

Selective Adsorption of Small Hydrocarbons Using MOFs

Abstract

This application note presents a study on the selective adsorption behavior of small molecule hydrocarbons—acetylene (C_2H_2), ethylene (C_2H_4), propane (C_3H_8), and propylene (C_3H_6)—on various metal-organic framework (MOF) materials. Using AMI's **Micro 300** for high-precision static adsorption isotherms, this work highlights the potential of MOFs in non-cryogenic, energy-efficient separation of light hydrocarbons. Although dynamic breakthrough testing was not performed in this study, AMI's **BTsorb 100** system is noted as an ideal platform for future validation under flow conditions.

Introduction

In the petrochemical industry, C_2 hydrocarbons are foundational to the production of downstream products including polymers, rubbers, and specialty chemicals. However, separating these components remains difficult due to their similar boiling points and molecular sizes. Conventional cryogenic distillation is energy-intensive and cost-prohibitive.

Recent studies have demonstrated that MOF materials—due to their tunable pore size and chemically functionalized internal surfaces—offer a promising solution for energy-efficient separation of these hydrocarbons. Examples include the **SIFSIX** series, known for acetylene/ethylene selectivity (**FIGURE 1**), and flexible frameworks like **sql-SIFSIX-bpe-Zn**, which undergo reversible transformations in the presence of C_2H_2 (**FIGURE 2**). Additionally, **MIL-142A**, a cross-linked Fe-MOF, has shown remarkable capacity and selectivity for C_3H_8 over CH_4 under ambient conditions (**FIGURE 3**).

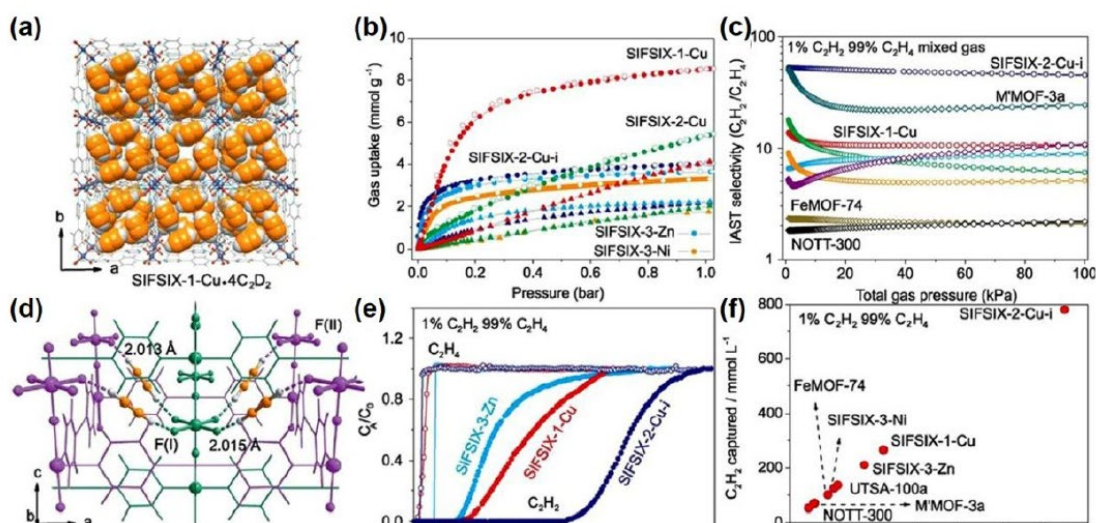


Figure 1: (a) SIFSIX-1-Cu-4C₂D₂ Structural Diagram and (b-f) C₂H₂ Adsorption and C₂H₂/C₂H₄ Separation Schematic

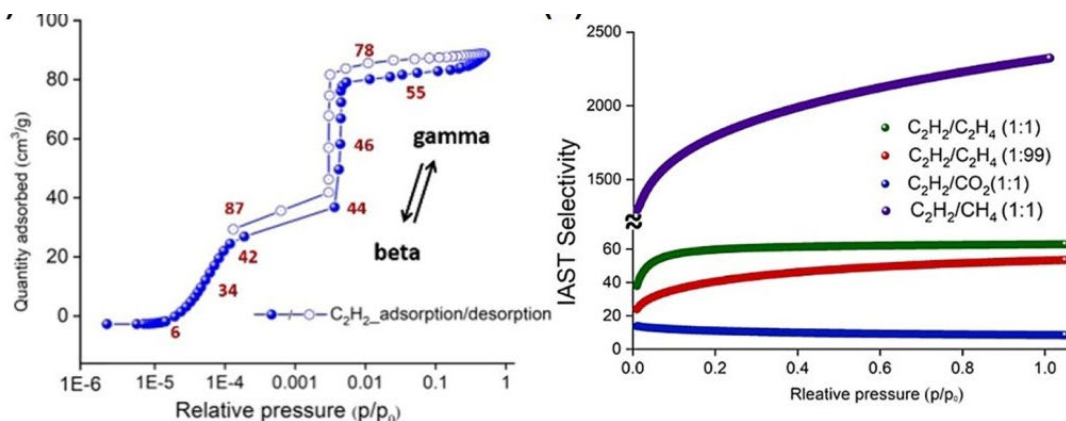


Figure 2: (Left) Adsorption Changes of C₂H₂ during the SC-SC Transition of the two-dimensional Flexible MOF Material sql-SIFSIX-bpe-Zn; (Right) C₂H₂/C₂H₄ Separation Ratio.

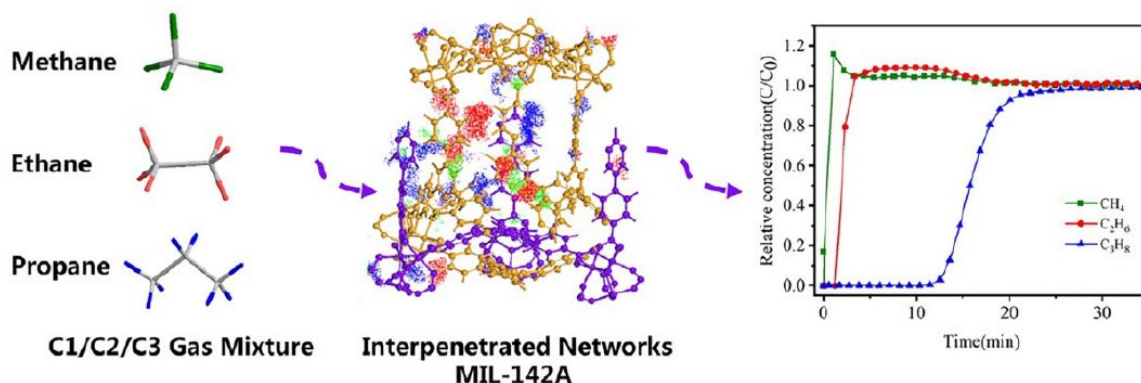


Figure 3: C1/C2/C3 Three-component Gas Separation Diagram of MIL-142A

Experimental Methods

Instruments

- AMI Micro 300: Used to collect static adsorption isotherms of gases on MOF samples at room temperature.
- AMI BTsorb 100: Identified as the intended platform for future dynamic breakthrough testing of gas mixtures under flow conditions.

Conditions

- Temperature: Ambient (~298 K)
- Pressure Range: Up to 100 kPa
- Gases Tested: C_2H_2 , C_2H_4 , C_3H_6 , C_3H_8
- MOF Samples: Labeled MOF-1, MOF-2, and MOF-3

Results and Discussion

C_2 Hydrocarbon Adsorption

Adsorption isotherms recorded on the AMI Micro 300 revealed a distinct difference in uptake behavior between acetylene and ethylene. For MOF-1, acetylene displayed a steep increase in adsorption between 4–6 kPa, followed by saturation (**FIGURE 4**). Ethylene, by contrast, showed negligible adsorption across the tested pressure range.

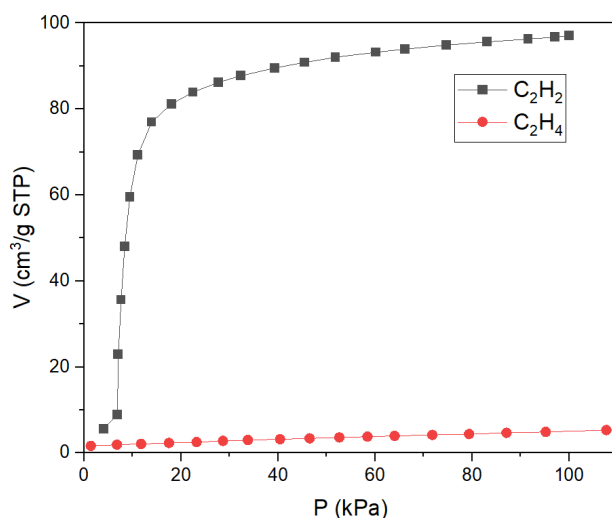


Figure 4: Adsorption Isotherm on Micro 300

These results are consistent with the known affinity of fluorinated MOFs for triple-bonded hydrocarbons, likely due to π -H interactions with exposed SiF_6^{2-} groups.

C_3 Hydrocarbon Selectivity

Further experiments evaluated the adsorption of propane and propylene on MOF-2 and MOF-3. Both materials exhibited strong uptake of propylene while showing no detectable adsorption of propane (**FIGURE 5**). The clear selectivity suggests that steric effects and kinetic diameter differences influence uptake behavior.

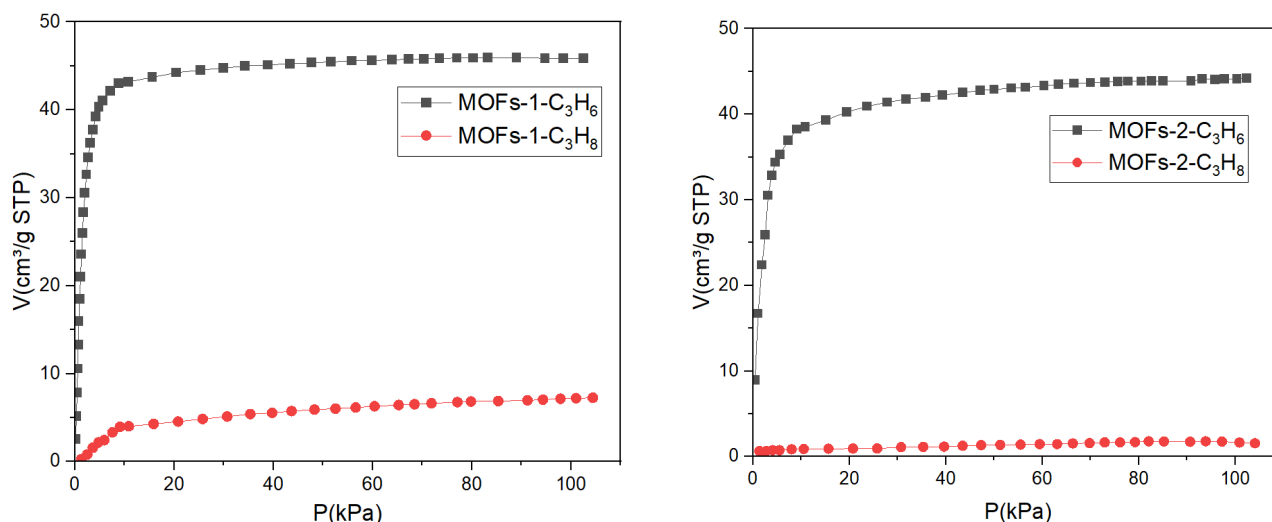


Figure 5: Adsorption Isotherm on Micro 300 of MOF 2 and 3

Note on Dynamic Testing

Although dynamic breakthrough testing was not conducted as part of this study, the **AMI BTsorrb 100** is designed for such evaluations and remains a valuable tool for future studies aimed at simulating industrial gas separation scenarios.

Applications

These findings indicate that:

- MOF-1 is suited for trace acetylene removal from ethylene streams in polymer production.
- MOF-2 and MOF-3 can selectively capture propylene, ideal for propylene recovery or purification from LPG mixtures.

By pairing AMI's **Micro 300** for equilibrium data and the **BTsorrb 100** for future dynamic testing, researchers can comprehensively assess adsorbent materials for industrial gas separation applications.

Conclusion

This study underscores the promise of MOF-based adsorbents for targeted separation of light hydrocarbons at ambient conditions. While this work focused on static adsorption behavior, AMI's suite of instruments—especially the **Micro 300** and **BTsorb 100**—provides a scalable, versatile platform for future full-cycle evaluation from material screening to process development.