# Aerogel Adsorbent Polymers for Direct Air Capture of $CO_2$

DE-FE0032251

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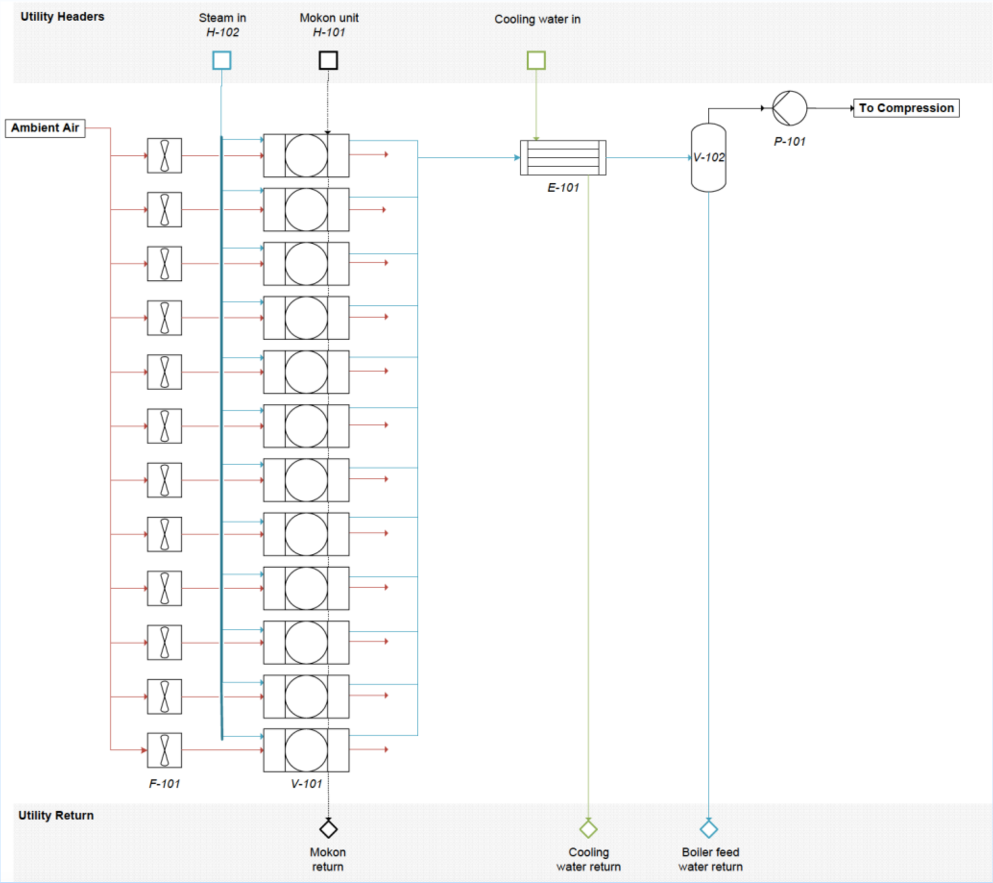
# Project Overview

- Funding: $2,999,642 Federal, $749,907 Cost Share
- Project Participants: Palo Alto Research Center, Lawrence Livermore National Laboratory
- Awaiting project kick-off
- Overall Project Objectives:
  - Optimize the structured adsorbent, contactor, and DAC system operation for improved volumetric productivity, pressure drop, and capacity fade towards the general target DAC cost of < $100/ton $CO_2$e.
  - Identify a low-cost, scalable manufacturing method for structured adsorbent production.
  - Develop a laboratory-scale DAC system with a continuous production rate of > 1 kg $CO_2$/day at a purity of > 90% $CO_2$, demonstrating < 0.005% / cycle capacity fade over 1,000 h of operation.

# DAC Process - TVSA




- The DAC system uses a TVSA process that adsorbs under ambient conditions and desorbs under moderate temperature (80-100 ˚C) and reduced pressure.
- Initial engineering model includes direct steam and/or indirect heat for regeneration.
- Several contactors in parallel (‘contactor bank’ or ‘module’) enable continuous $CO_2$ production.

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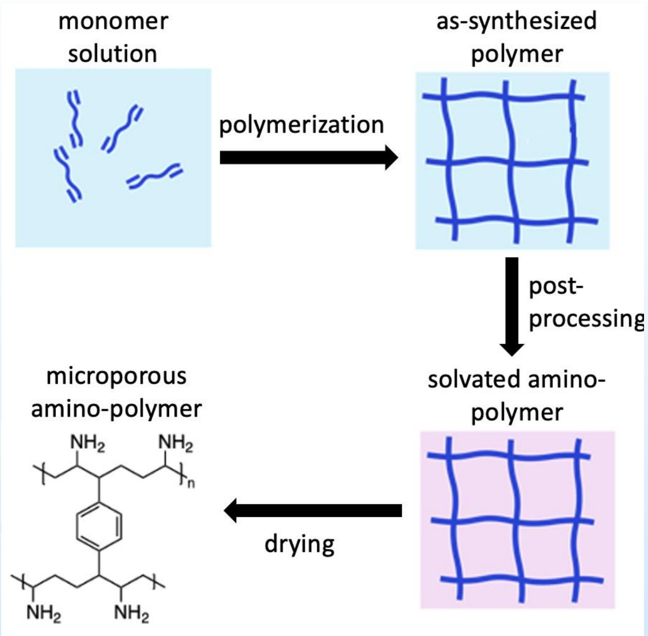
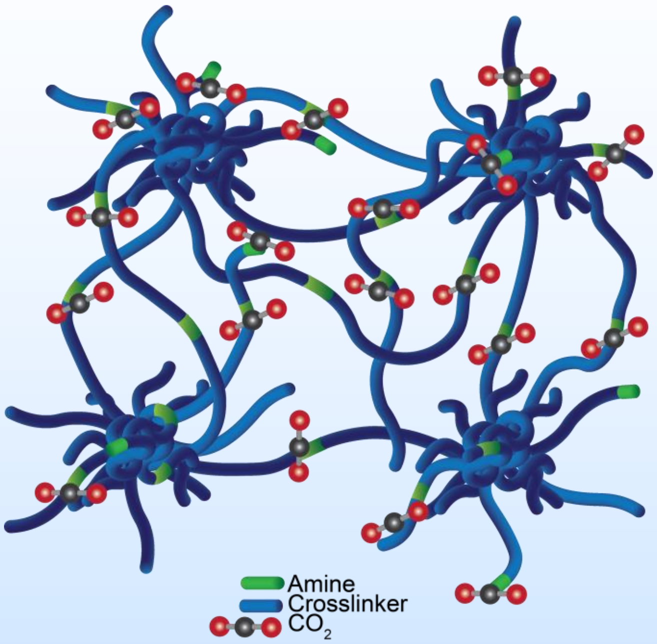
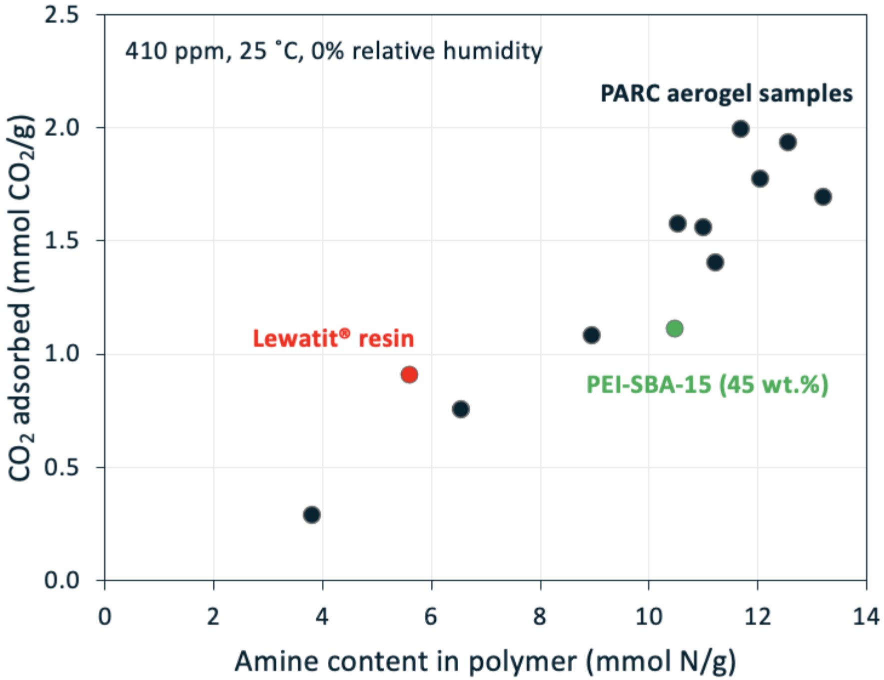
# Adsorbent Chemistry

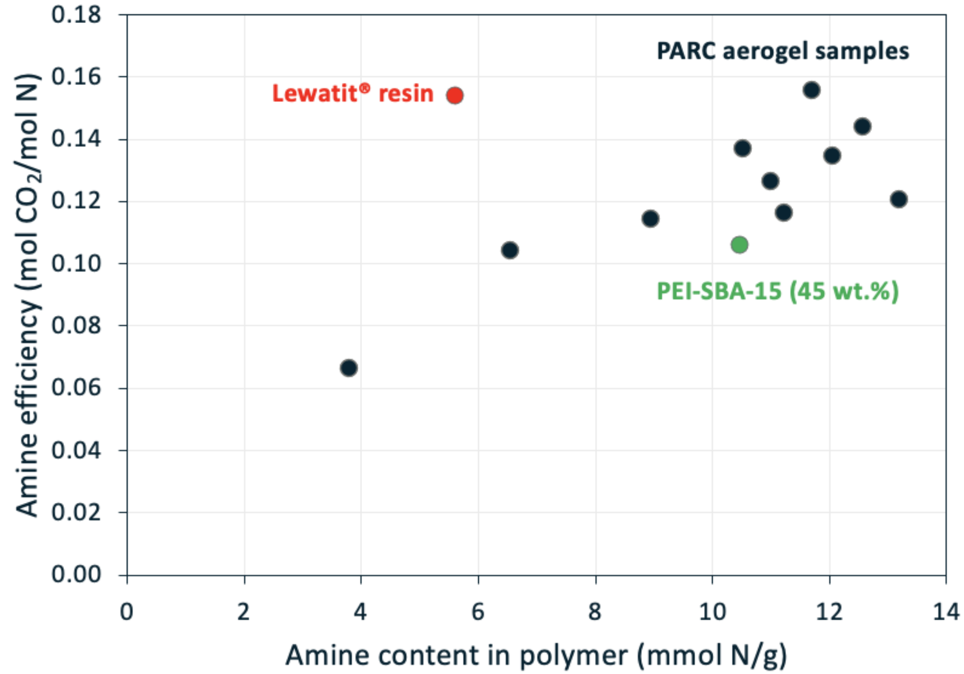



- Based upon work supported by Department of Energy under Award Number DE-FE0031951 (Tunable, Rapid Uptake Amino-Polymers for Direct Air Capture of Carbon Dioxide, TRAPS).
- Amine-containing polymer aerogel featuring high amine loading (> 10 mmol/g).
- Synthesized by radical polymerization of vinyl-containing monomers followed by post-functionalization and drying.

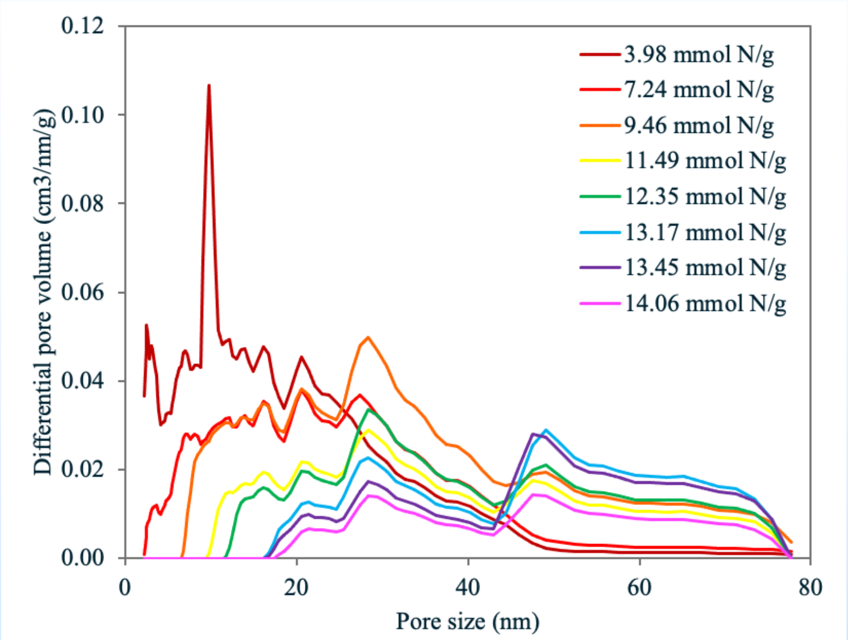
# Structure Property Relationship – $CO_2$ Adsorption & Amine Efficiency

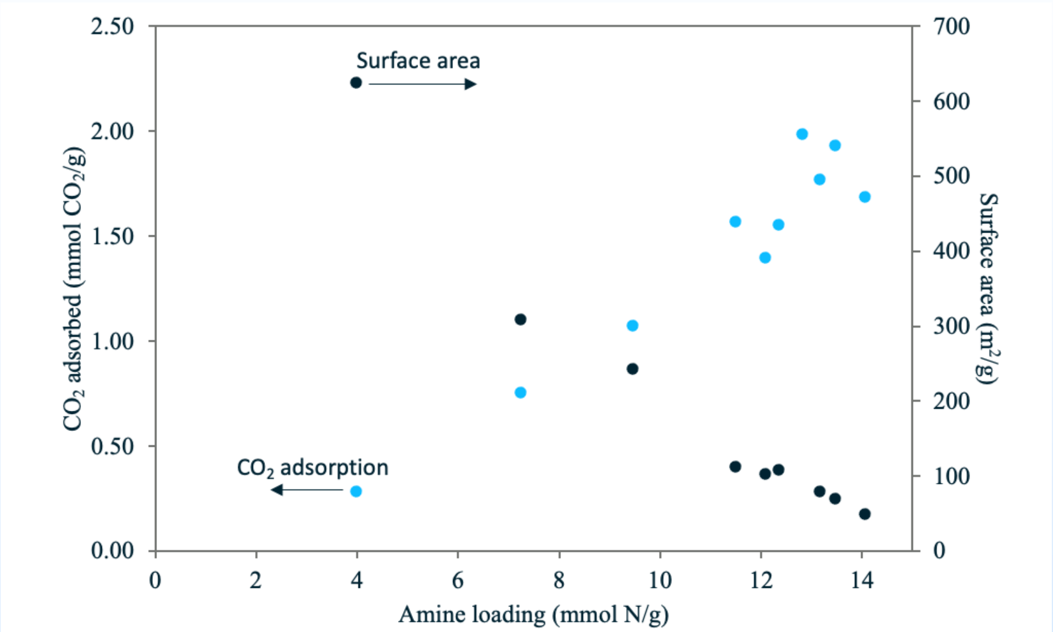



- Amine content is controlled by the monomer ratio in polymerization.
- Elemental analysis was used to determine N content in the material and thermogravimetric analysis (TGA) was used to measure $CO_2$ adsorption.

# Structure Property Relationship – Surface Area & Pore Structure




- Average pore size increases and pore volume decreases with increasing amine loading.
- $CO_2$ adsorption increases and surface area decreases with increasing amine loading in the polymer.

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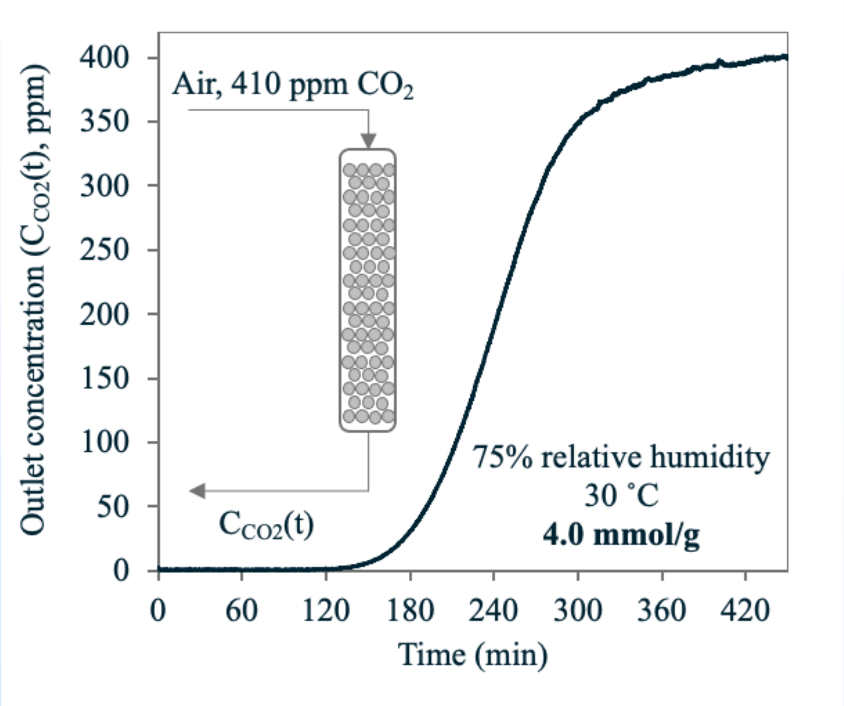
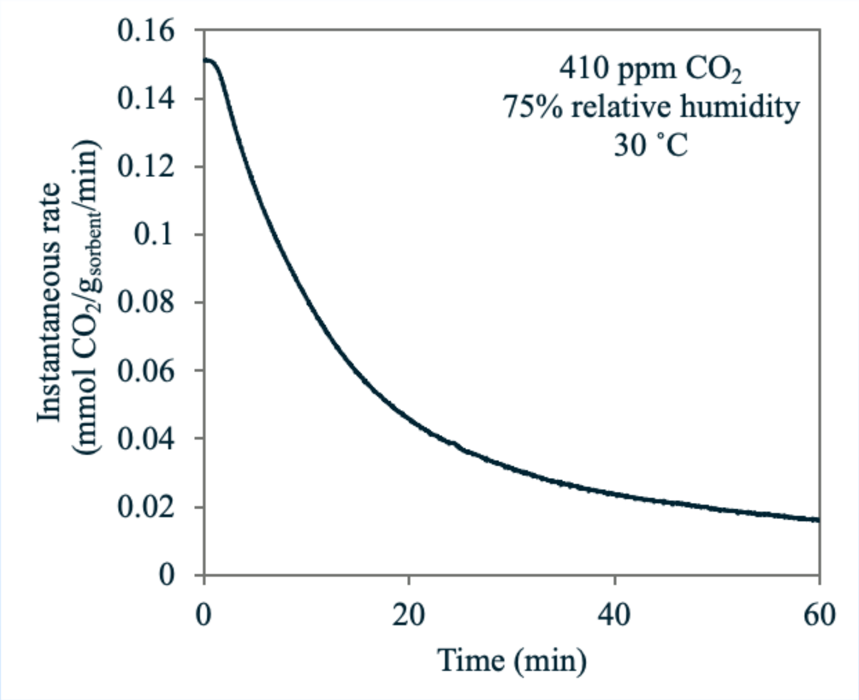
# Transient Breakthrough Testing




- $CO_2$ adsorption doubles under high relative humidity, reaching > 4 mmol $CO_2$/g equilibrium adsorption capacity.
- High flow rate testing revealed that 'extrinsic' mass transport is limiting the adsorption rate (increasing flow/mass ratio always increased adsorption rate).

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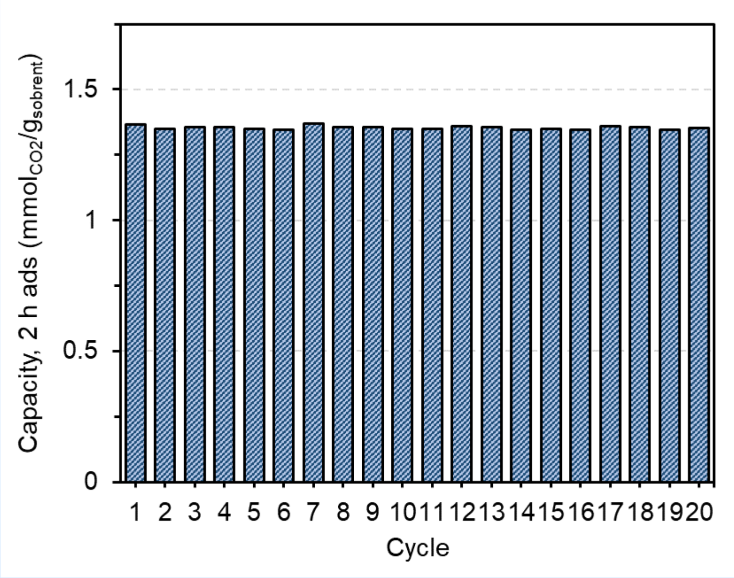
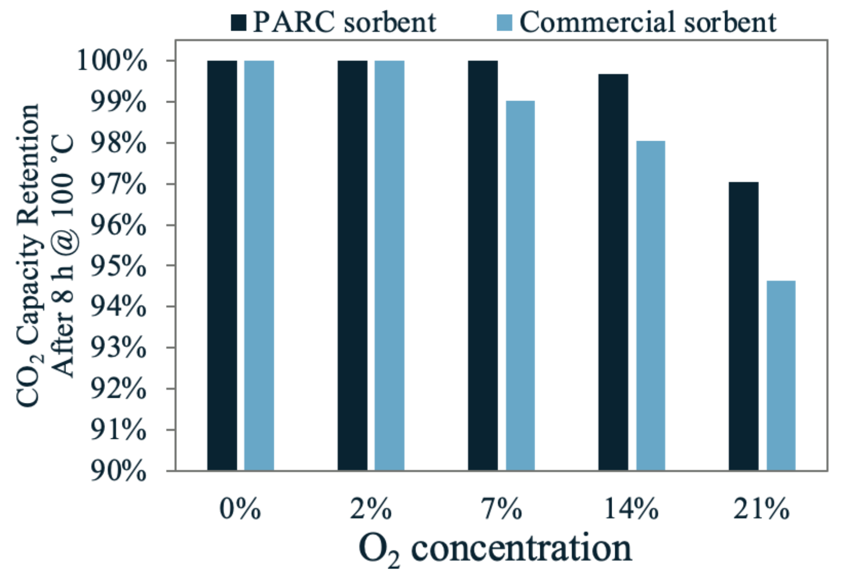
# Thermal & Oxidative Stability

TGA cycling (1 h, 100 ˚C under $N_2$)




Accelerated aging (8 h, 100 ˚C under $O_2$)




- No capacity loss is observed under inert regeneration at elevated temperature.
- Significant improvement in oxidative stability relative to the commercial adsorbent under accelerated aging conditions (0.0007 %/min capacity loss under 14% $O_2$ compared to 0.0041 %/min for the commercial material)

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# Technoeconomic Impact of Adsorbent Performance

- Increasing adsorption rate and working capacity results in fewer contactors required (based on 100,000 ton/year DAC facility):

| Parameter | PARC DAC | Baseline DAC | Units |
|---|---|---|---|
| Average adsorption rate | 0.087 | 0.03 | mol/kg/min |
| Adsorption time | 10 | 10 | min |
| Working capacity | 0.87 | 0.3 | mol/kg |
| Desorption time | 4.5 | 1.5 | min |
| Total cycle time | 14.5 | 11.5 | min |
| Contactors per bank | 12 | 12 | - |
| Number of contactor banks | 10 | 22 | - |
| Number of contactors | 120 | 264 | - |
| Number of blower fans | 120 | 264 | - |

- A lower sorbent requirement translates to lower capital and operational costs, resulting in a ~60% decrease in $CO_2$ capture cost relative to a baseline material.

| | PARC DAC | Baseline DAC | Units |
|---|---|---|---|
| Total cost of capture | $170 | $419 | $/ton $CO_2$ |
| Capital Expenditure | $17 | $39 | $/ton $CO_2$ |
| Sorbent Cost | $96 | $278 | $/ton $CO_2$ |
| Other Operating Cost | $16 | $23 | $/ton $CO_2$ |
| Utilities cost | $40 | $79 | $/ton $CO_2$ |

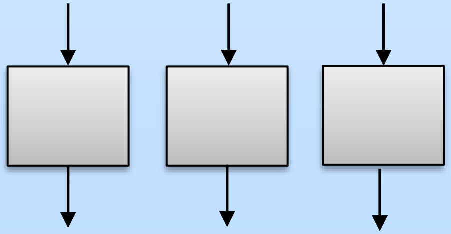
# Technical Approach - SWAAP

**BP 1: Contactor design and testing**

- Structured adsorbent optimization
- Contactor design
- Initial DAC system design

**BP 2: Contactor fabrication and DAC system commissioning**

- Large-area contactor fabrication
- Contactor optimization
- Single contactor cycling
- Large-scale contactor production design
- DAC system commissioning



**BP 3: Long-term, continuous process testing with ambient air**

- DAC system optimization
- Long-term cycle testing

# Success Criteria

| Budget Period 1 | Budget Period 2 | Budget Period 3 |
|---|---|---|
| • Demonstrate SA with > 1.35 mmol/g under 0% RH.<br>• Demonstrate contactor with 0.0435-0.087 mmol/g/min adsorption rate (0-75% RH).<br>• Establish baseline volumetric productivity, pressure drop, and capacity fade.<br>• Finalize contactor design and regeneration process for DAC system.<br>• Determine system requirements for 1 kg $CO_2$/day demonstration. | • Produce the structured adsorbent needed to construct laboratory DAC system.<br>• Build and commission DAC system.<br>• Demonstrate that the DAC system is capable of achieving > 1 kg $CO_2$/day at > 90% purity.<br>• Develop a scale-up design for structured adsorbent and contactor production. | • Optimize volumetric productivity and pressure drop on the DAC system.<br>• Demonstrate > 1 kg $CO_2$/day production, > 90% $CO_2$ purity, and < 0.005% /cycle capacity fade over 1,000 h of cumulative operation.<br>• Final TEA/LCA |

# Plans for Commercialization

- PARC's commercialization strategy is being executed in parallel with the Government project.
- Development of "next-gen" structured adsorbents, contactors, and DAC systems is occurring in-house, while working with partners to accelerate deployment of PARC's materials into $CO_2$ capture systems.
- Commercialization will be paced by adsorbent manufacturing scale-up while working with partners to deploy the material.
  - 2023: 100-300 g-scale
  - 2024: 20-80 kg-scale
  - 2025: 100-1,000 kg-scale

# Conclusions

- Our work demonstrates a novel $CO_2$ adsorbent, based on an amine-containing polymer aerogel, and its state-of-the-art performance under DAC conditions (> 4 mmol/g capacity, > 0.15 mmol/g/min adsorption rate).

- The adsorbent properties achieved are expected to substantially reduce the cost of DAC compared to currently available adsorbent materials.

- Our goal going forward is to develop a bench-scale DAC system with improved volumetric productivity and low pressure drop, using a scalable, low-cost structured adsorbent.

# Acknowledgements


- NETL, Office of Fossil Energy and Carbon Management
  - The material is based upon work supported by the Department of Energy under Award Number DE-FE0032251.
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- Palo Alto Research Center (PARC)
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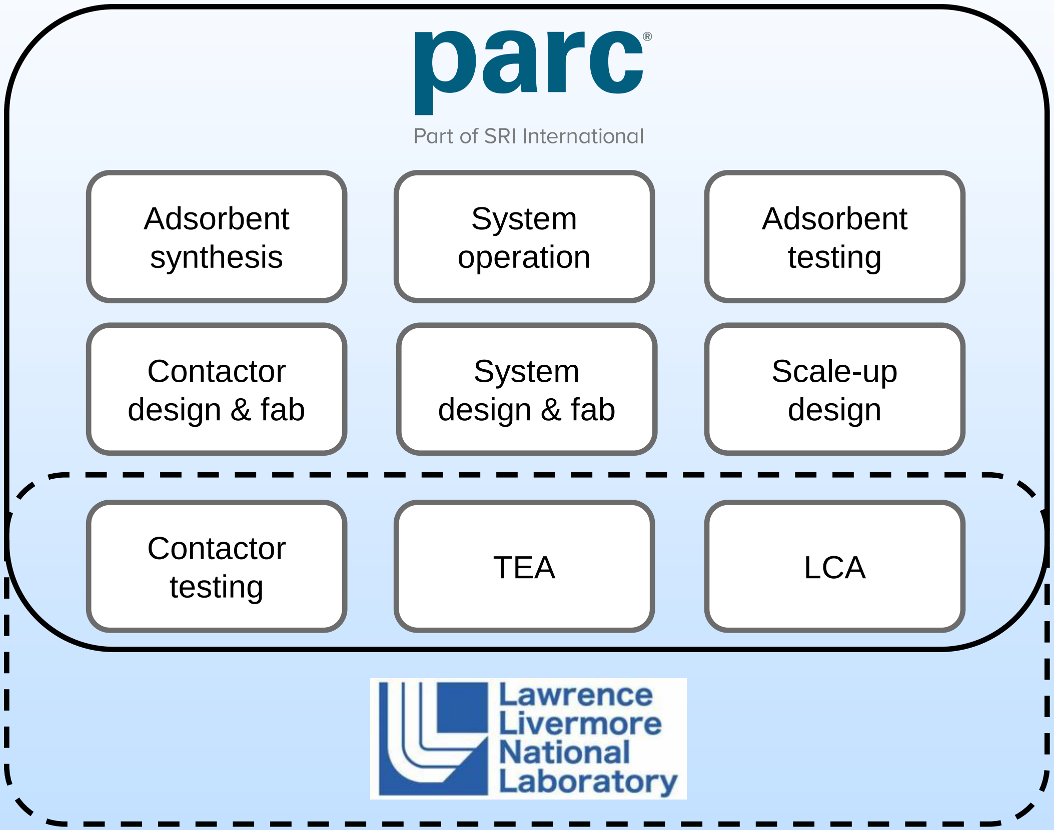
- SoCalGas and SRI International are acknowledged for cost share support.

# Appendix

# Organization Chart



# Gantt Chart

| | Overall quarter | 1 | | | 2 | | | 3 | | | 4 | | | 5 | | | 6 | | | 7 | | | 8 | | | 9 | | | 10 | | | 11 | | | 12 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **Year** | **1** | | | | | | | | | | | | **2** | | | | | | | | | | | | **3** | | | | | | | | | | | |
| | **Quarter** | **1** | | | **2** | | | **3** | | | **4** | | | **1** | | | **2** | | | **3** | | | **4** | | | **1** | | | **2** | | | **3** | | | **4** | | |
| **Task/subtask #** | **Task/subtask title** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **11** | **12** | **13** | **14** | **15** | **16** | **17** | **18** | **19** | **20** | **21** | **22** | **23** | **24** | **25** | **26** | **27** | **28** | **29** | **30** | **31** | **32** | **33** | **34** | **35** | **36** |
| 1 | Project management and planning | | | | | | | | | | D1 | | | | | | | | | | | | D1 | | | | | | | | | | | | | | |
| 1.1 | Project management plan | D1.1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1.2 | Technology maturation plan | | | D1.2 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | D1.2 | | | |
| 1.3 | State point data table | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | D1.3 | | | |
| 2 | Conduct Diversity, Equity, and Inclusion Activities (Year 1) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | Perform initial TEA | | | | D3 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | Perform initial LCA | | | | D4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | Perform preliminary contactor design and testing | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5.1 | Perform structured adsorbent optimization | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5.2 | Identify key parameters for contactor design | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5.3 | Develop an initial design of the DAC system | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | Conduct Diversity, Equity, and Inclusion Activities (Year 2) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | Construct contactors and DAC system | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7.1 | Fabricate contactors | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7.2 | Optimize single contactor | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7.3 | Conduct long-term cycling in single contactor | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7.4 | Conceptually design large scale adsorbent and contactor production | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7.5 | Integrate contactors with auxilliary components and comission DAC system | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | Conduct Diversity, Equity, and Inclusion Activities (Year 3) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | Complete final TEA | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 10 | Complete final LCA | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 11 | Complete technology EH&S risk assessment | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12 | Perform long-term, continuous process testing using ambient air | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12.1 | Optimize the DAC system operation | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12.2 | Conduct long-term cycle testing | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |