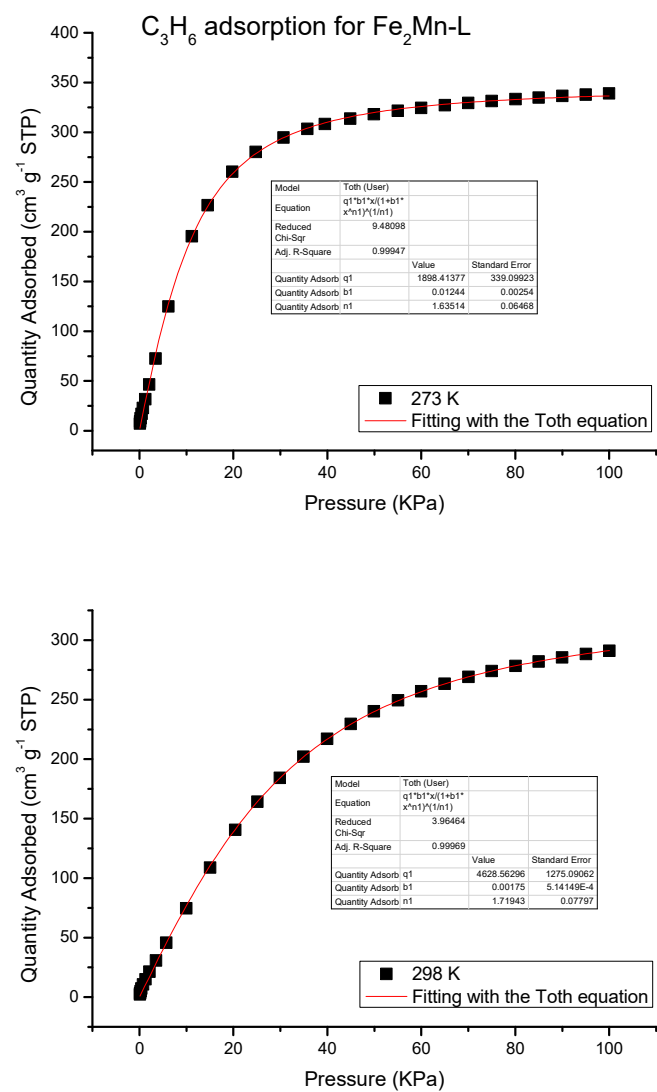


Figure S15. C₃H₆ adsorption isotherms of the Fe₂Mn-L sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

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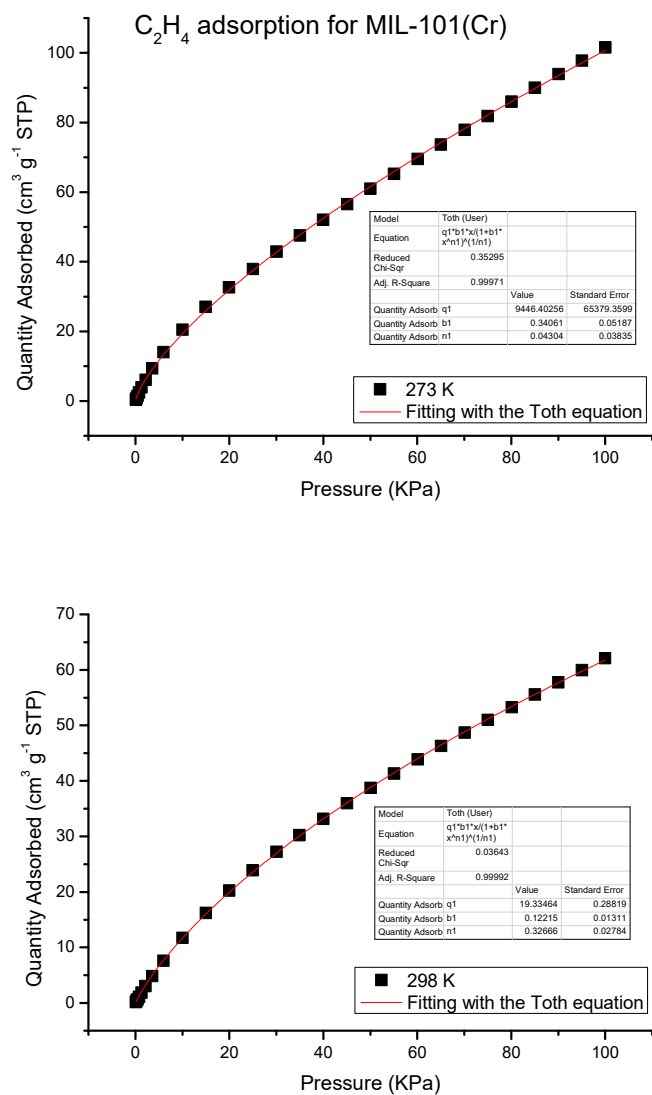


Figure S16. C₂H₄ adsorption isotherms of the MIL-101(Cr) sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

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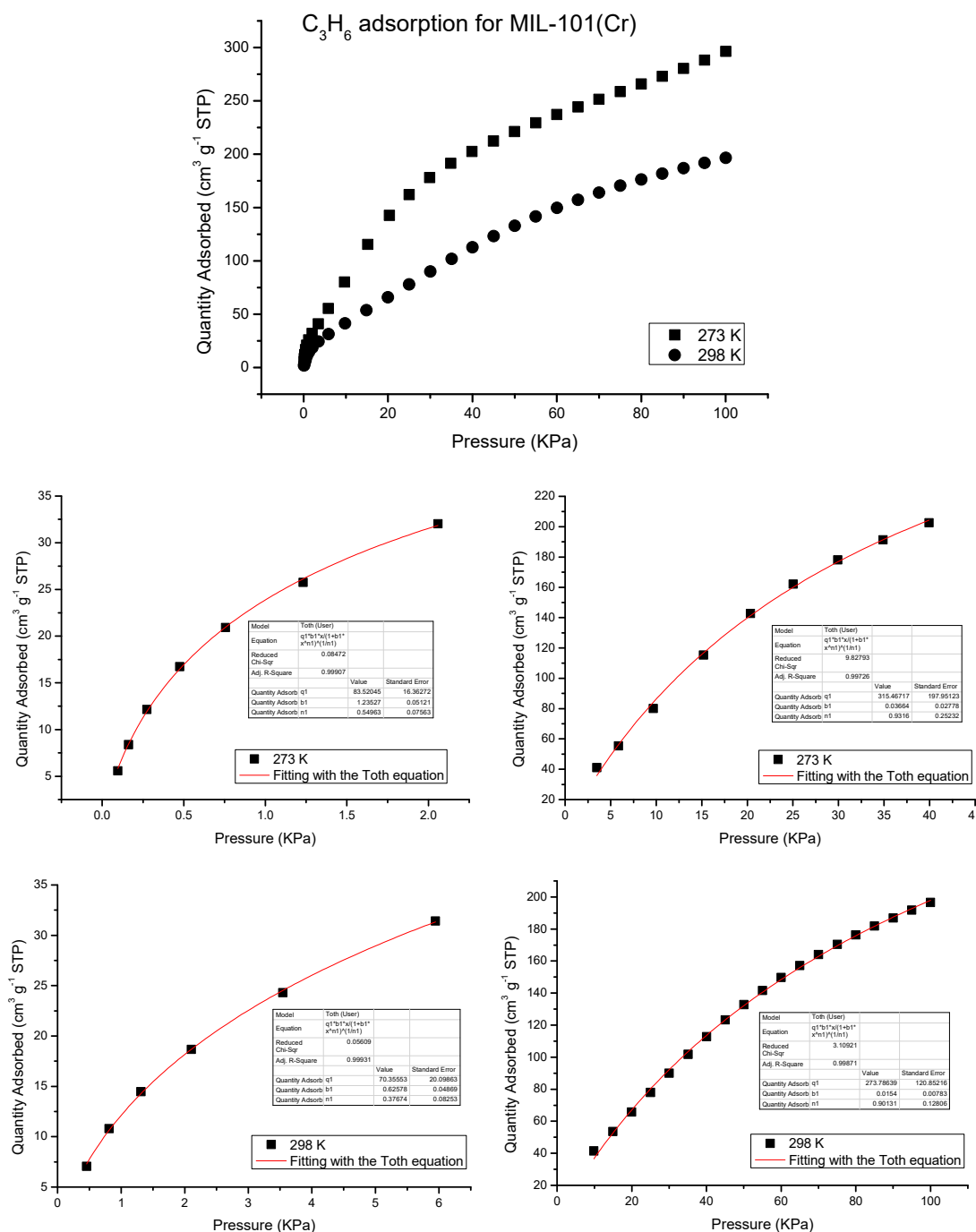


Figure S17. C_3H_6 adsorption isotherms of the MIL-101(Cr) sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation. To get better fitting results, the data at low pressure range and the data at high pressure range were fitted separately.

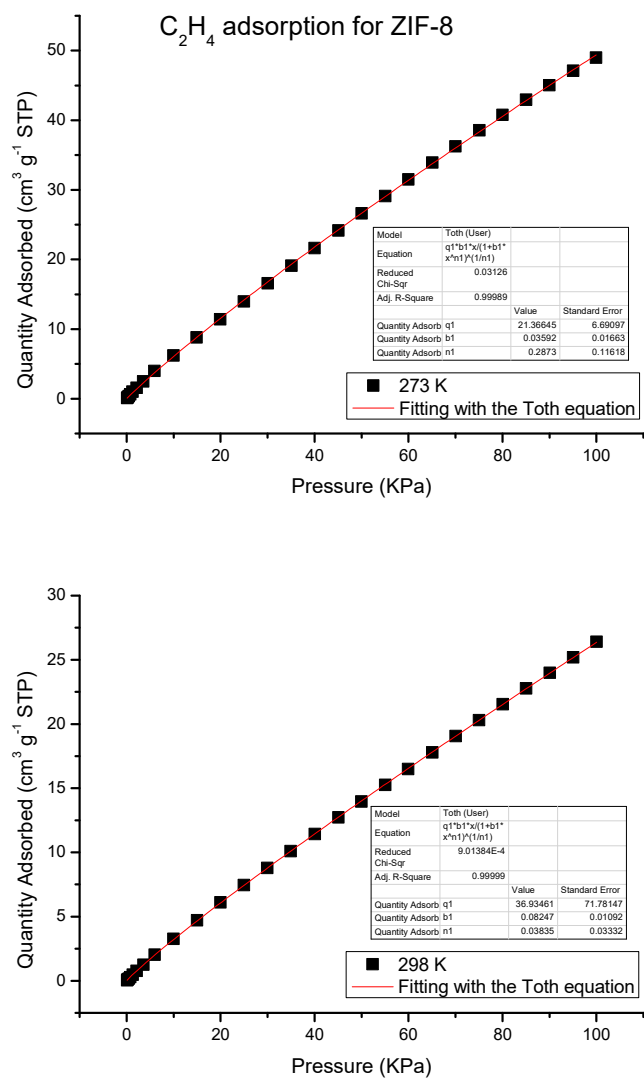


Figure S18. C₂H₄ adsorption isotherms of the ZIF-8 sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

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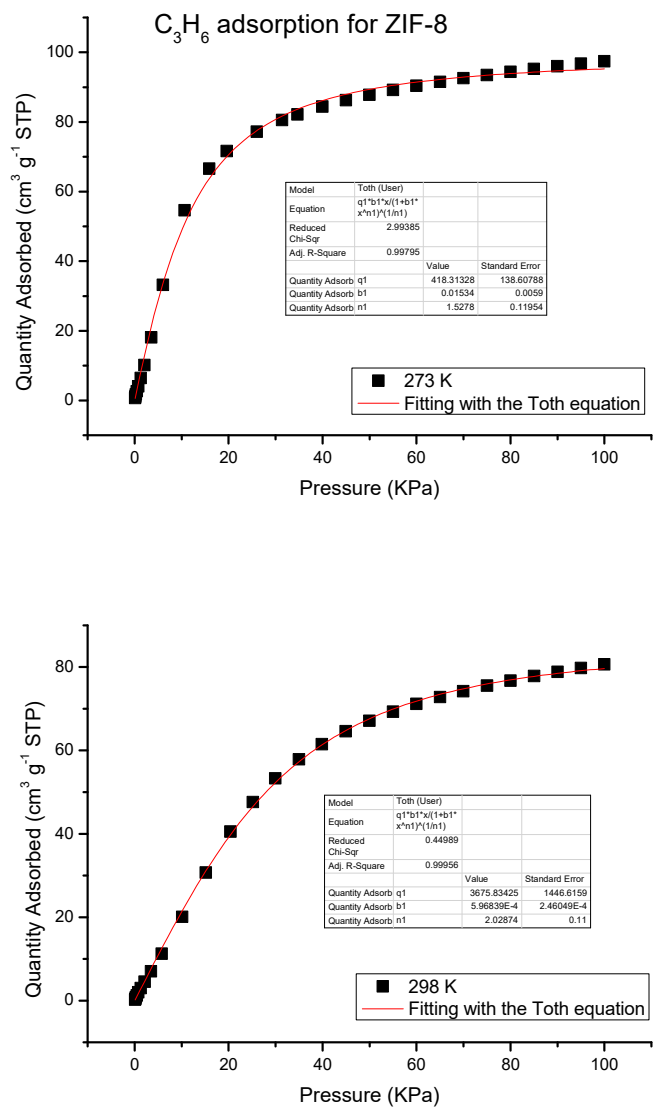


Figure S19. C3H6 adsorption isotherms of the ZIF-8 sample recorded at 273 and 298 K, and fitting results of the isotherms by the Toth equation.

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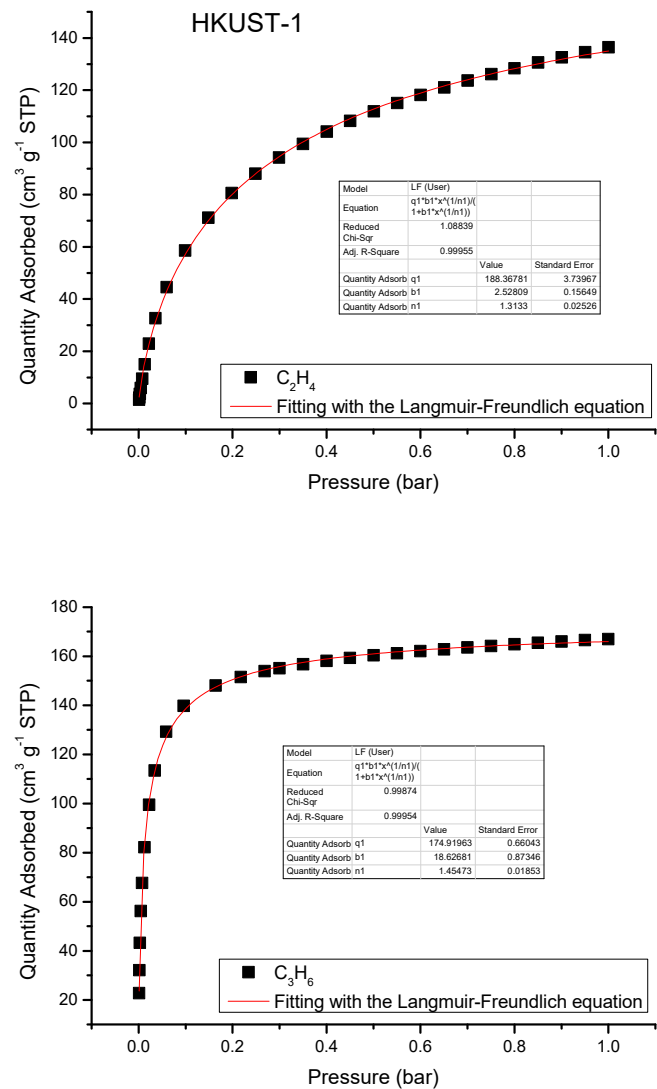


Figure S20. C₂H₄ and C₃H₆ adsorption isotherms of the prepared HKUST-1 sample recorded at 298 K, and fitting results of the isotherms by the Langmuir-Freundlich equation.

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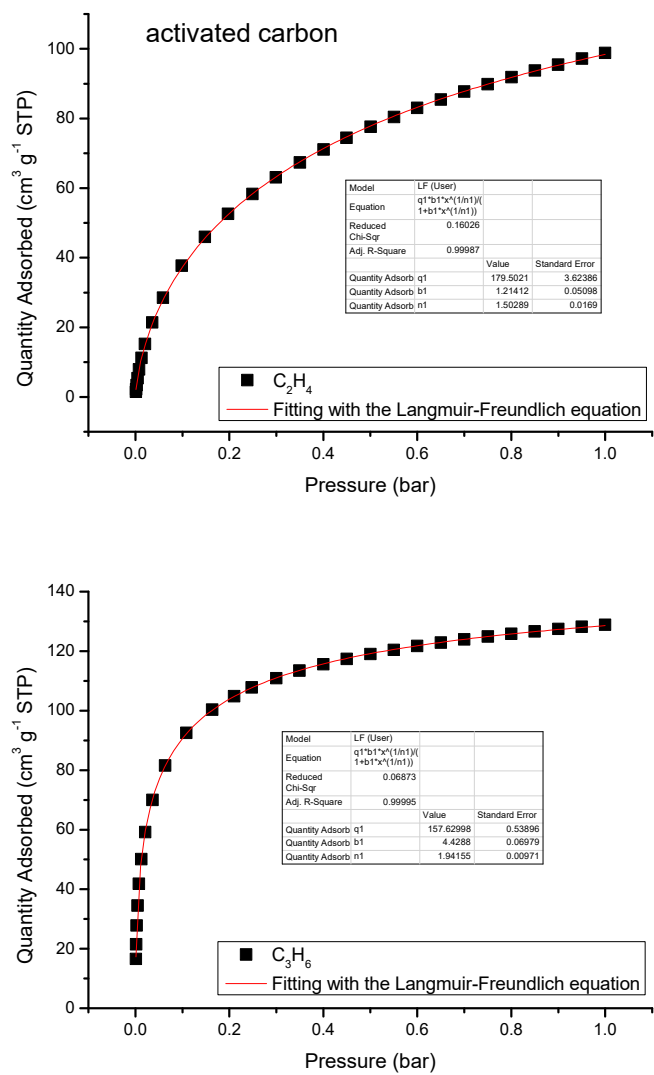


Figure S21. C₂H₄ and C₃H₆ adsorption isotherms of the activated carbon sample recorded at 298 K, and fitting results of the isotherms by the Langmuir-Freundlich equation.

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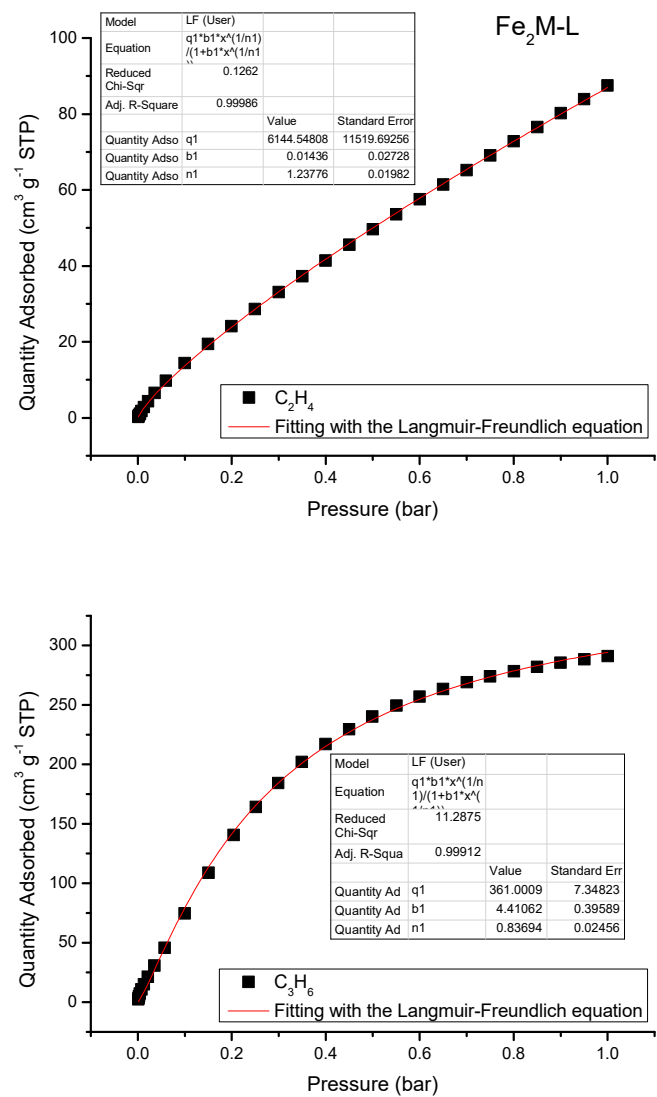


Figure S22. C₂H₄ and C₃H₆ adsorption isotherms of the prepared Fe₂M-L sample recorded at 298 K, and fitting results of the isotherms by the Langmuir-Freundlich equation.

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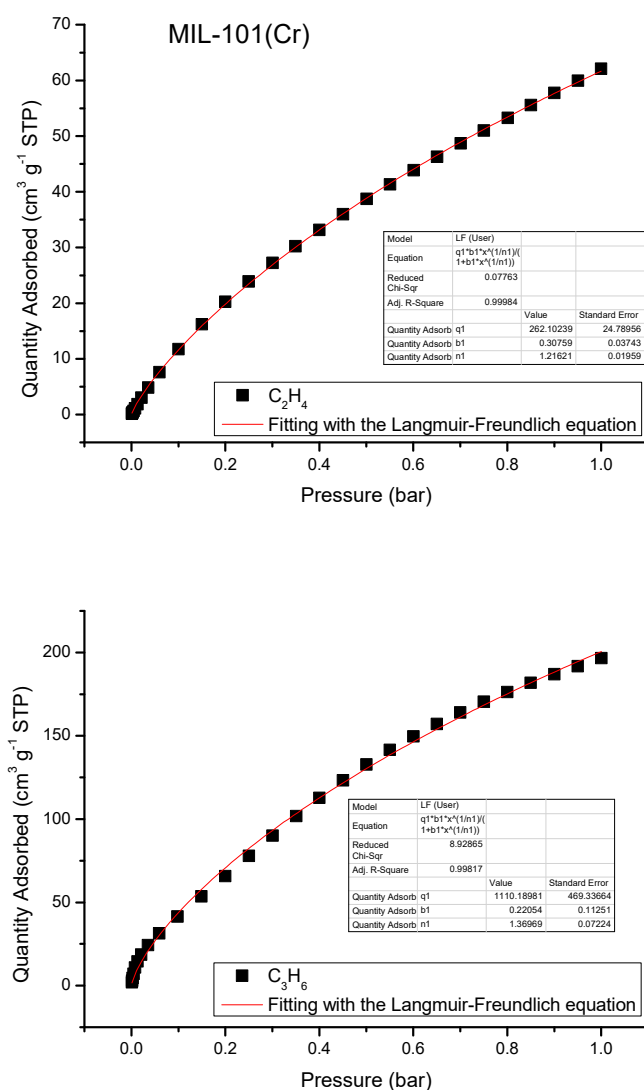


Figure S23. C_2H_4 and C_3H_6 adsorption isotherms of the prepared MIL-101(Cr) sample recorded at 298 K, and fitting results of the isotherms by the Langmuir-Freundlich equation.

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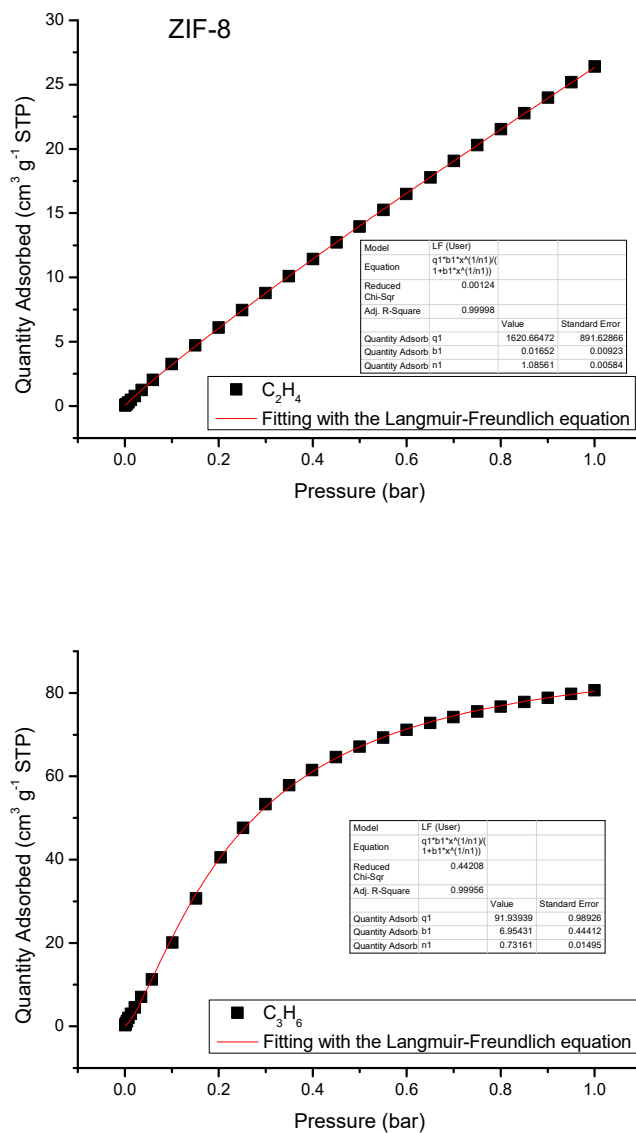


Figure S24. C_2H_4 and C_3H_6 adsorption isotherms of the prepared ZIF-8 sample recorded at 298 K, and fitting results of the isotherms by the Langmuir-Freundlich equation.