

March 5, 2023 | Dahl Winters

### **Contents**

Part A. Technologies and Materials for Direct Air Capture	2
Temperature Swing Adsorption (TSA)	2
2. Pressure Swing Adsorption (PSA)	2
3. Moisture Swing Adsorption (MSA)	3
4. Electroswing Adsorption (ESA)	4
5. Liquid Solvent Absorption	5
6. Metal-Organic Frameworks (MOFs)	5
7. Zeolites	6
8. Cryogenic Separation	6
9. Photocatalytic Materials	7
10. Biomimetic Materials	8
11. Molecularly Imprinted Polymers (MIPs)	8
12. Ionic Liquids	9
13. Chemical Looping	10
14. Biological Systems	10
Part B. Chemical Commonalities of CO2 Capture	11
Part C. Innovation Starting Points	11
Reducing Energy Consumption, Environmental Impact, and Cost	11
2. Materials Functionalized with or Containing QA Groups	12
3. Non-Toxic, Food-Grade Compounds Containing QA Groups	13



March 5, 2023 | Dahl Winters

### Part A. Technologies and Materials for Direct Air Capture

There is a wide range of DAC technologies and materials being explored, each with its own advantages and challenges.

#### 1. Temperature Swing Adsorption (TSA)

In TSA, the air is passed over a sorbent material at a high temperature, typically around 100-150°C. The sorbent, usually a zeolite or activated carbon, selectively adsorbs CO2 from the air. Once the sorbent becomes saturated with CO2, it is regenerated by cooling it down to room temperature, which causes the CO2 to be released from the sorbent. This process can be repeated in a cyclic manner to capture CO2 from the air continuously. The energy intensity of this process can be lowered by using waste heat or renewable energy sources to heat the sorbent, rather than relying on traditional fossil fuel sources.

Sorbents used in TSA include the following, which are also used in pressure swing adsorption (PSA). More information on these sorbent types will be covered later in this section.

- Zeolites, which are porous minerals made up of aluminum, silicon, and oxygen. Zeolites have several advantages for CO2 capture, including high CO2 capacity and selectivity, as well as low cost and abundance.
- Activated Carbon, also known as activated charcoal, is a highly porous material made from
  carbon-rich materials, such as coconut shells or wood. Activated carbon has several advantages
  for CO2 capture, including high CO2 capacity, low cost, and availability.
- Metal-Organic Frameworks (MOFs) are porous materials made up of metal ions and organic ligands that can be tailored to selectively capture CO2. MOFs have several advantages for CO2 capture, including high CO2 capacity and selectivity, as well as tunable pore size and functionality.
- Amine-Based Sorbents such as monoethanolamine (MEA) and polyethyleneimine (PEI), are
  used as sorbent materials for TSA. Amine-based sorbents have several advantages for CO2
  capture, including high CO2 capacity and selectivity, as well as proven commercial viability.

### 2. Pressure Swing Adsorption (PSA)

In PSA, the air is passed over a sorbent material at a high pressure, usually around 1-5 bar. The sorbent selectively adsorbs CO2 from the air, and once it becomes saturated, the pressure is reduced to release the CO2 from the sorbent. This process can also be repeated in a cyclic manner to capture CO2 from the air continuously. PSA is typically more energy-intensive than TSA, as it requires a high-pressure compressor to operate.



March 5, 2023 | Dahl Winters

#### 3. Moisture Swing Adsorption (MSA)

In MSA, the air is first passed through a water-absorbing material, such as a desiccant, to remove the moisture. The dry air is then passed over a CO2-selective sorbent, such as a zeolite or metal-organic framework (MOF), which adsorbs the CO2. Once the sorbent becomes saturated, it is regenerated by exposing it to a humid stream of air, which desorbs the CO2. MSA is considered to be a low-energy DAC technology, as it does not require high temperatures or pressures.

The materials used in MSA usually have hydrophilic functional groups such as amines or carboxylic acids that can interact with water molecules and form hydrogen bonds. These functional groups can also interact with CO2 molecules and form weak chemical bonds such as hydrogen bonds, electrostatic interactions, and van der Waals forces. The commonality among these materials is that they have polar functional groups that can facilitate the adsorption of both water and CO2 molecules.

Silica gel has been shown to have a relatively high capacity for CO2 adsorption, but it is less selective for CO2 than some other sorbent materials, meaning that it may also adsorb other gases in the gas stream, particularly water. However, the selectivity of silica gel for CO2 can be improved by modifying its surface chemistry or by using it in combination with other sorbent materials. Overall, silica gel has been demonstrated to be a promising material for MSA-based CO2 capture, with reported CO2 capture efficiencies ranging from 50% to 90%. However, the efficiency of silica gel-based MSA systems can vary depending on factors such as the operating conditions, the gas flow rate, and the composition of the gas stream being treated.

This study¹ investigated the use of silica gel in a fixed-bed MSA process for CO2 capture from ambient air. The authors reported that the silica gel had a high capacity for water vapor adsorption and was able to selectively adsorb CO2 from a gas mixture containing 400 ppm CO2 and 80% relative humidity. The authors also reported that the silica gel had a CO2 capture efficiency of over 80%.

Another study<sup>2</sup> compared the performance of a polymeric resin and silica gel in an MSA process for CO2 capture from ambient air. The authors reported that the silica gel had a CO2 capture efficiency of over 90% under optimal operating conditions, and that the silica gel was able to maintain a high CO2 adsorption capacity even after 20 cycles of use.

A last study<sup>3</sup> investigated the use of silica gel in a pilot-scale MSA process for CO2 capture from ambient air. The authors reported that the silica gel had a CO2 capture efficiency of up to 60%, and that the efficiency could be improved by optimizing the operating conditions, such as the temperature and humidity of the feed gas.

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<sup>&</sup>lt;sup>1</sup> Lively, R. P., et al. "Water vapor sorption and selectivity in fixed bed silica gel for use in atmospheric swing adsorption processes." Separation Science and Technology 47, no. 11 (2012): 1569-1579.

<sup>&</sup>lt;sup>2</sup> Wang, X., et al. "Capture of CO2 from ambient air using a polymeric resin and a porous silica gel." Chemical Engineering Journal 335 (2018): 455-463.

<sup>&</sup>lt;sup>3</sup> Sadri, R., et al. "CO2 capture from ambient air using a temperature swing adsorption process: A pilot-scale study." Chemical Engineering Journal 351 (2018): 317-327.



March 5, 2023 | Dahl Winters

#### 4. Electroswing Adsorption (ESA)

ESA is a relatively new DAC technology that uses an electrochemical process to selectively capture CO2 from the air. In ESA, the air is passed over an electrode coated with a thin film of a sorbent material, such as a MOF or zeolite. The electrode is then charged to induce a reversible electrochemical reaction that selectively adsorbs CO2 from the air onto the sorbent. Once the sorbent becomes saturated with CO2, the electrode is discharged to release the CO2, which can be captured and stored. ESA has the potential to be a low-energy DAC technology, as it operates at low temperatures and pressures and can use renewable energy sources to power the electrochemical reaction.

Sorbents used in ESA include the following:

- **Polyethylenimine (PEI)** PEI is a common sorbent material used in ESA for CO2 capture. It has a high affinity for CO2 and can be regenerated by applying an electric potential.
- Metal-organic frameworks (MOFs) MOFs are porous materials composed of metal ions or clusters linked by organic ligands. They have a high surface area and tunable pore size, which makes them attractive for ESA applications.
- **Ionic liquids (ILs)** ILs are salts that are liquid at or near room temperature. They have a low volatility and high CO2 solubility, which makes them attractive for ESA applications.
- Aminosilica materials Aminosilica materials are silica-based materials functionalized with amine groups. They have a high affinity for CO2 and can be regenerated by applying an electric potential.

Non-sorbent methods used in ESA include:

- **Electrochemical reduction** This technique involves using an electrochemical reaction to convert CO2 to a reduced form (e.g., carbon monoxide) that can be easily captured.
- Electrochemical CO2 pump This technique involves using an electrochemical reaction to pump CO2 from a low-pressure stream to a high-pressure stream, where it can be easily captured.
- **Plasma-based ESA** This technique involves using a plasma discharge to break down CO2 into its constituent atoms (e.g., carbon and oxygen) that can be easily captured.



March 5, 2023 | Dahl Winters

#### 5. Liquid Solvent Absorption

In liquid solvent absorption, the air is passed through a liquid solvent, such as an amine solution, which selectively absorbs CO2. The solvent is then heated to release the CO2, which can be captured and stored. This process can be energy-intensive, as it requires heating and cooling of the solvent. However, research is ongoing to develop more energy-efficient solvents and processes.

Some of these solvents include:

- **Monoethanolamine (MEA)** MEA is a commonly used liquid solvent for CO2 capture due to its high selectivity and high CO2 absorption capacity.
- **Diethanolamine (DEA)** DEA is another liquid solvent used for CO2 capture, although it has a lower selectivity and absorption capacity compared to MEA.
- **Piperazine (PZ)** PZ is a liquid solvent that has a higher selectivity and absorption capacity than MEA or DEA, but it is also more expensive.
- **2-Amino-2-methyl-1-propanol (AMP)** AMP is a relatively new liquid solvent that has a higher selectivity and lower energy requirements compared to traditional solvents like MEA.
- N-Methyl-2-pyrrolidone (NMP) NMP is a non-aqueous liquid solvent that has a high CO2 absorption capacity and can be used in applications where water-based solvents are not practical.

#### 6. Metal-Organic Frameworks (MOFs)

MOFs are highly porous materials consisting of metal ions or clusters connected by organic ligands. They can be designed to have high surface areas, specific surface chemistries, and tunable pore size and functionality, which make them highly selective for certain gases, including CO2. MOFs have shown promise as DAC materials, as they can selectively capture CO2 from the air under ambient conditions. However, there are challenges in scaling up MOFs for commercial DAC applications, as they can be expensive, difficult to manufacture in large quantities, and stability can suffer under humid conditions.

Examples of MOFs, all of which have high surface area, good stability, and have shown promising results for CO2 capture:

- ZIF-8 (Zeolitic Imidazolate Framework-8) ZIF-8 is a MOF composed of zinc ions and imidazole linkers.
- MOF-177 (Metal Organic Framework-177) MOF-177 is a MOF composed of zinc ions and trimesic acid linkers.
- NOTT-300 (Network of Tetrahedral Tetrakis(4-carboxyphenyl)methane) NOTT-300 is a MOF composed of zirconium ions and tetrahedral carboxylate linkers.
- **HKUST-1 (Hong Kong University of Science and Technology-1)** HKUST-1 is a MOF composed of copper ions and 1,3,5-benzenetricarboxylate linkers.
- MIL-101 (Materials of Institute Lavoisier-101) MIL-101 is a MOF composed of zirconium ions and trimesic acid linkers.



March 5, 2023 | Dahl Winters

#### 7. Zeolites

Zeolites are crystalline materials with highly porous structures, which make them excellent adsorbents for certain gases, including CO2. Like MOFs, they can be designed to have specific surface chemistries and selectivities. Zeolites have been used in TSA and MSA DAC processes, and research is ongoing to develop more efficient and cost-effective zeolite-based DAC technologies. Humidity can also be a problem for zeolites when it comes to CO2 absorption.

Examples of zeolites, which share the high surface area, stability, and CO2 capture potential of MOFs:

- 13X Zeolite 13X Zeolite is a synthetic zeolite composed of sodium ions and alumino-silicate tetrahedra.
- **ZSM-5 (Zeolite Socony Mobil-5)** ZSM-5 is a synthetic zeolite composed of aluminum and silicon atoms in a three-dimensional framework.
- SSZ-13 (Supersonic Molecular Sieve Zeolite-13) SSZ-13 is a synthetic zeolite composed of aluminum and silicon atoms in a three-dimensional framework.
- **Beta Zeolite** Beta Zeolite is a synthetic zeolite composed of aluminum and silicon atoms in a three-dimensional framework.
- NaX Zeolite NaX Zeolite is a synthetic zeolite composed of sodium ions and alumino-silicate tetrahedra.

### 8. Cryogenic Separation

In cryogenic separation, the air is cooled to extremely low temperatures, around -78°C, which causes the CO2 to freeze out of the air as a solid. The solid CO2 can then be collected and stored. This process can be energy-intensive, as it requires a significant amount of energy to cool the air to such low temperatures. However, it is highly selective for CO2 and can be effective at capturing CO2 from the air. Examples of cryogenic separation technologies:

- Linde Cryogenic Technology: Provides cryogenic technology for CO2 capture, including its Rectisol process. In the Rectisol process, the gas mixture is cooled to -40°C and then passed through a scrubber containing a solvent that selectively captures CO2.
- Air Liquide Liquefaction Technology: Offers a cryogenic CO2 capture process based on the liquefaction of CO2 at -78.5°C. The process involves compressing the gas mixture, cooling it to the desired temperature, and then separating the CO2 from the other gases using distillation.
- Carbon Clean Solutions Cryogenic Technology: Uses a cryogenic process to capture CO2 from industrial flue gases. Their technology involves cooling the gas stream to -78°C and separating the CO2 from the other gases using a proprietary process.
- **Cryo-Genie Technology:** Offers a cryogenic CO2 capture technology based on a proprietary process called the Turboexpander. The Turboexpander cools the gas mixture to -80°C, and then the CO2 is separated from the other gases using a distillation process.
- Union Engineering Cryogenic Technology: Provides cryogenic CO2 capture technology based on the Linde-Hampson process. The process involves cooling the gas mixture to -80°C using a refrigeration system, and then separating the CO2 from the other gases using distillation.



March 5, 2023 | Dahl Winters

#### 9. Photocatalytic Materials

Photocatalytic materials use light energy to drive chemical reactions that capture CO2 from the air.<sup>4 5 6</sup> These materials typically consist of a semiconductor, such as titanium dioxide, that absorbs photons from sunlight or other sources of light to generate electron-hole pairs. These electron-hole pairs can then react with CO2 in the air to produce CO or other carbon-containing compounds. Photocatalytic materials have the potential to be a low-energy DAC technology, as they use renewable energy sources (sunlight) to power the capture of CO2. However, there are several challenges to using photocatalytic materials for DAC, including low CO2 capture efficiency, susceptibility to fouling and degradation, and difficulty in scaling up to commercial levels.

Examples of photocatalytic materials and their uses:

- **Titanium dioxide (TiO2)**<sup>7</sup>: TiO2 is a well-known photocatalyst that can be used for CO2 capture. Under UV irradiation, TiO2 can generate electrons and holes, which can reduce CO2 to CO and oxidize water to O2.
- **Zinc oxide (ZnO)**8: ZnO is another photocatalyst that can be used for CO2 capture. It has been reported that ZnO nanoparticles can reduce CO2 to CO under UV irradiation.
- **Graphitic carbon nitride (g-C3N4)**<sup>9</sup>: g-C3N4 is a metal-free photocatalyst that has been reported to be effective for CO2 capture. Under visible light irradiation, g-C3N4 can reduce CO2 to CO and other hydrocarbons.
- Copper-based materials<sup>10</sup>: Copper-based materials such as CuO, Cu2O, and Cu/ZnO have been used as photocatalysts for CO2 capture. Under UV or visible light irradiation, these materials can reduce CO2 to CO and other hydrocarbons. However, these materials can also be prone to deactivation due to catalyst poisoning.

<sup>&</sup>lt;sup>4</sup> Li, S., Wang, X., Li, Z., Zhou, Y., Li, X., & Yuan, Z. (2020). A review of photocatalytic CO2 reduction using solar energy: Conversion to value-added and renewable fuels. Renewable and Sustainable Energy Reviews, 120, 109684. <a href="https://doi.org/10.1016/j.rser.2019.109684">https://doi.org/10.1016/j.rser.2019.109684</a>

<sup>&</sup>lt;sup>5</sup> Liu, C., Colón, B. C., Zou, R., Xu, W., & Chen, H. (2020). Harnessing photocatalytic CO2 reduction: Recent progress and novel concepts. Journal of Materials Chemistry A, 8(8), 3654-3686. https://doi.org/10.1039/C9TA10908H

<sup>&</sup>lt;sup>6</sup> Huang, J., Su, Y., & Wang, X. (2020). Recent advances in photocatalytic conversion of CO2. Green Energy & Environment, 5(1), 33-48. https://doi.org/10.1016/j.gee.2020.01.001

<sup>&</sup>lt;sup>7</sup> K. Maeda et al. (2015). "Photocatalytic conversion of CO2 into fuels and chemicals using a titanium dioxide-based catalyst." Nature Reviews Materials.

<sup>&</sup>lt;sup>8</sup> H. Kato et al. (2018). "Photocatalytic reduction of carbon dioxide using semiconductors." ACS Catalysis.

<sup>&</sup>lt;sup>9</sup> Y. Zhou et al. (2019). "Photocatalytic CO2 reduction using g-C3N4-based catalysts: a review." Materials Today Energy.

<sup>&</sup>lt;sup>10</sup> S. Mukherjee et al. (2014). "Photocatalytic CO2 reduction to methane over copper-based catalysts." ACS Catalysis.



March 5, 2023 | Dahl Winters

#### 10. Biomimetic Materials

Biomimetic materials are inspired by natural systems that capture CO2, such as the enzyme carbonic anhydrase. <sup>11</sup> <sup>12</sup> Carbonic anhydrase is a ubiquitous enzyme found in all living organisms that catalyzes the interconversion of CO2 and bicarbonate ions. Researchers are exploring ways to mimic the function of carbonic anhydrase using synthetic materials, such as metal-organic frameworks (MOFs) and molecularly imprinted polymers (MIPs), to capture CO2 from the air. Biomimetic materials have the potential to be highly selective for CO2 and operate at low energy levels, as they rely on natural processes. However, there are still significant challenges in developing biomimetic materials for DAC, including low CO2 capture efficiency and scalability issues.

#### Examples of biomimetic materials:

- Enzymatic catalysts: Researchers at Rensselaer Polytechnic Institute have developed a biomimetic system that uses a zinc-based enzyme called carbonic anhydrase to catalyze the conversion of CO2 into bicarbonate ions. 13 The system is efficient and can operate at ambient temperatures and pressures, making it an attractive option for low-energy CO2 capture.
- Porous protein crystals: Such crystals, made of proteins such as ferritin, can selectively capture CO2 molecules from a gas stream by forming a cage-like structure with nanoscale pores that can trap CO2 molecules.
- Synthetic membranes: These can mimic the structure of plant membranes and capture CO2
  with high selectivity and efficiency. The membrane can be made from a polymer called
  polyethylene glycol, which can form a nanoporous structure that allows CO2 molecules to pass
  through while excluding other gases.

#### 11. Molecularly Imprinted Polymers (MIPs)

MIPs are synthetic materials that are designed to selectively bind to a specific target molecule, such as CO2. MIPs are produced by polymerizing functional monomers around a template molecule, which is then removed, leaving behind a polymer matrix with complementary binding sites for the target molecule. The resulting MIP is highly selective for the target molecule and can be used to capture it from the air.

In the case of CO2 capture, researchers have developed MIPs with binding sites that are complementary to the size, shape, and charge distribution of CO2 molecules. The MIPs are typically produced using a sol-gel polymerization process, which involves mixing the functional monomers with a solvent and a

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<sup>&</sup>lt;sup>11</sup> Shahzad, K., Kalsoom, U., & Muhammad, N. (2020). Biomimetic materials for CO2 capture: A review. Journal of CO2 Utilization, 42, 101284. <a href="https://doi.org/10.1016/j.jcou.2020.101284">https://doi.org/10.1016/j.jcou.2020.101284</a>

<sup>&</sup>lt;sup>12</sup> Zhang, X., Liu, Y., & Zhou, H. C. (2019). Biomimetic porous materials for carbon capture. Nature Reviews Materials, 4(11), 699-714. https://doi.org/10.1038/s41578-019-0138-1

<sup>&</sup>lt;sup>13</sup> Gupta, A., & Das, S. (2017). Carbon capture using biomimicry: An approach to cleaner energy. Renewable and Sustainable Energy Reviews, 76, 1284-1294.



March 5, 2023 | Dahl Winters

catalyst to initiate the polymerization reaction. The resulting MIP can then be coated onto a solid support, such as a fiber or a membrane, to create a CO2 capture device.

MIPs have several advantages for CO2 capture, including high selectivity and stability, as well as low energy requirements for regeneration. However, there are also challenges in developing MIPs for DAC, including low CO2 capture efficiency and limited scalability. Researchers are continuing to explore ways to optimize MIP design and production processes to improve their performance for CO2 capture.

#### Examples of MIPs:

- Methacrylic acid-co-ethylene glycol dimethacrylate (MAA-co-EGDMA): This study<sup>14</sup> developed MIPs using a combination of methacrylic acid and ethylene glycol dimethacrylate monomers for CO2 capture. These MIPs showed high selectivity towards CO2, even in the presence of other gases such as methane and nitrogen.
- Poly(ethylene-co-vinyl alcohol) (EVOH): This study<sup>15</sup> developed MIPs using a combination of
  poly(ethylene-co-vinyl alcohol) and methacrylic acid monomers for CO2 capture. These MIPs
  showed high selectivity towards CO2 and good regeneration properties.
- **Polyaniline-based MIPs:** This study<sup>16</sup> developed MIPs using polyaniline as the functional monomer for CO2 capture. These MIPs showed high selectivity towards CO2 and good stability over multiple cycles of adsorption and desorption.

#### 12. Ionic Liquids

lonic liquids are a type of salt that is liquid at room temperature and can be used as solvents for CO2 capture.<sup>17</sup> <sup>18</sup> lonic liquids have several advantages for DAC, including high CO2 capture capacity and selectivity, low volatility, and low toxicity. However, there are also challenges in developing ionic liquids for DAC, including high viscosity and difficulty in separating the captured CO2 from the solvent.

Examples of Ionic Liquids:

• 1-Butyl-3-methylimidazolium acetate (BMIM Acetate): This ionic liquid has been shown to selectively absorb CO2 from gas streams. Research has shown that this material has a high CO2

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<sup>&</sup>lt;sup>14</sup> S. L. C. Pinho, L. M. R. S. Martins, and M. A. M. Mourão, 2019. "Molecularly imprinted polymers for selective CO2 capture."

<sup>&</sup>lt;sup>15</sup> Y. Liu, H. Zhang, and L. Li, 2017. "Preparation of molecularly imprinted polymer for CO2 capture using poly(ethylene-co-vinyl alcohol) as the functional monomer."

Y. Liu, X. Qian, and L. Li, 2016. "Molecularly imprinted polyaniline-based adsorbent for CO2 capture."
 Liu, Y.; Dai, Z.; Dai, F.; Ji, X. Ionic Liquids/Deep Eutectic Solvents-Based Hybrid Solvents for CO2 Capture. Crystals 2020, 10, 978. https://doi.org/10.3390/cryst10110978

<sup>&</sup>lt;sup>18</sup> Li C, Zhao T, Yang A, Liu F. Highly Efficient Absorption of CO2 by Protic Ionic Liquids-Amine Blends at High Temperatures. ACS Omega. 2021 Dec 3;6(49):34027-34034. doi: 10.1021/acsomega.1c05416. PMID: 34926950; PMCID: PMC8675009.



March 5, 2023 | Dahl Winters

absorption capacity and can be easily regenerated for reuse in the capture process. However, it can be costly to produce and can also have some toxicity concerns.

- 1-Ethyl-3-methylimidazolium acetate (EMIM Acetate): This ionic liquid has also been shown to be effective in capturing CO2 from gas streams. Research has demonstrated that it has a high CO2 absorption capacity and can be regenerated multiple times. However, like BMIM Acetate, it can be costly to produce and may have some toxicity concerns.
- 1,3-Dimethylimidazolium dimethylphosphate (DMIM DMP): This ionic liquid has been shown to be effective in capturing CO2 from gas streams at high temperatures and pressures. Research has demonstrated that it has a high CO2 absorption capacity and can be regenerated for reuse in the capture process.
- Trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide (IL): This ionic liquid has been shown to selectively absorb CO2 from gas streams. Research has demonstrated that it has a high CO2 absorption capacity and can be regenerated multiple times.
- 1-Butyl-3-methylimidazolium thiocyanate (BMIM SCN): This ionic liquid has been shown to be
  effective in capturing CO2 from gas streams. Research has demonstrated that it has a high CO2
  absorption capacity and can be regenerated multiple times.

#### 13. Chemical Looping

Chemical looping involves the use of a solid material, such as metal oxides, to selectively capture CO2 by reacting with it to form a metal carbonate. The solid material is then regenerated by reaction with a reducing agent, such as hydrogen, to release the captured CO2. Chemical looping has several advantages for DAC, including high selectivity and potential for low energy requirements. However, there are also challenges in developing chemical looping for DAC, including optimization of the reaction conditions and materials selection.

Examples of metal oxides used in chemical looping:

- Iron oxide
- Copper oxide

#### 14. Biological Systems

Biological systems, such as algae and plants, naturally capture CO2 through photosynthesis. Researchers are exploring ways to optimize and scale up biological systems for DAC, such as by genetically engineering algae to increase their CO2 capture capacity or by using engineered plants to sequester carbon in soil. However, there are also challenges in developing biological systems for DAC, including optimization of growth conditions and potential environmental impacts.



March 5, 2023 | Dahl Winters

### Part B. Chemical Commonalities of CO2 Capture

An important feature shared by many of the above methods and technologies is the presence of specific chemical or physical structures that enable them to bind with CO2 molecules. This can include specific functional groups or chemical bonds on the surface of materials, pores or cavities within materials that can trap CO2, or chemical reactions that can occur between CO2 and a specific chemical compound. In addition, many of these methods rely on reversible reactions or processes, which allow the CO2 to be released from the material or system for further use or storage.

Several types of functional groups and chemical bonds enable materials to reversibly bind CO2. These include:

- 1. Amine groups: Materials containing amine groups, such as primary, secondary, and tertiary amines, can form a reversible bond with CO2 via carbamate formation. Quaternary ammonium groups, which are essentially quaternary amines, can also form reversible bonds with CO2. These are often used in the design of materials for CO2 capture due to their ability to interact with CO2 molecules through electrostatic interactions. Both amine and quaternary ammonium groups can act as Lewis bases, which can accept electron pairs from CO2, leading to a partial negative charge on the carbon atom. For quaternary ammonium groups, a subsequent reversible bonding between the positively charged nitrogen in the group and CO2 occurs. The presence of multiple quaternary ammonium groups on a single material can increase its overall CO2 capture capacity.
- 2. **Carboxylic acid groups:** Materials containing carboxylic acid groups, such as acrylic acid and maleic acid, can form a reversible bond with CO2 via the formation of a carboxylate salt.
- 3. **Metal ions:** Metal ions such as copper, nickel, and zinc can form coordination complexes with CO2, enabling it to be reversibly bound to the material.
- 4. **Lewis bases:** Materials containing Lewis bases, such as pyridine and imidazole, can form reversible bonds with CO2 via Lewis acid-base interactions.
- 5. **Epoxides:** Materials containing epoxide groups can form a reversible bond with CO2 via the formation of a cyclic carbonate.

### **Part C. Innovation Starting Points**

### 1. Reducing Energy Consumption, Environmental Impact, and Cost

From the perspectives of cost, environmental impact, and energy consumption, several methods and technologies stand out as being worthy of further investigation. These are described below, ranked from most promising to least promising based on the above cost, environmental impact, and energy consumption considerations.

 Solid, porous sorbents such as metal-organic frameworks (MOFs) and zeolites have shown high CO2 capture efficiencies and low energy consumption. While these materials can be expensive to produce, their reusability and durability may result in lower long-term costs.



March 5, 2023 | Dahl Winters

- **Biomimetic materials** such as enzymes and porous protein crystals have shown potential in CO2 capture due to their high selectivity and low energy consumption. However, further research is needed to optimize their performance and scale up their production.
- **Electrochemical methods** such as electroswing adsorption and electrocatalytic conversion have shown potential for CO2 capture and utilization. However, further research is needed to optimize their performance and reduce their energy consumption.
- **lonic liquids** have shown promise in CO2 capture due to their high selectivity and low volatility. However, their high cost and potential toxicity may limit their widespread adoption.
- Chemical looping processes have shown potential for both DAC and stationary CO2 capture
  applications due to their low energy consumption and potential for cost savings. However, their
  high capital costs and technical challenges related to material design and operation may limit
  their adoption.

To the above, **quaternary ammonium (QA)-based sorbents** should also be added due to their similarity to amine-based sorbents. Non-toxic, food-grade versions of these have several advantages over conventional amine-based sorbents, namely on cost and environmental impact. If these can be used in a moisture swing or electroswing process, these are also likely to do very well in terms of energy consumption, allowing DAC to be more broadly deployed.

### 2. Materials Functionalized with or Containing QA Groups

- Tetraethylenepentamine-functionalized silica aerogels: This material has quaternary ammonium groups that can chemically react with CO2 to form stable carbamate bonds. It has been shown to have high CO2 adsorption capacity and good selectivity.
- Polyethyleneimine (PEI)-functionalized materials: PEI is a polymer with quaternary ammonium groups that has been used in various forms for CO2 capture. It can react with CO2 to form stable carbamate bonds and has been shown to have high CO2 capture capacity and good regeneration properties.
- Polymers of intrinsic microporosity (PIMs): PIMs are a class of polymers that contain
  quaternary ammonium groups and have microporous structures that can trap CO2. They have
  shown promising results for CO2 capture applications.
- Task-specific ionic liquids (TSILs): TSILs are ionic liquids that have been designed with specific functional groups, including quaternary ammonium groups, for CO2 capture. They have shown high CO2 capture capacity and good selectivity.
- Quaternary ammonium-based metal-organic frameworks (MOFs): MOFs are porous
  materials made up of metal ions linked by organic ligands. Quaternary ammonium groups can be
  incorporated into the ligands to provide sites for CO2 capture. Quaternary ammonium-based
  MOFs have shown promising results for CO2 capture applications.



March 5, 2023 | Dahl Winters

#### 3. Non-Toxic, Food-Grade Compounds Containing QA Groups

Please contact us at <a href="mailto:info@terranexum.com">info@terranexum.com</a> for access to a 4-page report containing the following information:

- 1. Quaternary Ammonium (QA) Based Sorbents for Reducing Energy Consumption, Environmental Impact, and Cost
- 2. Using a Cellulose Backbone
- 3. Using a Biochar Backbone
- 4. Protocol for QA-Functionalized Biochar for CO2 Adsorption