

Project Notes:

A Novel Approach to Capturing CO₂ Directly from the Air Using Metal-Organic Frameworks:

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Contents:

Knowledge Gaps:	2
Literature Search Parameters:	3
Tags:	3
Article #0 Notes: Template	4
Article #1: Will Better Superconductors Transform the World?	5
Article #2: Could allergies be 'deleted' someday?	7
Article #3: Sunlight-powered purifier could clean water for the impoverished	8
Article #4: Evidence of illegal emissions of ozone-depleting chemicals	10
Article #5 Notes: Utilizing CO ₂ as a strategy to scale up direct air capture may face fewer short-term barriers than directly storing CO ₂	12
Article #6 Notes: Water harvesting from air with metal-organic frameworks powered by natural sunlight	14
Article #7 Notes: A Strategy for Trapping Molecular Guests in MOF-5 Utilizing Surface-Capping Groups	17
Article #8 Notes: A scalable metal-organic framework as a durable physisorbent for carbon dioxide capture	19
Article #9 Notes: These 2 companies can pull CO ₂ straight from the air	21
Article #10 Notes: A review on metal-organic frameworks: Synthesis and applications	23
Patent #1 Notes: Activated carbon-metal organic framework composite materials with enhanced gas adsorption capacity and process for the preparation thereof	26
Patent #2 Notes: Gas adsorption on metal-organic frameworks	28
Article #11 Notes: Recent advances in metal-organic frameworks: Synthesis, application and toxicity	30
Article #12 Notes: Direct air capture of CO ₂ in designed metal-organic frameworks at lab and pilot scale	32
Article #13 Notes: Direct Capture of CO ₂ from Ambient Air	34
Article #14 Notes: Back to the Basics: Developing Advanced Metal-Organic Frameworks Using Fundamental Chemistry Concepts	36
Article #15 Notes: Recent progress in metal-organic frameworks (MOFs) for CO ₂ capture at different pressures	38

Article #16 Notes: Computational screening of metal-organic frameworks for ammonia capture from humid air	40
Article #17 Notes: How to Make Metal-Organic Frameworks (MOFs)	42
Article #18 Notes: Grand canonical Monte Carlo (GCMC) study on adsorption performance of metal organic frameworks (MOFs) for carbon capture	44
Article #19 Notes: Algorithms and tools for high-throughput geometry-based analysis of crystalline porous materials	46
Article #20 Notes: RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials	47

Knowledge Gaps:

This list provides a brief overview of the major knowledge gaps for this project, how they were resolved and where to find the information.

Knowledge Gap	Resolved By	Information is located	Date resolved

Literature Search Parameters:

These searches were performed between (Start Date of reading) and XX/XX/2019.

List of keywords and databases used during this project.

Database/search engine	Keywords	Summary of search

Tags:

#energyefficiency	#allergies
#wateravailability	#airpollution
#carboncapture	#DAC
#MOFs	#cappingreagent
#MOFsynthesis	#simulations

Article #0 Notes: Template

KEEP THIS BLANK AND USE AS A TEMPLATE

Source Title	
Source citation (APA Format)	
Original URL	
Source type	
Keywords	
#Tags	
Summary of key points + notes (include methodology)	
Research Question/Problem/ Need	
Important Figures	
VOCAB: (w/definition)	
Cited references to follow up on	
Follow up Questions	<ol style="list-style-type: none">1.2.3.

Article #1: Will Better Superconductors Transform the World?

Source Title	Will Better Superconductors Transform the World?
Source citation (APA Format)	Levin, J. (2024, May 9). <i>Will Better Superconductors Transform the World?</i> Quanta Magazine. https://www.quantamagazine.org/will-better-superconductors-transform-the-world-20240509/
Original URL	https://www.quantamagazine.org/will-better-superconductors-transform-the-world-20240509/
Source type	Website
Keywords	Superconductor, energy efficiency
#Tags	#energyefficiency
Summary of key points + notes (include methodology)	<p>This article from Quanta Magazine is an adapted version of an interview with a physicist who provides insight about the advances in superconductors. Regular conductors lose energy as electrons flow through them—one example being loss of energy in the form of heat. Superconductors, on the other hand, have no such loss of energy, so the discovery of a superconductor that could function in normal temperature and pressure conditions would have profound effects on energy efficiency. So far, superconductors are already used in CAT scans, MRI scans, and maglev trains; however, they are not more widespread because they only exist in low temperatures or under high pressure. Due to the BCS theory and the concept of Cooper pairs—electrons attract rather than repel under certain conditions—scientists have learned more about how superconductors work and have also discovered more clues hinting at the type of material a superconductor at regular conditions would be. Unfortunately, progress is slow, as even minute modifications to the composition of a substance alter its material properties, leading to repeating cycles of trial and error. Still, scientists are now closer than ever to finding superconductors at room temperature and normal pressure and improving energy efficiency in a way that could benefit the entire world.</p>
Research Question/Problem/Need	Can a superconductor be developed so that it can be used at regular conditions?
Important Figures	N/A
VOCAB: (w/definition)	Superconductor: a conductor that conducts without energy loss
Cited references to follow up on	https://www.quantamagazine.org/high-temperature-superconductivity-understood-at-last-20220921/ https://www.quantamagazine.org/room-temperature-superconductor-discovery-meets-with-resistance-20230308/
Follow up Questions	<ol style="list-style-type: none"> 1. Do the superconductors that have already been discovered function properly over long distances?

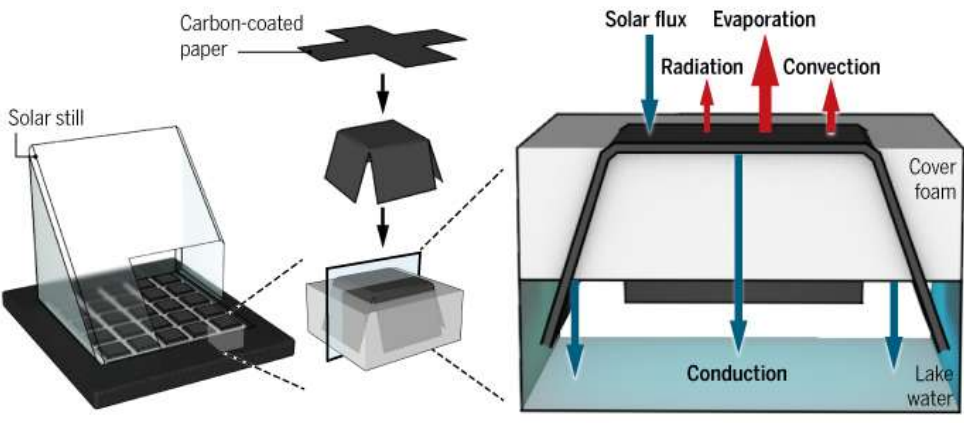
- | | |
|--|--|
| | <ol style="list-style-type: none">2. Could an encasement or coating be developed to keep the current low temperature or high-pressure superconductors in the required conditions to function properly?3. What types of materials or compositions seem to be the most promising in being a superconductor in regular conditions? |
|--|--|

Article #2: Could allergies be ‘deleted’ someday?

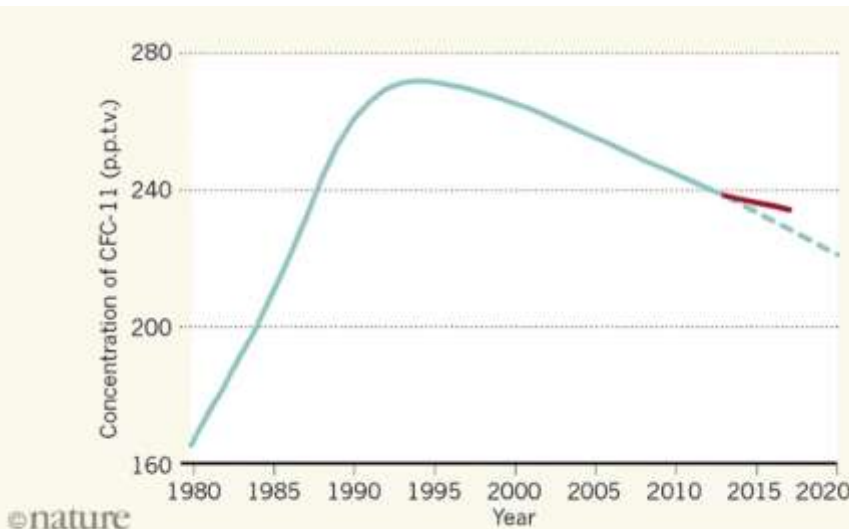
Source Title	Could allergies be ‘deleted’ someday?
Source citation (APA Format)	Sohn, R. (2024, February 16). <i>Could allergies be ‘deleted’ someday?</i> Live Science. https://www.livescience.com/health/allergies/what-do-some-allergies-last-a-lifetime-newly-described-immune-cells-to-blame
Original URL	https://www.livescience.com/health/allergies/what-do-some-allergies-last-a-lifetime-newly-described-immune-cells-to-blame
Source type	Science Website
Keywords	Allergies, Immune System, Immunoglobulin
#Tags	#allergies
Summary of key points + notes (include methodology)	This article from Live Science describes the discovery of a type of immune cell that explains the existence of long-term allergies. These memory B immune cells typically remember viruses, bacteria, and other threats, producing an antibody, immunoglobulin G (IgG), to attack the harmful threat; however, some of these immune cells remember allergens and produce immunoglobulin E (IgE), which attacks harmless proteins in the allergen, resulting in an allergic reaction when exposed to an allergen. Prior to this discovery, scientists had only discovered short-lived plasma cells that produced IgE, but it didn’t explain persisting allergies. Unlike the plasma cells, the immune cells can live for longer in one’s body, resulting in a longer lasting allergy than one caused by the plasma cells. This new knowledge could help develop better treatment of allergies, as previous medicine and techniques such as immunotherapy may reduce the reaction, but they do not address the root cause of allergies: the immune cells that switch to producing IgE.
Research Question/Problem/Need	What causes short-term and long-term allergies?
Important Figures	N/A
VOCAB: (w/definition)	Immunoglobulin: antibodies, which are proteins meant to fight off perceived threats to the body
Cited references to follow up on	https://www.ncbi.nlm.nih.gov/books/NBK27117/ https://www.ncbi.nlm.nih.gov/books/NBK541058/
Follow up Questions	<ol style="list-style-type: none"> 1. How effective is immunotherapy in reducing the symptoms of allergies? 2. What causes oral allergy syndrome? (related to allergies in general) 3. What sorts of medicine can be used to address IgE?

Article #3: Sunlight-powered purifier could clean water for the impoverished

Source Title	Sunlight-powered purifier could clean water for the impoverished
Source citation (APA Format)	Service, R. F. (2017, February 2). <i>Sunlight-powered purifier could clean water for the impoverished</i> . Science. https://www.science.org/content/article/sunlight-powered-purifier-could-clean-water-impoverished
Original URL	https://www.science.org/content/article/sunlight-powered-purifier-could-clean-water-impoverished
Source type	Science Journal
Keywords	Solar still, clean water
#Tags	#wateravailability
Summary of key points + notes (include methodology)	<p>This article describes a new faster way of using solar energy to generate clean water for those who don't have access to it. Solar stills use the sun's energy to evaporate water—leaving behind pollutants—and then collect the clean evaporated water. They have been around for a long time, but they are extremely inefficient in both speed and energy use. Researchers have sought to eliminate these problems by creating a design that only heats and evaporates the top portion of the water, which reduces energy consumption. They also experimented with using light-absorbing nanomaterials to increase the absorption of solar energy; however, the material is quite expensive. The cost led researchers to seek cheaper alternatives. One design is made up of thick paper coated in carbon black, polystyrene foam, and a clear acrylic cover. The polystyrene foam is cut into blocks that float in the unclean water. The thicker paper is placed on top of the foam but folded in such a way that it soaks up the water the foam is floating in, which then evaporates from the paper and is replaced with more water. This process not only speeds up and regulates the evaporation but increases the efficiency of the solar energy being used. The acrylic cover collects the evaporated water and leads it to a collection compartment.</p>
Research Question/Problem/Need	How can solar energy generate clean water at a cheaper price?

<p>Important Figures</p>	 <p>A solar still is made by placing carbon-coated paper (center) atop sections of a polystyrene block that floats on a water source to be purified (left).</p> <p>Water wicks up the ends of the carbon-coated paper to the top surface. Incoming sunlight evaporates water that is collected for drinking.</p> <p>The figures above detail the design of the product.</p>
<p>VOCAB: (w/definition)</p>	<p>Nanomaterial: a material with at least one dimension that is 1-100nm in length</p>
<p>Cited references to follow up on</p>	<p>https://onlinelibrary.wiley.com/doi/full/10.1002/gch2.201600003 https://www.science.org/content/article/solar-still-made-bubble-wrap-could-purify-water-poor?adobe_mc=MCMID%3D50007176715608129752738862016995515621%7CMORGID%3D242B6472541199F70A4C98A6%2540AdobeOrg%7CTS%3D1724033013</p>
<p>Follow up Questions</p>	<ol style="list-style-type: none"> 1. How large would such a solar still have to be to supply a family of four for a day? 2. How easy and cheap is it to manufacture this product and get it to people who need it? 3. Is it possible to increase the rate of evaporation through other methods?

Article #4: Evidence of illegal emissions of ozone-depleting chemicals

Source Title	Evidence of illegal emissions of ozone-depleting chemicals
Source citation (APA Format)	Hegglin, M. I. (2018). Evidence of illegal emissions of ozone-depleting chemicals. <i>Nature</i> , 557(7706), 317+. http://dx.doi.org.ezpv7-web-p-u01.wpi.edu/10.1038/d41586-018-05110-3
Original URL	http://dx.doi.org.ezpv7-web-p-u01.wpi.edu/10.1038/d41586-018-05110-3
Source type	Scientific Journal
Keywords	Ozone layer, chlorofluorocarbons
#Tags	#airpollution
Summary of key points + notes (include methodology)	Historically, chlorofluorocarbons such as CFC-11 have caused massive damage to the ozone layer when they were emitted into the atmosphere, leading to an international ban; however, scientists have recently discovered evidence proving that new CFC-11 emissions have entered the atmosphere since then. CFCs are very long-lasting, but their concentration in the atmosphere has been steadily decreasing since the ban until recently, when the decrease has been slowing. After taking all factors into account, scientists believe that the only possible cause of the slowing decrease are new, additional emissions of CFC, and they are now searching for a potential source of the chemical pollutants.
Research Question/Problem/Need	How are scientists trying to protect and preserve the ozone layer?
Important Figures	 <p>The figure above shows the predicted decrease of CFC concentration compared to the actual concentration (in red), revealing that something is wrong.</p>

VOCAB: (w/definition)	Chlorofluorocarbon: organic compounds that were previously used until it was discovered that they are harmful to the ozone layer
Cited references to follow up on	https://www-nature-com.ezpv7-web-p-u01.wpi.edu/articles/s41586-018-0106-2 https://www-nature-com.ezpv7-web-p-u01.wpi.edu/articles/249810a0
Follow up Questions	<ol style="list-style-type: none">1. How can scientists check if the ozone layer is recovering?2. Are there any other ways to destroy CFCs in the atmosphere without harming the ozone layer?3. How can you trace chemical pollutants in air or water back to their original source?

Article #5 Notes: Utilizing CO₂ as a strategy to scale up direct air capture may face fewer short-term barriers than directly storing CO₂

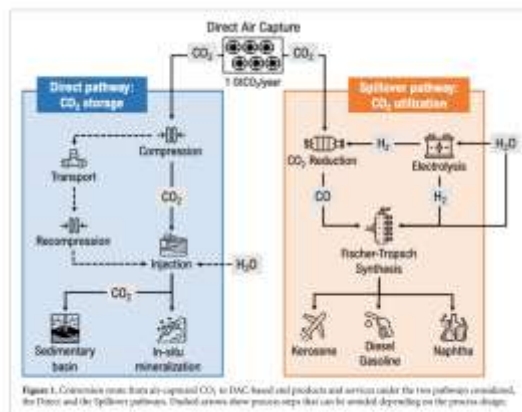
Source Title	Utilizing CO ₂ as a strategy to scale up direct air capture may face fewer short-term barriers than directly storing CO ₂
Source citation (APA Format)	Brazzola, N., Moretti, C., Sievert, K., Patt, A., & Lilliestam, J. (2024). Utilizing CO ₂ as a strategy to scale up direct air capture may face fewer short-term barriers than directly storing CO ₂ . <i>Environmental Research Letters</i> , 19(5), 054037. https://doi.org/10.1088/1748-9326/ad3b1f
Original URL	https://www.proquest.com/esdb/docview/3045481979/8A5EE6428F5D4414PQ/3?accountid=29120&sourcetype=Scholarly%20Journals
Source type	Scholarly Journal
Keywords	Direct air capture of carbon, net-zero emissions
#Tags	#DAC #carboncapture
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - DAC is needed to achieve Paris climate goals - 2 pathways: “Direct” is better in the long-term, “Spillover” is better in the short-term - Climate goal = net-zero carbon emissions, eventually net-negative - DACCS = direct air carbon capture & storage, expensive, but mostly because of the DAC process - DACCU = DACC utilization, requires hydrogen supply and additional machinery to make fuel & chemical intermediate, but fuel creation could support fuel demand - Most previous studies only look at these two pathways individually, no comparison / combining - Aim to fill knowledge gap by comparing 2 possibilities for “initial development and scale-up of DAC”, also taking into account govt policies etc, examining beyond resource use or economic effects - Direct = CO₂ is captured, compressed, and stored - Spillover = CO₂ is used to make synthetic fuels or chemical intermediates - Used very detailed operational definitions to aim to objectively compare the two pathways and identify potential short-term bottlenecks - Overall, Direct is better resources/technology-wise, but Spillover performs better when taking policies, societal factors, etc into account <p>There are two potential pathways of what to do with carbon dioxide captured by DAC: use it (Direct pathway) or store it (Spillover pathway). By using detailed operational definitions, the researchers compare the two paths and conclude that Spillover is better in the short term while Direct is better in the long term. Direct is scalable but requires policy changes and Spillover will be easier to implement at</p>

first, but due to energy and resource consumption, is not as easily scalable.

Research Question/Problem/Need

Is using carbon dioxide from DAC a good alternative to storing carbon dioxide?

Important Figures



The figure above shows the different processes of Direct vs Spillover.

ELEMENTS	ENABLING FACTORS	DIRECT PATHWAY	SPILLOVER PATHWAY
U.S. TECHNICAL FACTORS	<ul style="list-style-type: none"> • 10x range 0-11 • Lowest TRL of key component: 1 	<ul style="list-style-type: none"> • Lower life-cycle emissions, and less electricity, heat, and water intensity • No to low reliance on new CO₂ transport infrastructure • CO₂ pipeline investment: \$ 200 billion 	<ul style="list-style-type: none"> • 10x range 0-11 • Lowest TRL of key component: 2 • Higher life-cycle emissions, and use electricity, heat, and water intensity • No to low reliance on new CO₂ and H₂ transport infrastructure • CO₂ pipeline investment: \$ 20 billion & H₂ pipeline investment: \$0.5-1 billion • Existing pipeline suitable for H₂ transport
U.S. POLITICAL FACTORS	<ul style="list-style-type: none"> • Existing markets are needed to create price/discount creation of industrial facilities to create its own energy • Government policy support needed to complete with cheaper natural resources • Current regulations can increase deployment • New regulations needed before deployment 	<ul style="list-style-type: none"> • Current regulations can increase deployment • New regulations needed before deployment 	<ul style="list-style-type: none"> • Policy support needed to phase out fossil resources and to compete with existing • Current regulations may not accelerate deployment • New regulations needed before deployment
International agreements	<ul style="list-style-type: none"> • Current international agreements partially include DACCS • Additional international agreements needed for DACCS deployment 	<ul style="list-style-type: none"> • Current international agreements partially include DACCS 	<ul style="list-style-type: none"> • Current international agreements may not include DACCS • Only national agreements needed for 1 DACCS deployment
Global and national policies	<ul style="list-style-type: none"> • More clear policies, but partially aligned with current existing policies • Potential exists 	<ul style="list-style-type: none"> • Lack of clarity, but the existence of relatively high public acceptance 	<ul style="list-style-type: none"> • No to low clarity, but the existence of relatively high public acceptance

Legend: Blue = Best suited, lowest energy intensity pathway (Direct); Orange = No to low clarity, but the existence of relatively high public acceptance; Green = No to low clarity, but the existence of relatively high public acceptance.

The figure above shows which pathway performed better or worse in each criterion determined by the researchers.

VOCAB: (w/definition)

No new vocab

Cited references to follow up on

- <https://www.cell.com/joule/fulltext/S2542-43511830225-3> (how DAC works)
- <https://www.frontiersin.org/journals/energy-research/articles/10.3389/fenrg.2020.00092/full> (more on how DAC works)
- <https://pure.iiasa.ac.at/id/eprint/19787/1/The-State-of-Carbon-Dioxide-Removal-2Edition.pdf> (lengthy scholarly report on current methods of carbon removal)

Follow up Questions

1. Are there other less-resource-heavy products that can be created from captured carbon dioxide?
2. What are some ways to optimize the creation of green hydrogen or synthesis of synthetic fuels?
3. Are there methods to incentivize the purchase of carbon credits in countries such as the US (different marketable product for the Direct pathway)?

Article #6 Notes: Water harvesting from air with metal-organic frameworks powered by natural sunlight

Source Title	Water harvesting from air with metal-organic frameworks powered by natural sunlight
Source citation (APA Format)	Kim, H., Yang, S., Rao, S.R., Narayanan, S., Kapustin E.A., Furukawa, H., Umans, A.S., Yaghi, O.M., & Wang, E.N. (2017). Water harvesting from air with metal-organic frameworks powered by natural sunlight. <i>Science</i> , 356(6336), 430-434. https://doi.org/10.1126/science.aam8743
Original URL	https://www.science.org/doi/10.1126/science.aam8743
Source type	Scholarly Journal
Keywords	Metal-Organic Frameworks, water shortages, direct air harvesting
#Tags	#MOFs #wateravailability
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - New method of addressing water shortages - Dewing is ineffective (RH must be 100% of too much energy) and other competitors do not work for low RHs - Water harvesting through vapor absorption w microcrystalline powder - MOFs are easily modifiable, developed & then tested under certain conditions to optimize for specific goal (prelim data) - Main issue is releasing water from MOF, use solar energy to power that - Release water during the day when the sun is out, absorb water during the cooler night - MOF-801 works the best @ RH20% - Vapor adsorbed by diffusion, solar assisted desorption (cooled to condense water vapor into droplets that can then be collected) - Ran simulations + tested out various factors to optimize the product, then tested the final prototype and collected 2.8L water / kg MOF / day; Technically tested once, but ran simulation that the experimental data matched pretty closely <p>Previously, there was no method of harvesting water directly from the air that functions in an effective manner in conditions of low RH. The researchers decided to address that issue by developing and optimizing and MOF that could harvest water at RH 20%. Through preliminary tests, simulations, and a final test of the optimized product, they were able to create a prototype that was able to harvest 2.8L water / kg MOF / day.</p>
Research Question/Problem/Need	How can water be harvested through metal-organic frameworks (MOFs)?
Important Figures	Preliminary data:

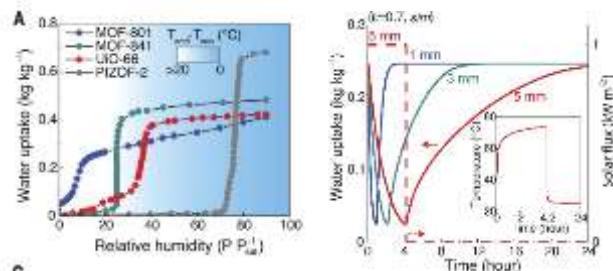
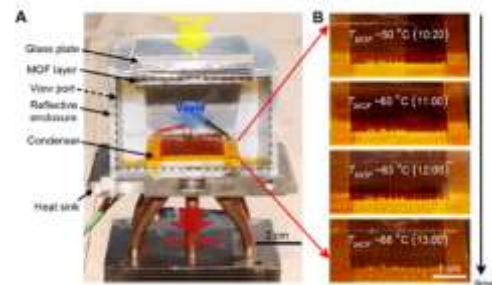
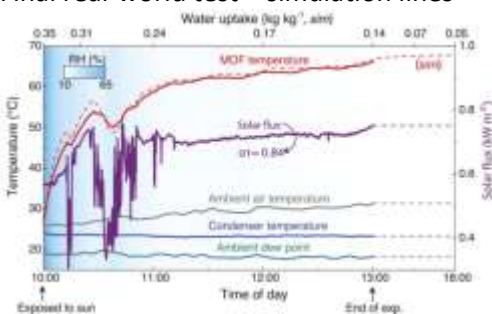


Diagram of product



Final real-world test + simulation lines

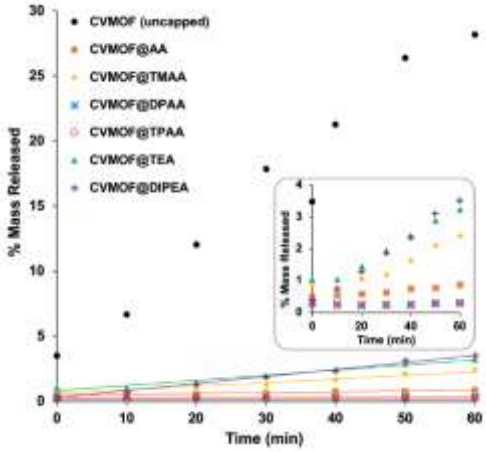


<p>VOCAB: (w/definition)</p>	<p>Adsorption = substance is distributed only on surface Absorption = substance is distributed into other material; soaked in Desorption = substance is released from material that absorbed it</p>
<p>Cited references to follow up on</p>	<p>https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201000431?casa_token=p7At4AAs2QQAAAAA%3AHA9vpfm5gRq8lL4TOqb6vP_feNShkMqT4GeUKA_sy_7rQDnBcKs1UrrEDxw8-KTepc8TLKCTc_L08rHo https://www.science.org/doi/full/10.1126/science.1067208?casa_token=gz5vwWqOU30AAAAA%3A1GHSYoa6ys9bUxVIXEm-vqOudRI1sPO6kqDy1EiWlw8K_gdUIqAJWR7A-ijkjinfJtLDQRYAjRH5CmVs https://www.science.org/doi/full/10.1126/science.1230444?casa_token=Zip3V8fM6TAAAAA%3AFEoiurPSc4tClqW2z69LyWFif5fj9rNB7zdd7xzO8TwOMdlqTKRH6YC3qxeUz3WtTfKGCTMrfo4I</p>
<p>Follow up Questions</p>	<ol style="list-style-type: none"> 1. Can MOFs be used / optimized for the harvesting of carbon dioxide directly from the air? 2. Can the final prototype be altered to be portable and cost-effective for families experiencing water shortages? Can it be sold to consumers as a product?

- | | |
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| | <p>3. Can such a product support a family of four living in a relative humidity of 20% for a week?</p> |
|--|--|

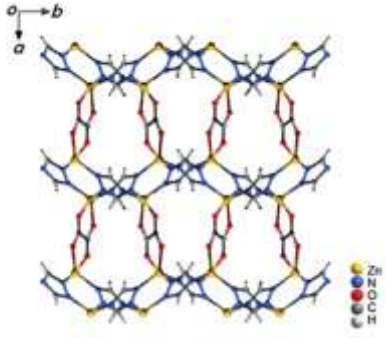
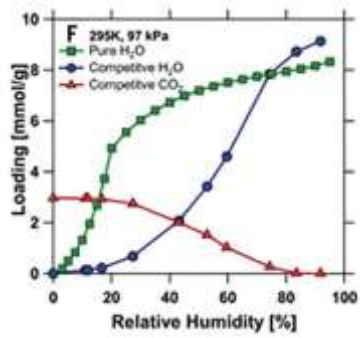
Article #7 Notes: A Strategy for Trapping Molecular Guests in MOF-5 Utilizing Surface-Capping Groups

Source Title	A Strategy for Trapping Molecular Guests in MOF-5 Utilizing Surface-Capping Groups
Source citation (APA Format)	Homan, R. A., Hendricks, D. S., Rayder, T. M., Thein, U. S., Fossum, K. J., Claudio-Vázquez, A. P., Yan, J., Grimm, R. L., Burdette, S. C., & MacDonald, J. C. (2019). A Strategy for Trapping Molecular Guests in MOF-5 Utilizing Surface-Capping Groups. <i>Crystal Growth & Design</i> , 19(11), 6331-6338. https://doi.org/10.1021/acs.cgd.9b00818
Original URL	https://pubs.acs.org/doi/10.1021/acs.cgd.9b00818
Source type	Scholarly Paper
Keywords	MOF, sorption, capping reagents
#Tags	#MOF #cappingreagent
Summary of key points + notes (include methodology)	By testing the ability of different capping reagents in their ability to trap crystal violet (CV) in MOF-5, the researchers found that carboxylic acids such as triphenylacetic acid and diphenylacetic acid, with the addition of a substituent such as zinc nitrate, released no CV over 60 minutes, This reveals that the capping reagents and substituents fully covered the pores of MOF-5 and was successful in trapping CV in MOF-5. The other reagents tested were much smaller than TPAA and DPAA and shouldn't have affected the release of CV as much as they did in the experiment did, but the researchers do not know what specific mechanism is causing the partial blocking of pores seen through the tests of other capping reagents. This experiment overall serves as a proof-of-concept that molecular storage and trapping in MOFs is possible, and further avenues include finding a more accurate way to predict pore coverage / post synthesis pore size adjustments.
Research Question/Problem/Need	What is the feasibility of using capping reagents to trap guest molecules in MOF-5?

Important Figures	 <p>This table demonstrates how each of the tested capping reagents performed; the less % mass released, the better the capping reagent performed at trapping CV in MOF-5</p>
VOCAB: (w/definition)	<p>Hydrothermal = crystallizing substances at high temperatures or high vapor pressures</p> <p>Reagent = substance added to a system to cause a chemical reaction</p>
Cited references to follow up on	<p>https://www.science.org/doi/epdf/10.1126/science.1067208?src=getftr</p> <p>https://www.science.org/doi/epdf/10.1126/science.1230444?src=getftr</p> <p>https://pubs.rsc.org/en/content/articlelanding/2018/cs/c8cs00688a</p>
Follow up Questions	<ol style="list-style-type: none"> 1. How can capping reagents be used, not to block pores, but to resize them? 2. Are there other capping reagents that don't require the addition of a substituent to maximize pore coverage? 3. Are there other methods of post synthesis pore size alteration that do not involve capping pores?

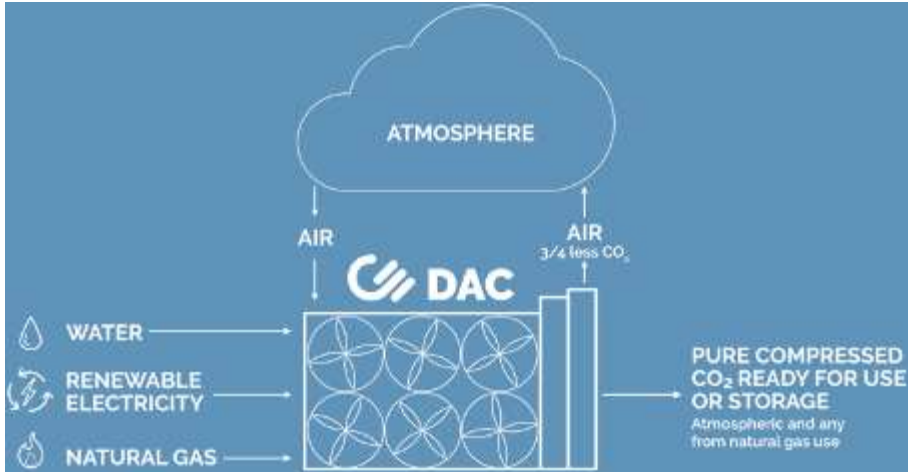
Article #8 Notes: A scalable metal-organic framework as a durable physisorbent for carbon dioxide capture

Source Title	A scalable metal-organic framework as a durable physisorbent for carbon dioxide capture
Source citation (APA Format)	Lin, J., Nguyen, T., Vaidhyanathan, R., Burner, J., Taylor, J. M., Durekova, H., Akhtar, F., Mah, R. K., Ghaffari-Nik, O., Marx, S., Fylstra, N., Iremonger, S. S., Dawson, K. W., Sarkar, P., Hovington, P., Rajendran, A., Woo, T. K., & Shimizu, G. K. H. (2021). A scalable metal-organic framework as a durable physisorbent for carbon dioxide capture. <i>Science</i> , 374(6574), 1464-1469 https://doi.org/10.1126/science.abi7281
Original URL	https://www.science.org/doi/10.1126/science.abi7281
Source type	Scholarly Journal
Keywords	Selectivity, adsorption
#Tags	#carboncapture #postcombustion #MOF
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - Flue gas is essentially power plant emissions; low CO₂ concentration, also has N₂, H₂O, and acid gases - Pre-existing post combustion carbon capture method: amine & solvent system, CO₂ absorbing liquid but energy intensive - More recently, ppl have been examining solid sorbents, but increased effectiveness tends to mean increased energy usage - It is more common for MOF carbon capture systems to have selectivity over N₂, not as common selectivity over water vapor - Why metal-organic frameworks? Wide variety of shapes, pore sizes, surface properties, etc allow for detailed optimization; many are stable in the presence of water; overall, MOFs hold potential to make carbon capture a lot less \$\$\$ - To optimize: high volume productivity and low regen energy - CALF-20!! High capacity and selectivity for CO₂, stable to steam and wet acid gases - ~38% void volume - Since selectivity over N₂ is more common, researchers examined selectivity over water vapor - From the graphs, you can see that CALF-20 outperforms a lot of other frameworks - 80% MOF + 20% polysulfone = structured CALF-20 - Used Grand Canonical Monte Carlo (GCMC) simulation, helped to identify binding sites for both water and CO₂ to determine that CO₂ actually suppresses water binding until RH40ish - Essentially, CO₂ is better at adsorbing to empty pores than water, while water is better at sticking once at least one water molecule has adsorbed

	<p>to a pore, explaining why at first, CO₂ precluded water from being adsorbed compared to regular water adsorption without competing with CO₂</p> <ul style="list-style-type: none"> - No competitors have this suppression feature, so none are as effective at not adsorbing water - CALF-20 also stays stable even after used for a week, no significant performance loss
Research Question/Problem/Need	<p>How can MOFs be used for post-combustion carbon capture with little impact from water vapor?</p>
Important Figures	<div style="display: flex; justify-content: space-around; align-items: flex-start;"> <div style="text-align: center;"> <p>B</p>  </div> <div style="text-align: center;"> <p>F 295K, 97 kPa</p>  </div> </div> <p>The figure on the left displays the structure of the MOF. The figure on the right displays the MOF's absorption of water alone, compared to when water needs to compete with CO₂, displaying the MOF's selectivity of CO₂ over water, until ~RH40%.</p>
VOCAB: (w/definition)	<p>Physisorb = sticking to/adsorbing without chemical bonding (caused by weak Van der Waal forces) Å is an Ångström, 10⁻¹⁰m</p>
Cited references to follow up on	<p>https://onlinelibrary.wiley.com/doi/full/10.1002/adsu.201800080 https://pubs.acs.org/doi/full/10.1021/acsami.9b08487 https://www.nature.com/articles/natrevmats201745</p>
Follow up Questions	<ol style="list-style-type: none"> 1. Can CALF-20s efficiently desorb the captured carbon? 2. What are some potential uses of the captured carbon from the MOF? 3. Can such an MOF be used to harvest CO₂ in a non-post-combustion situation?

Article #9 Notes: These 2 companies can pull CO₂ straight from the air

Source Title	These 2 companies can pull CO ₂ straight from the air
Source citation (APA Format)	Myers, J. (2020, Jun 26). <i>These 2 companies can pull CO₂ straight from the air</i> . World Economic Forum. https://www.weforum.org/agenda/2020/06/direct-air-capture-co2-environment-climate/
Original URL	https://www.weforum.org/agenda/2020/06/direct-air-capture-co2-environment-climate/
Source type	Website
Keywords	DAC, adsorption/absorption
#Tags	#carboncapture #DAC
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - DAC is different from typical methods of carbon capture bc it captures CO₂ directly from air rather than from flue gas released from power plant (point source capture / post-combustion capture) - Two considered companies use fans to collect air - Company 1: Adsorption of CO₂ by a filter material, collector is closed and temp increased to release high concentration CO₂ - Company 2: Uses potassium hydroxide solution to bind w CO₂ molecules, forms carbonate salt, then salt is processed to produce CO₂ - CO₂ can be stored or used, underground storage or synthetic fuels - Not mentioned in the article, but some of the flaws in these systems seem to be with taking the air in (in order for CO₂ to be captured) and with the release process of the CO₂ (high temperatures etc in order to get the CO₂ out of the filter or liquid sorbent) <p>This article explains two methods two companies are using to capture carbon directly from regular air. They both got air by using fans, but the first company used a filter material to adsorb CO₂ while the second used a liquid sorbent. They appeared to have not fully optimized the air intake portion of this method, or the CO₂ desorption portion.</p>
Research Question/Problem/Need	How are some companies capturing carbon dioxide directly from the air rather than at a point source?

Important Figures	 <p>The diagram illustrates the Direct Air Capture (DAC) process. It shows a cycle where air is drawn from the atmosphere into a DAC unit. This unit uses water, renewable electricity, and natural gas as inputs. The output is air with 3/4 less CO₂ and pure compressed CO₂ ready for use or storage. The CO₂ can be sourced from atmospheric air or natural gas use.</p> <p>Diagram of basic DAC process</p>
VOCAB: (w/definition)	N/A
Cited references to follow up on	https://carbonengineering.com/our-technology/ https://news.climate.columbia.edu/2019/05/29/co2-utilization-profits/ https://climeworks.com/direct-air-capture
Follow up Questions	<ol style="list-style-type: none"> 1. How can the intake of air of this system be further improved/optimized? 2. How can the CO₂ desorption process of this system be further optimized? 3. How can the effectiveness of CO₂ (% of CO₂ successfully removed from air) be further increased?

Article #10 Notes: A review on metal-organic frameworks: Synthesis and applications

Source Title	A review on metal-organic frameworks: Synthesis and applications
Source citation (APA Format)	Safael, M., Foroughi, M. M., Ebrahimpoor, N., Jahani, S., Omid, A., & Khatami, M. (2019). A review on metal-organic frameworks: Synthesis and applications. <i>TrAC Trends in Analytical Chemistry</i> , 118, 401-425. https://doi.org/10.1016/j.trac.2019.06.007
Original URL	https://www.sciencedirect.com/science/article/abs/pii/S0165993619301840
Source type	Scholarly Journal
Keywords	MOF applications
#Tags	#MOFs
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - MOF = metal ions or clusters connected by organic ligands - 3 main: topology of framework, metal ion center, organic linkers - MOF pore size and porosity can vary a lot - By changing the metal ions / clusters or organic ligands, physical and chemical properties and be changed for higher selectivity for a specific chemical reaction - Polyamines, carboxylates, pyridyl and cyano groups, crown ethers, and phosphonates are common ligands - There are a variety of methods of MOF synthesis and a variety of uses of these frameworks, including removing toxic pollution from water, gas adsorption, and serving as a catalyst - 5 areas: adsorption, catalysts, sensors, electrochemical charge storage (batteries), and drug delivery systems <p>MOFs are an emerging new material that has a lot of potential in a lot of fields, such as adsorption, catalysts, sensors, batteries, and drug delivery.</p>
Research Question/Problem/Need	What are some uses of MOFs?

Important Figures

Table 2
Selected applications of metal-organic framework.

MOF	Synthetic method	Application	Ref.
PSA@Zr-MOF@Fe ₂ O ₄	Hydrothermal	Determination of glyphosate, glufosinate, malathion, and their main metabolites	[101]
UMCM-151	Hydrothermal	Adsorption of light hydrocarbons	[102]
MOF@ML-100-B	Solvothermal	Determination of the endogenous catecholamines	[103]
Fe ₃ O ₄ @TMU-21	Hydrothermal	Absorbent for pyrethroids	[104]
ZIF-8	Ultrasound assisted	Removal of tetracycline and oxytetracycline antibiotics	[105]
ML-53 (Fe)	Solvothermal	Absorbent for ciprofloxacin antibiotic	[106]
Fe ₂ O ₃ /MOF-74	Hydrothermal	Removal of arsenic	[107]
ML-53(O)-CO	Hydrothermal	Removal of arsenic	[108]
UIO-66 (HP-UIO-66)	Hydrothermal	Extraction of uranium	[109]
[Me ₂ NH ₂] ₂ [Zn ₂ (μ-O)] ₂ (ad) ₄ (BPDC) ₄	Hydrothermal	Uranium sorption	[110]
Zr-CAU-24	Hydrothermal	Detection of aflatoxin B1	[111]
HPW/Zr-BTC	Hydrothermal	Absorption of benzothiofene	[112]
ML-101 (Fe) @PDDa@Fe ₃ O ₄	Solvothermal	Absorption of methyl red and malachite green	[113]
Fe ₃ O ₄ -NH ₂ @HKUST-1@PDES-MSPE	Hydrothermal	Separation of anionic dyes	[114]
P,W @ MIL-101(G)	Hydrothermal	Removal of organic dyes	[115]
[[(CH ₃) ₂ NH ₂] ₂ [Zn ₂ (μ-OH)] ₂ (μ-O)(NSBPDC) ₂ (H ₂ O) ₂]	Hydrothermal	Absorption and separation of organic dyes	[116]
DMF-12(H ₂ O) ₂			
Mn(II)-MOF (I)	Solvothermal	Absorption of dyes	[117]
ZU-66	Hydrothermal	CO ₂ separation	[118]
[Zn ₂ (NDC) ₂ (DABCO)] _n	Hydrothermal	CH ₄ /CO ₂ gas separation	[119]
ML-101@M-X-Y	Hydrothermal	CO ₂ and H ₂ S Adsorption	[120]
[Co(TCP) ₂ (H ₂ O)] _n (DMF) _n	Solvothermal	CO ₂ Adsorption	[121]
ZIF-12	Hydrothermal	Rn Adsorption	[122]
[Cr(4,4'-bpy) ₂ (H ₂ O)] ₂ [CO ₃] ₂ (2,4'-bpy) ₂ H ₂ O	Hydrothermal	Gas adsorption	[123]
0.4M-Cu@ML-100(Fe)	Solvothermal	Adsorptive separation of C ₃ H ₂ C ₂ H ₄ mixtures	[124]
[In ₂ O ₃] ₂ (CDBA) ₂ 18DMF-3H ₂ O	Solvothermal	Gas adsorption	[125]
Fe ₃ O ₄ @ZIF-8	Hydrothermal	Oxygen Reduction Catalysis	[126]
Cu ₂ -PDA ₂ /ML-101-NH ₂	Hydrothermal	Catalytic activity for the generation of hydrogen from formic acid	[127]
Ru ₂ -NHC-MOF	Solvothermal	catalytic hydrogenation of CO ₂ to formic acid	[128]
VNU-21 (Fe ₂ BTC)(EDB) ₂ (12.27 H ₂ O)	Solvothermal	heterogeneous catalyst	[129]
ML-53(A) (Al(OH) ₃)-O ₂ -C ₂ H ₄ -CO ₂ (I)	Solvothermal	Cobalt catalyst	[130]
[CH ₃ COOH] ₂ [M](HSO ₄) ₂ H-UIO-66	Hydrothermal	Catalyst in biodiesel synthesis	[131]
ML-101-NH ₂	Hydrothermal	Catalyst for the synthesis of 3-ary-2-oxazolidinones	[132]
IL@PUBN	Post impregnation	Catalyst for the cycloaddition of epoxides to CO ₂	[133]
UNMOF] ₂ -C ₂ H ₄	Ultrasound assisted	Photocatalytic H ₂ production	[134]
NH ₂ -ML-125	Solvothermal	Photocatalytic H ₂	[135]
Co-MB	Hydrothermal	Photocatalysis for hydrogen production	[136]
[Zn ₂ (L) ₂ (bta) ₂] _n (1)	Hydrothermal	Photocatalytic degradation Rhodamine B	[137]
[Cu ₂ (L) ₂ (DMF) ₂ (1)	Hydrothermal	photocatalyst for the photodegradation of organic dyes	[138]
Au@PDA@MOF-74, Pt@MOF-74 and Pt/Au@PDA@MOF-74	Solvothermal	photoactivated CO ₂	[139]
NH ₂ -ML-125(Ti)	Hydrothermal	Photoelectrochemical water oxidation	[140]
Zn@ MOF@ZnO	Hydrothermal	photoelectrochemical water oxidation	[141]
AC/ML-88B (Fe)	Hydrothermal	catalysts to degrade Reactive Red 198	[142]
Pt@PNSMOF	Hydrothermal	Oxygen electrocatalysis	[143]
Fe-ML-88B	Solvothermal	Electrocatalysts for Oxygen	[144]
MoS ₂ /Co-MOF	Hydrothermal	Electrocatalytic hydrogen evolution reaction	[145]
Ni(Fe)-MOF	Solvothermal	Electrocatalytic Water Oxidation	[146]
CUP-1-Ni	Hydrothermal	Electrocatalytic Water Oxidation	[147]
rGO/C65/SNC	Hydrothermal	Electro-catalytic oxygen	[148]
V ₂ O ₅ /C	Solvothermal	Electro-catalytic N ₂	[149]
Fe ₃ O ₄ /Ni-BTC	Hydrothermal	Biocatalyst for biosynthesis of S-adenosylmethionine	[150]
MOF-808	Hydrothermal	Biocatalyst	[151]
[Cu ₂ (nbt) ₂ (H ₂ O) ₂ (OH) ₂](DMF) ₂ (H ₂ O) (1)	Solvothermal	Cyanosilylation of aldehydes and ablation of human laryngocarcinoma cells	[152]
UIO-68 NMOF	Hydrothermal	Biocatalytic decomposition of the duplex capping units	[153]
[ML-101(Cr)]	Hydrothermal	Biocatalyst for Clean synthesis of benzoxazoles	[154]
ML-101-NH ₂ -SO ₃ H	Solvothermal	Humidity sensing	[155]
ML-125/TiO ₂	Hydrothermal	QCM humidity sensor	[156]
HKUST-1	Hydrothermal	OH-MOF sensor	[157]
[Eu ₂ (TMC)(OH) ₂](DMF) ₂ (H ₂ O) ₂ (2DMF, 7H ₂ O)	Solvothermal	Sensing of Cu ²⁺ and UO ₂ ²⁺	[158]
Cu/Tb@Zn-MOF	Hydrothermal	Sensor for detection of aspartic acid	[159]
Fe ₃ O ₄ @ML-100(Fe)	Hydrothermal	Electrochemical sensor for chlorogenic acid	[160]
Zn-BDC-TED	Hydrothermal	Immunosensing for C-reactive protein	[161]
[Co(NPDC)(bpe) ₂](DMF, 2H ₂ O)	Solvothermal	Luminescent sensing for MnO ²⁺ and Hg ²⁺	[162]
[Tb(pdb)(phen)(ox) ₂] _n	Hydrothermal	luminescent probe for the 2-thiazolidinethione-4-carboxylic acid	[163]
Zr-UIO-66-N ₂ H ₄	Solvothermal	Fluorescent sensor for phosphate and 4-nitrobenzaldehyde	[164]
[Eu ₂ (NO) ₂] ₂ (μ ₄ -OH) ₂ Cl ₂ (H ₂ O)] _n (NO ₂) ₂ (H ₂ O) ₂	Solvothermal	Sensor for detection of nitro pollutants	[165]
Ce-MOF@COF	Hydrothermal	Aptasensor for detection of oxytetracycline residues	[166]
ML-101	Solvothermal	Aptasensor for extraction of ochratoxin A	[167]
Zn-Ag ₂ O@PEDOT:PSS	Solvothermal	Battery can be safely charged by wind energy	[168]
UIO-66	Solvothermal	Electrolyte additive for Li-metal battery	[169]

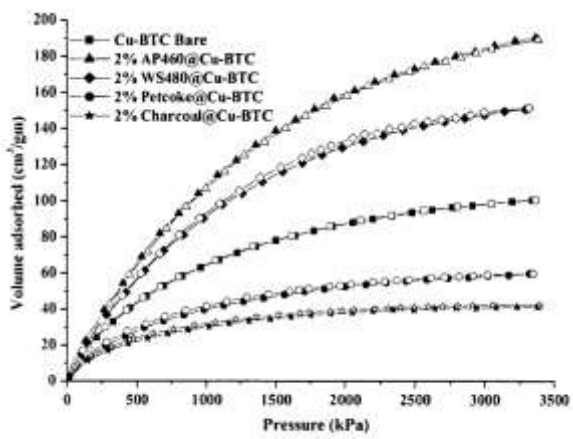
(continued on next page)

Table 2 (continued)

MOF	Synthetic method	Application	Ref.
Cu ₂ (CUTCP)	Solvothermal	lithium-sulfur battery	[170]
ZIF-670@MnO ₂	Hydrothermal	Lithium-selenium battery	[171]
Li-UIO-66(MDO)	Mechanochemical	Lithium sulfur battery	[172]
Zn-POMCF	Electrochemical	Lithium-ion batteries	[173]
MOFSDC	Hydrothermal	Sodium-ion battery	[174]
Ni-MOF	Solvothermal	Fabricated supercapacitor electrodes	[175]
NiCo-LDH@Ni-CAT	Hydrothermal	Supercapacitor	[176]
CoCuNS-bdc	Hydrothermal	Supercapacitor	[177]
Co-MOF	Hydrothermal	Supercapacitor	[178]
Ni-MOF	Hydrothermal	Supercapacitor	[179]
[Fe(C ₂ N ₄ O ₂)] ₂ (H ₂ O) ₂	Solvothermal	proton-exchange membrane fuel cells	[180]
[[(Me ₂ NH ₂) ₂ (SO ₄) ₂] ₂ [Zn ₂ (ox) ₂] _n]	Solvothermal	Fuel cells	[181]
CNC(MOF-5)GO	Hydrothermal	Drug delivery	[182]
ZIF-8@alginate NPs	Mechanochemical	Drug delivery	[183]
[Gd(BTC)(DMF)] ₂ (H ₂ O) ₂	Solvothermal	Drug delivery	[184]
[Dy(HABA)(ABA) ₂ (DMA) ₂] _n	Solvothermal	Drug delivery	[185]
Cu-MOF@BLNPGM	Mechanochemical	Drug delivery	[186]
NU-1000 and NU-501	Hydrothermal	Drug delivery	[187]
CD-MOF-1 and CD-MOF-2	Solvothermal	Drug delivery	[188]
CD-MOF	Vapor diffusion	Drug delivery	[189]

	The table above displays various MOFs and their potential uses/applications
VOCAB: (w/definition)	N/A
Cited references to follow up on	https://doi.org/10.1039/C8NJ04947E https://doi.org/10.1021/acssuschemeng.8b04916 https://doi.org/10.1016/j.inoche.2018.12.003
Follow up Questions	<ol style="list-style-type: none">1. How long lasting are certain MOFs, and does the method of synthesis play a factor in why?2. How are the materials that make up MOFs produced?3. How can the stability/life of MOFs be extended/optimized?

Patent #1 Notes: Activated carbon-metal organic framework composite materials with enhanced gas adsorption capacity and process for the preparation thereof

Source Title	Activated carbon-metal organic framework composite materials with enhanced gas adsorption capacity and process for the preparation thereof
Source citation (APA Format)	Bajaj, H. C., Somani, R. S., Rallapalli, P. B., Patil, D., Prasanth, K. P., Manoj, C. R., & Choudary, N. V. (2016). <i>Activated carbon-metal organic framework composite materials with enhanced gas adsorption capacity and process for the preparation thereof</i> (U.S. Patent No. 9,433,919). U.S. Patent and Trademark Office. https://patents.google.com/patent/US9433919B2/en
Original URL	https://patents.google.com/patent/US9433919B2/en
Source type	Patent
Keywords	MOF synthesis, carbon, gas adsorption
#Tags	#MOF
Summary of key points + notes (include methodology)	The researchers used a “void space filling method” in MOFs, which was essentially to add activated carbon to an MOF (Cu-BTC) during MOF synthesis to create a new MOF with increased gas adsorption (of methane).
Research Question/Problem/Need	How can carbon be used to improve MOF adsorption of gas?
Important Figures	 <p style="text-align: center;">FIG. 2</p> <p>The table above displays how the same MOF with different activated carbons added to them performed against each other, which helped them decide which activated carbon was the best choice.</p>

VOCAB: (w/definition)	Activated carbon = carbon that is processed to be very porous
Cited references to follow up on	https://patents.google.com/patent/US8227375B2/en https://patents.google.com/patent/US8883676B1/en?peid=6243676a77d90%3A612%3Af0926196 https://patents.google.com/patent/CN112705167A/en?peid=624367945dad8%3A705%3A72df2da6
Follow up Questions	<ol style="list-style-type: none">1. Can other molecules be added to MOFs to improve gas adsorption?2. How efficient or costly is the synthesis of this new MOF?3. Can this product be optimized for other gases such as CO₂?

Patent #2 Notes: Gas adsorption on metal-organic frameworks

Source Title	Gas adsorption on metal-organic frameworks																																																							
Source citation (APA Format)	Willis, R. R., Low, J. J., Faheem, S. A., Benin, A. I., Snurr, R. Q., & Yazaydin, A. O. (2012). <i>Gas adsorption on metal-organic frameworks</i> (U.S. Patent No. 8,227,375). U.S. Patent and Trademark Office. https://patents.google.com/patent/US8227375B2/en																																																							
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Source type	Patent																																																							
Keywords	MOF, hydration																																																							
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Summary of key points + notes (include methodology)	After water treatment, the MOF Cu-BTC displayed significantly larger gas adsorption abilities than Cu-BTC that was not hydrated.																																																							
Research Question/Problem/Need	How does the hydration of an MOF impact its efficiency at gas adsorption?																																																							
Important Figures	<p>The figure is a scatter plot with 'pressure, atm' on the x-axis (ranging from 0 to 5) and 'CO₂ loading, wt-%' on the y-axis (ranging from 0 to 80). The legend indicates four data series: hydrated_CuBTC_EXPT (filled diamonds), dry_CuBTC_EXPT (filled triangles), hydrated_CuBTC_SIM (open diamonds), and dry_CuBTC_SIM (open triangles). The hydrated series show a clear upward trend in CO₂ loading as pressure increases, while the dry series show much lower and more scattered loading values.</p> <table border="1"> <caption>Approximate data points from the CO₂ loading vs. pressure plot</caption> <thead> <tr> <th>Pressure (atm)</th> <th>hydrated_CuBTC_EXPT (wt-%)</th> <th>dry_CuBTC_EXPT (wt-%)</th> <th>hydrated_CuBTC_SIM (wt-%)</th> <th>dry_CuBTC_SIM (wt-%)</th> </tr> </thead> <tbody> <tr><td>0.3</td><td>16</td><td></td><td></td><td></td></tr> <tr><td>0.5</td><td>28</td><td></td><td>18</td><td>7</td></tr> <tr><td>0.8</td><td></td><td>22</td><td></td><td></td></tr> <tr><td>1.0</td><td>37</td><td></td><td>24</td><td>11</td></tr> <tr><td>1.5</td><td></td><td>32</td><td>27</td><td>15</td></tr> <tr><td>2.0</td><td></td><td></td><td>31</td><td>20</td></tr> <tr><td>2.3</td><td>55</td><td>39</td><td></td><td></td></tr> <tr><td>3.0</td><td>62</td><td>44</td><td>36</td><td>28</td></tr> <tr><td>3.7</td><td>64</td><td>48</td><td></td><td></td></tr> <tr><td>4.7</td><td>68</td><td></td><td></td><td></td></tr> </tbody> </table> <p>The table above demonstrates how a hydrated MOF (Cu-BTC) outperforms its dry form both in the simulation and experiment, and the experiment does better the expected performance too.</p>	Pressure (atm)	hydrated_CuBTC_EXPT (wt-%)	dry_CuBTC_EXPT (wt-%)	hydrated_CuBTC_SIM (wt-%)	dry_CuBTC_SIM (wt-%)	0.3	16				0.5	28		18	7	0.8		22			1.0	37		24	11	1.5		32	27	15	2.0			31	20	2.3	55	39			3.0	62	44	36	28	3.7	64	48			4.7	68			
Pressure (atm)	hydrated_CuBTC_EXPT (wt-%)	dry_CuBTC_EXPT (wt-%)	hydrated_CuBTC_SIM (wt-%)	dry_CuBTC_SIM (wt-%)																																																				
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VOCAB: (w/definition)	N/A																																																							

Cited references to follow up on	https://pubmed.ncbi.nlm.nih.gov/17177438/ https://patents.google.com/patent/US20050154222A1/en?peid=62436bf0e8a38%3A143%3A4c48cfd2 https://patents.google.com/patent/US20070248852A1/en?peid=62436c0508400%3A146%3A98efe13f
Follow up Questions	<ol style="list-style-type: none">1. Does water treatment have the same gas adsorption improving effect on other MOFs as well?2. Why does MOF gas adsorption increase after water treatment?3. Can treatment with other molecules/substances produce similar beneficial results?

Article #11 Notes: Recent advances in metal-organic frameworks: Synthesis, application and toxicity

Source Title	Recent advances in metal-organic frameworks: Synthesis, application and toxicity																																																																																																																																																																																																																																																																																																																																																																																																								
Source citation (APA Format)	Zhang, Q., Yan, S., Yan, X., & Lv, Y. (2023). Recent advances in metal-organic frameworks: Synthesis, application and toxicity. <i>Science of the Total Environment</i> , 902. https://doi.org/10.1016/j.scitotenv.2023.165944																																																																																																																																																																																																																																																																																																																																																																																																								
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Summary of key points + notes (include methodology)	There are four main types of MOFs (IR-MOF, MIL, ZIF, UiO). Some existing MOF synthesis methods include hydro/solvothermal, microwave-assisted, sonochemical, mechanochemical, electrochemical, among others, though most involve the use of a solvent and special environmental conditions during the synthesis. There are many different applications of MOFs, though I am mostly interested in the gas adsorption, gas storage, or gas separation properties of MOFs. MOFs can be inhaled and absorbed into the bloodstream, but the toxicity of MOFs if ingested or absorbed is not as studied.																																																																																																																																																																																																																																																																																																																																																																																																								
Research Question/Problem/Need	What are some methods of MOF synthesis, applications of MOFs, and downsides to MOFs regarding their toxicity?																																																																																																																																																																																																																																																																																																																																																																																																								
Important Figures	<div style="display: flex; justify-content: space-between;"> <div style="width: 48%;"> <p>Table 2 The synthesis methods of MOFs.</p> <table border="1"> <thead> <tr> <th>Method</th> <th>Reaction time</th> <th>Reaction pressure</th> <th>Advantages</th> <th>Disadvantages</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>Hydrothermal/solvothermal method</td> <td>Long</td> <td>Yes</td> <td>High conversion - High yields - Before the particles have been washed, are considered as waste (impurities)</td> <td>Low cost - Difficult to separate large scale production</td> <td>[1] (Zhang et al., 2023) [2] (Zhang et al., 2023) [3] (Zhang et al., 2023)</td> </tr> <tr> <td>Microwave-assisted method</td> <td>Short</td> <td>Yes</td> <td>High conversion rate of raw material - High yield - Recently considered as cleaner synthesis</td> <td>High energy consumption - High energy consumption</td> <td>[4] (Zhang et al., 2023) [5] (Zhang et al., 2023)</td> </tr> <tr> <td>Mechanochemical 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₂	Storage	[38] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[39] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[40] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[41] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[42] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[43] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[44] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[45] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[46] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[47] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[48] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[49] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[50] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[51] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[52] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[53] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[54] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[55] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[56] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[57] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[58] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[59] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[60] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[61] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[62] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[63] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[64] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[65] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[66] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[67] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[68] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[69] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[70] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[71] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[72] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[73] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[74] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[75] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[76] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[77] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[78] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[79] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[80] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[81] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[82] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[83] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[84] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[85] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[86] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[87] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[88] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[89] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[90] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[91] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[92] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[93] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[94] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[95] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[96] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[97] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[98] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[99] (Zhang et al., 2023)	MOF-5, HKUST-1	CO ₂	Storage	[100] (Zhang et al., 2023)
Method	Reaction time	Reaction pressure	Advantages	Disadvantages	Reference																																																																																																																																																																																																																																																																																																																																																																																																				
Hydrothermal/solvothermal method	Long	Yes	High conversion - High yields - Before the particles have been washed, are considered as waste (impurities)	Low cost - Difficult to separate large scale production	[1] (Zhang et al., 2023) [2] (Zhang et al., 2023) [3] (Zhang et al., 2023)																																																																																																																																																																																																																																																																																																																																																																																																				
Microwave-assisted method	Short	Yes	High conversion rate of raw material - High yield - Recently considered as cleaner synthesis	High energy consumption - High energy consumption	[4] (Zhang et al., 2023) [5] (Zhang et al., 2023)																																																																																																																																																																																																																																																																																																																																																																																																				
Mechanochemical method	Short	No	Low energy consumption - Environment friendly - The rate of synthesis - Low consumption of solvents - Better safety can be used as raw material	General product obtained - Difficult to control product	[6] (Zhang et al., 2023) [7] (Zhang et al., 2023) [8] (Zhang et al., 2023)																																																																																																																																																																																																																																																																																																																																																																																																				
Electrochemical method	Short	No	High conversion - High yield - Low energy consumption - Low consumption of raw material - High safety can be used as raw material	Low cost - High energy consumption - The safety issue of synthesis will reduce the large-scale production	[9] (Zhang et al., 2023) [10] (Zhang et al., 2023)																																																																																																																																																																																																																																																																																																																																																																																																				
Other method	Long	Yes	High conversion - High yields - Before the particles have been washed, are considered as waste (impurities)	Low cost - Difficult to separate large scale production	[11] (Zhang et al., 2023) [12] (Zhang et al., 2023)																																																																																																																																																																																																																																																																																																																																																																																																				
MOF species	Gas	Application	Reference																																																																																																																																																																																																																																																																																																																																																																																																						
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<p>Table 1 depicts various synthesis methods of MOFs and provides further papers in which these methods were tested. Table 3 depicts some MOFs with known adsorption or separation properties and further papers that tested those properties.</p>																																																																																																																																																																																																																																																																																																																																																																																																									

VOCAB: (w/definition)	Hydrothermal: relating to hot water Solvothermal: relating to high temperatures or pressures Sonochemical: using ultrasound (in synthesis)
Cited references to follow up on	CO ₂ /CH ₄ separation: https://doi.org/10.1039/d2qm00802e CO ₂ /C ₂ H ₂ separation: https://doi.org/10.1039/d2ta07473g CO ₂ /N ₂ separation: https://doi.org/10.1016/j.memsci.2022.121107 CO ₂ /H ₂ separation: https://doi.org/10.1021/acssuschemeng.1c03443
Follow up Questions	<ol style="list-style-type: none">1. Which synthesis method is generally the most environmentally friendly and how can it be optimized for greater time efficiency?2. Which synthesis method is the most time efficient and how can it be optimized to have a lesser impact on the environment?3. What methods of MOF synthesis are used in industrial settings and how can industries make a shift to a more optimized method?

Article #12 Notes: Direct air capture of CO₂ in designed metal-organic frameworks at lab and pilot scale

Source Title	Direct air capture of CO ₂ in designed metal-organic frameworks at lab and pilot scale																																				
Source citation (APA Format)	Zhang, X., Zhao, H., Yang, Q., Yao, M., Wu, Y., & Gu, Y. (2023). Direct air capture of CO ₂ in designed metal-organic frameworks at a lab and pilot scale. <i>Carbon Capture Science & Technology</i> , 9. https://doi.org/10.1016/j.ccst.2023.100145																																				
Original URL	https://www.sciencedirect.com/science/article/pii/S2772656823000490?via%3Di%3Dhub																																				
Source type	Scholarly Journal																																				
Keywords	MOF, direct air capture																																				
#Tags	#DAC #MOF																																				
Summary of key points + notes (include methodology)	Direct air capture (DAC) has to selectively absorb CO ₂ from a mixture with a far lower concentration of carbon dioxide than its counterpart, point-source capture that captures CO ₂ directly from power plant emissions. The paper explains some of the thermodynamics behind CO ₂ capture and then certain strategies that can be used to optimize a MOF, introducing hybrid ultramicroporous materials (HUMs) and their potential to capture CO ₂ without energy-consuming chemical reactions involved. They also emphasize the importance of the selectivity of CO ₂ /H ₂ O and the potential for CO ₂ and H ₂ O co-capturing and end off explaining how the discussed topics could be applied, eventually, in an industrial setting.																																				
Research Question/Problem/Need	How can MOFs be optimized for DAC and what are some current impediments or promising findings?																																				
Important Figures	<p>Table 1 Volume fractions and main physicochemical properties of CO₂ and other typical components of air [60].</p> <table border="1"> <thead> <tr> <th>Gas</th> <th>CO₂</th> <th>N₂</th> <th>O₂</th> <th>Ar</th> <th>H₂O</th> </tr> </thead> <tbody> <tr> <td>Volume fraction</td> <td>~400 ppm</td> <td>78.084 %</td> <td>20.946 %</td> <td>0.934 %</td> <td>0-4 %</td> </tr> <tr> <td>Kinetic diameter (Å)</td> <td>3.3</td> <td>3.64-3.80</td> <td>3.467</td> <td>3.542</td> <td>2.641</td> </tr> <tr> <td>Boiling point (K)</td> <td>194.7</td> <td>77.15</td> <td>90.15</td> <td>87.25</td> <td>373.15</td> </tr> <tr> <td>Polarizability (× 10⁻²⁵ cm³)</td> <td>29.11</td> <td>17.403</td> <td>15.812</td> <td>16.411</td> <td>14.5</td> </tr> <tr> <td>Quadrupole moment (× 10²⁶ esu cm²)</td> <td>4.30</td> <td>1.52</td> <td>0.39</td> <td>0</td> <td>-</td> </tr> </tbody> </table> <p>Table 1 shows many of the different properties or characteristics of some of the main components of air.</p>	Gas	CO ₂	N ₂	O ₂	Ar	H ₂ O	Volume fraction	~400 ppm	78.084 %	20.946 %	0.934 %	0-4 %	Kinetic diameter (Å)	3.3	3.64-3.80	3.467	3.542	2.641	Boiling point (K)	194.7	77.15	90.15	87.25	373.15	Polarizability (× 10 ⁻²⁵ cm ³)	29.11	17.403	15.812	16.411	14.5	Quadrupole moment (× 10 ²⁶ esu cm ²)	4.30	1.52	0.39	0	-
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Table 3The uptake capacity, Q_{st} , and mechanisms of MOFs for DAC.

MOFs	Uptake		Q_{st} (kJ/mol)	Main mechanisms	Desorption condition	Ref.
	Uptake capacity (mmol/g)	CO ₂ (ppm)				
Mg-MOF-74	0.088	400	47	OMSs	180 °C	[34]
Mg-IRMOF-74-II	0.53	390	44	OMSs	Not available	[63]
HKUST-1	0.05	400	34	OMSs	140 °C	[34]
UIO-66	0.02	400	Not available	OMSs	100 °C	[57]
ZIF-8	0.05	400	27	OMSs	100 °C	[57]
MIL-101(Cr)	0.02	400	Not available	OMSs	100 °C	[57]
SIFSIX-3-Cu	1.24	400	54	Kinetic sieving / Lewis interactions	Vacuum, 323K	[64]
SIFSIX-3-Zn	0.13	400	45	Kinetic sieving / Lewis interaction	Not available	[64]
SIFSIX-3-Ni	0.29	400	51	Kinetic sieving / Lewis interaction	Not available	[64]
SIFSIX-2-Cu-i	0.68	400	32	Kinetic sieving / Lewis interaction	Not available	[64,65]
NbOFFIVE-1-Ni	1.30	400	54	Kinetic sieving / Lewis interaction	Vacuum, 328 K	[5]
SIFSIX-18-Ni-β	0.96	400	52	Kinetic sieving / hydrophobic interaction	Not available	[66]
TIFSIX-3-Ni	1.15	400	53	Kinetic sieving / Lewis interaction	Not available	[66]
TIFSIX-3-Co	1.05	400	Not available	Kinetic sieving / Lewis interaction	Not available	[67]
GeFSIX-3-Ni	1.07	400	56	Kinetic sieving / Lewis interaction	Not available	[68]
GeFSIX-3-Co	0.30	400	39	Kinetic sieving / Lewis interaction	Not available	[68]
[Zn(ZnOH) ₄ (bibta) ₃]	2.20	400	42	Covalent interactions	100 °C	[69]
Zn ₂ (OH) ₄ (btdd) ₃	1.54	400	Not available	Covalent interactions	100 °C	[70]
Mg ₂ (dobdc)-en	1.51	400	Not available	Covalent interactions	120 °C, Ar purge	[71]
Mg ₂ (dobdc)(N ₂ H ₄) _{1.8}	3.89	400	118	Covalent interactions	Not available	[72]
Mg ₂ (dobpdc)-en	2.83	390	Not available	Covalent interactions	Simulated air purge, 150 °C	[73]
Mg ₂ (dobpdc)-mmen	3.00	400	74	Covalent interactions	N ₂ purge, 150 °C	[63,74]
Cr-MIL-101-SO ₃ H-TETA	1.12	400	87	Covalent interactions	Not available	[75]
NbOFFIVE-1- Ni@PA	1.44	400	Not available	Covalent interactions	Water vapor, 378 K	[76]
MIL-101(Cr)-TREN	0.35	400	Not available	Covalent interactions	Not available	[77]
MIL-101(Cr)-PEI-800	1.20	400	Not available	Covalent interactions	Not available	[77]

Table 3 shows the CO₂ uptake of many different MOFs and their associated properties, as well as the sources/paper that back up the data.

VOCAB: (w/definition)

Isosteric: has the same number of electrons

Entropy: unavailable energy in a closed thermodynamic system

Cited references to follow up on

[http://refhub.elsevier.com/S2772-6568\(23\)00049-0/sbref0118](http://refhub.elsevier.com/S2772-6568(23)00049-0/sbref0118)

[http://refhub.elsevier.com/S2772-6568\(23\)00049-0/sbref0131](http://refhub.elsevier.com/S2772-6568(23)00049-0/sbref0131)

[http://refhub.elsevier.com/S2772-6568\(23\)00049-0/sbref0066](http://refhub.elsevier.com/S2772-6568(23)00049-0/sbref0066)

Follow up Questions

1. What are the pros and cons or using HUMs instead of MOFs in DAC?
2. What specific changes to MOF structure have demonstrated improvements in CO₂ capture efficiency and why?
3. What specific changes to MOF structure have demonstrated an increase in CO₂ selectivity over H₂O?

Article #13 Notes: Direct Capture of CO₂ from Ambient Air

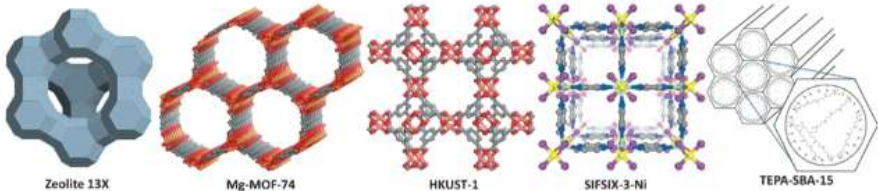
Source Title	Direct Capture of CO ₂ from Ambient Air
Source citation (APA Format)	Sanz-Pérez, E. S., Murdock, C. R., Didas, S. A., & Jones, C. W. (2016). Direct Capture of CO ₂ from Ambient Air. <i>Chemical Reviews</i> , 116, 11840–11876. https://doi.org/10.1021/acs.chemrev.6b00173
Original URL	https://pubs.acs.org/doi/10.1021/acs.chemrev.6b00173
Source type	Scholarly Journal
Keywords	Direct air capture of carbon, CO ₂ emissions
#Tags	#DAC
Summary of key points + notes (include methodology)	The article provides many different approaches for scalable DAC including aqueous hydroxide sorbents, solid alkali carbonates, and organic-inorganic hybrid sorbents, the latter of which MOFs fall under. It provides a lot of justification as to why CO ₂ emissions need to be reduced, and why DAC in particular is a very promising path to explore. It also explains why physisorbent materials such as MOFs are gaining attention: compared to chemisorbent materials, much less energy is needed for the regeneration of physisorbent materials because no chemical interactions occur between the sorbent and the sorbate. The article introduces the possibility of amine tethered MOFs to further increase the CO ₂ uptakes of certain MOFs, highlighting EN-Mg 2(dobpdc).
Research Question/Problem/Need	What are the pros and cons of some approaches to DAC?
Important Figures	 <p>Figure 19. Range of physisorbents investigated by Zaworotko and co-workers. Reprinted with permission from ref 186. Copyright 2015 Wiley. The figure above shows visually depicts some of the physisorbent MOFs that have been previously studied for their ability to absorb CO₂.</p> <p>The figure below depicts the absorption capacity of various MOFs, some with amines.</p>

Table 5. MOFs Used for Direct Air Capture; Amine-Tethered (If Applicable) And Experimental Conditions Are Noted As Well^a

MOF	amine	T (°C)	CO ₂ (ppm)	adsorption capacity (mmol of CO ₂ /g of sorbent)	method	ref
SIFSIX-3-Cu		25	400	1.24	vol.	191
SIFSIX-3-Zn		25	400	0.13	vol.	210
SIFSIX-3-Ni		23	400 ^b	0.18	TPD	186
HKUST		23	400 ^b	0.05	TPD	186
Mg-MOF-74		23	400 ^b	0.14	TPD	186
Mg-MOF-74	EN	22 ^c	400	1.51	TGA	205
Mg ₂ (dobpdc)		25	390	0.13 ^d	vol.	206
Mg ₂ (dobpdc)	MMEN	25	390	2.0 ^d	vol.	206
Mg ₂ (dobpdc)	EN	25	390	2.83 ^d	vol.	209

^bApproximate value. Samples exposed to lab atmosphere with an average $T = 23.4$ °C and 49% RH. ^cApproximate value. Room temperature denoted in manuscript. ^dAdsorption capacities interpolated from a pure CO₂ isotherm. ^eEN, ethylenediamine; MMEN, *N,N'*-dimethylethylenediamine; vol., volumetric; TPD, temperature-programmed desorption; TGA, thermogravimetric analysis.

VOCAB: (w/definition)

Physisorbent: absorbs with physical interactions rather than chemical interactions
 Chemisorbent: absorbs with chemical interactions rather than physical interactions
 Sorbate: the substance being absorbed

Cited references to follow up on

<https://pubmed.ncbi.nlm.nih.gov/20730980/>
<https://pubmed.ncbi.nlm.nih.gov/26440308/>
<https://pubs.rsc.org/en/content/articlelanding/2014/ee/c3ee42328j>

Follow up Questions

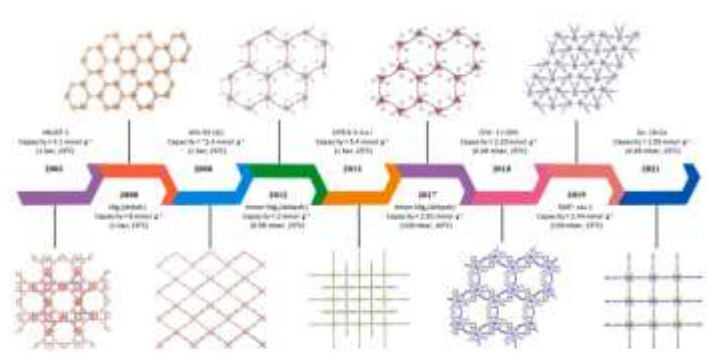
1. Why might amines increase CO₂ uptake?
2. What particular properties are common among beneficial amines and the MOFs they are tethered to?
3. How does the regeneration of chemisorbents differ from the regeneration of physisorbents like MOFs?

Article #14 Notes: Back to the Basics: Developing Advanced Metal-Organic Frameworks Using Fundamental Chemistry Concepts

Source Title	Back to the Basics: Developing Advanced Metal-Organic Frameworks Using Fundamental Chemistry Concepts
Source citation (APA Format)	Kirlikovali, K. O., Hanna, S. L., Son, F. A., & Farha, O. K. (2023). Back to the Basics: Developing Advanced Metal-Organic Frameworks Using Fundamental Chemistry Concepts. <i>ACS Nanoscience Au</i> , 3(1), 37-45. https://doi.org/10.1021/acsnanoscienceau.2c00046
Original URL	https://pubs.acs.org/doi/10.1021/acsnanoscienceau.2c00046
Source type	Scholarly Journal
Keywords	Metal-organic frameworks, chemistry, stability
#Tags	#MOF
Summary of key points + notes (include methodology)	This paper explains the history of MOFs and also explores the chemistry behind how these frameworks function. The stability of a MOF is reliant on chemistry concepts such as the HSAB theory and the crystalline structure of MOFs can be further improved by adding modulators during synthesis. This paper focuses less on applications and more on ways one can increase stability by employing certain methods during synthesis.
Research Question/Problem/Need	How can chemistry concepts be applied to increase the stability of MOFs by making changes during synthesis?
Important Figures	<p>The figure above depicts how modulators work during synthesis. The figure below depicts some of the causes for different types of stability.</p>

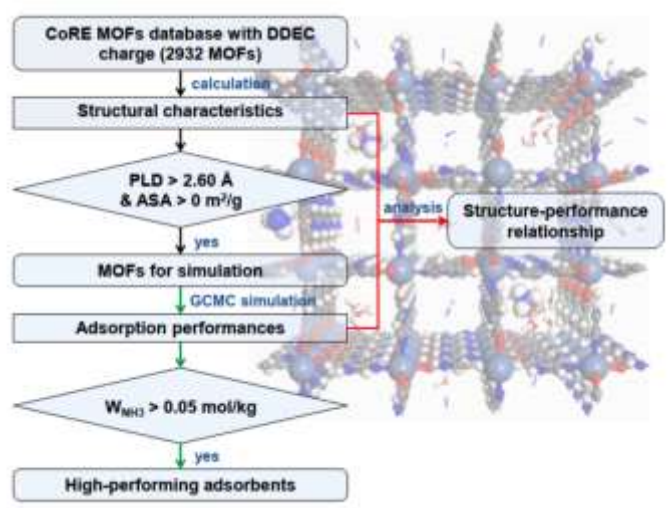
VOCAB: (w/definition)	<p>“Chemically robust”: essentially means something is stable even under fairly extreme conditions</p> <p>Hydrolytic: relating to reactions with water</p>
Cited references to follow up on	<p>https://doi.org/10.1038/ncomms15369</p> <p>https://doi.org/10.1021/acsami.1c01329?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as</p> <p>https://doi.org/10.1126/science.aaz8881</p>
Follow up Questions	<ol style="list-style-type: none"> 1. What sorts of modulators have shown promise in increasing the stability of certain MOFs? 2. What effects does the inclusion of modulators during synthesis have on the CO₂ uptake of certain MOFs? 3. Are there any solvents that appear to improve the stability of MOFs?

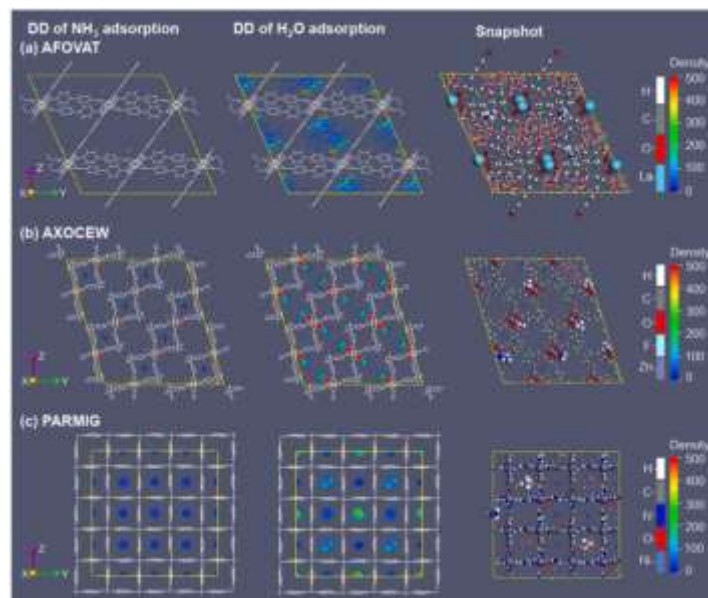
Article #15 Notes: Recent progress in metal-organic frameworks (MOFs) for CO2 capture at different pressures

Source Title	Recent progress in metal-organic frameworks (MOFs) for CO2 capture at different pressures
Source citation (APA Format)	Mahajan, S. & Lahtinen, M. (2022). Recent progress in metal-organic frameworks (MOFs) for CO2 capture at different pressures. <i>Journal of Environmental Chemical Engineering</i> , 10(6). https://doi.org/10.1016/j.jece.2022.108930
Original URL	https://www.sciencedirect.com/science/article/pii/S2213343722018036
Source type	Scholarly Journal
Keywords	Metal-organic framework, chemisorption or physisorption
#Tags	#MOFs
Summary of key points + notes (include methodology)	The paper explores a variety of different techniques to increase the CO2 uptake of MOFs, including using open metal sites (OMSs), which could have amines attached to it in order to chemisorb CO2 from the atmosphere. Regarding MOF stability in the presence of water, the article proposes metalated-ligand exchange (MLE), which has to do with exchanging the typical ligand bdc with another ligand and a collection of metal ions, and also HUMs due their physisorptive properties resulting from bridging anions.
Research Question/Problem/Need	What are some strategies that can be employed to increase the CO2 absorption of MOFs?
Important Figures	 <p>Fig. 3. Illustration of CO₂ capture capacities for some well-known MOFs: (a) HKUST-1 (187) [Cu] (Mg/Al) (b) UiO-66 (108) [Zr] (c) MIL-53 (109) [Al] (d) ZIF-8 (109) [Zn] (e) MOF-5 (109) [Al]. The diagram also shows the chemical structures of the MOFs and their corresponding CO₂ capture capacities.</p>
VOCAB: (w/definition)	N/A
Cited references to follow up on	https://doi.org/10.1002/cssc.201601545

	https://doi.org/10.1007/s10450-019-00118-1 https://doi.org/10.1016/j.micromeso.2013.06.023
Follow up Questions	<ol style="list-style-type: none">1. How might certain MOF structures influence stability in the presence of water or chemical stability?2. How do certain structures promote chemisorption or physisorption of CO₂?3. How does reuse of MOFs affect its stability or CO₂ uptake?

Article #16 Notes: Computational screening of metal-organic frameworks for ammonia capture from humid air


Source Title	Computational screening of metal-organic frameworks for ammonia capture from humid air
Source citation (APA Format)	Liu, Z., Wang, X., Liu, Y., Li, L., & Li, S. (2021). Computational screening of metal-organic frameworks for ammonia capture from humid air. <i>Microporous and Mesoporous Materials</i> , 331. https://doi.org/10.1016/j.micromeso.2021.111659
Original URL	https://www.sciencedirect.com/science/article/pii/S1387181121007848?via%3Dihub
Source type	Scholarly Journal
Keywords	MOFs, ammonia capture, computational screening
#Tags	#simulations #MOFs
Summary of key points + notes (include methodology)	In order to identify potential MOFs to be used in the capture of ammonia directly from the air, this paper used computational methods in order to test a variety of MOFs from the CoRE database in order to find the best candidates for ammonia capture. Using the data from the CoRE database, they ran GCMC simulations of ammonia absorption and then tested its selectivity over water too, developing a complex system of equations attempting to quantify different criteria and their effect on overall MOF performance. They used RASPA 2.0 for a more visual view.
Research Question/Problem/Need	What MOFs can be used in the direct air capture of ammonia?
Important Figures	 <p>Fig. 1. Schematic diagram of the computational screening strategy for ammonia capture from humid air.</p> <p>The figure above depicts the computational methodology used in the paper</p>



The figure above shows the density distributions of ammonia and water in three of the tested MOFs, simulated with RASPA 2.0.

VOCAB: (w/definition)	N/A
Cited references to follow up on	http://refhub.elsevier.com/S1387-1811(21)00784-8/sref26 http://refhub.elsevier.com/S1387-1811(21)00784-8/sref23 http://refhub.elsevier.com/S1387-1811(21)00784-8/sref33
Follow up Questions	<ol style="list-style-type: none"> 1. Why do some areas of a MOF tend to absorb more of a substance over other areas? 2. What properties are exhibited by sites with higher densities of ammonia? 3. Does higher selectivity for ammonia tend to correlate with higher ammonia uptake overall?

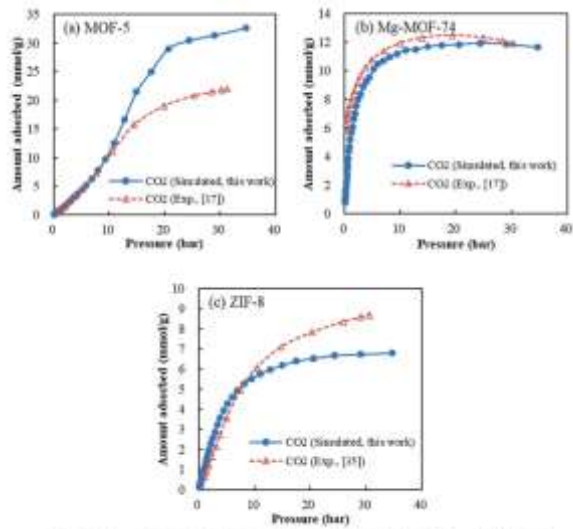
Article #17 Notes: How to Make Metal-Organic Frameworks (MOFs)

Source Title	How to Make Metal-Organic Frameworks (MOFs)
Source citation (APA Format)	Wood, A. (n.d.). <i>How to Make Metal-Organic Frameworks (MOFs)</i> . Ossila. https://www.ossila.com/pages/how-to-make-metal-organic-frameworks
Original URL	https://www.ossila.com/pages/how-to-make-metal-organic-frameworks
Source type	Website
Keywords	MOF synthesis,
#Tags	#MOFsynthesis
Summary of key points + notes (include methodology)	This website depicts many methods of synthesis and provides visual aids for better comprehension. Similarly to article #14, it mentions MOF modulators that help control MOF crystallization, increasing stability, and it lists several modulators including acetic acid, water, ammonia, hydrochloric acid, and sulfuric acid. It explains the conditions needed for each method of synthesis, as well as commonly used solvents and commonly synthesized MOFs that use that method.
Research Question/Problem/Need	What are some methods used to synthesis MOFs and what are some of their pros and cons?
Important Figures	 <p style="text-align: center;">General synthesis of MOFs</p> <p>The figure above depicts a general synthesis process for MOFs.</p> <p>The table below lists some of the pros and cons of each synthesis method.</p>

	<table border="1"> <thead> <tr> <th>Synthetic Method</th> <th>Advantages</th> <th>Disadvantages</th> </tr> </thead> <tbody> <tr> <td>Solvothermal/Hydrothermal</td> <td> <ul style="list-style-type: none"> One-step synthesis Can access single crystals Moderate temperature </td> <td> <ul style="list-style-type: none"> Long reaction time (hrs/days) Requires more solvent Easy to produce unwanted by-products </td> </tr> <tr> <td>Microwave-assisted</td> <td> <ul style="list-style-type: none"> Rapid (mins) High purity Uniform morphology Eco-friendly </td> <td> <ul style="list-style-type: none"> Difficult to get single crystals Not yet scalable </td> </tr> <tr> <td>Electrochemical</td> <td> <ul style="list-style-type: none"> No need for metal salts Mild reaction conditions Quick (hrs) </td> <td> <ul style="list-style-type: none"> Requires N₂ atmosphere Varied structure Lower yield </td> </tr> <tr> <td>Mechanochemical</td> <td> <ul style="list-style-type: none"> Room temperature Less hazardous by-products Rapid (mins) Eco-friendly </td> <td> <ul style="list-style-type: none"> Decreased pore volume Lower crystallinity Lower yield </td> </tr> <tr> <td>Sonochemical</td> <td> <ul style="list-style-type: none"> Quick (less of mins) Eco-friendly </td> <td> <ul style="list-style-type: none"> Difficult to get single crystals </td> </tr> </tbody> </table> <p>There are also many additional figures depicting each method of synthesis that I will refer to when I'm simulating synthesis.</p>	Synthetic Method	Advantages	Disadvantages	Solvothermal/Hydrothermal	<ul style="list-style-type: none"> One-step synthesis Can access single crystals Moderate temperature 	<ul style="list-style-type: none"> Long reaction time (hrs/days) Requires more solvent Easy to produce unwanted by-products 	Microwave-assisted	<ul style="list-style-type: none"> Rapid (mins) High purity Uniform morphology Eco-friendly 	<ul style="list-style-type: none"> Difficult to get single crystals Not yet scalable 	Electrochemical	<ul style="list-style-type: none"> No need for metal salts Mild reaction conditions Quick (hrs) 	<ul style="list-style-type: none"> Requires N₂ atmosphere Varied structure Lower yield 	Mechanochemical	<ul style="list-style-type: none"> Room temperature Less hazardous by-products Rapid (mins) Eco-friendly 	<ul style="list-style-type: none"> Decreased pore volume Lower crystallinity Lower yield 	Sonochemical	<ul style="list-style-type: none"> Quick (less of mins) Eco-friendly 	<ul style="list-style-type: none"> Difficult to get single crystals
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VOCAB: (w/definition)	N/A																		
Cited references to follow up on	https://doi.org/10.1021/acsomega.2c05310 https://doi.org/10.1021/acsnanoscienceau.2c00046 https://doi.org/10.1039/D1MA00719J																		
Follow up Questions	<ol style="list-style-type: none"> 1. How do the listed modulators effect MOF synthesis and improve MOF crystallinity? 2. Which synthesis method appears to be the most scalable and why? 3. Which synthesis method has the most room for growth/improvement and what are some methods to improve it? 																		

Article #18 Notes: Grand canonical Monte Carlo (GCMC) study on adsorption performance of metal organic frameworks (MOFs) for carbon capture

Source Title	Grand canonical Monte Carlo (GCMC) study on adsorption performance of metal organic frameworks (MOFs) for carbon capture
Source citation (APA Format)	Tao, Y. R., Zhang, G. H., & Xu, H. J. (2022). Grand canonical Monte Carlo (GCMC) study on adsorption performance of metal organic frameworks (MOFs) for carbon capture. <i>Sustainable Materials and Technologies</i> , 32. https://doi.org/10.1016/j.susmat.2021.e00383
Original URL	https://www.sciencedirect.com/science/article/pii/S221499372100138X?ref=pdf_download&fr=RR-2&rr=8eef35e7ccee3045
Source type	Scholarly Journal
Keywords	GCMC, carbon capture
#Tags	#MOFs #simulation
Summary of key points + notes (include methodology)	This paper uses Grand Canonical Monte Carlo simulations to analyze the CO ₂ absorption of three MOFs: MOF-5, Mg-MOF-74, and ZIF-8. The parameters inputted into the simulations were generated from the Cambridge Crystallographic Data Center, and many of the equations used are provided in the article. After the simulation, the results were checked against pre-existing experimental studies. The selectivity of CO ₂ /N ₂ was then tested and they determined that overall, Mg-MOF-74 seemed to perform the best out of the three.
Research Question/Problem/Need	How can GCMC methods be used in simulating the CO ₂ absorption of different MOFs?

Important Figures	 <p data-bbox="568 745 1071 766">Fig. 3. Force field verification for CO₂ adsorption in (a) MOF-5, (b) Mg-MOF-74 and (c) ZIF-8 (3 mmol = 10⁻³ mol).</p> <p data-bbox="519 766 1494 840">The graphs above compare the experimental results to the simulated results. The simulated data matched the experimental data well especially in for Mg-MOF-74.</p>
VOCAB: (w/definition)	N/A
Cited references to follow up on	http://refhub.elsevier.com/S2214-9937(21)00138-X/rf0075 http://refhub.elsevier.com/S2214-9937(21)00138-X/rf0120 http://refhub.elsevier.com/S2214-9937(21)00138-X/rf0180
Follow up Questions	<ol style="list-style-type: none"> <li data-bbox="568 1071 1494 1134">1. What are some potential causes for the discrepancy between the simulated results and the experimental results of MOF-5 and ZIF-8? <li data-bbox="568 1144 1494 1176">2. Why might experimental ZIF-8 have outperformed the simulated results? <li data-bbox="568 1186 1494 1239">3. How can MOF stability under normal conditions / exposure to water be factored into a simulation?

Article #19 Notes: Algorithms and tools for high-throughput geometry-based analysis of crystalline porous materials

Source Title	Algorithms and tools for high-throughput geometry-based analysis of crystalline porous materials
Source citation (APA Format)	Willems, T. F., Rycroft, C. H., Kazi, M., Meza, J. C., & Haranczyk, M. (2012). Algorithms and tools for high-throughput geometry-based analysis of crystalline porous materials. <i>Microporous and Mesoporous Materials</i> , 149(1), 134-141. https://doi.org/10.1016/j.micromeso.2011.08.020
Original URL	https://www.sciencedirect.com/science/article/pii/S1387181111003738
Source type	Scholarly Journal
Keywords	Algorithms and tools, porous materials
#Tags	#simulation
Summary of key points + notes (include methodology)	This paper compiles many different tools that can be used to calculate the pore size of many porous materials including metal-organic frameworks. They describe various existing methods people used, including a Monte Carlo approach that generates probes into the molecular structure to determine the volume that can be absorbed, though it fails to account for channels that may open up to larger areas but are too small for specific molecules to fit through, causing the simulation to count areas the molecule can technically fit in though it may not be able to get into the area in the first place. The paper then introduces the Voronoi network, which considers how various particles might interact or block each other in a porous material, which ultimately helps with visualizing the surface area, volume, and overall structure of porous materials.
Research Question/Problem/Need	What are some algorithms or tools that can be used to computationally analyze the properties of porous materials?
Important Figures	N/A
VOCAB: (w/definition)	N/A
Cited references to follow up on	https://www.tandfonline.com/doi/abs/10.1080/08927022.2011.562502
Follow up Questions	<ol style="list-style-type: none"> 1. What are some further applications of the Voronoi network beyond calculating surface area or volume? 2. Can the existing Monte Carlo system be altered in order to account for its limitations? 3. What are some limitations or pitfalls of the Voronoi network and how can they be addressed?

Article #20 Notes: RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials

Source Title	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials
Source citation (APA Format)	Dubbeldam, D., Calero, S., Ellis, D. E., & Snurr, R. Q. (2016). RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. <i>Molecular Simulation</i> , 42(2), 81-101. https://doi.org/10.1080/08927022.2015.1010082
Original URL	https://www.tandfonline.com/doi/full/10.1080/08927022.2015.1010082
Source type	Scholarly Journal
Keywords	Simulation software, nanoporous materials
#Tags	#simulation
Summary of key points + notes (include methodology)	RASPA is a software that combines MC (Monte Carlo) simulations with MD (molecular dynamics) simulations, based upon calculations involving force fields. This article lists the numerous applications of RASPA, including simulating adsorption into different types of structures, screening, and diffusion, which is important to MOFs because diffusion of a substance into a MOFs is as important as adsorption. In addition, equations used in this simulation are provided, and further information about the simulation's code or other details are provided in the references.
Research Question/Problem/Need	What is RASPA and some of its applications?
Important Figures	N/A
VOCAB: (w/definition)	N/A
Cited references to follow up on	http://dx.doi.org/10.1080/08927020601156418 https://www.sciencedirect.com/science/article/pii/S0010854511000701 http://dx.doi.org/10.1021/jp051771y
Follow up Questions	<ol style="list-style-type: none"> 1. Can RASPA help to visualize adsorption and diffusion in nanoporous materials? 2. Why were configurational-bias MC and continuous fractional component MC chosen over GCMC? 3. What are some drawbacks or areas of improvement for RASPA?