

Enabling Machine Learning-Assisted Discovery of Polyamines for Solid- State CO₂ Capture

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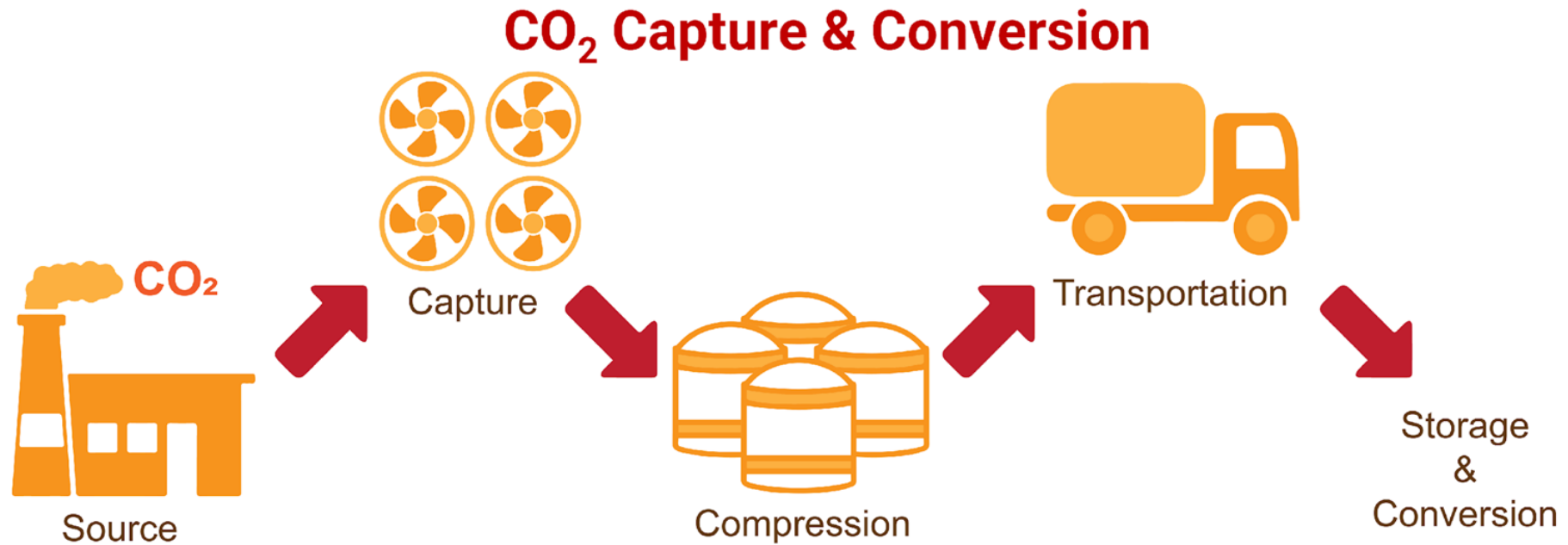
Background



Rise in
atmospheric
 CO_2

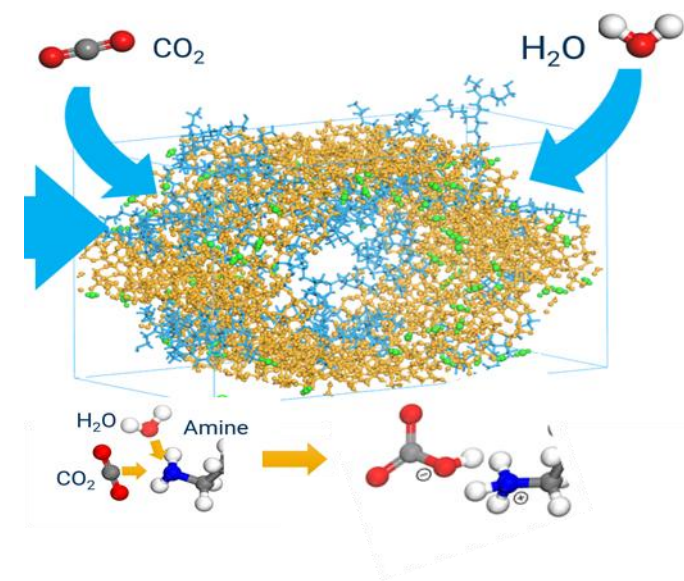
Need for active removal through
Carbon Capture and Storage (CCS)

Direct Air Capture (DAC)



Polyamine Sorbent

- Need for highly selective sorbent for DAC.
- **Why solid amine sorbents?**
 - Performance is governed by accessibility of amine group, not by the surface area
 - critical under sub-1vol% CO₂ conditions

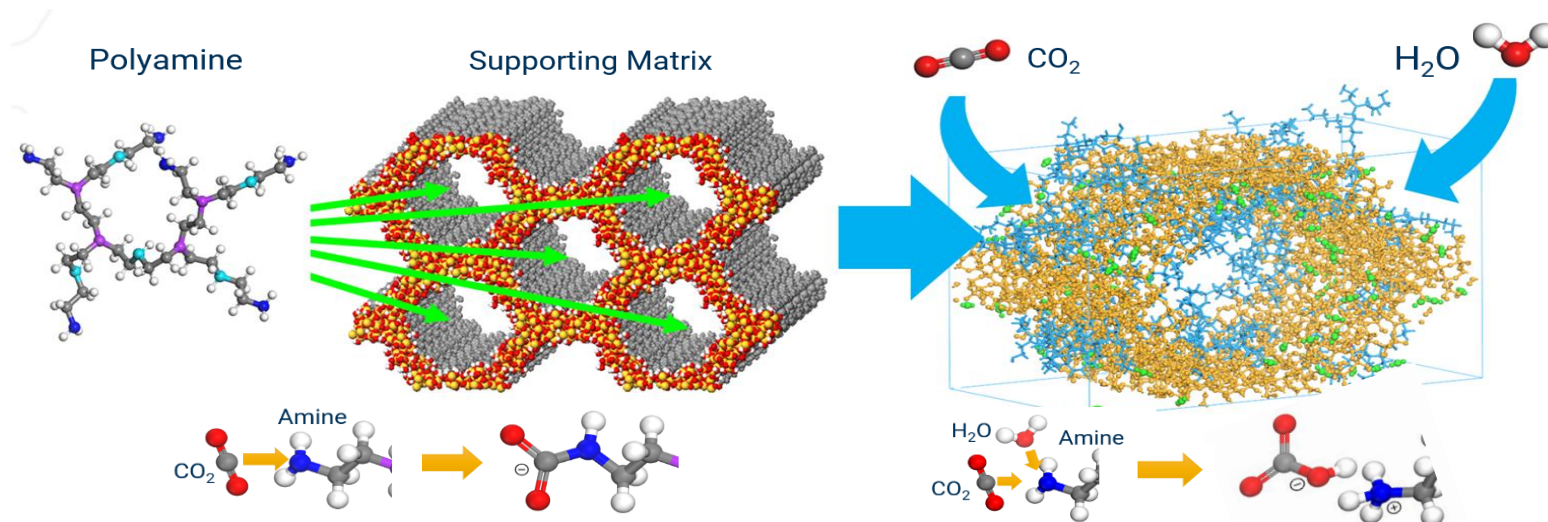
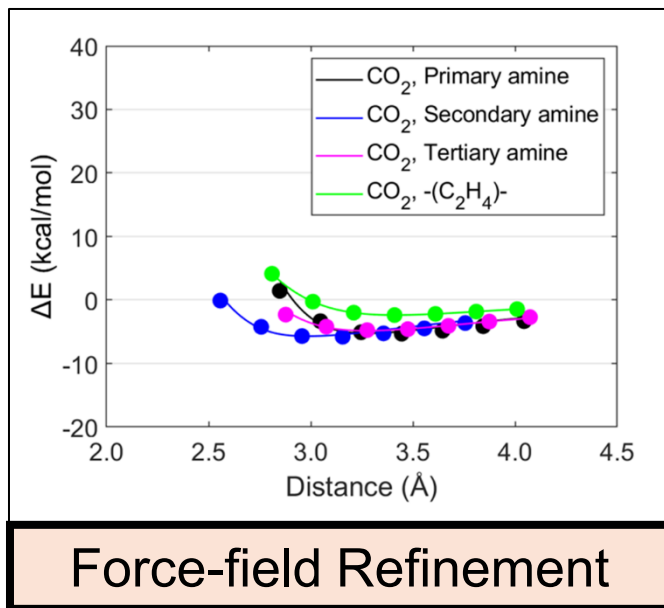


Our Contribution

1

Computationally efficient simulation pipeline for CO₂ uptake estimates

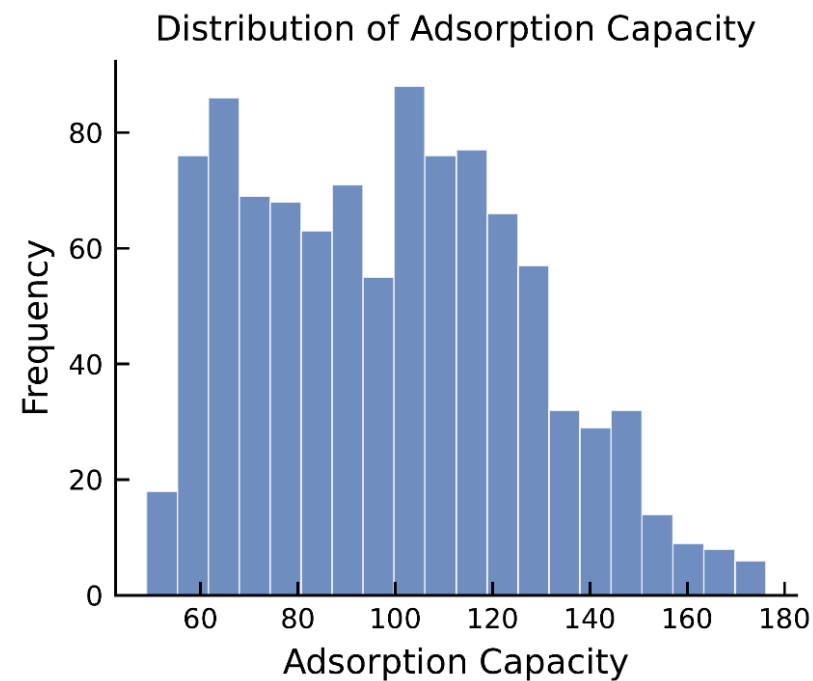
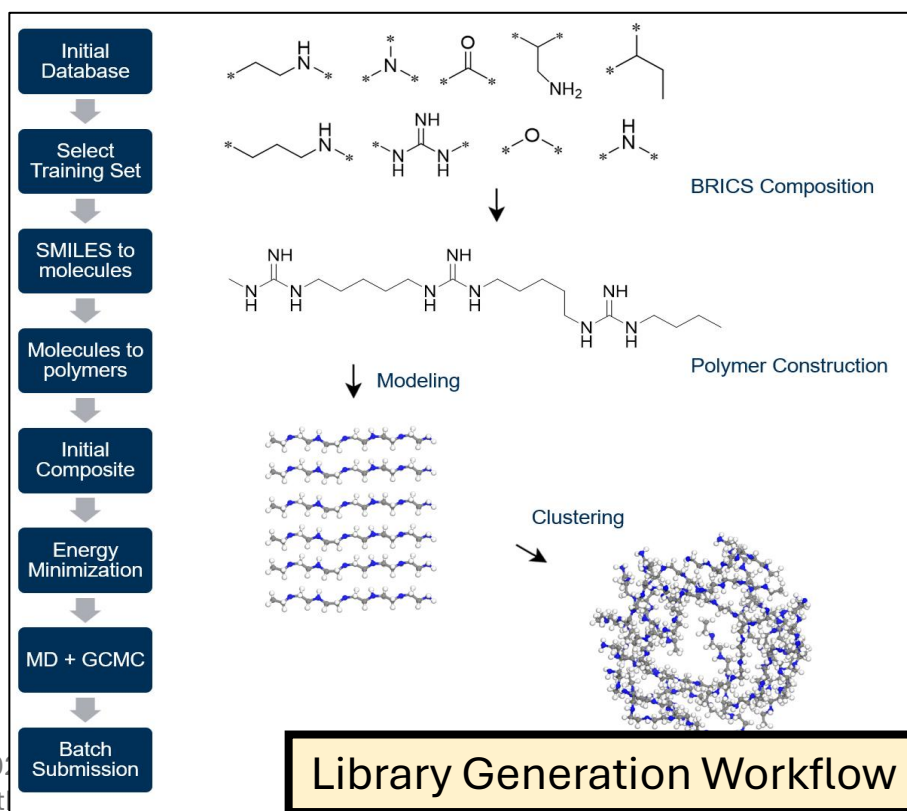
- fast MD relaxations + grand canonical Monte Carlo (GCMC)



Our Contribution

2

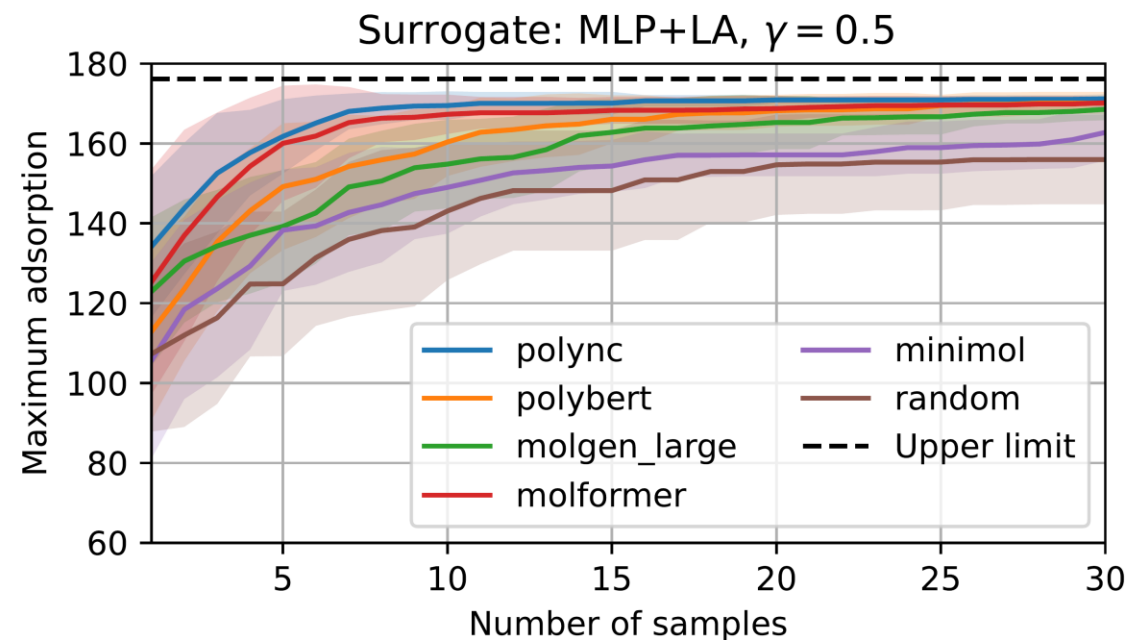
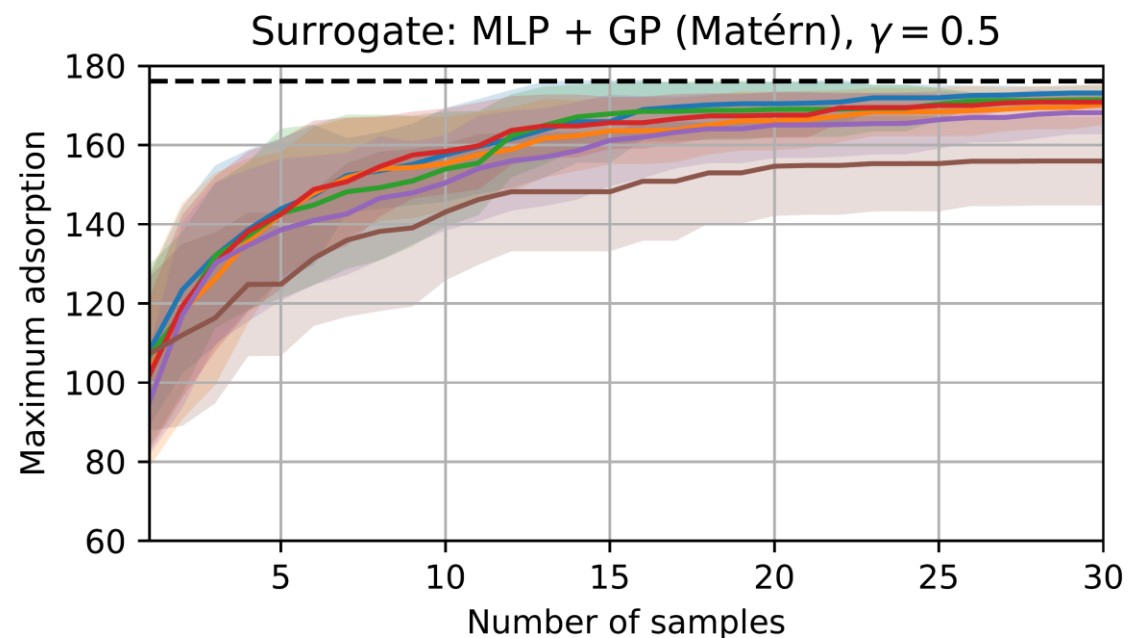
Diverse library of 1000 hypothetical polymers with estimated CO₂ adsorption capacity.



Our Contribution

3

Retrospective investigation of **Bayesian optimization (BO)** in accelerating discovery of polymer with **optimized adsorption capacity**



Key Takeaways

- **Outcome:** Polymer library and CO₂ adsorption simulation pipeline
- **Insight:** BO showed promise in accelerating the high-performance polymer identification under small computational budget.
- **Future work:**
 - Requires validation by long-timescale MD simulation.
 - Need for exploration beyond linear polymers.

Thank you!

Queries/Comments:

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