Investigating Gas Adsorption and Diffusion Dynamics in Zeolite-Based Membranes for Post-Combustion CO_2 Capture

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Introduction

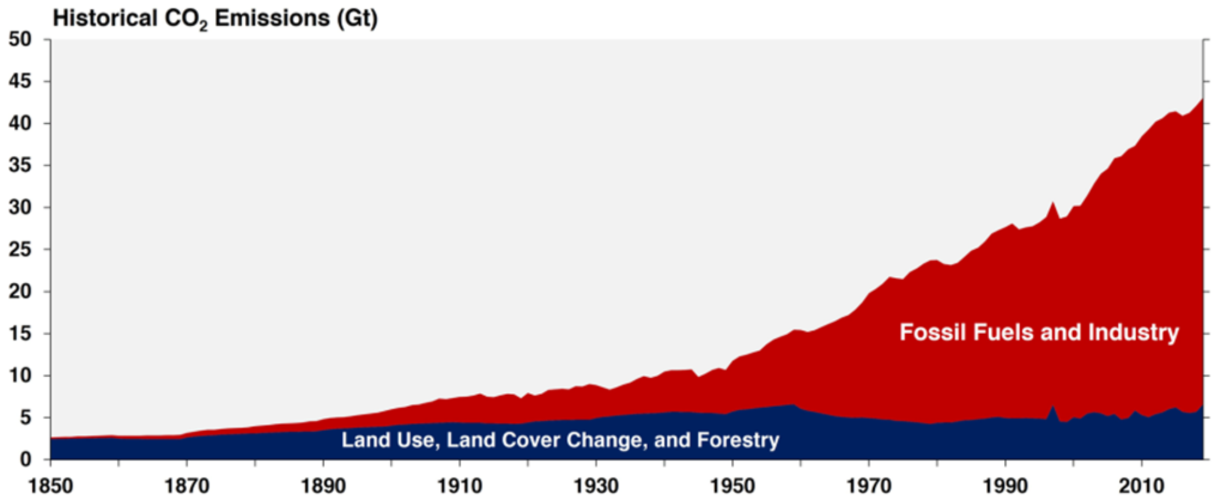
Global CO_2 Emission

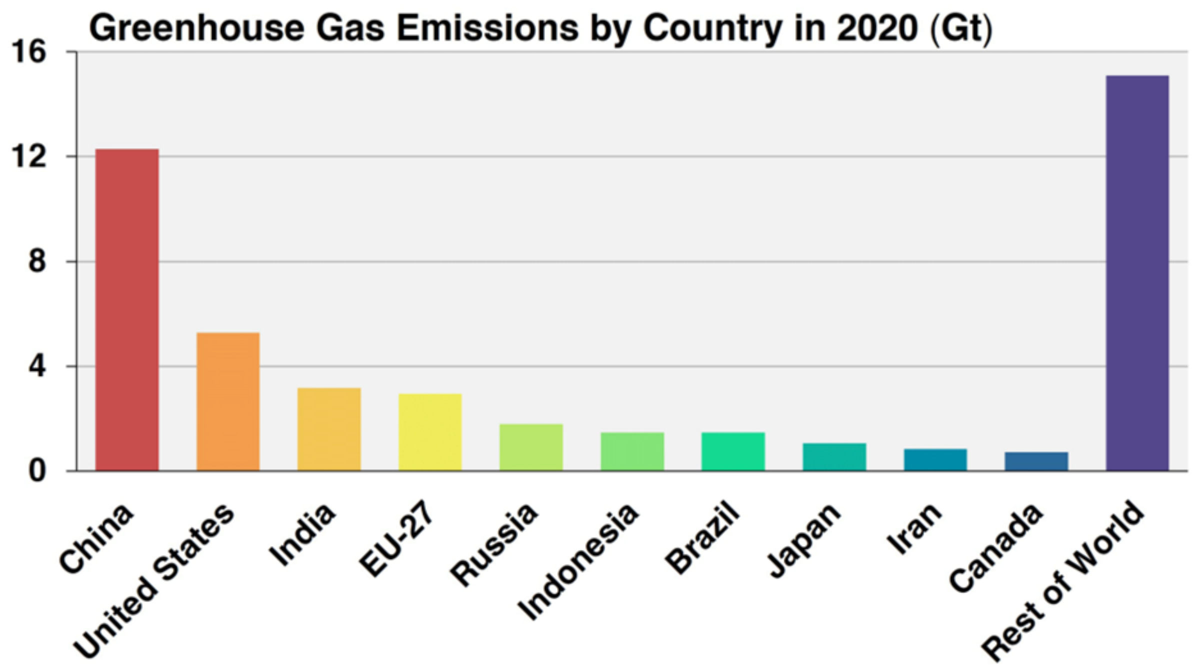
- CO_2 is the primary greenhouse gas contributing to global warming

- Power plants and industrial processes are significant sources of emissions

Importance of CCS

- - CCS as a vital strategy for reducing greenhouse gases.
- - Focus on post-combustion CO_2 capture, which captures CO_2 from flue gases.





Background:
Post-Combustion Carbon Capture

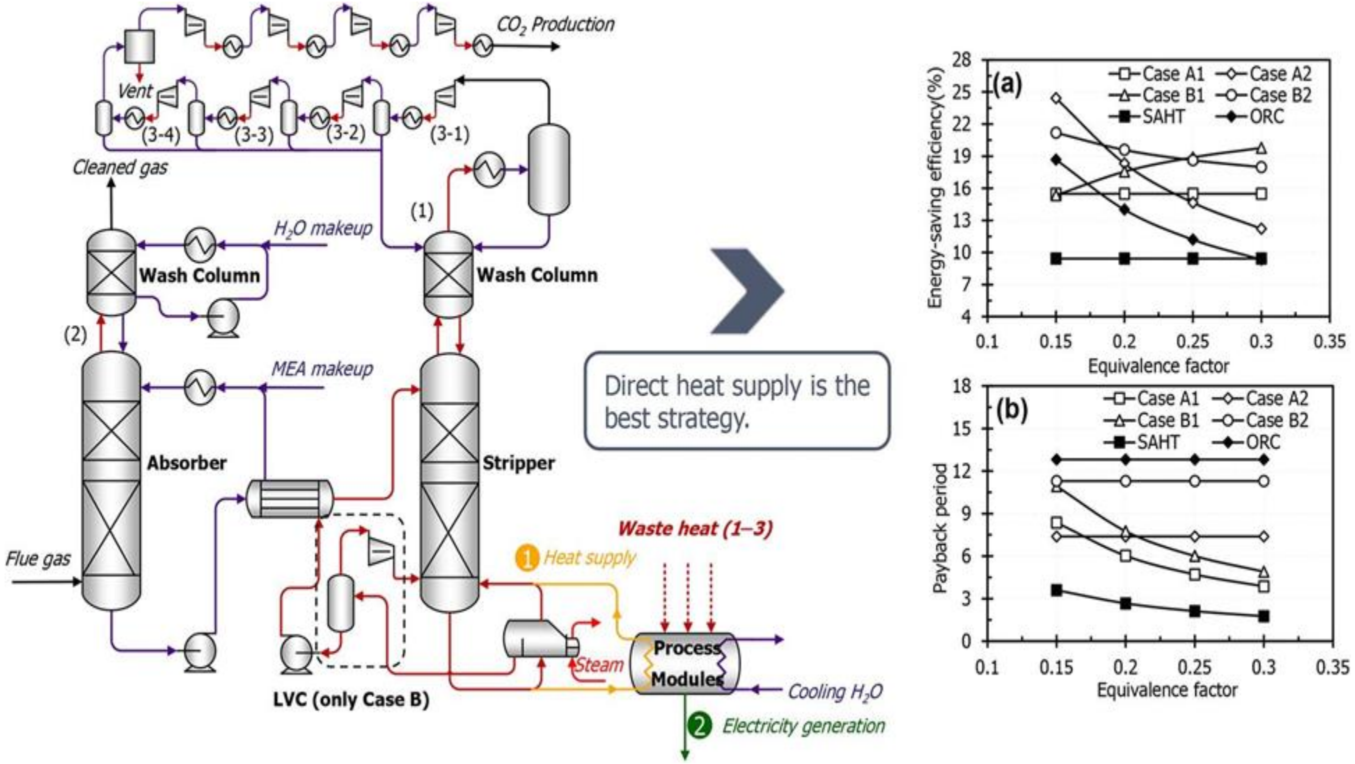
- Used in power plants to capture CO_2 after fuel combustion.

  - Conventional techniques like amine scrubbing: limitations in large-scale use (high energy consumption, solvent degradation).

Savings-to-investment ratio (SIR) and payback period (PBP) depended on EF and electricity prices

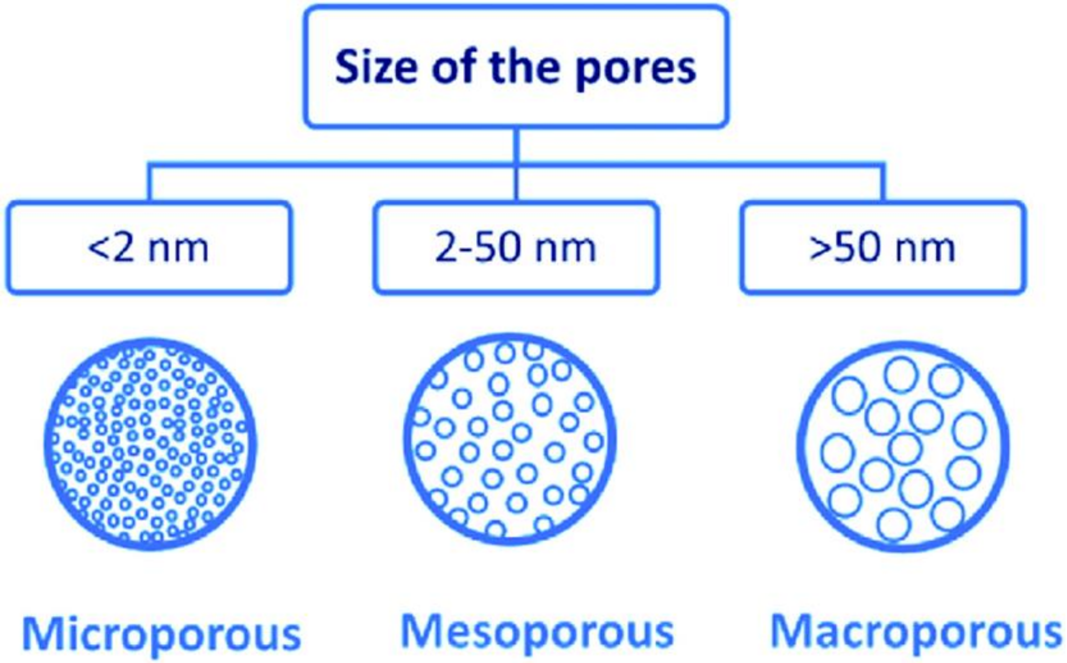
Need for Advanced Solutions

  - Current technologies are not energy-efficient or economically viable for long-term

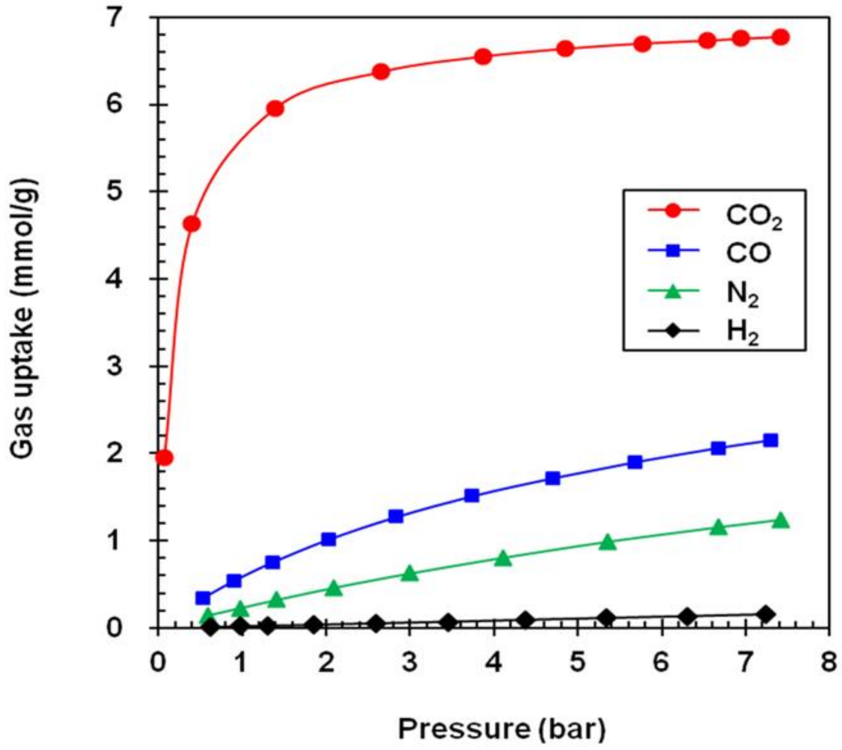


Zeolites in CCS:
Advantages over conventional techniques (lower energy consumption, material stability).

tunable pore sizes, high adsorption capacity selective CO_2 separation



Molecular sieving and diffusion studies in gas separation by zeolites



Problem Statement

Challenges in Current CO_2 Capture Technologies leading to increase in atmospheric CO2 concentration

- High energy consumption and operating costs in solvent-based systems.
- Limitations in scalability for industrial applications.

Need for Efficient Solutions

- There's a pressing need to improve the efficiency and cost-effectiveness of CCS systems
- **Key Question**: How can zeolite-based membranes enhance post-combustion CO_2 capture while minimizing energy and operational costs?

Research objectives

Primary objective

- To Investigate the gas adsorption and diffusion dynamics in zeolite-based membranes for enhanced post-combustion CO_2 capture

Specific Objectives

i. To optimize CO_2 selectivity and separation efficiency in zeolite-based membranes.

ii. To reduce energy consumption during the CO_2 capture and regeneration process.

iii. To evaluate the economic and environmental feasibility of using zeolite membranes in large-scale CCS applications

Hypothesis

Working Hypothesis

- Zeolite-based membranes can outperform conventional CO_2 capture techniques by providing higher selectivity, efficiency, and lower energy demands for CO_2 separation and regeneration

Methodology

1. Experimental Setup

Zeolite Membrane Selection

Select zeolite membranes based on pore size, surface area, and adsorption characteristics.

- Measure CO_2 adsorption capacity using gas chromatography and breakthrough experiments.
- Evaluate diffusion rates through zeolite membranes using Fick's law.
- Analyze selectivity of CO_2 vs other gases (N_2, O_2) under various temperatures and pressures.

2. Modeling and Simulation

- Computational models to predict gas diffusion dynamics within zeolite pores.
- Simulate adsorption and regeneration cycles to assess energy efficiency

Theoretical Framework

Adsorption Theory

- Langmuir and BET isotherms for describing gas adsorption on zeolite surfaces

Diffusion Dynamics

- Fick's laws of diffusion to model gas transport through the zeolite membrane.
- The impact of pore size and structure on diffusion rates and selectivity

Expected Results

- **Efficiency Gains**

  - Zeolite membranes will show higher CO_2 selectivity and lower energy use for regeneration.

- **Economic Benefits**

  - The cost per ton of CO_2 captured will be reduced compared to conventional techniques.

- **Scalability**

  - Zeolite-based membranes will demonstrate potential for large-scale applications in industrial settings.

Significance of the Study

- **Contribution to CO_2 Capture Technologies**

  - This study will advance the development of more efficient and cost-effective CO_2 capture systems.

- **Environmental Impact**

  - Successful implementation could significantly reduce greenhouse gas emissions.

- **Industry Relevance**

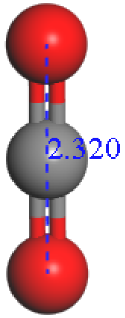
  - Findings can be applied to power plants, cement production, and other industries with high CO_2 output.

Conclusion

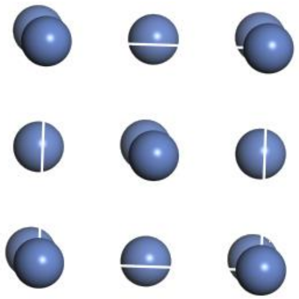
- Zeolite-based membranes offer a promising alternative to traditional CO_2 capture methods.
- They enhance selectivity, reduce energy demands, and present a sustainable solution for long-term CO_2 capture

Backup

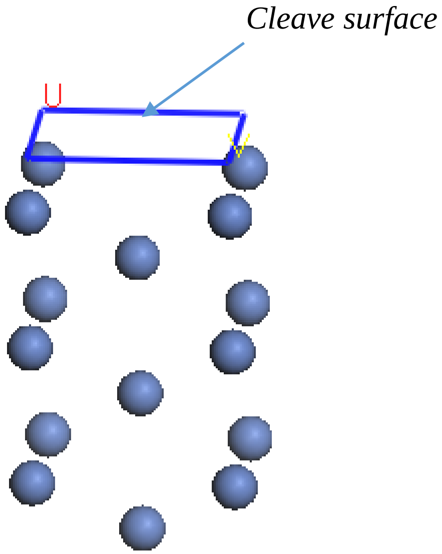
High-Throughput Evaluation of Earth abundant metal Catalysts for CO2 conversion to methane Using Machine Learning and Molecular Simulations



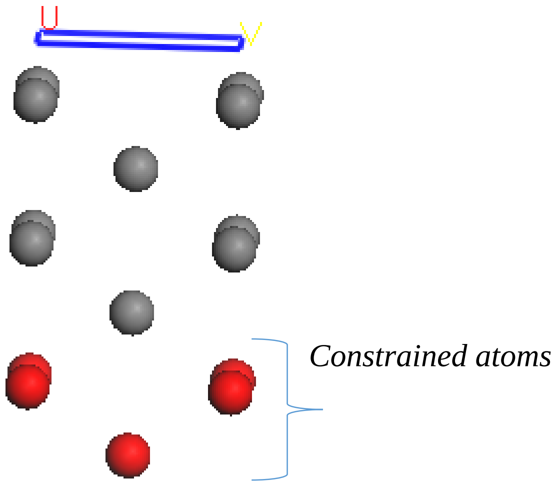
a) CO2 molecule *(O-O bond length = 2.320 Ang)*



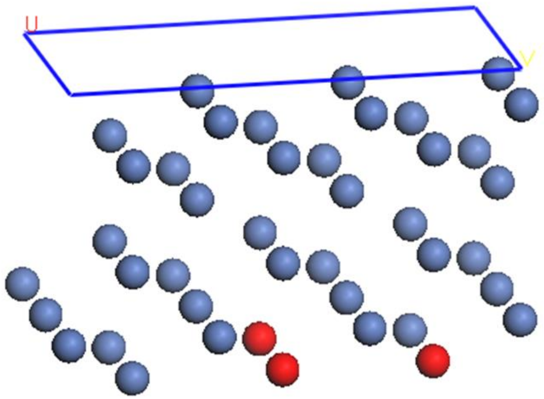
b) Ni catalyst



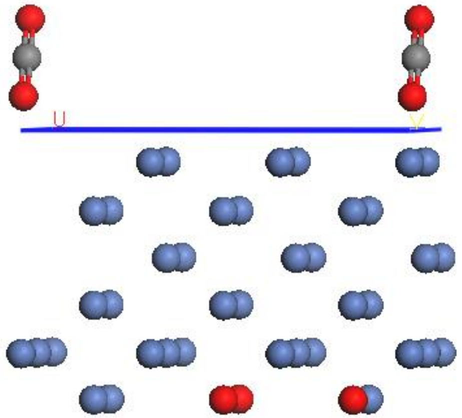
c) Ni catalyst with the cleaved surface



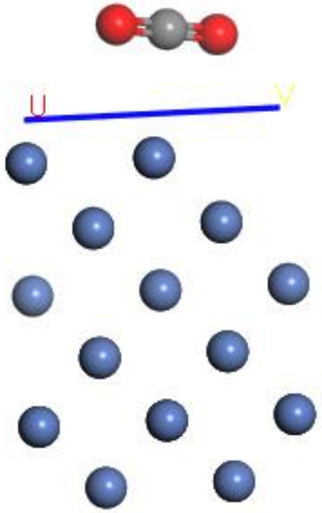
d) Constrained atoms are shown in red



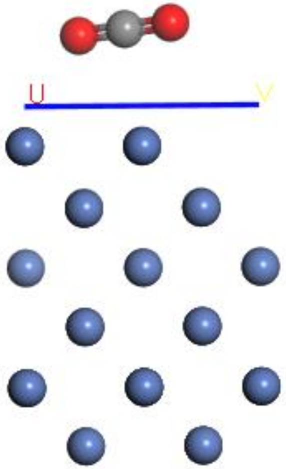
a) Optimized 3x2 Ni structure



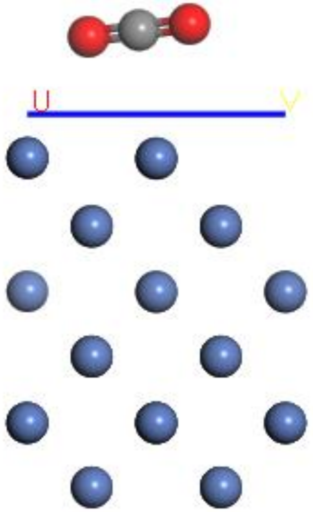
b) Perpendicular orientation on the surface



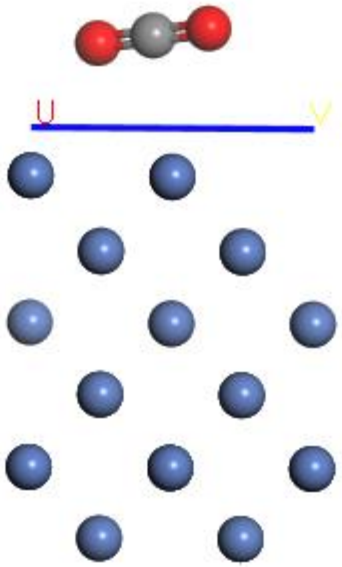
a) BE = -9.75490171eV



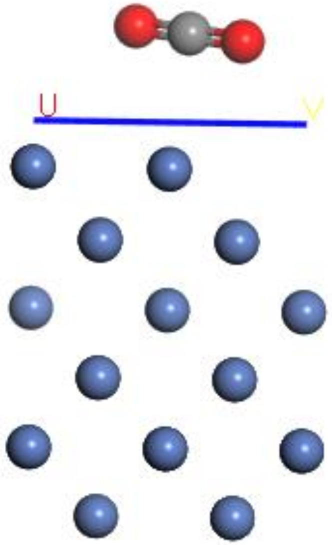
b) BE = -9.74915627eV



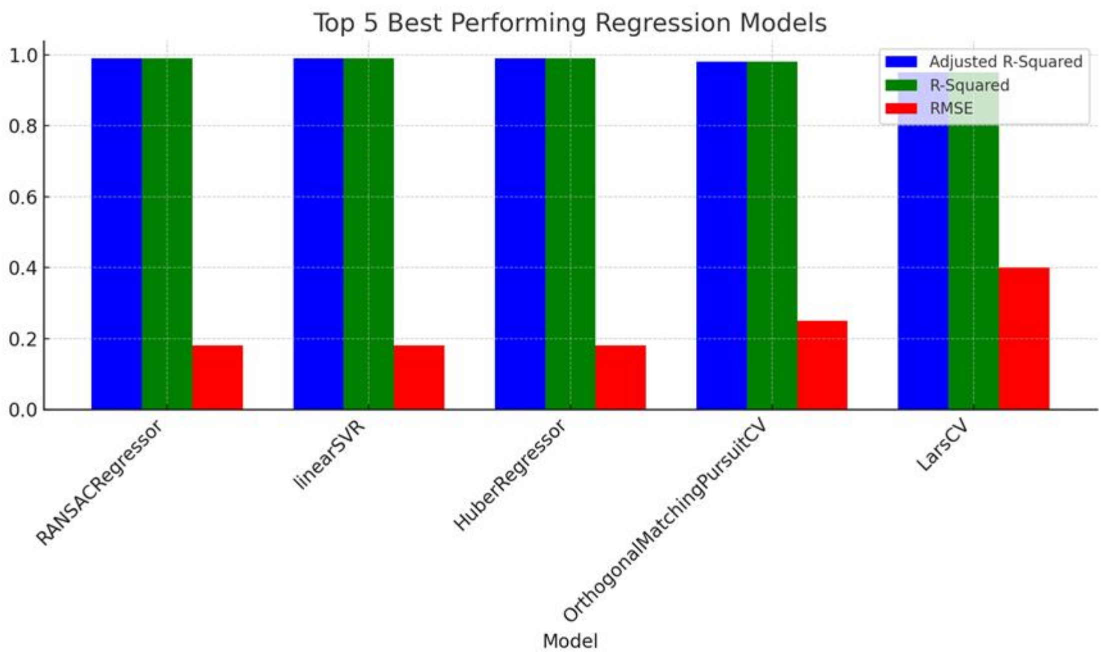
c) BE = -9.75611590eV

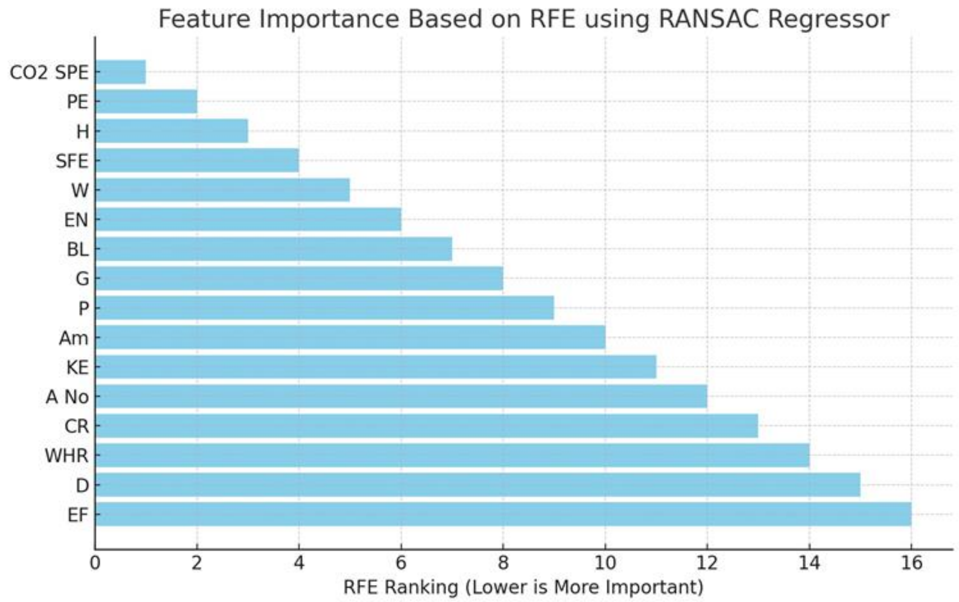


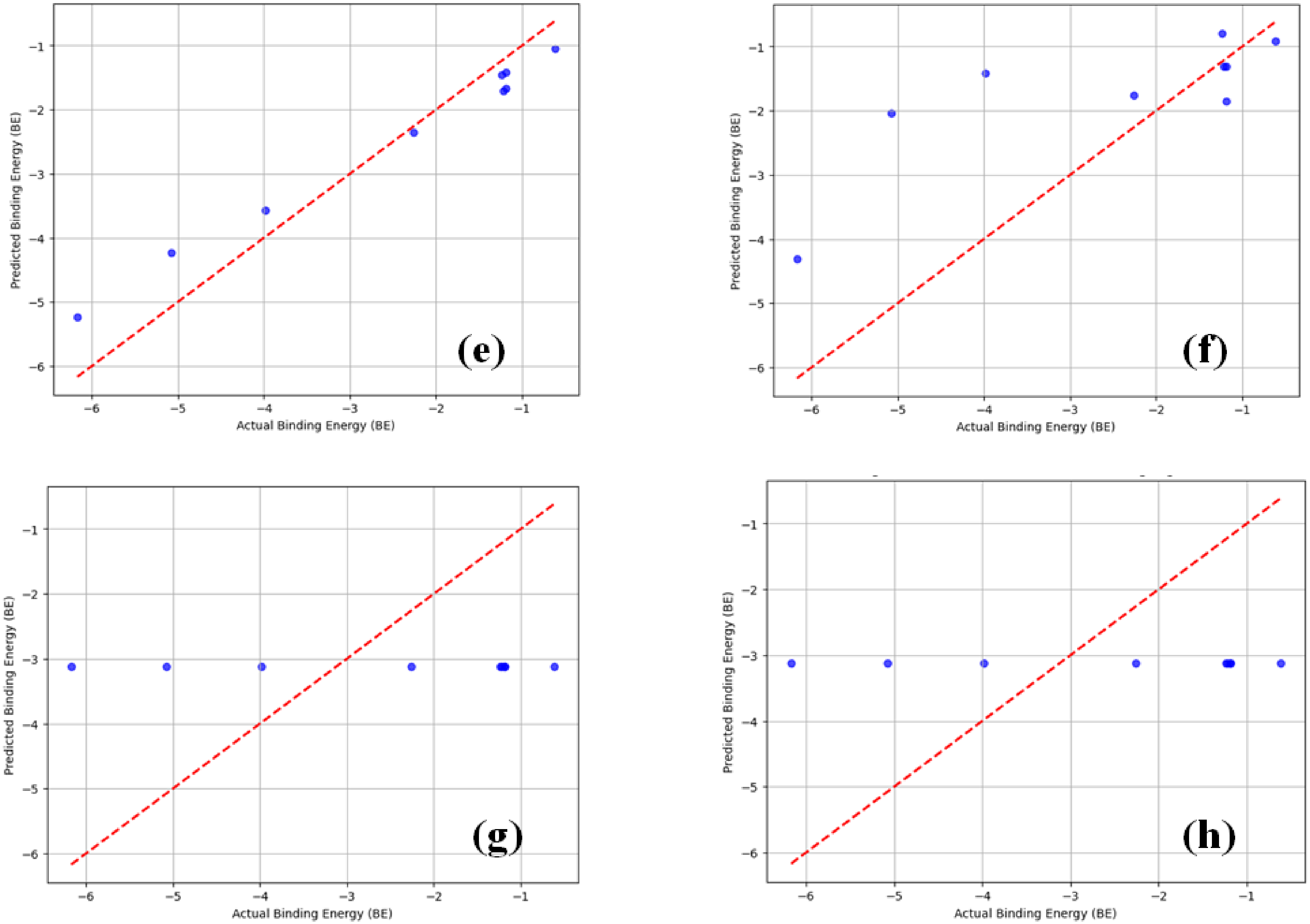
d) BE = -9.75088002eV

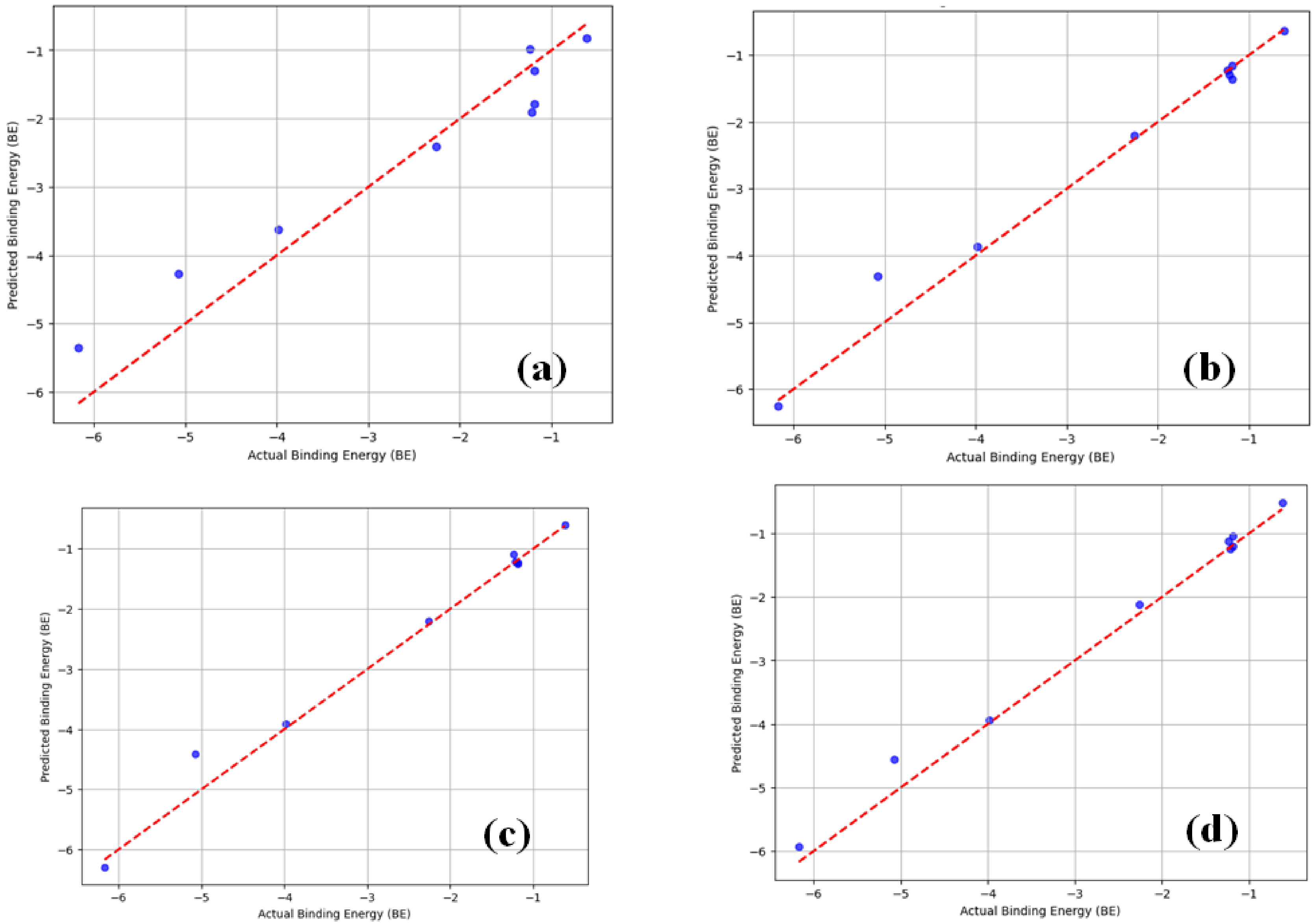


e) BE = -9.74872344eV


Top 5 Best Performing Regression Models
Adjusted R-Squared
R-Squared
RMSE
1.0
0.8
0.6
0.4
0.2
0.0
RANSACRegressor
linearSVR
HuberRegressor
OrthogonalMatchingPursuitCV
LarsCV
Model


Feature Importance Based on RFE using RANSAC Regressor
CO2 SPE
PE
H
SFE
W
EN
BL
G
P
Am
KE
A No
CR
WHR
D
EF
0
2
4
6
8
10
12
14
16
RFE Ranking (Lower is More Important)


(e)
(f)
(g)
(h)
Predicted Binding Energy (BE)
Actual Binding Energy (BE)
−1
−2
−3
−4
−5
−6



(a)
(b)
(c)
(d)
Predicted Binding Energy (BE)
Actual Binding Energy (BE)
−1
−2
−3
−4
−5
−6