



Zeolitic Imidazolate Framework-8 (ZIF-8) Membranes for Kr/Xe Separation

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Xe and Kr Separation in Nuclear Reprocessing

Separating Krypton (Kr) from Xenon (Xe) is a critical step during treatment of spent nuclear fuel

- ^{85}Kr -> **radioactive**
- **10Xe:1Kr**

Need to store ^{85}Kr for 100 years

- Separating Xe and Kr can save space and money!

Xe used in lighting, medical applications, including neuroprotection, imaging, and anesthesia

- Currently expensive

Benchmark separation technology: cryogenic distillation

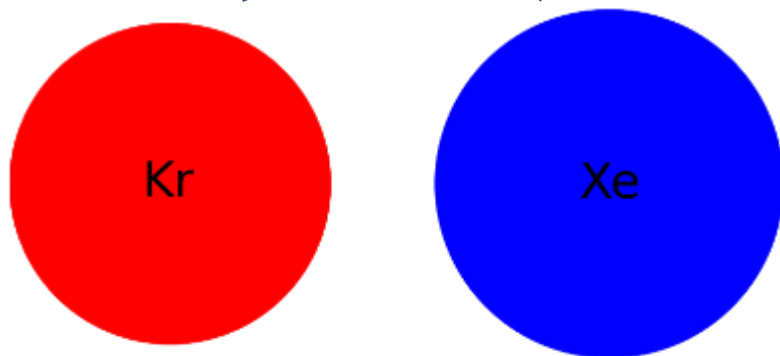
- Energy intensive and expensive process.

Distinguishing Xe and Kr



Membrane Separation
(size)

← No phase transformation!



Kr

Xe

Diameter = 0.37 nm
Boiling point = -153.4 °C

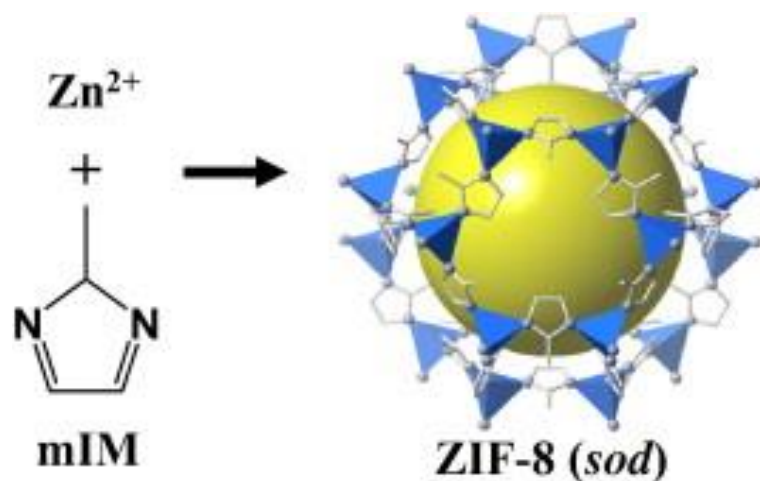
Diameter = 0.41 nm
Boiling point = -108.1 °C

Cryogenic Distillation
(temperature)

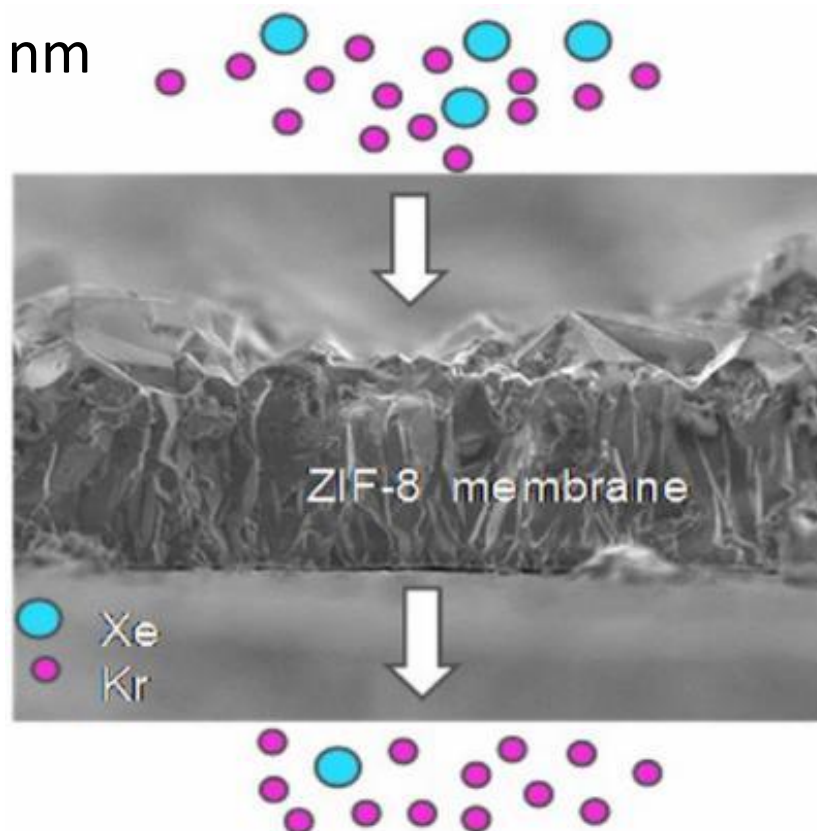
Physical properties	Kr	Xe
Kinetic diameter (nm)	0.366	0.405
Polarizability (10^{-25} cm^3)	24.844	40.44
Dipole moment (esu cm)	0	0
Quadruple moment (esu cm^2)	0	0

ZIF-8

- Family of Metal–organic frameworks (MOFs)
- Zeolitic imidazolate framework, thermally and chemically stable
- Effective aperture size of 0.4–0.42 nm



Crystal structure of ZIF-8: Zn (polyhedral), N (sphere), and C (line)



Gas Separation Process



- Adsorption: electrostatic interaction
- Molecular sieving: membrane and gas size
- Diffusion: molecular radii and weight

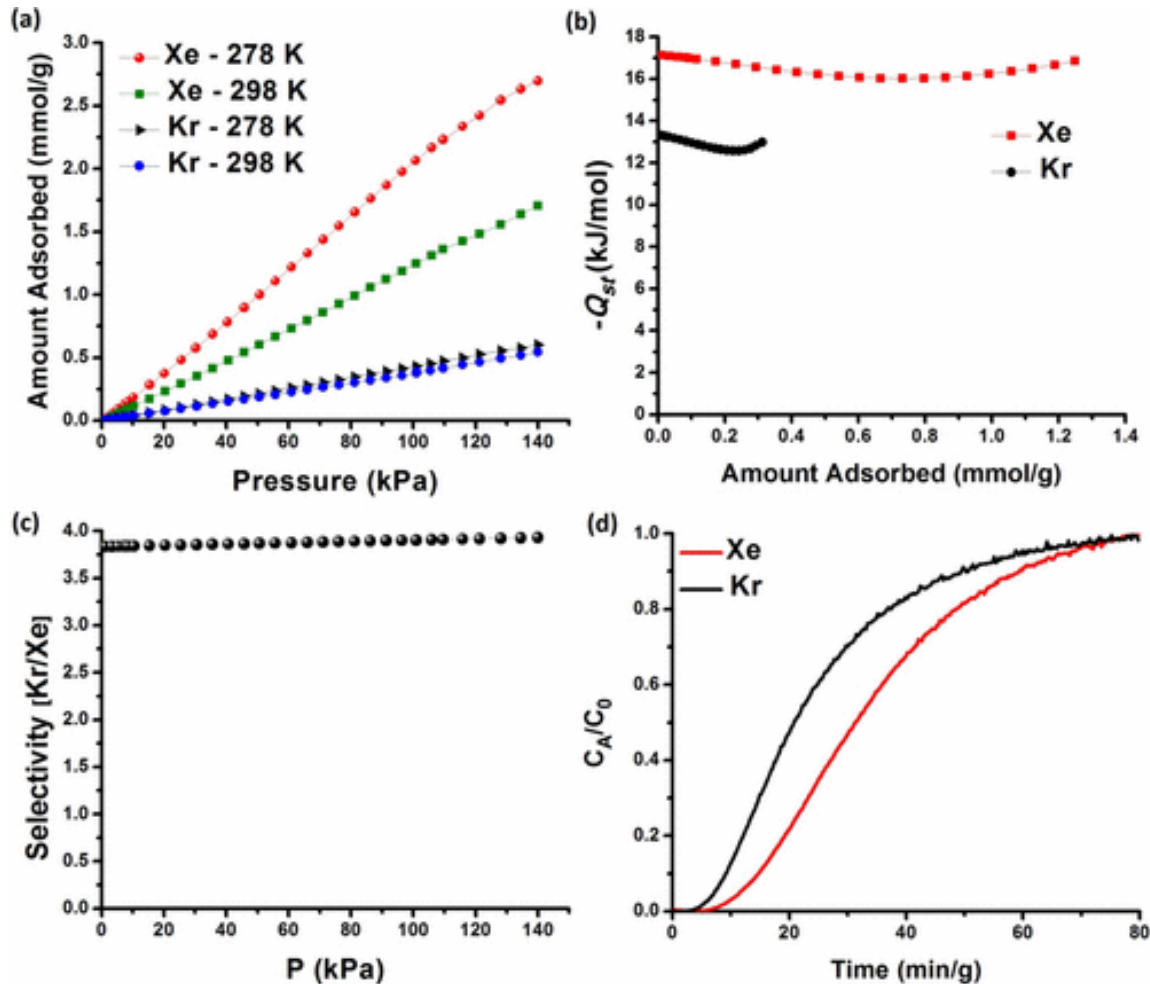


● Kr (0.37 nm)

● Xe (0.41 nm)

== membrane

ZIF-8 Adsorption and Diffusion Selectivity



Diffusion is the dominant mechanism

Membrane Preparation



chemicals and solvent



Place support in mixed solution, then in a Teflon liner



solvothermal treatment



120 °C
4-12 hours

Crystallization



Membrane Separation Results

Permeance = pressure - normalized flux, membrane property

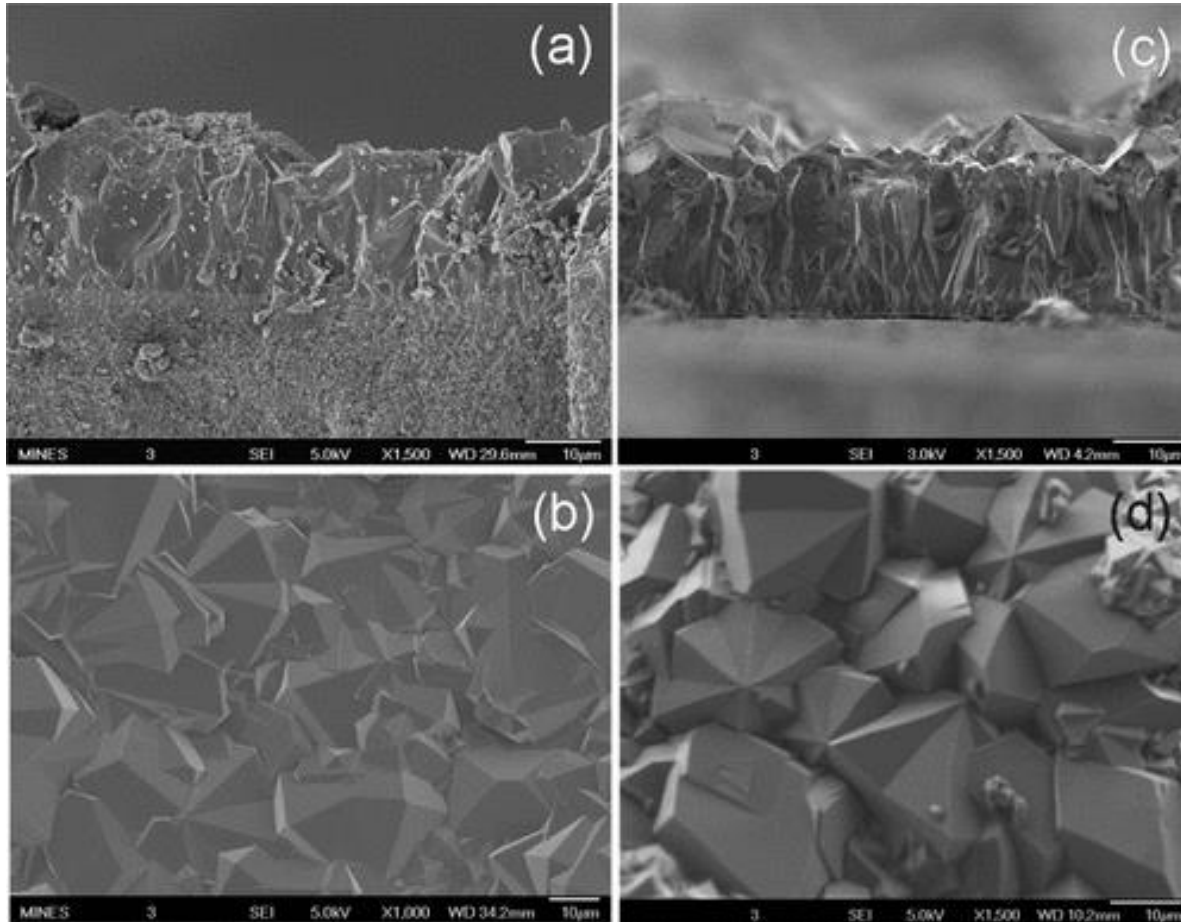
Separation factor α for a ratio of Kr permeance/Xe permeance.

Kr/Xe separation performance over ZIF-8 membranes. Molar gas mixture composition: 92:8 Kr/Xe. Transmembrane pressure 138 kPa.

Membrane ID ^a	Kr permeance (mol/m ² ·s·Pa) ^b	Separation selectivity (α)	Separation index (π) ^c	
1A	0.33x10 ⁻⁸ (9.9)	5.9	13.6 x10 ⁻⁴	} 2-layer
1B	0.17x10 ⁻⁸ (5.1)	10.8	13.9 x10 ⁻⁴	
2A	1.7x10 ⁻⁸ (50.8)	12.3	162 x10 ⁻⁴	
2B	1.3x10 ⁻⁸ (38.8)	16.1	164 x10 ⁻⁴	
3	0.5x10 ⁻⁸ (14.9)	7.9	28.9 x10 ⁻⁴	— 3-layer

^a 1A, 1B, 2A, 2B are two layer membranes. 3 is three-layer membrane. ^b Numbers in parentheses indicate Gas permeation units (GPU). ^c $\pi = \text{Kr permeance} \times (\text{selectivity}-1) \times \text{permeate pressure}$

SEM Images of ZIF-8 2-Layer Membranes





Conclusion and Future work

- Successfully synthesized continuous ZIF-8 membranes and first to demonstrate Kr/Xe gas separation with MOF membrane
 - Average Kr permeances as high as $1.5 \times 10^{-8} \pm 0.2$ mol/m²s Pa and average separation selectivities of 14.2 ± 1.9 for molar feed compositions in air ratio
 - Molecular sieving, competitive adsorption, and differences in diffusivities were the prevailing separation mechanisms.
 - Promising alternative to the benchmark technology cryogenic distillation currently employed to separate Kr/Xe
- Next step:
 - Optimize synthesis parameters to improve selectivity and permeance

Thank you!

Advisor: Prof. Moises Carreon

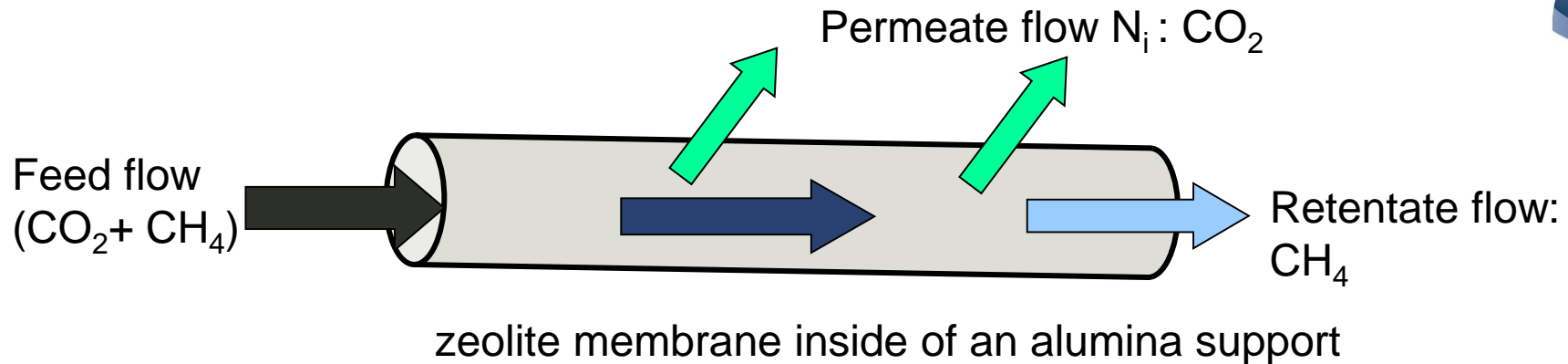


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- Kr: 83.798 g/mol
- Xe: 131.293 g/mol

Membrane Performance Parameters



Permeance= pressure - normalized flux, membrane property

$$\prod_i (\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}) = \frac{N_i}{\Delta P_i}$$

Permeability=permeance*membrane thickness, material property

$$P_i (\text{mol} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}) = \prod_i l$$

Separation factor α for a binary mixture of component A(CO₂) and B(CH₄):

$$\alpha_{A/B} = \frac{(c_A / c_B)_{\text{permeate}}}{(c_A / c_B)_{\text{feed}}}$$