# Direct Air Reactive Capture and Conversion for Utility-Scale Energy Storage

FWP-FEW0277


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Lawrence Livermore National Laboratory


U.S. Department of Energy
National Energy Technology Laboratory
Carbon Management Project Review Meeting
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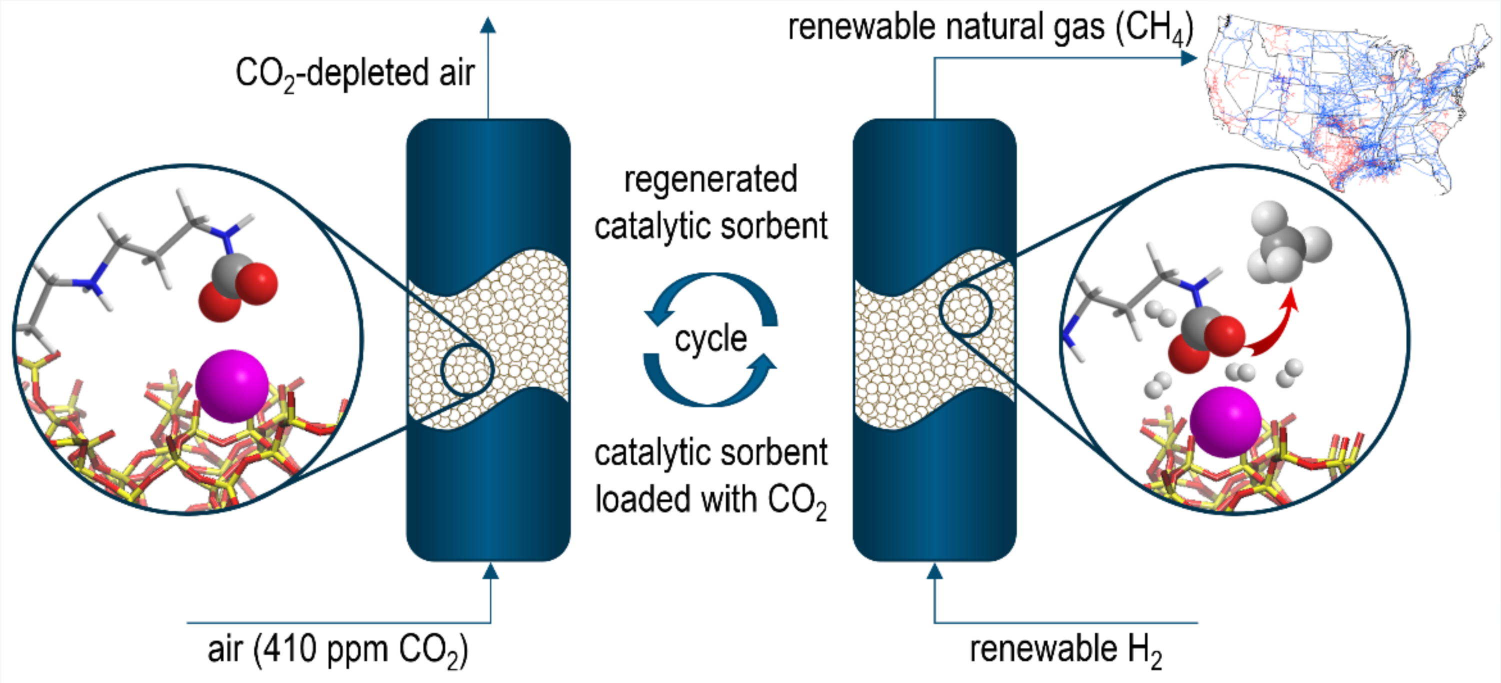
# Direct Air Reactive Capture and Conversion for Utility-Scale Energy Storage

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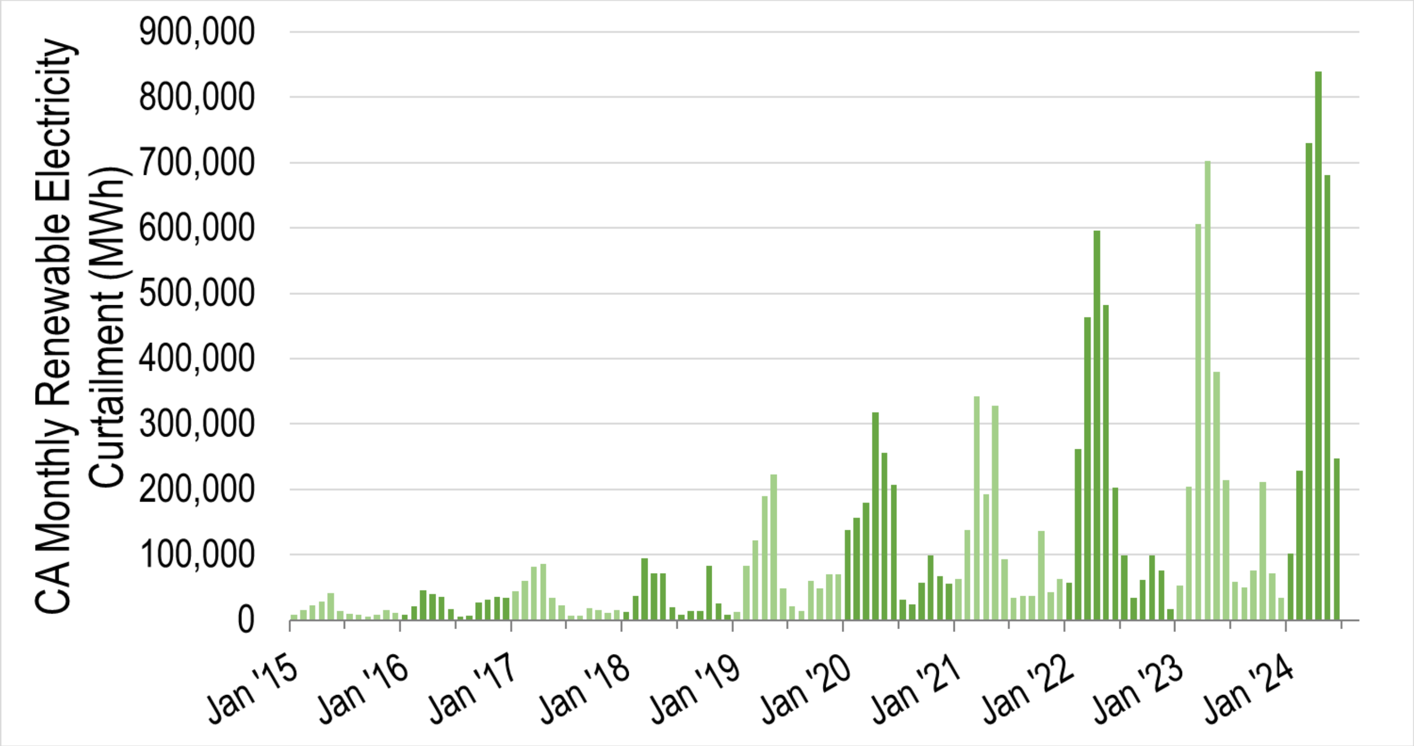
NATIONAL RENEWABLE ENERGY LABORATORY

***Reactive Capture & Conversion R&D***
***FEW0277:*** \$3,000k over FY22–FY24(+)
10/1/2021 – 12/31/2024
Project Manager: Gregory Imler

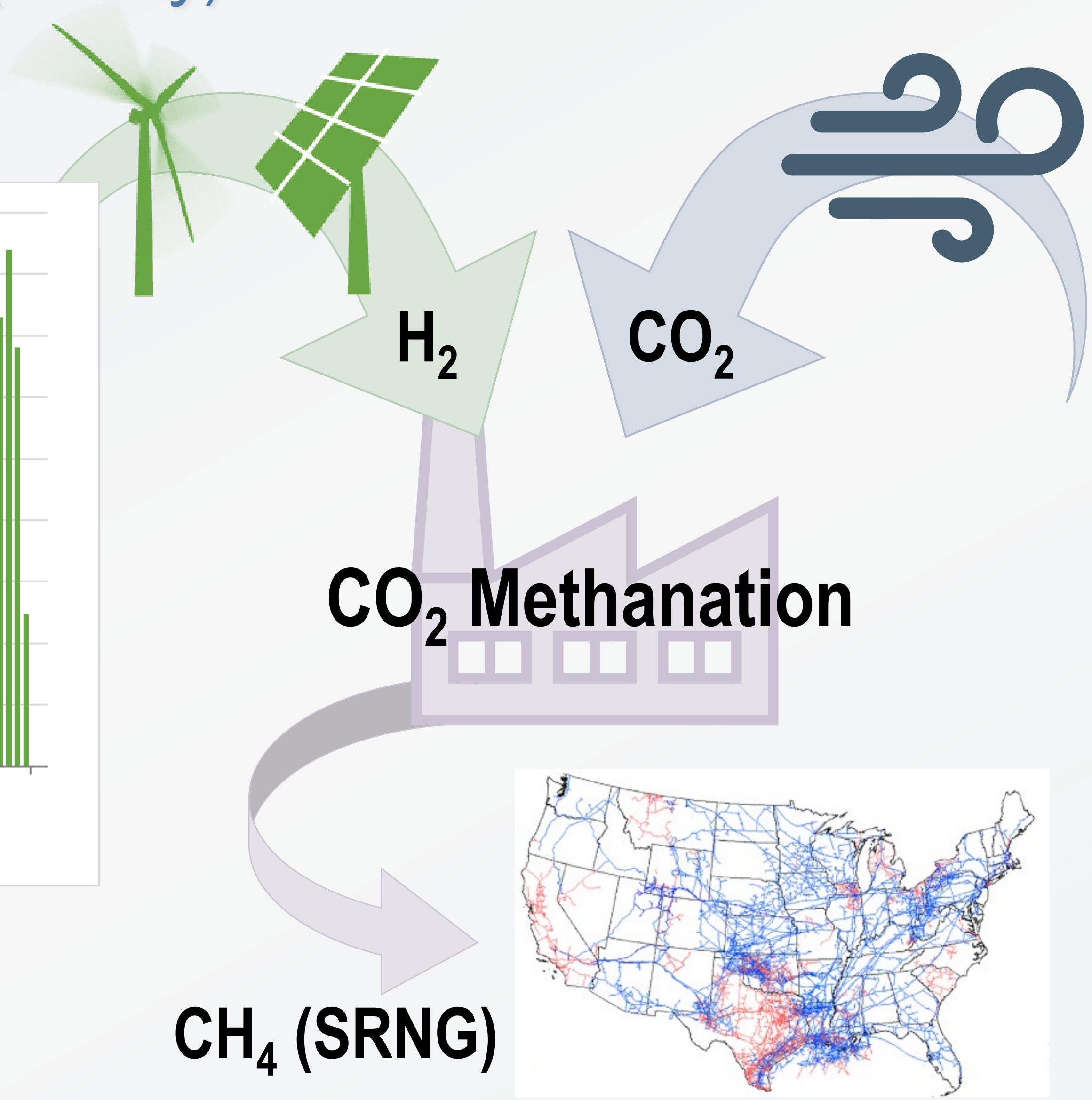
***Goal: develop dual-functional material and process for capturing $CO_2$ from the air and converting it to RNG***

Four parallel tracks in direct air capture materials synthesis/characterization, catalysts for $CO_2$ conversion, mechanistic investigations via *ab initio* simulations, and process modeling and systems analysis

# Methanation of $CO_2$ from the air can provide a distributable source of long-duration energy storage using a (nearly) carbon-neutral fuel

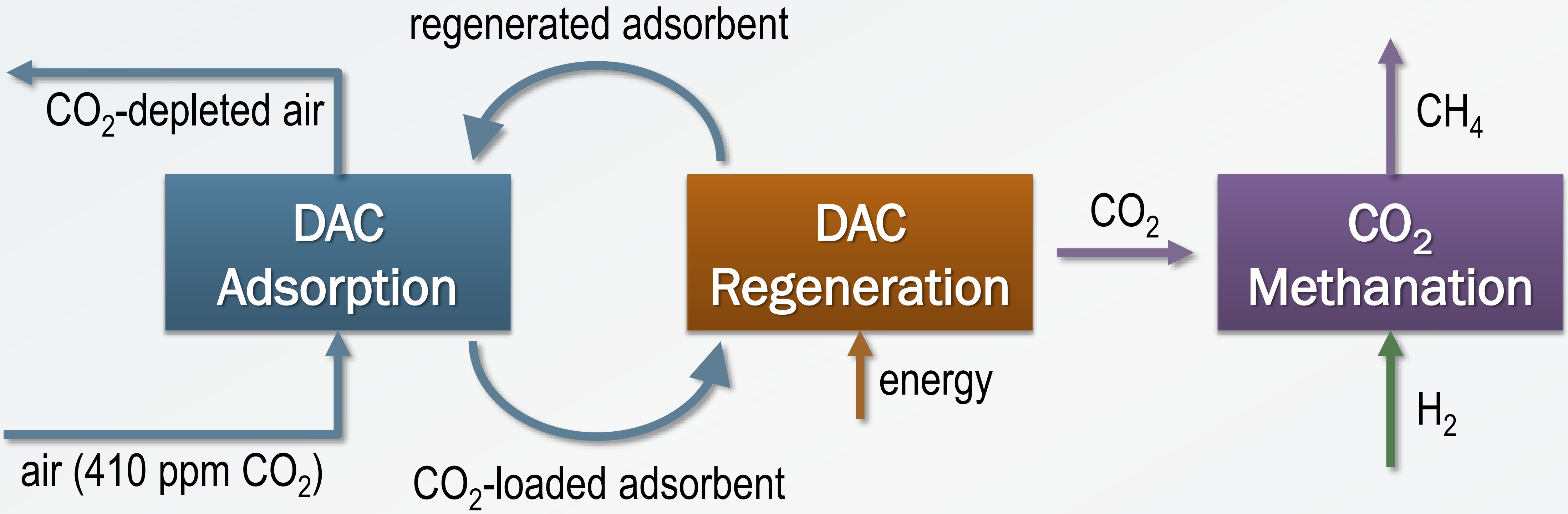



*Renewable electricity curtailed over the last year could have powered over 200,000 homes in CA*



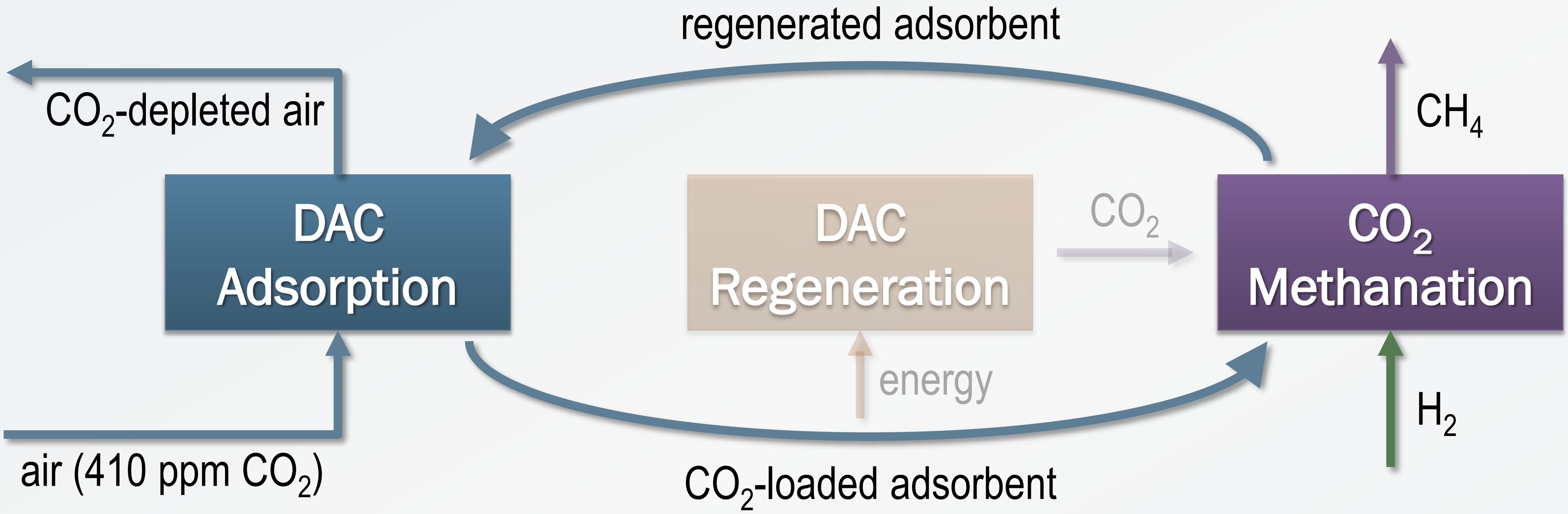
# Our goal is to develop a material and process to directly convert captured $CO_2$ into methane without explicitly requiring desorption

*Separate Direct Air Capture and $CO_2$ Methanation*



# Our goal is to develop a material and process to directly convert captured $CO_2$ into methane without explicitly requiring desorption

*Direct Air Reactive Capture and Methanation*



# Project Overview

### *Direct air capture*

- Graft capture agent on commercial oxides
- Evaluate adsorption performance (gravimetric and flow/breakthrough)

Measured DAC capacity and kinetics for hybrid materials

~~Q3, Q8~~

### *Catalytic methanation*

- Deposit highly dispersed metal catalysts
- Evaluate $CO_2$ conversion performance (continuous and cyclic)

Achieved high $CO_2$ conversion and $CH_4$ selectivity

~~Q4, Q9~~

Downselected materials and achieved stable performance with extended cyclic operation

~~Q6, Q11~~

### *Atomistic mechanism*

- Simulate interaction between capture agent and oxide surface
- Simulate interaction between captured $CO_2$ and metal catalyst surface
- Simulate interaction at triple solid phase boundary

Developed mechanism of bound-$CO_2$ methanation

~~Q5~~

### *Reactive capture analysis*

- Develop M&EB, TEA, LCA for baseline scenarios
- Develop reactive capture process model for comparison

Impact of fractional $CO_2$ conversion

~~Q8~~

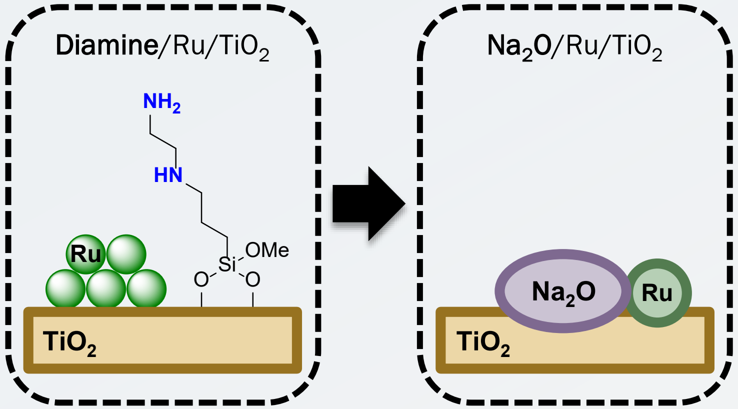
Demonstrated improvement for reactive capture

~~Q6~~, **Q13**

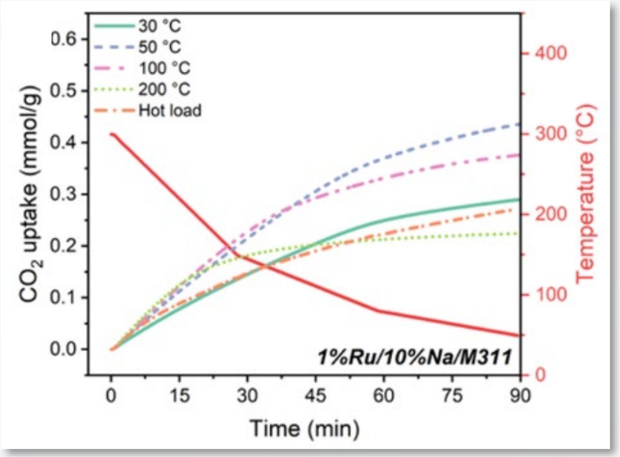
***End-of-project success criteria:*** demonstrate 15% relative improvement in RNG Minimum Fuel Selling Price and Carbon Intensity using a reactive capture process compared to baseline scenario(s)

# Our project has developed materials and protocols for thermal reactive capture, converting $CO_2$ from the air into methane

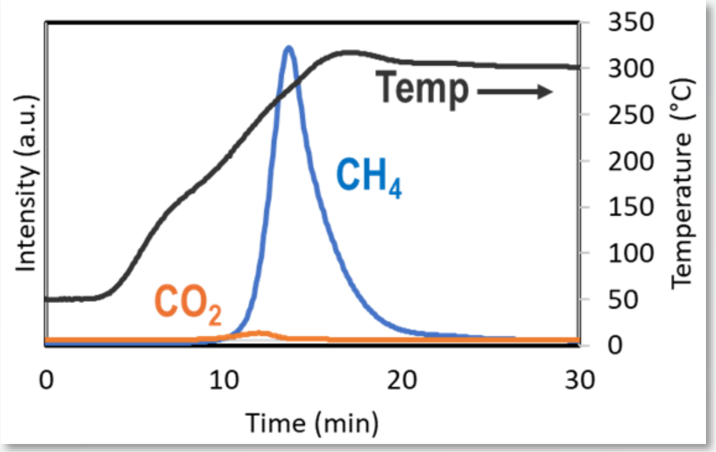
*Budget Period 1* *Budget Period 2*

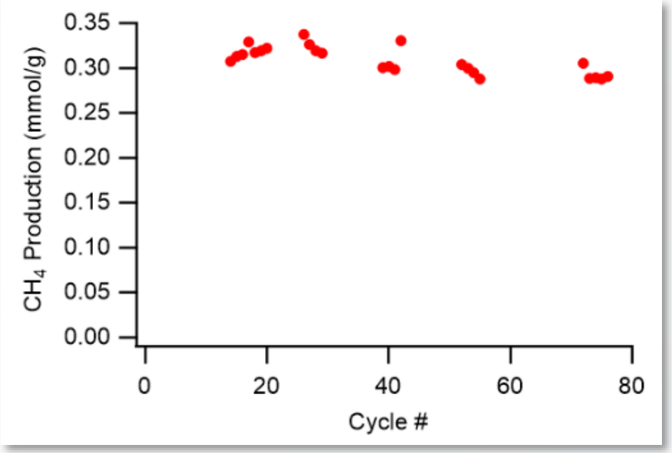



## *Effective air adsorbents*

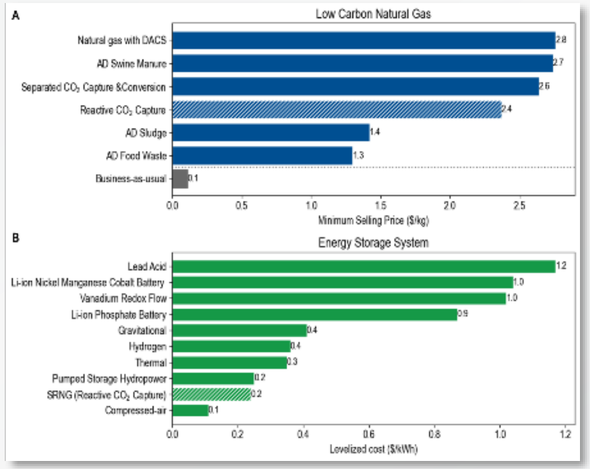


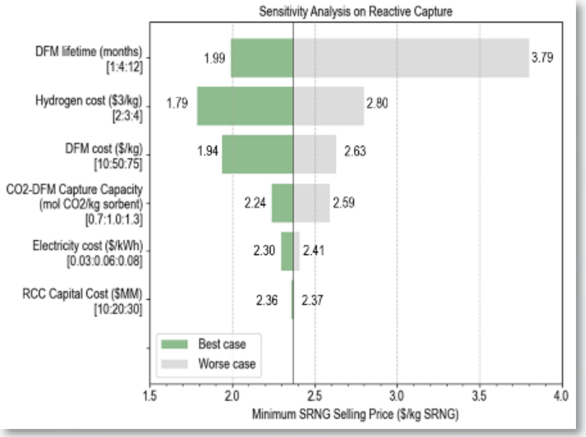

## *Materials/process for high-$CO_2$-conversion methanation*



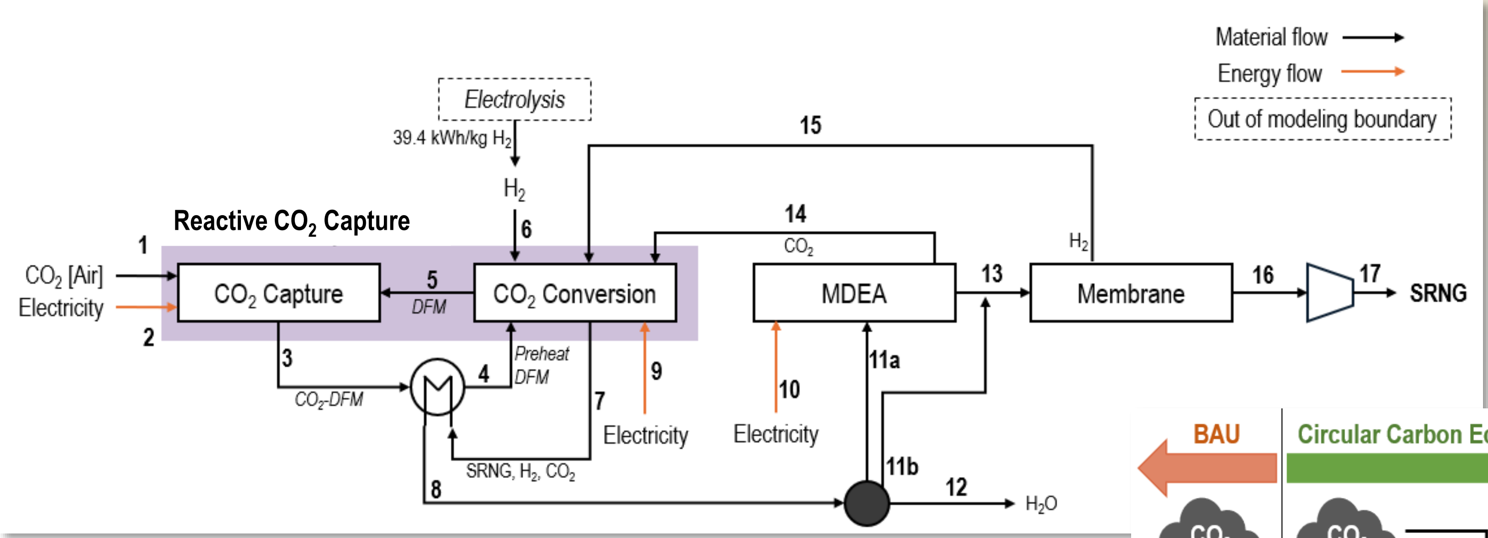



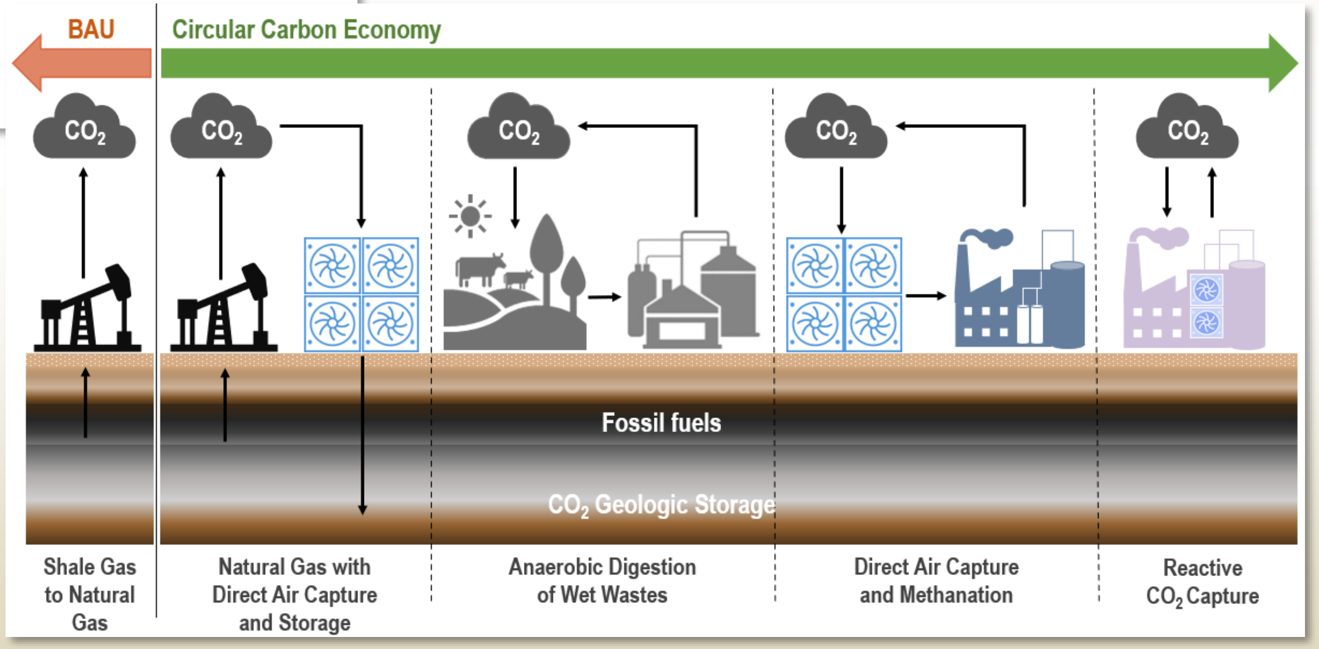

## *Process modeling and analysis to identify benefits*



# We developed a high-level process model for reactive capture and compared methods for creating renewable natural gas

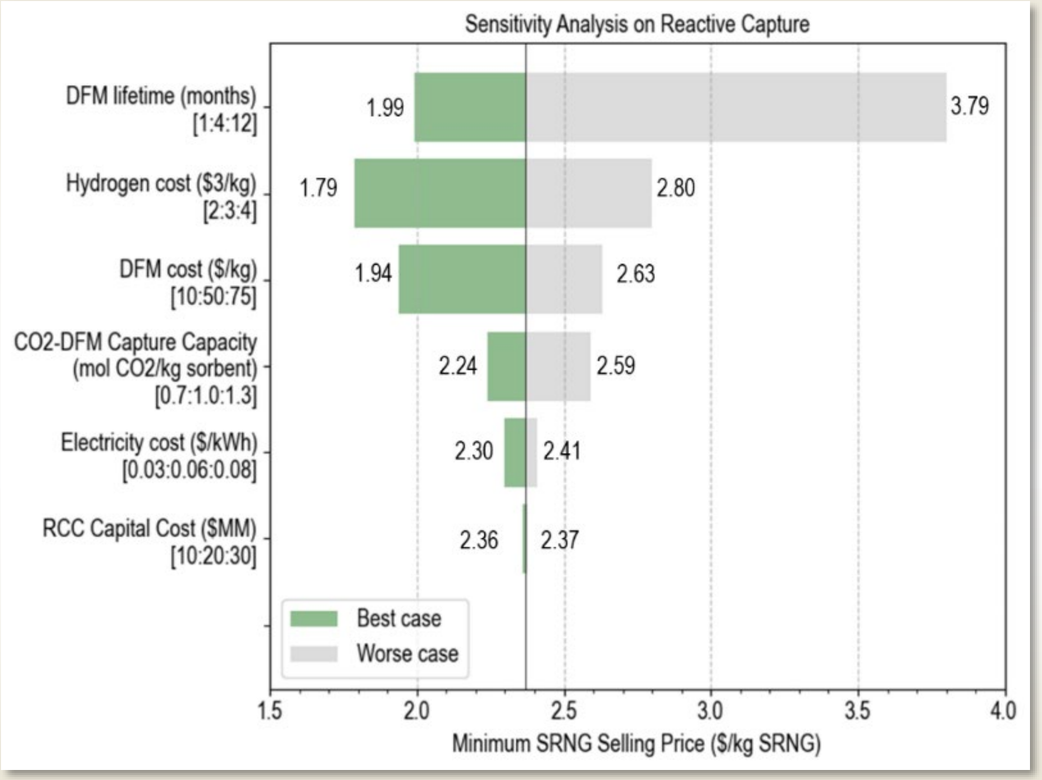


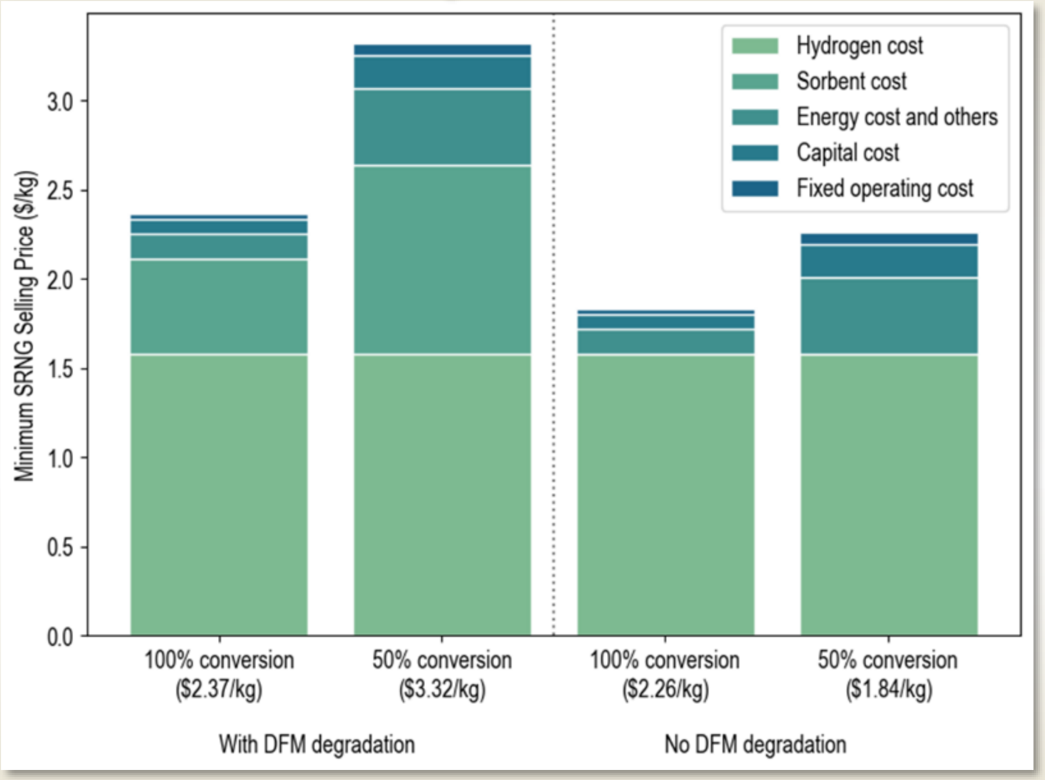






A. Aui, S.H. Pang, et al. *in preparation*

# Milestone 8: Demonstrated impact of $CO_2$ adsorption capacity and fractional conversion on RNG MFSP

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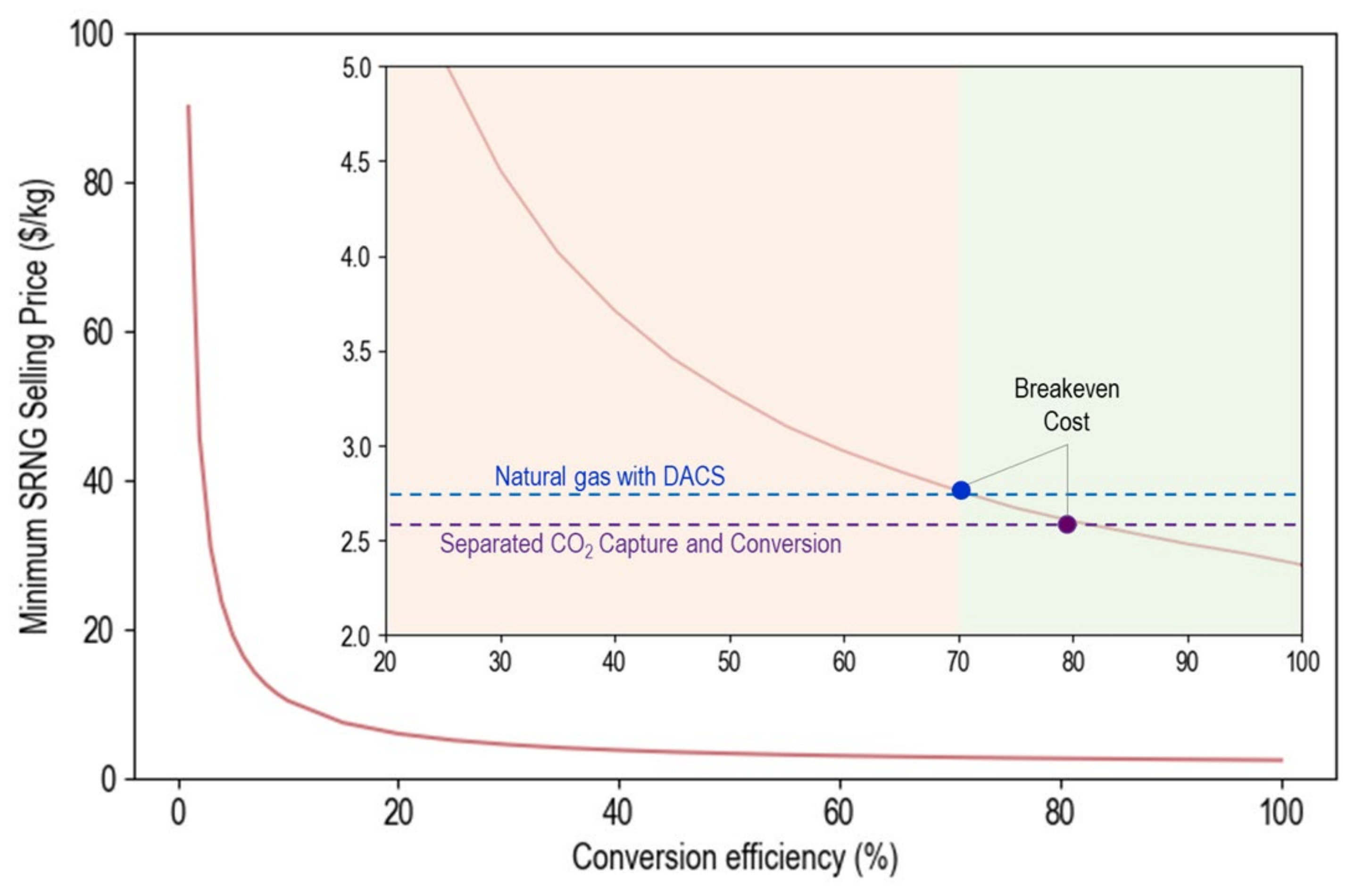
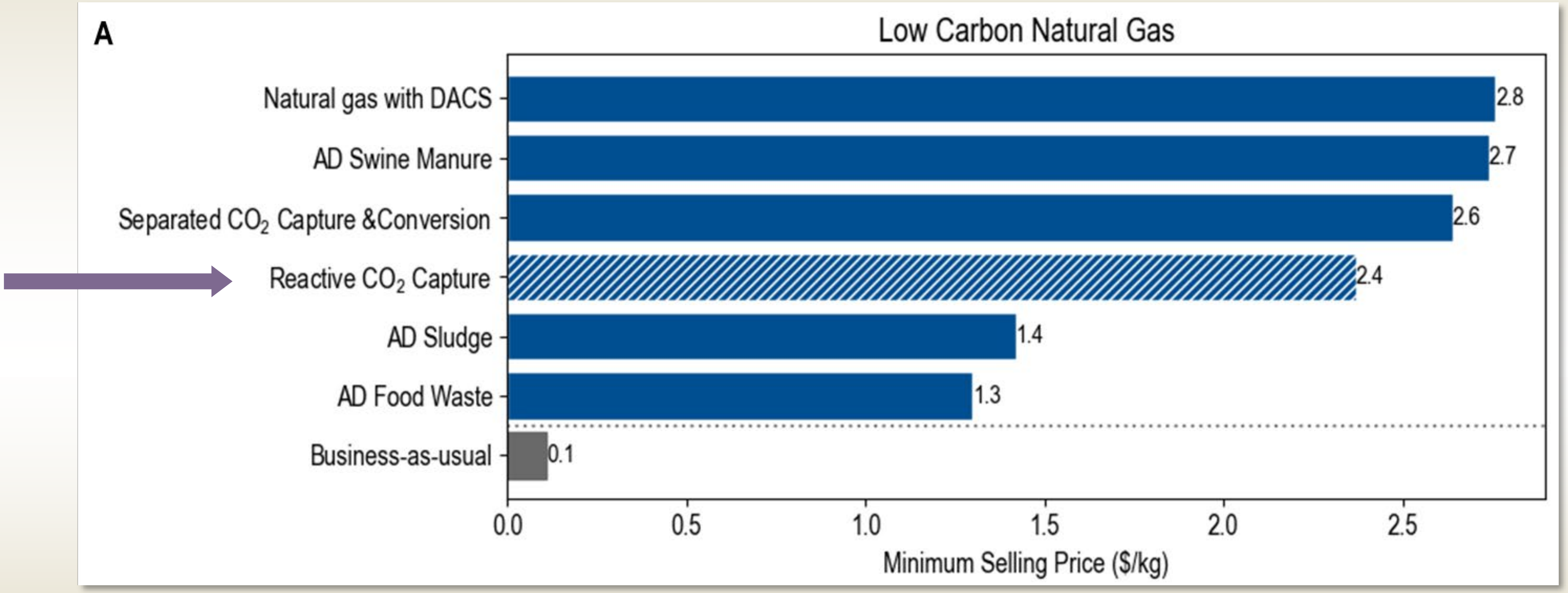
# The economics of reactive capture are dependent on achieving high conversion of $CO_2$ to avoid downstream separations






A. Aui, S.H. Pang, et al. *in preparation*

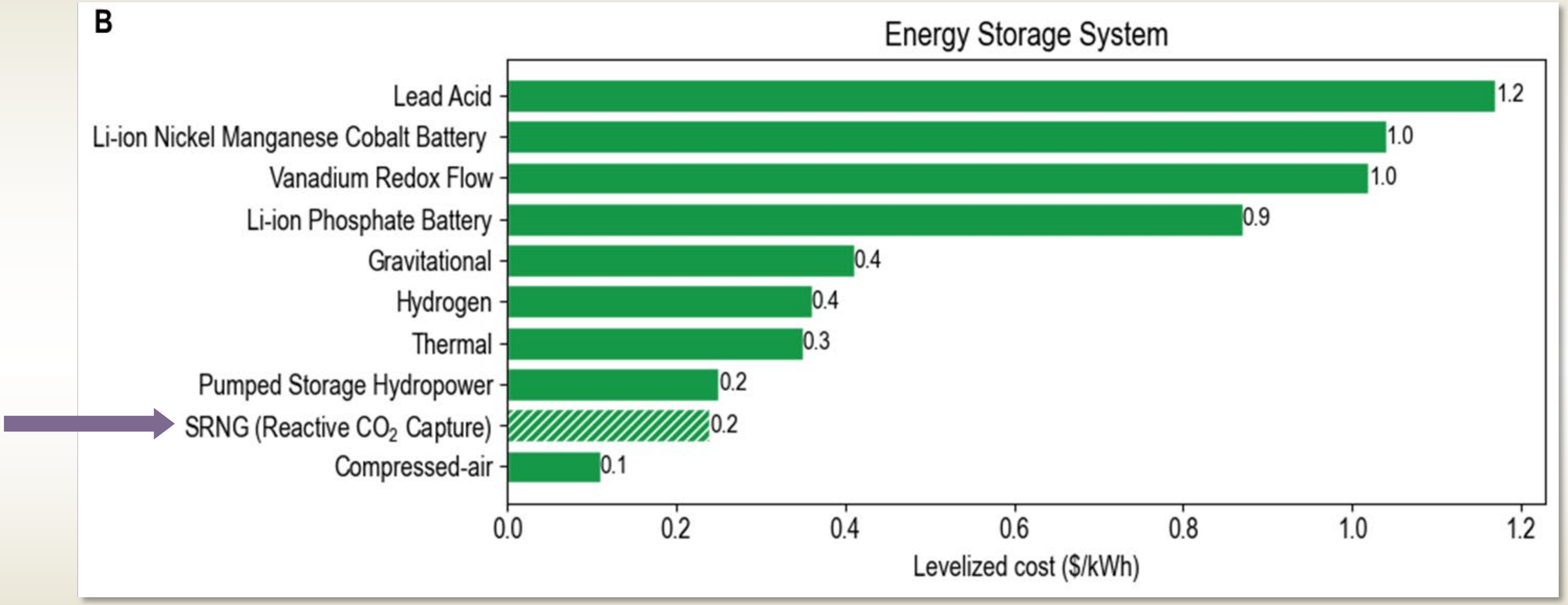
# Our reactive capture strategy is cost comparable to other methods for forming renewable natural gas






A. Aui, S.H. Pang, et al. *in preparation*

# Storing energy as methane created via reactive capture is competitive with other forms of long-duration energy storage

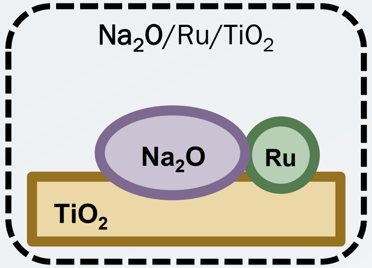


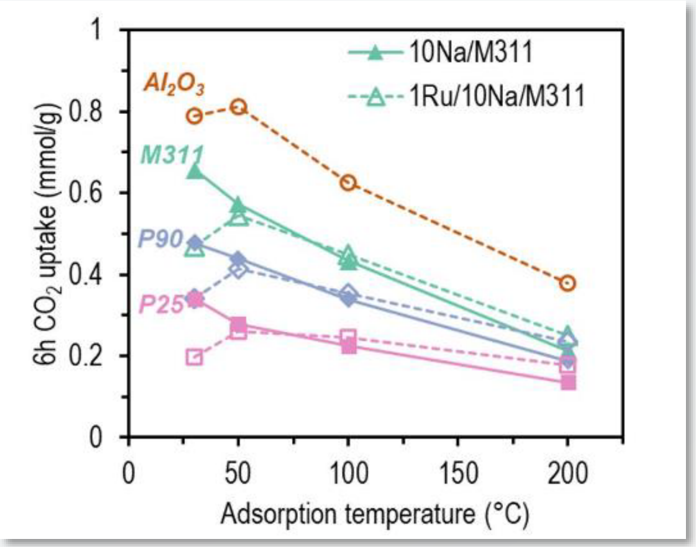

***If properly executed, reactive capture to methane could provide inexpensive long-duration energy storage***

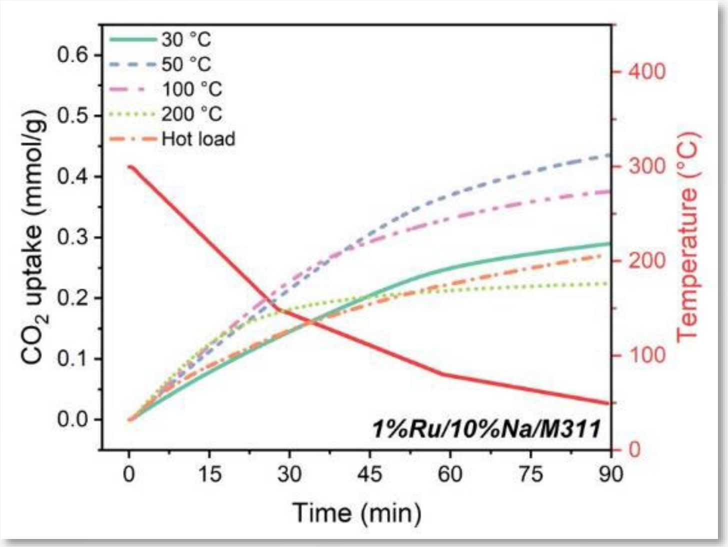


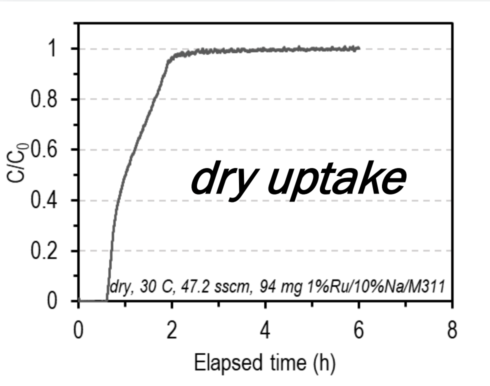
A. Aui, S.H. Pang, et al. *in preparation*

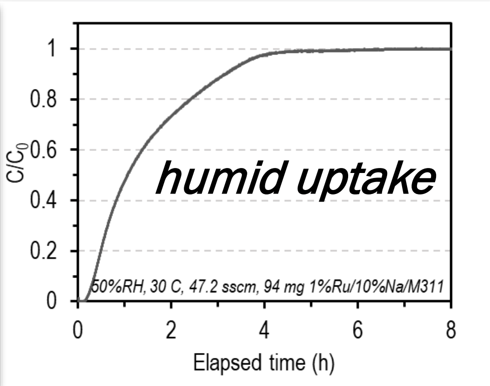
# Milestone 5: Measured DAC adsorption capacity >0.40 mol $CO_2$/kg



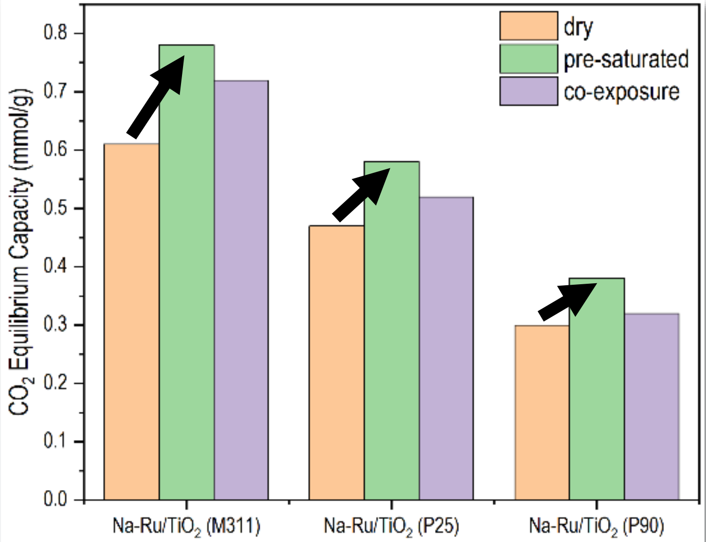



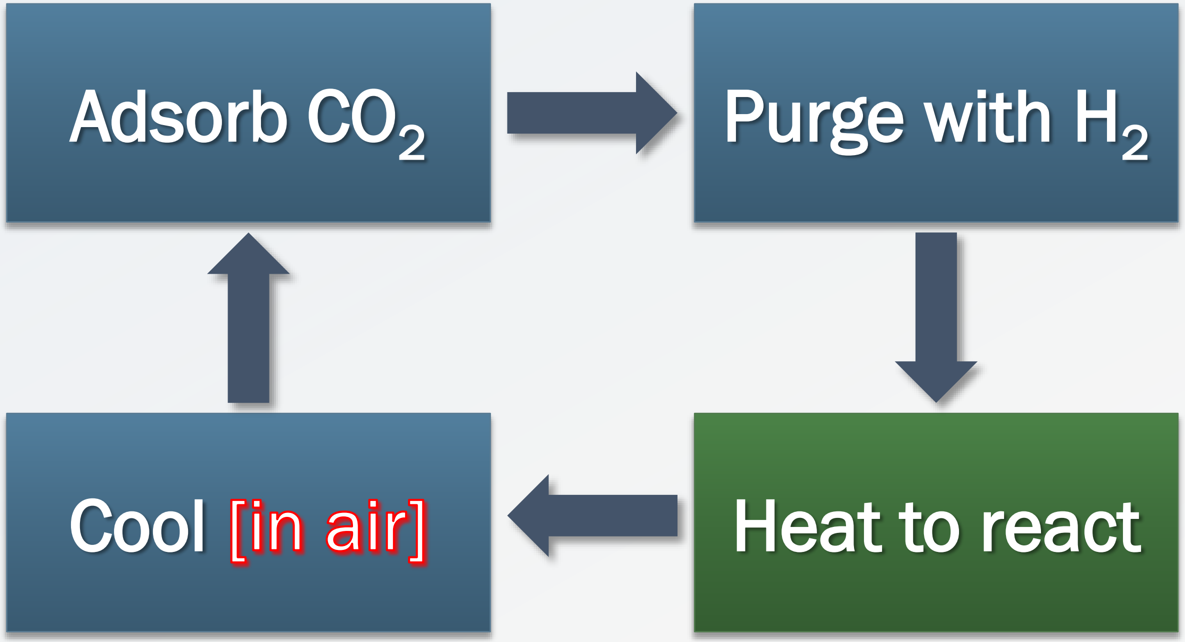



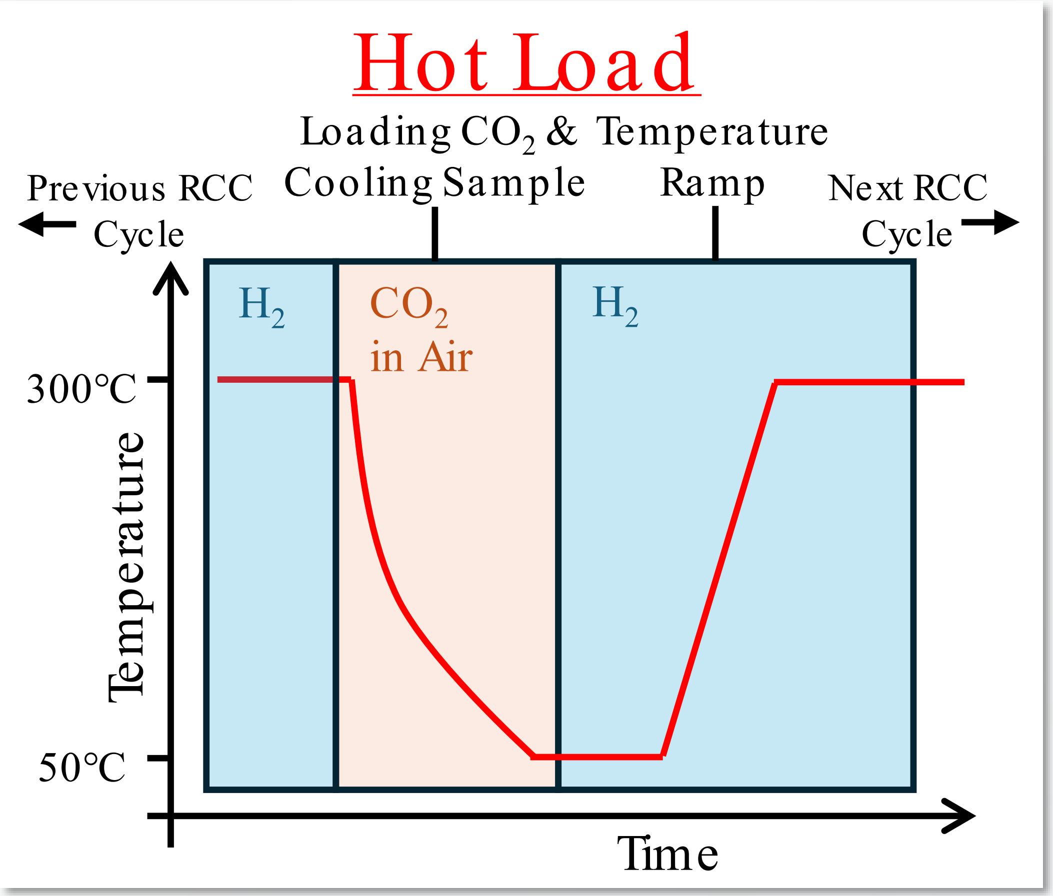




*Adsorption temperature or temperature profile impacts $CO_2$ uptake under DAC conditions*

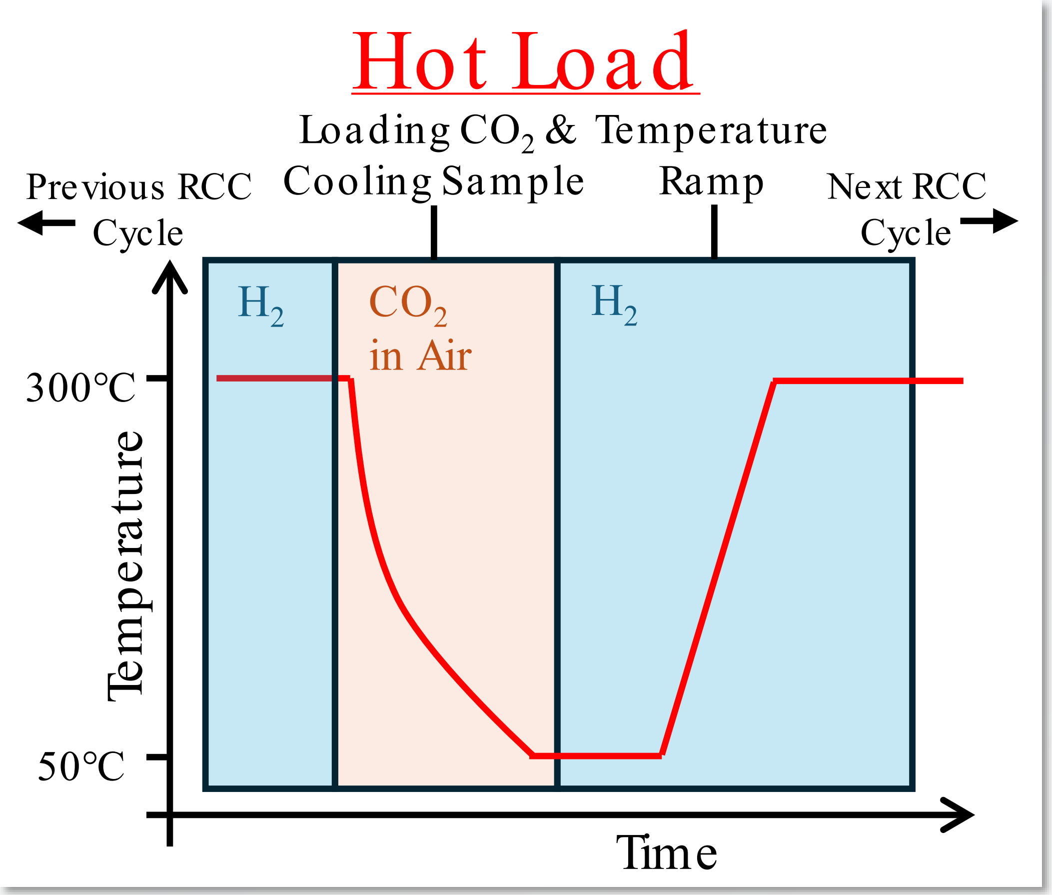


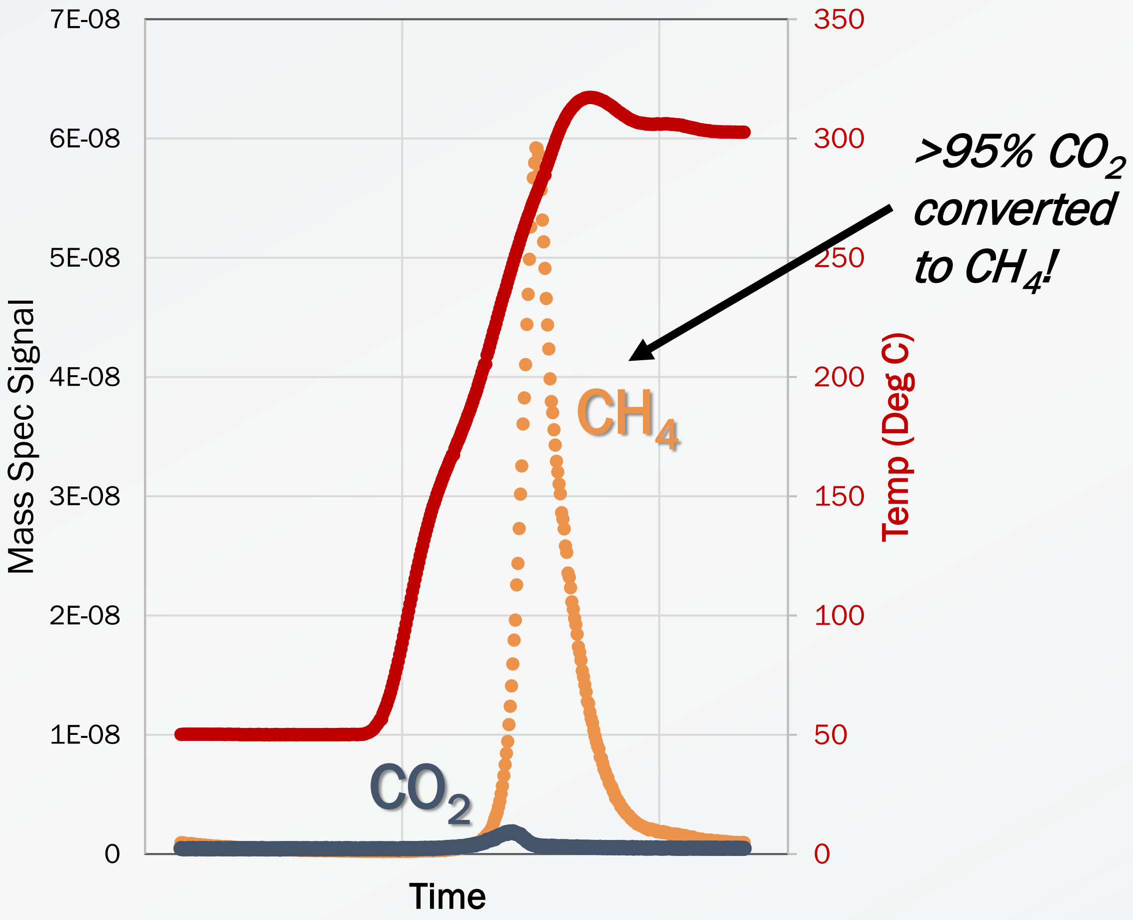
# A candidate reactive capture cycle exposes captured $CO_2$ to reactant gases while heating to convert it into products



# Milestone 6: Converted >50% of captured $CO_2$ into $CH_4$

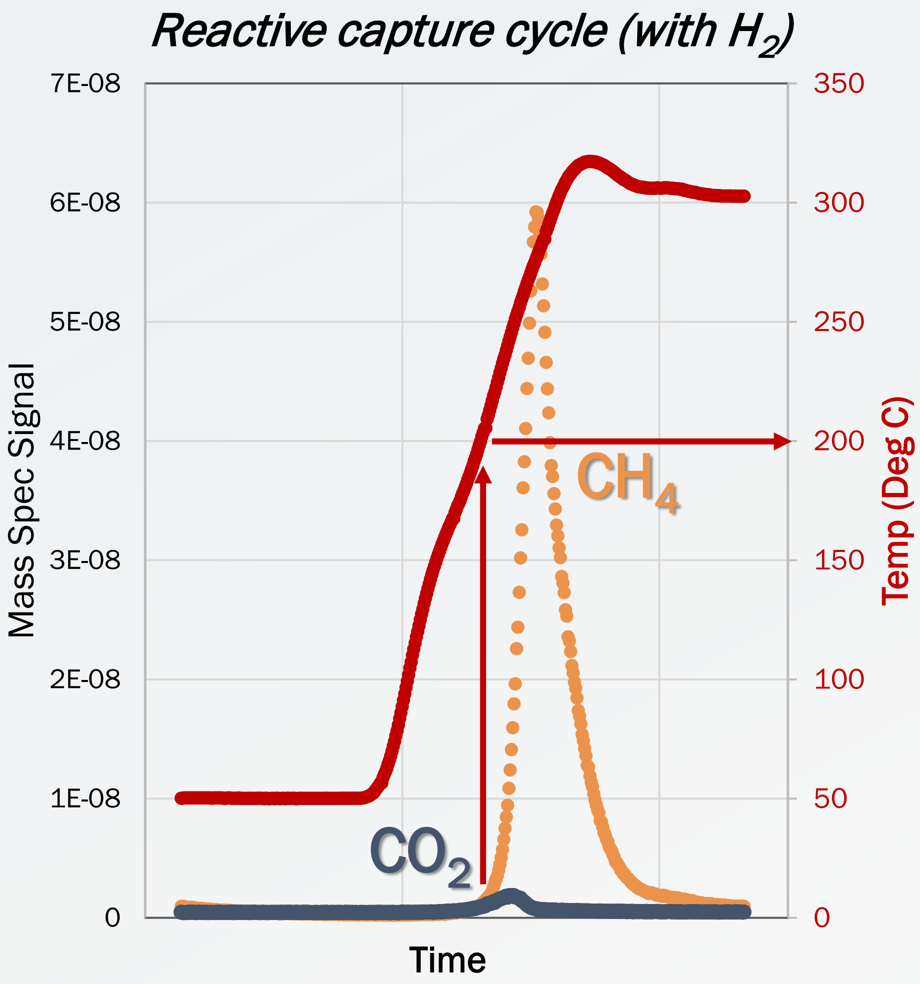


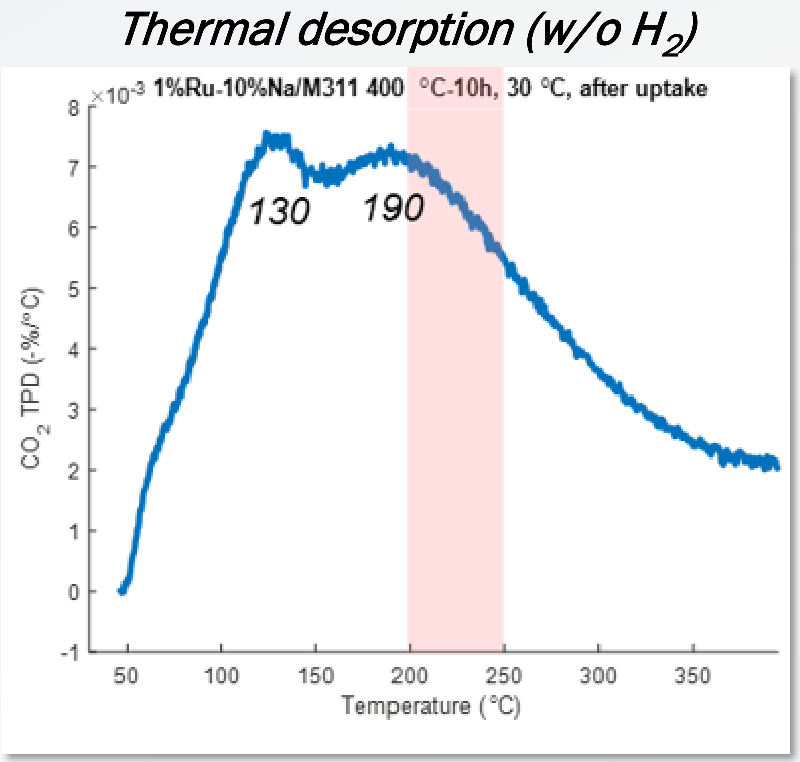



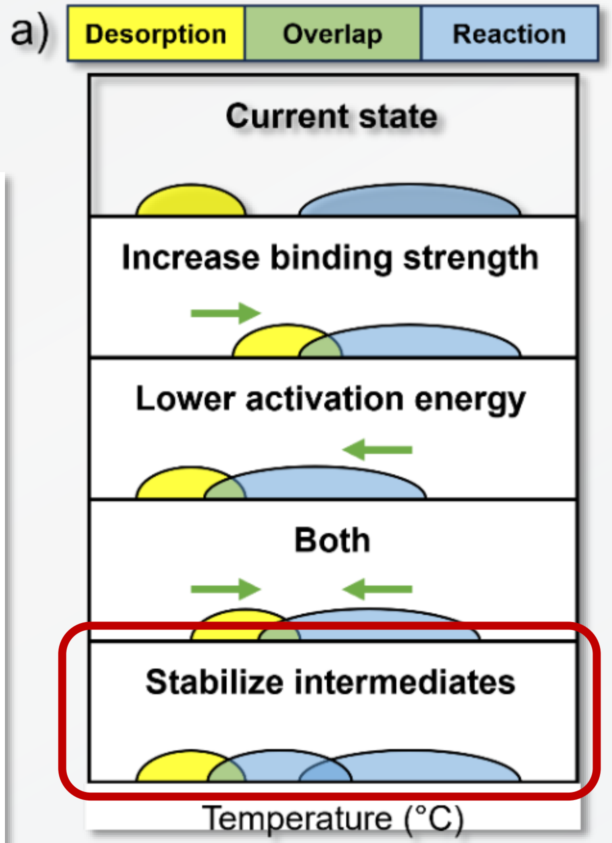



M. Rasmussen, S. Halingstad, M.M. Yung, S.H. Pang, et al. *in preparation*

# Formation of methane occurs at higher temperature than $CO_2$ desorption, suggesting formation of stable intermediate species



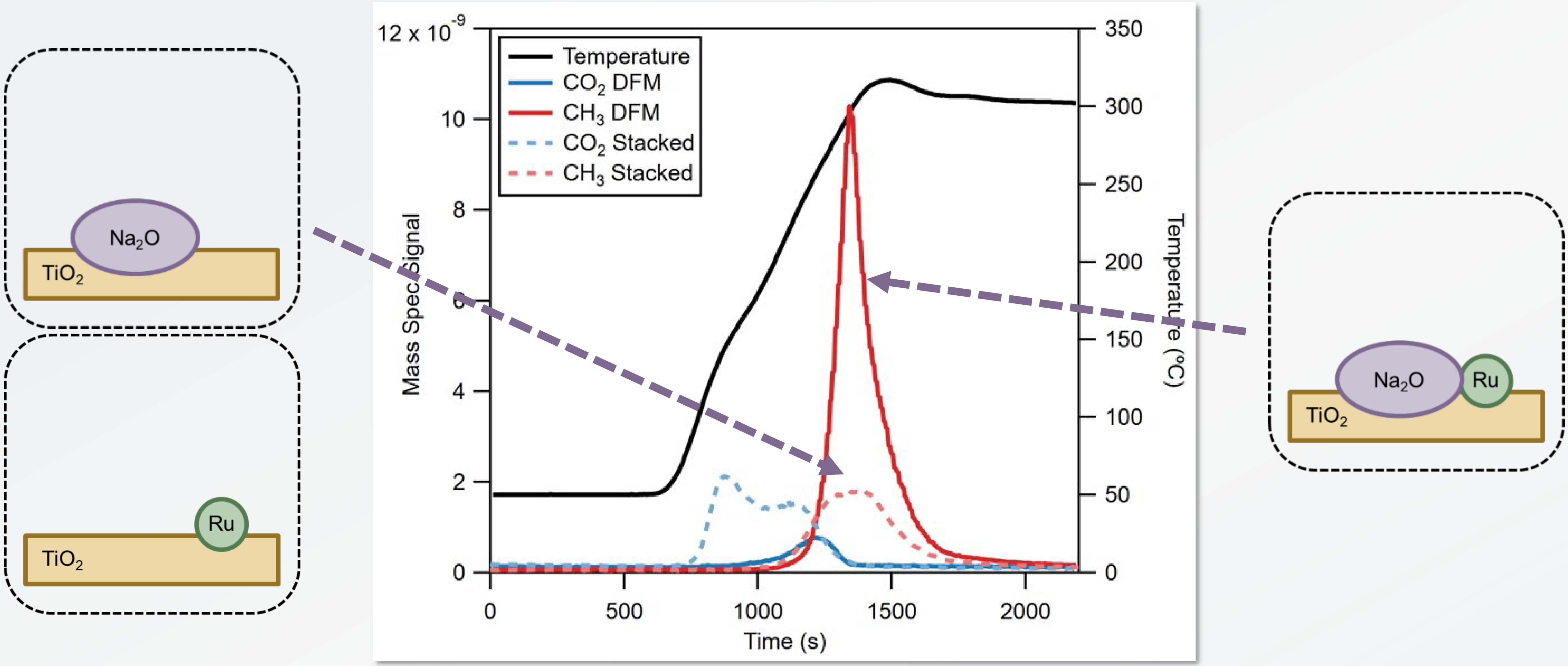





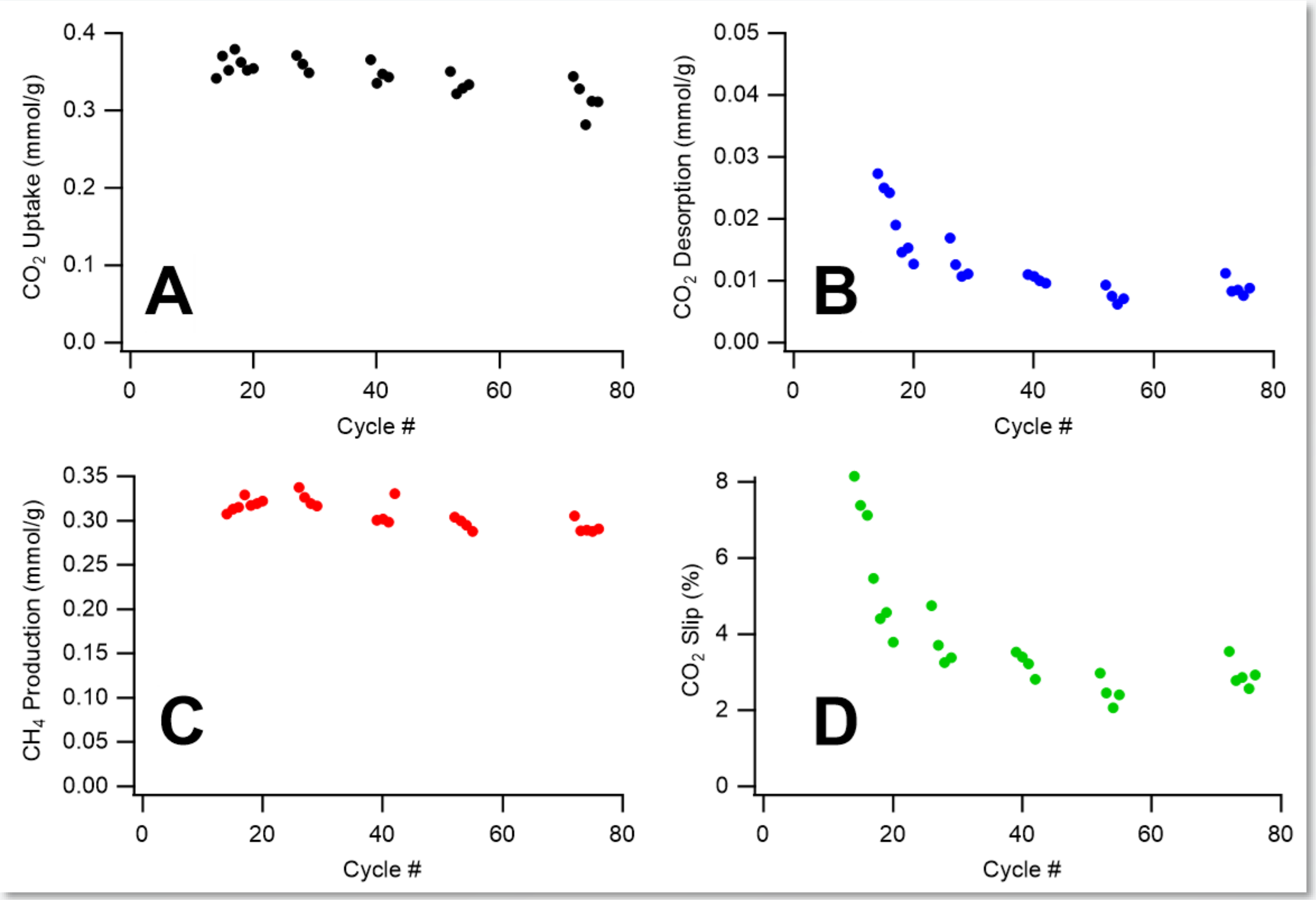

M. Rasmussen, S. Halingstad, M.M. Yung, S.H. Pang, et al. *in preparation*

# Reactor bed configuration studies suggest synergy between captured $CO_2$ and catalytic Ru site leading to higher conversion




M. Rasmussen, S. Halingstad, M.M. Yung, S.H. Pang, et al. *in preparation*

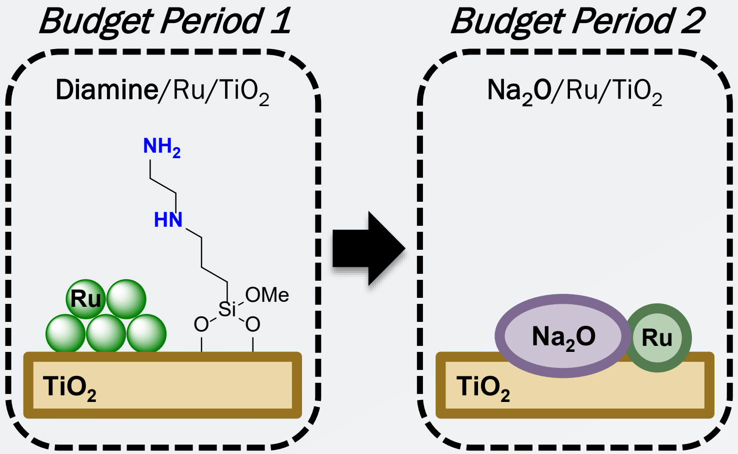
# Milestone 7: Retained >75% performance after extended cyclic operation



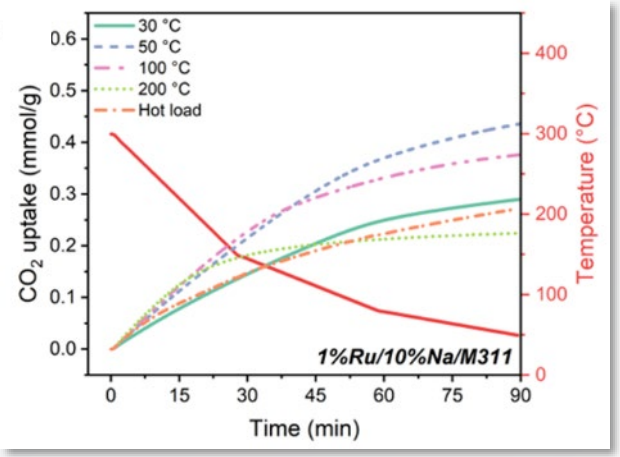

*Cyclic adsorption/reaction tests indicate long-term stability for $CH_4$ production and slight improvement in $CO_2$ conversion*

M. Rasmussen, S. Halingstad, M.M. Yung, S.H. Pang, et al. *in preparation*

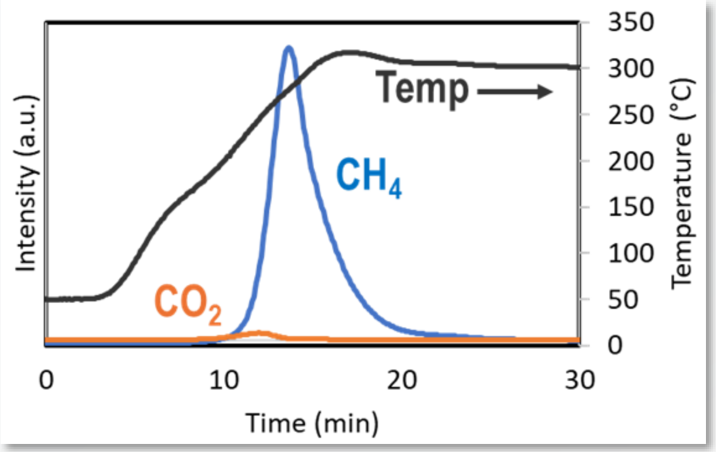
# Our project has developed materials and protocols for thermal reactive capture, converting $CO_2$ from the air into methane

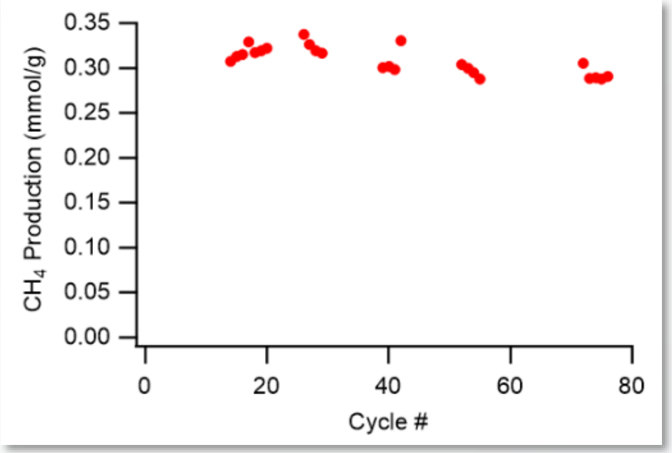



## *Effective air adsorbents*




## *Materials/process for high-$CO_2$-conversion methanation*

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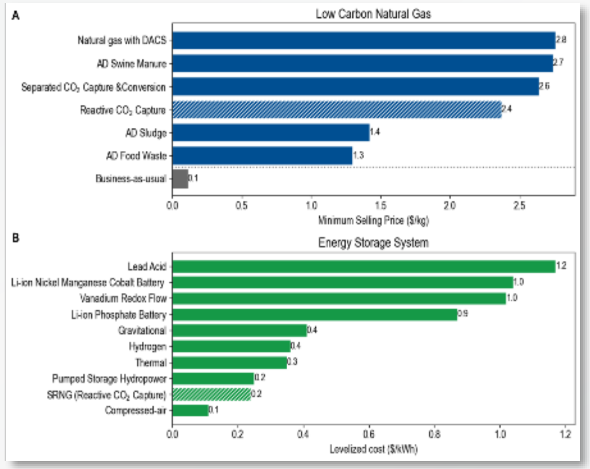


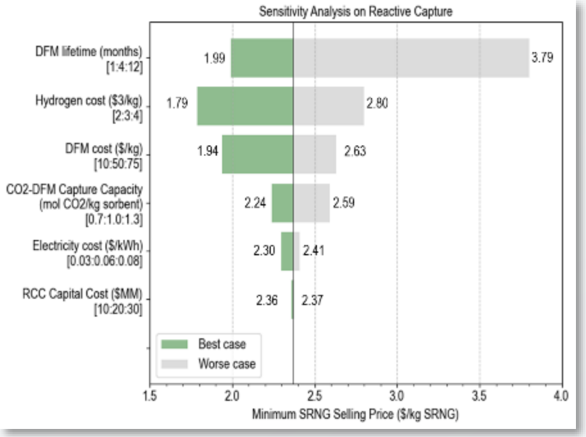

# Project Impact

### *Peer-reviewed publications*

- Jue, M. L.; Ellebracht, N. C.; Rasmussen, M. J.; Hunter-Sellars, E.; Marple, M. A. T.; Yung, M. M.; Pang, S. H.* Improving the Direct Air Capture Capacity of Grafted Amines via Thermal Treatment. *Chem. Comm*. 2024, *60*, 7077–7080.
- Crawford, J. M.*; Rasmussen, M. J.; McNeary, W. W.; Halingstad, S.; Hayden, S. C.; Dutta, N. S.; Pang, S. H.; Yung, M. M.* High Selectivity Reactive Carbon Capture over Zeolite Dual-Functional Materials. *ACS Catal.* 2024, *14*, 8541–8548. Front cover article.
- Freyman, M. C.; Huang, Z.; Ravikumar, D.; Duoss, E. B.; Li, Y.*; Baker, S. E.*; Pang, S. H.*; Schaidle, J. A.* Reactive $CO_2$ Capture: A Path Forward for Process Integration in Carbon Management, *Joule* 2023, 7, 631–651.
- Crawford, J. M.*; Petel, B.; Rasmussen, M. J.; Ludwig, T.; Miller, E. M.; Halingstad, S.; Akhade, S. A.; Pang, S. H.; Yung, M. Influence of Residual Chlorine on Ru/TiO2 Active Sites During $CO_2$ Methanation. *Appl. Catal. A: General* 2023, 663, 119292.
- McNeary, W. W.*; Ellebracht, N. C.; Jue, M. L.; Rasmussen, M. J.; Crawford, J. M.; Yung, M. M.; To, A. T.; Pang, S. H.* Application of Solid-Supported Amines for Thermocatalytic Reactive $CO_2$ Capture. *Submitted*.
- Aui, A.; Goldstein, H.; Ellebracht, N. C.; Li, W.; Pang, S. H.* Comparative Systems Analysis of Reactive $CO_2$ Capture to Synthetic Natural Gas. *In preparation.*

### *External presentations*

- M. M. Yung, et al. "$TiO_2$-based Dual Functional Materials for Reactive Carbon Capture Methanation." Presented at the International Congress on Catalysis, Lyon, France, July 2024.
- S. H. Pang, et al. "Durability and Design of Materials for Direct Air $CO_2$ Capture and Conversion." Presented at Heriot-Watt University, Research Centre for Carbon Solutions, Edinburgh, Scotland, June 2024.
- M. M. Yung, et al. "Harnessing renewable electricity to enable the power-to-gas process: Developing a sustainable energy pathway through catalytic methanation of $CO_2$ to produce renewable natural gas." Presented at the Spring 2024 Meeting of the American Chemical Society, New Orleans, LA, March 2024.
- S. Halingstad, et al. "Renewable natural gas production from $CO_2$ methanation for energy storage." Presented at the Rocky Mountain Catalysis Society Meeting, Albuquerque, NM, March 2024.
- A. Aui, et al. "Techno-economic and Carbon Footprint Analysis of Reactive $CO_2$ Capture to Renewable Natural Gas." Presented at the 2023 American Institute of Chemical Engineers Annual Meeting, Orlando, FL, Nov 7, 2023.
- N. C. Ellebracht, et al. "Direct air reactive capture and conversion: the benefits and limitations of familiar chemistries." Presented at the Fall 2023 Meeting of the American Chemical Society, San Francisco, CA, Aug 13, 2023.
- J. M. Crawford, et al. "Importance of Chlorine Removal from Ru/$TiO_2$ Methanation Catalysts." Presented at the 28th North American Catalysis Society Meeting, Providence, RI, June 18–23, 2023.
- S. H. Pang, et al. "Direct Air Reactive Capture and Conversion of $CO_2$ to Methane." Presented at the Gordon Research Conference on Carbon Capture Utilization and Storage, Les Diablerets, Switzerland, May 28 – June 2, 2023.
- J. M. Crawford, et al. "Reactive Carbon Capture: Routes to Renewable Natural Gas (RNG)." Presented at the Colorado School of Mines, Chemical & Biological Engineering Seminar, Golden, CO, Feb 7, 2023.

### *Intellectual property*

- Provisional patent application (joint between LLNL and NREL) filed.

THE LLNL **CARBON** INITIATIVE


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Direct Air Capture Pillar Lead, LLNL Carbon Initiative

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.



Lawrence Livermore National Laboratory

# Appendix

| Tasks, Milestones, and Deliverables | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Budget Period:** | BP 1 | | | | | | BP 2 | | | | | | |
| **Project Year:** | FY 2022 | | | | FY 2023 | | | | FY 2024 | | | | '25 |
| **Project Quarter:** | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| **Task 0**: Project management and planning | | | | | | | | | | | | | |
| **Task 1**: Synthesize hybrid adsorbent-catalyst materials | | | | | | | | | | | | | |
| **Task 2**: Evaluate adsorption performance with dilute $CO_2$ | | | | | | | | | | | | | |
| ***Milestone 1***: Measured DAC adsorption capacity >0.25 mol $CO_2$/kg | | | ✓ | | | | | | | | | | |
| **Task 3**: Characterize catalysts and perform methanation with dilute $CO_2$ | | | | | | | | | | | | | |
| ***Milestone 2***: Achieved >25% $CO_2$ single-pass conversion from dilute $CO_2$ | | | | ✓ | | | | | | | | | |
| **Task 4**: Simulate interaction between captured $CO_2$ and single-atom catalyst site | | | | | | | | | | | | | |
| ***Milestone 3***: Established energetics for conversion of captured $CO_2$ into $CH_4$ | | | | | ✓ | | | | | | | | |
| **Task 5**: Develop preliminary technoeconomic assessment | | | | | | | | | | | | | |
| ***Deliverable 1*****:** Report detailing preliminary technoeconomic assessment | | | | | | ✓ | | | | | | | |
| **Task 6**: Develop preliminary life cycle assessment | | | | | | | | | | | | | |
| ***Deliverable 2*****:** Report detailing preliminary life cycle assessment | | | | | | ✓ | | | | | | | |
| ***Milestone 4***: Downselected material composition | | | | | | ✓ | | | | | | | |
| ***Success Criteria BP1:*** Demonstrate 10% improvement in RNG MFSP and CI compared to baseline | | | | | | ✓ | | | | | | | |
| **Task 7**: Synthesize second-generation materials | | | | | | | | | | | | | |
| **Task 8**: Evaluate adsorption performance and material durability with humidity | | | | | | | | | | | | | |
| ***Milestone 5***: Measured DAC adsorption capacity >0.40 mol $CO_2$/kg | | | | | | | | ✓ | | | | | |
| **Task 9**: Develop cyclic air capture-methanation process and test performance | | | | | | | | | | | | | |
| ***Milestone 6***: Converted >50% of captured $CO_2$ into $CH_4$ | | | | | | | | ✓ | | | | | |
| ***Milestone 7***: Retained >75% performance after extended cyclic operation | | | | | | | | | | ✓ | | | |
| **Task 10**: Simulate adsorption and conversion processes with humidity | | | | | | | | | | | | | |
| **Task 11**: Refine technoeconomic and life cycle analyses | | | | | | | | | | | | | |
| ***Milestone 8*****:** Demonstrated impact of $CO_2$ adsorption capacity and fractional conversion on RNG MFSP | | | | | | | | ✓ | | | | | |
| ***Deliverable 3*****:** Report documenting refined TEA and LCA for DAC-RCC process | | | | | | | | | | | | | |
| ***Success Criteria BP2:*** Demonstrate 15% improvement in RNG MFSP and/or CI compared to baseline | | | | | | | | | | | | | |