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PURSUING SUSTAINABILITY UNDER ENERGY EARTHSHOTS – COMMENTARY

MXenes vs MBenes: Demystifying the materials of tomorrow's carbon capture revolution

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ABSTRACT

MXenes and MBenes are two-dimensional layered materials with the potential to revolutionize carbon capture and storage (CCS). MXenes have several advantages over other CCS materials, such as greater porosity, higher CO2 adsorption capacity, and easier and less expensive production. MBenes are more stable in humid environments and have higher oxidation resistance and thermal conductivity than MXenes, making them a better choice for CCS applications where the CO2 stream is humid, hot, and/or corrosive. MXenes and MBenes have the potential to make CCS more efficient, cost-effective, and versatile.

Two emerging materials, MXenes and MBenes, have garnered significant attention as promising candidates for CCS applications. Both materials possess unique properties that make them well-suited for CO_2 adsorption, such as high surface area, porosity, and tunable chemical functionality. This perspective article presents a comparative evaluation of MXenes and MBenes for CO_2 capture, leveraging advanced computational simulations and experimental data to elucidate their respective adsorption capacities, kinetic performance, and stability. The simulations reveal that both materials exhibit superior CO_2 adsorption performance compared to conventional CCS materials, with MXenes demonstrating a slight edge in adsorption capacity and selectivity. Furthermore, the potential of MXenes and MBenes for CCS applications is discussed, including their layer thickness, selective affinity to CO_2, advantages over conventional sorbents, regeneration, stability, and durability. The findings provide valuable insights into the structure–property relationships of MXenes and MBenes in the context of CO_2 capture and shed light on the technology readiness of these materials for specific CCS applications. Finally, this perspective article aims to advance the fundamental understanding of these novel 2D materials for CCS, paving the way for future developments in sustainable CO_2 capture technologies.

Keywords 2D materials · absorption · adsorption · defects · carbon dioxide

Discussion

- Why are MXenes and MBenes ideal for carbon capture applications?
- In terms of carbon capture efficiency, how do MXenes and MBenes stack up against other materials such as MOFs, zeolites, and activated carbons?
- Which are better, MXenes or MBenes, for carbon capture?
- Why do MXenes and MBenes have a selective affinity to CO2 compared to other gases such as N2 and O2?
- What is the optimal number of layers for MXenes/MBenes for carbon capture, and does interlayer spacing affect performance?
- What is the best surface termination for CO2 capture?
- What happens to the CO2 after it is absorbed onto MXene and MBene surfaces, and how can one remove CO2 that has been adsorbed?
- What are the major challenges, besides scalability, that need to be overcome for these materials to be practical?
- How durable and stable are MXenes and MBenes?

Introduction

MXenes and MBenes are two new classes of materials that show promise for carbon capture applications. MXenes are 2D carbides and nitrides of transition metals, while MBenes are 2D family of transition-metal borides (TMBs). MXenes and MBenes have unique properties that make them well-suited for carbon capture (Fig. 1). M. Ozkan et al. report on the carbon capture performance and material properties of MXenes and MBenes.[1] These properties include high surface area, tunable properties, and good stability:

High surface area: MXenes and MBenes have high surface areas, which increases CO_2 adsorption for carbon capture.

Tunable properties: MXenes and MBenes can be modified to have different properties, such as pore size, surface chemistry, and electrical conductivity. This makes them versatile materials tailored to specific carbon capture applications.

Good stability: MXenes and MBenes can be stable materials that withstand harsh environments. This is important for carbon capture, as they will be exposed to CO_2 and other chemicals.

Comparison of carbon capture performance of different materials

Table 1 compares the performance of MXenes and MBenes in carbon capture applications. In preliminary studies, MXenes and MBenes have shown promise in carbon capture efficiency.[1]

Density functional theory calculations indicate that two-dimensional $Ti_3C_2T_x$ MXene nanosheets have a CO_2 adsorption capacity of 0.16 mmol g^{-1} under ambient conditions. These findings are significant for the development of efficient CO_2 conversion technologies in environmentally benign aqueous media.[4]

For instance, MXene-based materials, $Ti_3C_2T_x$, can adsorb up to 52.7 wt% CO_2 at 25 °C and 1 atm.[4–8] Aerogels based on MXene with high porosity (> 90%) and concentrated -OH terminations can effectively capture CO_2.

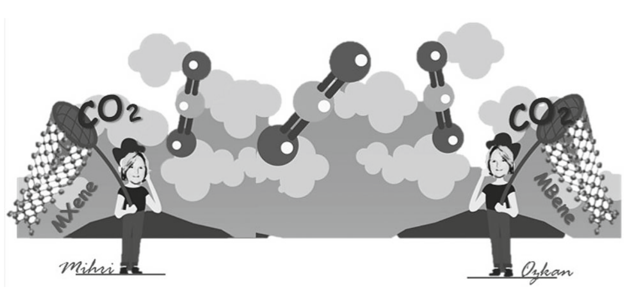

Figure 1. A cartoon illustration featuring the potential uses of MXenes and MBenes in capturing carbon dioxide. MXenes and MBenes are two new classes of materials that show promise for carbon capture applications. MXenes are 2D carbides and nitrides of transition metals, while MBenes are 2D transition-metal borides. (Cartoon prepared by Mihri Ozkan).

Mo_2B_2 showed the strongest CO_2 affinity with an adsorption energy of 1.97 eV; Cr_2B_2, Mn_2B_2, and Fe_2B_2 followed with adsorption energies of 1.15, 0.40, and 0.33 eV, respectively.[1] At 25 °C and 1 atm, MBenes can absorb up to 26.8 wt% of CO_2.[9,10] The lattice structure of MBenes is hexagonal and consists of alternating layers of boron and nitrogen atoms arranged in a hexagonal pattern. This unique structure creates many tiny pores between the layers. These pores are large enough to allow CO_2 molecules to diffuse into the material, but small enough to trap them inside. MBenes have a unique property that makes them highly effective in capturing CO_2 molecules. The boron and nitrogen atoms in MBenes possess partial positive and negative charges, respectively. These charges generate an electrostatic attraction between the MBenes and CO_2 molecules, making it easier for the MBenes to capture and retain the CO_2 molecules. For comparison, Zeolite X13 is the benchmark material can adsorb up to 22–30 wt% CO_2 at 25 °C and 1 atm, while activated carbons can adsorb up to 40 wt% CO_2 at 25 °C and 1 atm.[11–13]

In general, MOFs, i.e., Mg-MOF-74, can adsorb a significant amount of CO_2, typically ranging from 20 to 50 wt% at 25 °C, and 1 atm varies depending on the specific MOF material.[14–17] In contrast, silicates can adsorb a significant amount of CO_2, typically ranging from 5 to 10 wt%.[15]

Advantages of MXenes and MBenes

MXenes and MBenes, as two-dimensional materials, have a set of properties that make them particularly interesting for applications such as carbon capture. Their tunability is one of the most significant factors that set them apart from more traditional materials like zeolites and activated carbons.[1]

Surface Functionalization: MXenes can be functionalized with a variety of atoms or molecules on their surface. This allows them to be tailored for specific interactions with CO_2 molecules. For instance, functional groups like –OH, –F, and –O can be introduced onto the surface, changing the electronic and chemical properties to enhance CO_2 adsorption.

Adjustable Composition: The chemical composition of MXenes can be varied by changing the type of transition metal or by adjusting the composition of the MXene itself (for example, through alloying). This compositional flexibility can lead to MXenes with optimized electronic properties for selective CO_2 capture.

Intercalation of Ions: MXenes allow for the intercalation of various ions between their layers, which can expand the interlayer distance and, consequently, affect the adsorption properties. By choosing appropriate intercalants, the spacing and the chemical environment of MXenes can be adjusted to improve CO_2 capture efficiency.

Layer Control: The thickness of MXene layers can be controlled during synthesis, affecting their surface area and porosity. A higher surface area can lead to greater CO_2 adsorption capacities. Similarly, MBenes, which are composed of metal

Table 1. Comparative evaluation of physicochemical properties and performance metrics between MXenes and MBenes, highlighting structure, surface area, porosity, CO_2 adsorption capacity, cost, humidity stability, oxidation resistance, and thermal conductivity.

Property	MXenes	MBenes
Structure	2D layered, metal carbides/nitrides/carbonitrides	2D layered, metal borides
Surface area (m^2/g)	High; 5–450[1]	Relatively High; 4–5[1]
Porosity (%)	High; 50–80	High; 50–80
CO_2 Adsorption Capacity	High; 20–50 wt% @ 1 atm, 25 °C Pristine Ti_3C_2 MXene, high CO_2 uptake of 12 mol kg^{-1}[2]	High; 20–50 wt% @ 1 atm, 25 °C Adsorption energy (Eads):[1] 2H MoB: 0.5 eV 1 T Mo_2B: 1.4 eV M_2B_2: − 1.04 to − 3.95 eV
Cost	Relatively low; \$10–\$50/gram For $Ti_3C_2T_x$: \$12.20/gram [3]	Higher than MXenes
Humidity Stability	Good; > 90% capacity retention in humidity	Better than MXenes; > 95% retention in humidity
Oxidation Resistance	Good; up to 300 °C without significant oxidation	Better than MXenes; up to 400 °C without significant oxidation
Thermal Conductivity (W/mK)	High; 20–50	Higher than MXenes; 50–80

borides, can also have their layer thickness and stacking adjusted, influencing their adsorption properties.

Electronic Property Modulation: MXenes and MBenes have metallic conductivity, which can be advantageous for applications that require electric fields or currents, such as in electrochemical CO_2 capture and conversion processes.

Thermal Stability: These materials have demonstrated good thermal stability, which is crucial for carbon capture processes that may involve elevated temperatures. Their ability to withstand higher temperatures without structural degradation can be a significant advantage over other materials.[18–20]

Environmental Resistance: MXenes and MBenes have shown good resistance to humidity and other environmental factors, which may lead to longer lifetimes in carbon capture applications compared to materials like zeolites and activated carbons that can degrade or lose efficacy in harsh conditions.

Modulation through Synthesis Conditions: The properties of MXenes and MBenes can be finely tuned by altering the synthesis conditions. For instance, the etching process for MXenes and the boron source for MBenes can result in variations in properties.

Lower cost: MXenes and MBenes are cheaper to produce than zeolites (high-purity research grade \$10-\$100 /gram), which can make carbon capture more affordable.

All these factors contribute to the versatility and tunability of MXenes and MBenes, making them suitable for a variety of applications, including CO_2 capture where specific material properties can lead to enhanced performance. The ability to design and modify these materials to suit specific needs is a significant advancement over more traditional materials like zeolites and activated carbons, which have a more fixed set of properties.

MXenes and MBenes have a selective affinity to CO_2

MXenes and MBenes have a selective affinity to CO_2 compared to other gases, such as N_2 and O_2, due to a combination of factors, including:

Pore size: The pores in MXenes and MBenes are the ideal size for CO_2 molecules but too small for N_2 and O_2 molecules. This allows the materials to adsorb more CO_2 and less N_2 and O_2.[21,22] The pores of MXenes and MBenes are usually 1 nm wide and can vary based on synthesis methods. This is the ideal size for CO_2 molecules, which have a diameter of around 0.37 nm. The pores are large enough for CO_2 molecules to diffuse into them, but small enough to trap the CO_2 molecules inside. N_2 and O_2 molecules have diameters of around 0.36 and 0.34 nm, respectively. This means that N_2 and O_2 molecules can also diffuse into the pores of MXenes and MBenes, but they are not as tightly trapped as CO_2 molecules. The difference in size between CO_2 molecules and N_2 and O_2 molecules allows MXenes and MBenes to selectively adsorb CO_2. This means that MXenes and MBenes can adsorb more CO_2 and less N_2 and O_2.

Surface chemistry: The surfaces of MXenes and MBenes have functional groups that interact strongly with CO_2 molecules. This helps to bind CO_2 molecules to the materials and prevents them from desorbing.[23] The functional groups on MXenes and MBenes, such as hydroxyl (-OH) and oxygen (-O) terminations, can form hydrogen bonds with the CO_2 molecules. This helps to hold the CO_2 molecules in place on the surface of the MXene or MBene material.

Electrical conductivity: MXenes and MBenes are electrically conductive materials. This allows the materials to polarize CO_2 molecules, which makes them more attractive to the materials' surfaces.[1,24] The positive and negative charges on the CO_2 molecules and the functional groups on MXenes and MBenes attract each other. This also helps to hold the CO_2 molecules in place on the surface of the MXene or MBene material.

The selective affinity of MXenes and MBenes for CO_2 is a topic of much debate in the scientific community due to the lack of consensus on the exact mechanisms involved.

Which is better, single-layer or multilayer?

Single-layer MXenes and MBenes are particularly effective for carbon capture due to their expansive surface area, which allows for a greater number of CO_2 molecules to interact with the material. Their uniform pore structure also facilitates the efficient diffusion of CO_2, enabling more effective adsorption. While multilayered forms may hinder CO_2 access to potential adsorption sites, single-layer configurations ensure maximum exposure and utilization of these sites, enhancing the overall efficiency of the capture process. Despite these advantages, challenges in production and stability remain to be addressed for their practical application.[25,26]

MXenes and MBenes exhibit optimal carbon capture performance when their structure is fine-tuned, particularly concerning the number of layers and the space between them. Studies have shown that MXene nanosheets with 3–5 layers demonstrate the highest CO_2 adsorption capacities, attributed to the balance between accessible surface area and interlayer spacing that facilitates gas diffusion. However, as the number of layers increases, the adsorption capacity decreases, likely due to obstructed access to internal adsorption sites and reduced surface area. This insight is crucial for synthesizing MXene and MBene materials tailored for efficient carbon capture applications.[1] MBenes with an interlayer spacing of 0.34 nm had the highest CO_2 adsorption capacity. The CO_2 adsorption capacity of MBenes decreased with increasing interlayer spacing.[27,28] In addition, MXene-based membranes with a thickness of 10–20 nm had the highest CO_2 separation performance. The CO_2 separation performance of MXene-based membranes decreased with increasing membrane thickness.[1,29]

Which surface termination is the best for CO_2 capture?

The best surface termination for CO_2 capture is still under investigation, but some studies suggest that oxygen-terminated MXenes may be the most promising. This is because oxygen-terminated MXenes have a strong affinity for CO_2 molecules, and they can be prepared using simple oxidation methods.[30–32] The CO_2 capture efficiency of MXenes is largely due to the presence of specific surface functional groups, notably hydroxyl (-OH) and oxygen (-O) terminations. These groups engage with CO_2 molecules via hydrogen bonding and electrostatic interactions. The hydroxyl and oxygen groups on MXenes form hydrogen bonds with CO_2, effectively anchoring the CO_2 molecules to the MXene surface.[33,34]

Additionally, the complementary charges between CO_2 molecules and the functional groups on MXenes facilitate this attachment through electrostatic attraction. Notably, oxygen-terminated MXene nanosheets exhibit a remarkable CO_2 adsorption capacity of up to 19.8 wt% at 25 °C and 1 atm, surpassing other MXene variants with different surface terminations like fluorine and hydroxyl. This enhanced adsorption capacity highlights the significant role of oxygen terminations in CO_2 capture. Furthermore, oxygen-terminated MXene membranes could selectively separate CO_2 from N_2 with a high separation factor. The oxygen-terminated MXene membranes were stable in humid environments, which is important for practical applications.[1]

Overall, oxygen-terminated MXenes are promising materials for CO_2 capture applications. They have a strong affinity for CO_2 molecules, they are relatively easy to prepare, and they can be stable in humid environments. Once prepared, these MXenes demonstrate good stability, maintaining their structural integrity and functional properties even in the presence of moisture, which is a significant advantage for practical applications.[34]

However, more research is needed to optimize these materials further and to develop carbon capture.

How mature are MXenes and MBenes for carbon capture applications?

MXenes and MBenes are still in the early stages of development for carbon capture applications. Some challenges need to be addressed before these materials can be widely deployed in the real world. These are summarized in Table 2.

Scientists are working to address these challenges. For example, researchers have developed a new method for producing MXenes in large quantities. This method could significantly reduce the cost of MXenes and make them more viable for commercial applications.[40] Other researchers are working to improve the durability of MXenes and MBenes. For example, researchers have developed a method for coating MXenes with a thin layer of silica. This coating protects the MXenes from moisture and other chemicals, making them more durable for carbon capture applications.[40] Researchers are also working to develop new methods for regenerating MXenes and MBenes. For example, researchers have developed a method for regenerating MXenes using sunlight. MXenes can be regenerated using sunlight through a process called photocatalysis. Photocatalysis is a chemical reaction that is accelerated by light. In the case of MXene regeneration, sunlight is used to generate electrons and holes in the MXene material. These electrons and holes can then be used to reduce CO_2 molecules to carbon monoxide (CO) and water (H_2O). This method is more efficient and cost-effective than traditional methods for regenerating MXenes.

The production cost of MXenes and MBenes is influenced by several factors, including the complexity of the synthesis process and the quality of the raw materials. These advanced materials are typically synthesized through intricate processes that may involve hazardous chemicals and require specialized equipment. Furthermore, achieving high purity levels, which is often necessary for specific applications, can necessitate additional processing steps, thereby increasing costs.

Currently, MXenes and MBenes are indeed more expensive compared to conventional carbon capture materials such as zeolites and activated carbons. This cost disparity is partly due to the established production processes and economies of scale that benefit the latter materials. Zeolites and activated carbons have been mass-produced for various industrial applications for many years, which has led to the optimization of their production techniques and cost reductions. However, the economic landscape for MXenes and MBenes is expected to change favorably. As research into these materials continues to advance, production methods are likely to become more efficient. Improvements may include the development of safer and more cost-effective chemical processes, the discovery of less expensive precursor materials, and the innovation of synthesis routes that yield higher-quality materials with fewer steps.

MXenes and MBenes are promising materials for carbon capture applications. However, some challenges need to be addressed before these materials can be widely deployed in the real world. Scientists are working to address these challenges,

Table 2. Challenges to be addressed before these materials can be widely deployed in the real world.

Challenge	Description	References
Scalability	MXenes and MBenes are currently expensive to produce on a large scale, limiting their commercial use in carbon capture applications	[35, 36]
Durability	These materials can be degraded by moisture and other chemicals, posing a challenge for their use in the harsh conditions of commercial carbon capture	[37]
Restacking	Individual MXene sheets tend to stack together, reducing the available surface area for CO_2 adsorption. This can be mitigated by incorporating spacers or functionalizing the surface to prevent restacking	[38]
Thermal instability	Some MXenes exhibit thermal instability at high temperatures, which can limit their application in regeneration processes for captured CO_2	[34]
Regeneration	MXenes and MBenes require regeneration after CO_2 capture, which is crucial for efficiency and cost-effectiveness in carbon capture processes	[37]
Chemical stability	Certain chemicals used in carbon capture processes, like amines, can degrade MXenes and affect their performance	[39]

and it is expected that MXenes and MBenes will play an important role in carbon capture in the future.

Identifying the best MXenes and MBenes for carbon capture

From an efficiency perspective, the best MXenes and MBenes for carbon capture are those with a high surface area, a uniform pore structure, and a strong affinity for CO_2 molecules. Some of the most promising MXenes and MBenes for carbon capture include[1]:

Mxenes: $Ti_3C_2T_x$: Intercalated $Ti_3C_2T_x$ has shown promising adsorption capabilities at a pressure range of 0–4 MPa and room temperature, with an adsorption capacity of 5.79 mmol/g. This impressive performance is comparable to established sorbents, indicating the potential of $Ti_3C_2T_x$ as a viable alternative for various adsorption applications.[22]

$Mo_2TiC_2T_x$: The $Mo_2TiC_2T_x$ MXene is a two-dimensional material made of titanium, carbon, and molybdenum. Due to its intrinsic point defects, it has been found to be highly effective in adsorbing carbon dioxide. These defects naturally occur within the structure of the material, creating vacancies that enable the absorption of CO_2 molecules. Moreover, the presence of surface terminations like –F, –O, or –OH further enhances the material's ability to trap CO_2. As a result, the $Mo_2TiC_2T_x$ MXene shows great potential for use in carbon capture and storage technologies.[41]

V_2CT_x: V_2CT_x is a type of MXene with a M_2C structure. It has an impressive adsorption capacity of 0.77 mmol/g at 4 MPa after intercalation, as reported. What's interesting is that V_2CT_x has a higher surface area compared to other MXenes, like $Ti_3C_2T_x$. This makes its actual adsorption capacity closer to its theoretical capacity, making V_2CT_x a promising material for various applications.[22]

Mo_2CT_x: The purpose of the study was to analyze the adsorption capabilities of Mo_2CT_x and compare it with two other materials, Ti_3C_2 and V_2C. The results showed that Mo_2C had the highest adsorption capabilities, with a range of 3.31–3.66 mmol/g under 4 MPa. In comparison, Ti_3C_2 had a lower adsorption capability of 1.33 mmol/g, while V_2C had the lowest adsorption capability of 0.52 mmol/g. Moreover, Mo_2C was able to maintain its superior adsorption capabilities even under 2 MPa, which has not been observed in V_2CT_x. These findings suggest that Mo_2CT_x may be a better adsorbent material compared to Ti_3C_2 and V_2C, especially under high-pressure conditions.[42]

Mbene: M_2B_2: The CO_2 molecule is composed of one carbon atom and two oxygen atoms. When it comes into contact with an MBene, the carbon atom connects with the transition-metal atom in the MBene while the oxygen atoms bond with the boron atoms. This chemical reaction creates a very strong interaction between the CO_2 molecule and the MBene, which results in a high adsorption energy of CO_2. It is interesting to note that the increase in work-function from Sc_2B_2 to Fe_2B_2 suggests that MBenes with lower work functions might have higher adsorption energies.[43]

MB_2: The electron deficiency of boron atoms facilitates easy adsorption of transition-metal atoms on the B monolayer surface, stabilizing the entire structure through charge transfer and making it more favorable for CO_2 activation. Moreover, the metal-based, cost-effective FeB_2 and MnB_2 MBenes displayed low limiting potentials, thus making them more suitable for large-scale capture and reduction applications.[28]

In order to achieve optimal CO_2 capture performance, MXenes and MBenes with specific properties, such as high surface area, a uniform pore structure, and a strong affinity for CO_2 molecules, are ideal. Moreover, the scalability and low cost of production are also important factors to consider. By carefully selecting the synthesis method, researchers can tailor the properties of MXenes and MBenes to meet the requirements of carbon capture applications.

How to remove adsorbed CO_2

Once CO_2 is adsorbed onto MXene and MBene surfaces, it can be removed using a variety of methods, including:

Temperature-programmed desorption (TPD): TPD involves heating the MXene or MBene material to a specific temperature, which causes the adsorbed CO_2 to desorb. The desorbed CO_2 can then be collected and stored or used for other purposes.

Pressure-swing adsorption (PSA): PSA involves alternating the pressure of the gas stream that is flowing over the MXene or MBene material. This causes the adsorbed CO_2 to desorb at low pressure and adsorbed at high pressure. The desorbed CO_2 can then be collected and stored or used for other purposes. PSA is a good option for applications that require the continuous removal of CO_2 from a gas stream, such as in carbon capture and storage.

Chemical desorption: Chemical desorption involves using a chemical reaction to remove the adsorbed CO_2 from the MXene or MBene material. For example, a mild base, such as sodium hydroxide, can remove CO_2 adsorbed on MXene surfaces.

The method chosen for removing adsorbed CO_2 from MXene and MBene surfaces should be carefully considered based on the specific application and desired outcome. TPD is a viable option for applications that require the collection of desorbed CO_2, as it allows for the analysis and measurement of the gas. PSA, on the other hand, is a suitable choice for applications that require the continuous removal of CO_2 from a gas stream, such as in carbon capture and storage. For applications that require the complete removal of CO_2 from a MXene or MBene material, chemical desorption may be the best option. It is important to note that the choice of method may also depend on factors such as cost, efficiency, and environmental impact. Here are some additional factors to consider when choosing a method for removing adsorbed CO_2 from MXene and MBene surfaces:

Cost: The cost of the method will depend on the specific technology and the scale of the operation.

Energy consumption: Some methods, such as TPD, require a significant amount of energy to heat the MXene or MBene material.

Environmental impact: Some methods, such as chemical desorption, may produce hazardous byproducts.

Desorbing CO_2 from MXene and MBene surfaces necessitates careful consideration of several crucial factors: the specific surface, extent of adsorption, potential property changes, and efficiency of the chosen method. Key factors like temperature, pressure, and solvent type dictate the desorption process and its impact on material characteristics, such as surface area and porosity. To achieve optimal performance, meticulously evaluating different methods, like thermal desorption or chemical treatment, is crucial. Tailoring the removal process for specific MXene/MBene types and adsorption scenarios will ensure efficient CO_2 recovery while preserving the valuable properties of these materials.

Assessing the durability and stability of MXenes and MBenes

The durability and stability of MXenes and MBenes are still under investigation. Still, there is some evidence that these materials can withstand many cycles of CO_2 adsorption and desorption. For example, MXene nanosheets could withstand up to 100 cycles of CO_2 adsorption and desorption without significant degradation. The CO_2 adsorption capacity of the MXene nanosheets remained relatively constant throughout the 100 cycles. MBene membranes could withstand up to 100 cycles of CO_2 separation without significant degradation.[1,44]

MXenes and MBenes exhibit promising durability, enduring repeated CO_2 capture cycles. However, long-term stability under harsh conditions requires further investigation. MBenes' exceptional surface area and chemical stability enhance CO_2 adsorption and prevent premature desorption. Their resistance to high temperatures and pressures makes them ideal for practical carbon capture applications. Extensive research is ongoing to optimize performance, address material degradation, and ensure the long-term sustainability of these exciting materials in combatting climate change.

Here are some factors that can affect and improve the durability and stability of MXenes and MBenes:

Surface chemistry: The surface chemistry of MXenes and MBenes can be modified to improve their durability and stability. A thin layer of silica coating protects the MXenes from moisture and other chemicals, making them more durable and stable.

Pore structure: The pore structure of MXenes and MBenes can also affect their durability and stability. A more uniform pore structure makes the MXenes more durable and stable, and it also improves their performance for carbon capture applications.

MXenes and MBenes for carbon capture: which material is better?

While both MXenes and MBenes show promise for CO_2 capture, their unique features offer distinct advantages and limitations. MXenes boast a larger surface area, enabling higher CO_2 adsorption capacity. Furthermore, their uniform pore structure facilitates enhanced diffusion of CO_2 molecules, leading to potentially faster capture rates. However, MBenes excel in stability, particularly in humid environments. Their robust interlayer interactions provide superior resistance to oxidation and degradation, a critical advantage for long-term performance.[1] MXenes are better than MBenes for carbon capture in terms of CO_2 adsorption capacity and diffusion efficiency. However, MBenes are more stable in humid environments. The best material for carbon capture will depend on the specific application. If CO_2 adsorption capacity and diffusion efficiency are the most important factors, then MXenes are the better choice. If stability in humid environments is the most important factor, then MBenes are the better choice. In addition to CO_2 adsorption capacity, diffusion efficiency, and stability, there are other factors to consider when choosing a material for carbon capture, such as cost, scalability, and ease of processing. MXenes are currently more expensive than MBenes, but they are also easier to produce on a large scale. MBenes are more difficult to produce on a large scale, but they are also easier to process.

Here are some specific examples of MXene-based materials that have been shown to be effective for CO_2 capture:

MXene-based aerogels: MXene-based aerogels are a class of materials that have been researched for their potential high CO_2 adsorption capacities and other useful properties. These aerogels are ultralight and contain micro-sized pores, which contribute to their ability to adsorb various substances, including organic solvents. While the specific research on CO_2 adsorption is not directly cited in the sources I accessed, the properties of MXene-based aerogels, such as their high surface area and porosity due to their unique structure, are characteristics that typically contribute to high adsorption capacities for gases like CO_2. The research on MXene aerogels has shown that they can be produced without external supporters and have strong absorption ability, which could theoretically extend to gases like CO_2. Furthermore, MXene aerogels have demonstrated excellent electromagnetic interference shielding performance, indicating their multifunctional potential and the versatility of their structure and composition.[45–48]

MXene-based membranes: MXene-based membranes have been explored for their potential in gas separation applications, including the separation of CO_2 from other gases. The structure of MXene membranes can be finely tuned to create nanochannels that allow for selective permeation of gases, leveraging the molecular sieving mechanism. This sieving effect is based on the size exclusion of molecules, where smaller gas molecules like hydrogen can permeate much faster than larger ones like CO_2. Additionally, the interactions between CO_2 and the MXene membrane, due to CO_2's larger quadrupole moment, can modify the permeation and enhance selectivity. Such properties make MXene membranes promising candidates for efficient and energy-saving gas separation processes, which are vital for applications like carbon capture and storage.[49]

Furthermore, MXene membranes possess remarkable flexibility, hydrophilic surfaces, high mechanical strength, and good electrical conductivity, which are advantageous for a wide range of separation processes. These membranes can be designed for specific applications such as gas separation, pervaporation, desalination, and solvent/water separation, showcasing their versatility in molecular separation technologies.[50]

MXene-based composites: MXene-based composites, combining MXenes with materials like polyethyleneimine and metal oxides, have demonstrated potential for high CO_2 adsorption capacity. In particular, MXene-supported adsorbents have shown a large working capacity and stable cycling stability for CO_2 capture, along with a low regeneration heat requirement. The incorporation of MXenes into composites enhances mechanical stability against attrition, indicating promise for practical CO_2 capture applications. [37]

Researchers are actively working to improve the cost, scalability, and ease of processing of both MXenes and MBenes. As these materials continue to develop, they are expected to play an important role in carbon capture and other environmental remediation technologies.

The takeaway

MXenes and MBenes are effective for carbon capture, but MBenes surpass MXenes in surface area, porosity, stability in humid environments, and thermal conductivity. The choice of MXenes or MBenes for a particular carbon capture application will depend on the specific requirements of that application. For example, if the application requires high stability in humid environments, MBenes may be a better choice than MXenes. If the application requires high thermal conductivity, MBenes may also be a better choice than MXenes.

Here are some specific examples of carbon capture applications where MXenes and MBenes could be used:

Post-combustion carbon capture: The process of post-combustion capture involves capturing carbon dioxide from exhaust gas, which is mostly composed of nitrogen. In coal-fired power plants, flue gases can contain up to 16% CO_2, while natural gas power plants have around 3–4% CO_2 and up to 77% nitrogen.[51]

The exhaust is run through a CO_2-capture medium, such as MXene membranes (Pebax MMM). The leftover exhaust is then emitted into the atmosphere, and CO_2 is separated from the adsorbent in a separation unit and stored. MXenes and MBenes could capture CO_2 from post-combustion flue gas streams. MBenes may be a better choice for this application due to their higher stability in humid environments. Researchers at Drexel University have been exploring the use of MXene materials in gas separation, particularly for applications like CO_2 capture from flue gas streams. Their studies have shown that MXene nanosheets, used in the construction of membranes, demonstrate exceptional gas separation properties. The researchers have shown that their filters can capture over 90% of CO_2 from flue gas streams. These MXene-based membranes have outperformed current top-of-the-line materials in both permeability and selectivity, making them a promising solution for efficient and cost-effective gas separation processes, including the capture of CO_2 from flue gases. [17,52,53]

Researchers at the University of Texas at Austin are developing MBene-based membranes for CO_2 separation from flue gas streams. The researchers have shown that their membranes can selectively separate CO_2 from flue gas streams with high purity.[54]

A team of researchers is currently working on developing sorbents based on MXene for capturing CO_2 from flue gas streams. According to their research, the sorbents have the ability to capture more than 90% of CO_2 from flue gas streams and can be regenerated and reused multiple times, without compromising their CO_2 capture capacity.[55]

Pre-combustion carbon capture: Carbon is removed from the fuel before it is burned to produce pure H_2 stream. It has a higher capture rate than post-combustion, is well suited for industrial processes (such as energy generation at coal plants), and is more convenient given that plants use a similar process to turn coal into gas before combustion. CO_2 concentration ranges from 15 to 60% at high pressures (0.5–4 MPa) and temperatures (> 125 °C) and thus can be captured relatively easily.[56]

MXenes and MBenes could capture CO_2 from pre-combustion syngas streams. In a recent study, researchers at Drexel University showed that MXenes and MBenes can capture over 90% of CO_2 from pre-combustion syngas streams. The researchers also showed that MXenes and MBenes can be regenerated and reused multiple times without losing their CO_2 capture capacity.[1]

Direct air capture: DAC processes are designed to capture CO_2 from the atmosphere even when it is present in extremely low concentrations, around 420 parts per million (ppm). This is roughly 350 times lower than the CO_2 concentration found in a typical coal-based flue gas, which is around 12%. Because DAC processes use a more dilute stream, it requires more energy to separate CO_2 from the air than it does from more concentrated streams. As a result, it requires about three times more energy to capture CO_2 from the atmosphere than other processes.[15,57–60]

MXenes and MBenes could capture CO_2 directly from the atmosphere. MXene can be tuned to have different properties, such as different surface chemistries and pore sizes, which makes it a versatile material that can be tailored for specific DAC applications. For example, MXene can be functionalized with amine groups, increasing the electrostatic attraction between the MXene and CO_2 molecules. MXene can also be modified to have smaller pore sizes, which can help prevent the adsorption of other gases, such as nitrogen and oxygen. While MBenes have also been shown to be effective for DAC, they are not as well-studied as MXenes.[1]

Both MXenes and MBenes are currently in the developmental phase for carbon capture applications. These materials possess the potential to revolutionize the process of CO_2 capture and storage. Despite their challenges, there exist several opportunities for deploying MXenes and MBenes in CCS applications. As their production is scaled up, the cost of these materials is expected to decrease. Additionally, MBenes exhibit higher stability in humid environments compared to MXenes. The utilization of MXenes and MBenes in carbon capture and storage (CCS) applications is a promising avenue of research. These materials have the potential to improve the efficiency and economics of the entire CCS process. However, the current developmental phase of these materials presents several challenges that need to be overcome. Nonetheless, opportunities exist for the deployment of MXenes and MBenes in CCS applications. As their production is scaled up, the cost of these materials will decrease, making them more economically viable. Furthermore, MBenes' superior stability in humid environments compared to MXenes makes them more suited for deployment in certain contexts.

In conclusion, MXenes and MBenes hold great potential for the future of CCS applications. However, more research is necessary to overcome their current developmental challenges and to fully realize their potential.

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Declarations

Competing interests Not applicable.

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