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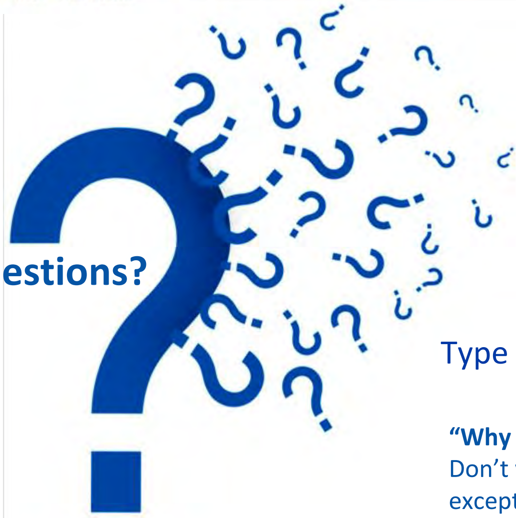

Type them into questions box!

"Why am I muted?"
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ACS Chemistry for Life®

Fecha: Miércoles, 27 de Octubre de 2021 @ 2-3pm ET
Ponente: David Quintanar Guerrero, Universidad Nacional Autónoma de México
Moderadora: Maria del Jesus Rosales Hoz, Cinvestav

Registrarse Gratuitamente

Lo Que El Público Aprenderá:

- Conceptos básicos de Nanotecnología y Química Verde
- Tendencias en el desarrollo de una Nanotecnología más sustentable
- Desarrollos e investigación nanotecnológicos relacionados con una tendencia amigable con el ambiente

This Spanish Language broadcast is co-produced with the Sociedad Química de México and *Chemical & Engineering News*.

Date: Thursday, October 28, 2021 @ 2-3:15pm ET
Speaker: Theresa Stotesbury, Ontario Tech University
Moderator: Monica Mattesi, Stony Brook University

Register for Free!

What You Will Learn:

- The forensic chemistry utilized by a bloodstain pattern analyst
- How biomolecule degradation is critical for "aging" a bloodstain
- What forensic blood substitutes are and how they are used in forensic science

Co-produced with: ACS Reactions

Date: Thursday, November 4, 2021 @ 2-3pm ET
Speakers: Jessica Martin, ACS Division of Chemical Health and Safety / Kali Miller, ACS Division of Chemical Health and Safety / Monica Nyansa, ACS Division of Chemical Health and Safety / Sarah Zin, ACS Division of Chemical Health and Safety
Moderator: Ralph Stuart, ACS Division of Chemical Health and Safety

Register for Free!

What You Will Learn:

- The motivation behind graduate student-led safety initiatives
- How lab productivity is often inextricably linked to lab housekeeping
- How LSTs can empower future lab leaders to collaborate on resolving safety continuity challenges

Co-produced with: ACS Division of Chemical Health and Safety ACS Committee on Chemical Safety

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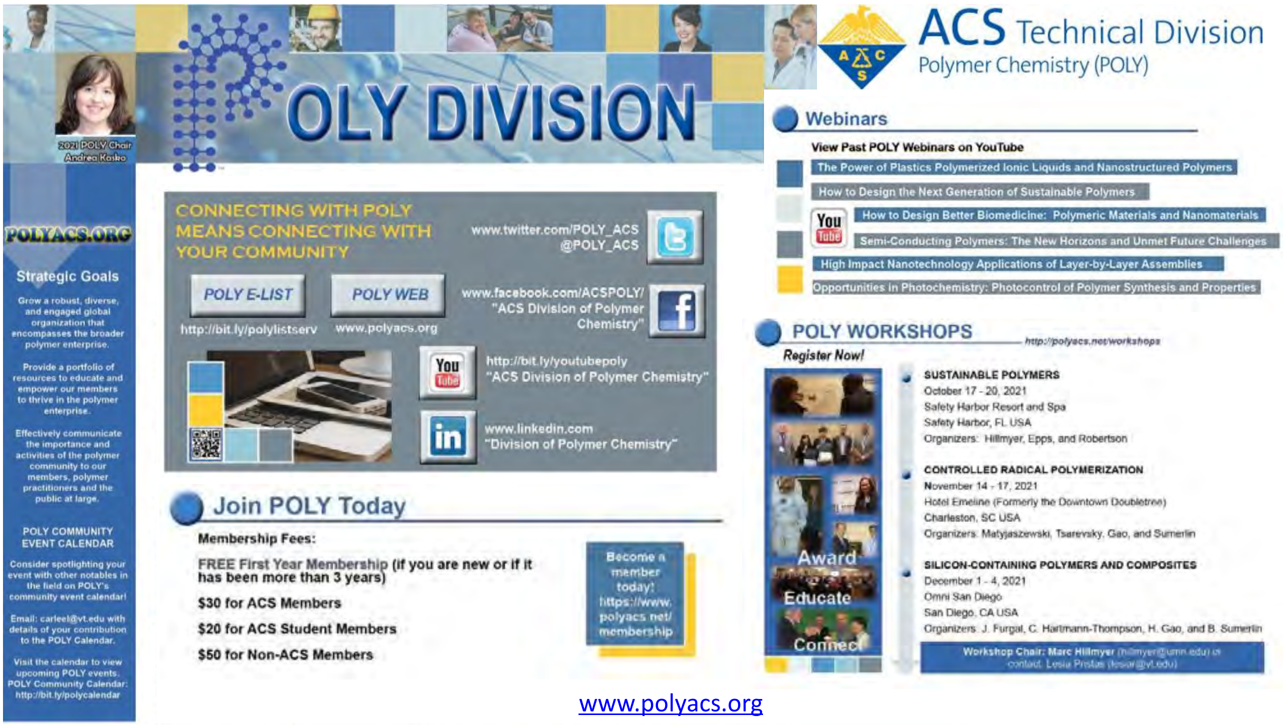
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Andrea Kasko
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Strategic Goals
Grow a robust, diverse, and engaged global organization that encompasses the broader polymer enterprise.
Provide a portfolio of resources to educate and empower our members to thrive in the polymer enterprise.
Effectively communicate the importance and activities of the polymer community to our members, polymer practitioners and the public at large.
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Semi-Conducting Polymers: The New Horizons and Unmet Future Challenges
High Impact Nanotechnology Applications of Layer-by-Layer Assemblies
Opportunities in Photochemistry: Photocontrol of Polymer Synthesis and Properties
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Organizers: Hillmyer, Epps, and Robertson
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November 14 - 17, 2021
Hotel Emeline (Formerly the Downtown Doubletree)
Charleston, SC USA
Organizers: Matyjaszewski, Tsarevsky, Gao, and Sumerlin
SILICON-CONTAINING POLYMERS AND COMPOSITES
December 1 - 4, 2021
Omni San Diego
San Diego, CA USA
Organizers: J. Furgal, C. Hartmann-Thompson, H. Gao, and B. Sumerlin
Workshop Chair: Marc Hillmyer
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By Capturing Atmospheric Carbon and Storing it Safely
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Achieving Climate Goals by Capturing Atmospheric Carbon and Storing it Safely

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Director of Science and Technology, Polymer Chemistry Innovations

EMILY PENTZER
Associate Professor, Department of Chemistry and the Department of Materials Science and Engineering, Texas A&M University

JOHANN PLANK
Chair for Construction Chemistry and Full Professor, Department of Chemistry, Technical University of Munich

Presentation slides are available now! The edited recording will be made available as soon as possible.
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This ACS Webinar is co-produced with ACS Division of Polymer Chemistry.

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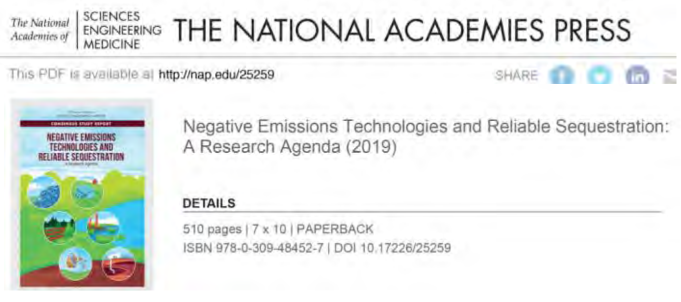
Carbon Dioxide and Global Climate Change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Negative Emissions Technologies and Reliable Sequestration: A Research Agenda (2019)

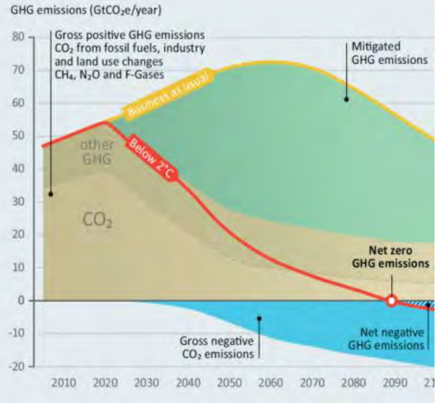
DETAILS

510 pages | 7 x 10 | PAPERBACK
ISBN 978-0-309-48452-7 | DOI 10.17226/25259

Negative emission technologies focus on taking CO_2 out of the atmosphere and putting it into geological reservoirs or terrestrial ecosystems
Less disruptive, less expensive

Over the last 300 years there has been an increase of 120 ppm of atmospheric CO_2

10 gigatones of atmospheric CO_2 must be removed annually by 2050 to stay below a temperature rise of 1.5 °C

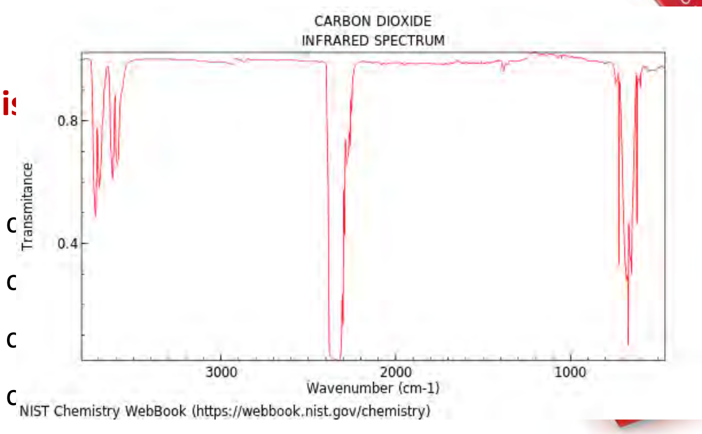


Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Where is ... **num?**

- 3000 c
- 1000 c
- 1700 c
- 2300 c



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Question

Where is the absorption profile of CO_2 gas at a maximum?

a) 3000 cm^{-1}

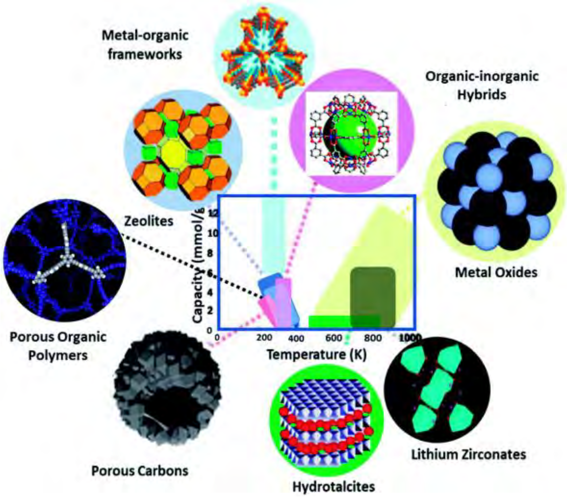
b) 1000 cm^{-1}

c) 1700 cm^{-1}

d) 2300 cm^{-1}

Adsorption of CO_2: Porous Materials

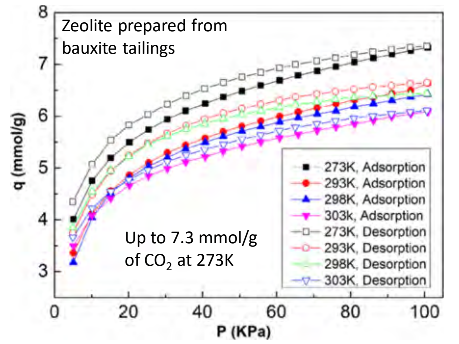
Adsorption of CO_2 onto porous structure: zeolites, metal–organic frameworks (MOFs), mesoporous silica, clay, porous carbons, porous organic polymers (POPs), etc.



RSC Advances, 2021, 11, 12658-12681

Properties to Consider:

- Capacity under adsorption conditions
- Selectivity
- Regenerability



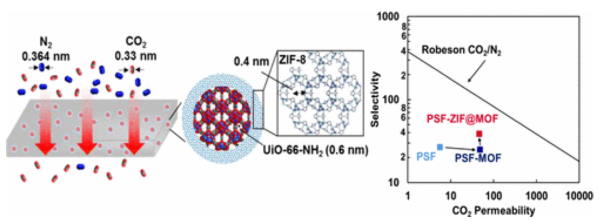
Energy & Fuels, 2019, 33, 6641-6649

Adsorption of CO_2: Mixed Matrix Membranes (MMMs)

Combine the mechanical properties and processability of polymers with permeability and selectivity of the filler

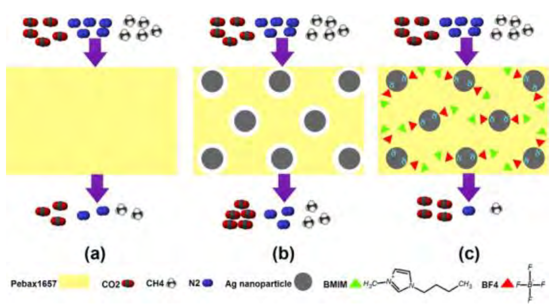
J. Mater. Chem. A, 2019, 7, 24738-24759

Core-shell MOF-ZIF blended with polysulfone
Tailored composition showed higher CO_2 permeability and better selectivity



Nano Lett, 2017, 17, 6752

Poly(ether-block-amide) with silver nanoparticles and ionic liquid (IL); ternary blend increased permeability and selectivity



ACS Appl. Mater. Interfaces, 2017, 9, 10094

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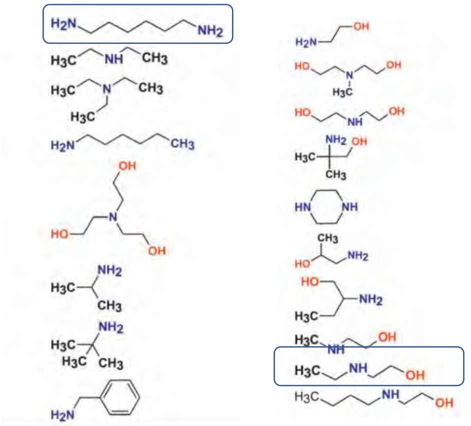
CO_2 Absorbing Liquids: Amines

Aqueous Amines (30 wt%)

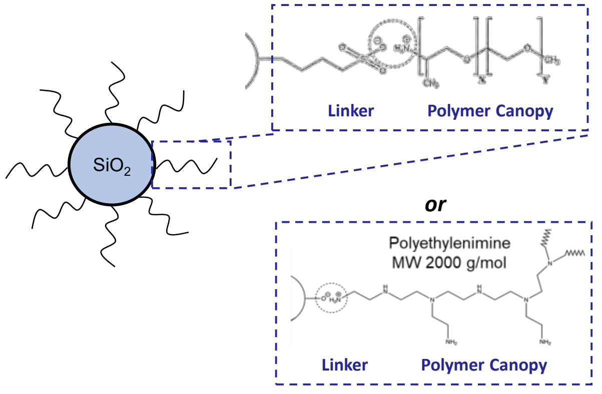
Energy intensive process, need to recover solvent vapor, corrosive



Applied Energy, 2017, 185, 1433-1449

Nanoparticle Organic Hybrid Materials (NOHMs)

Integrate amine or PEG functionalities in polymer canopy of nanoparticles



Phys. Chem. Chem. Phys. 2011, 13, 18115-18122

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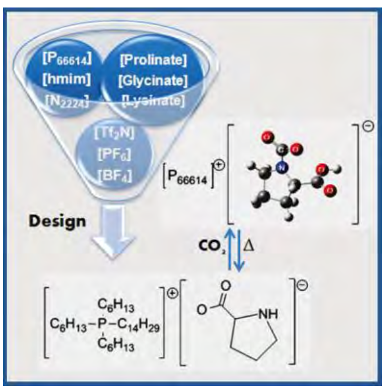
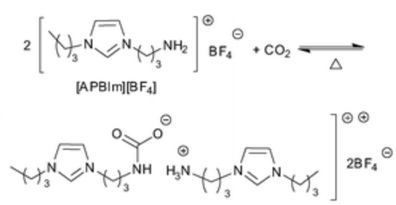
CO_2 Absorbing Ionic Liquids

Ionic Liquids

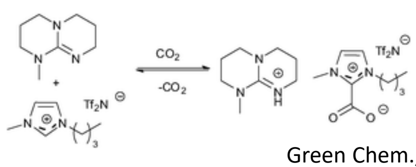
Water lean solvent with chemical flexibility allows tuning properties



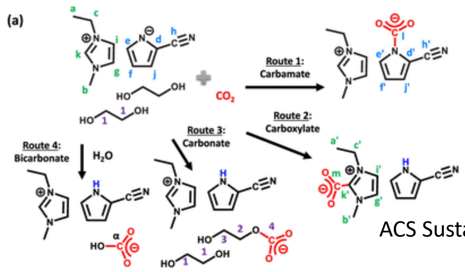
J. Phys. Chem. Lett. 2010, 1, 3459-3464



J. Am. Chem. Soc. 2002, 124, 926-927



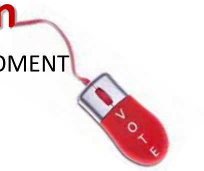
Green Chem., 2010, 12, 2019-2023



ACS Sustainable Chem. Eng. 2021, 1090-1098

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



What is the price of the Ionic Liquids [Bmim][PF6] when buying 5g, in USD?

70956-5G	5 G	Available to ship on October 21, 2021 - FROM	$70.30
70956-50G	50 G	Estimated to ship on January 25, 2022	$278.00
70956-250G	250 G	Only 2 left in stock (more on the way) - FROM	$929.00

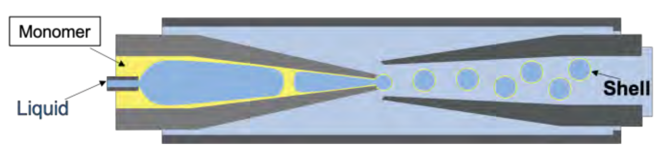
- ~$0.50/g
- ~$5/g

Encapsulation of CO_2 Sorbent Liquids

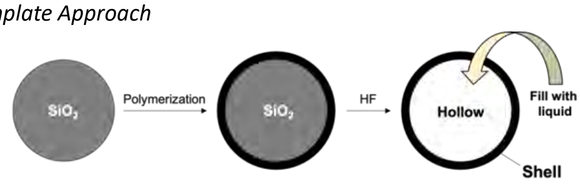
Encapsulation addresses issues with high viscosities or changes in physical properties of liquids

Can greatly increase surface area and CO_2 absorption rate *provided shell is permeable (selective)*

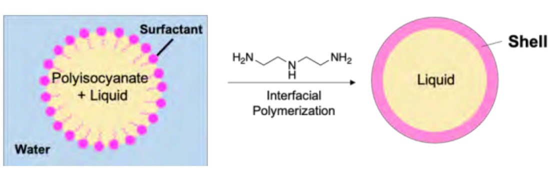
Microfluidic Approach



Hard Template Approach



Soft Template Approach



Encapsulation of CO_2 Sorbent Liquids

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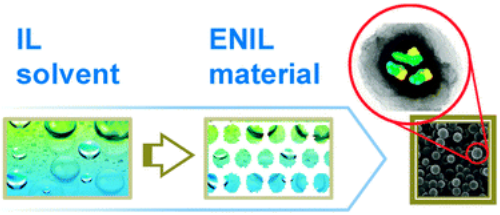
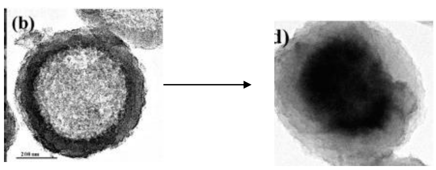
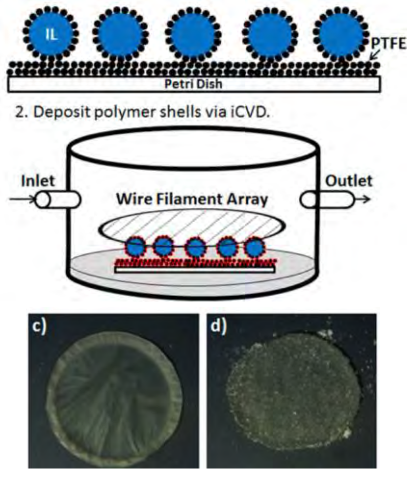
Encapsulated Ionic Liquids (ENILs)
Impregnate carbon with ionic liquid in acetone





Chem. Commun. 2012, 48, 10046-10048

Growth of polymer by CVD around droplets of IL with PTFE particles

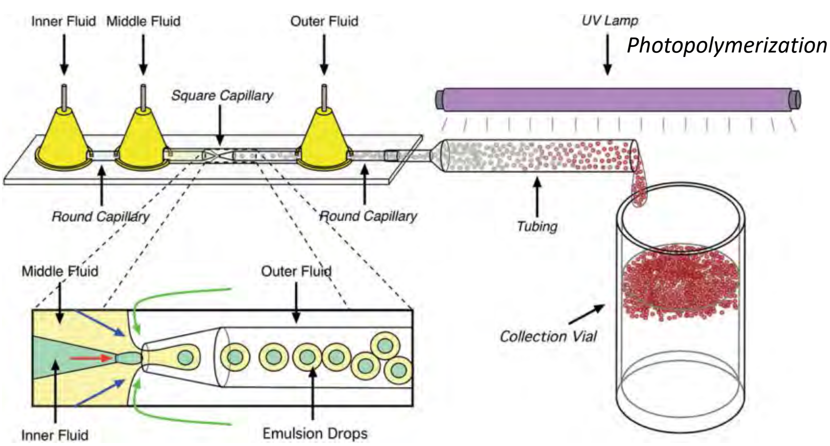


Langmuir, 2012, 28, 10276

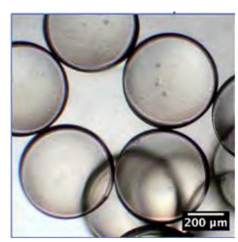
Encapsulation of CO_2 Sorbent Liquids

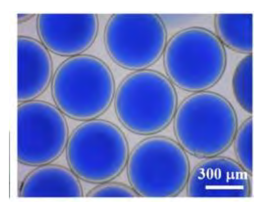
22

Microfluidic device used to encapsulate ionic liquids or CO_2-binding organic liquids (CO_2-BOLs)



Faraday Discuss. 2016, 192, 271-281

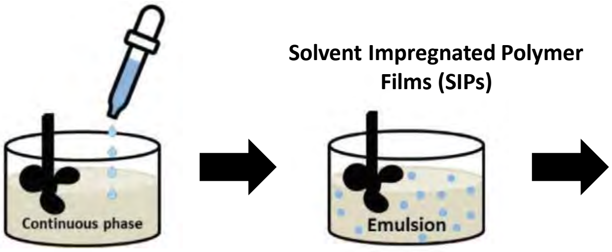


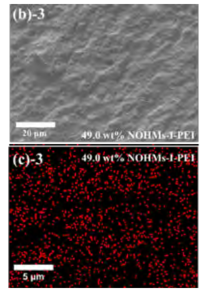


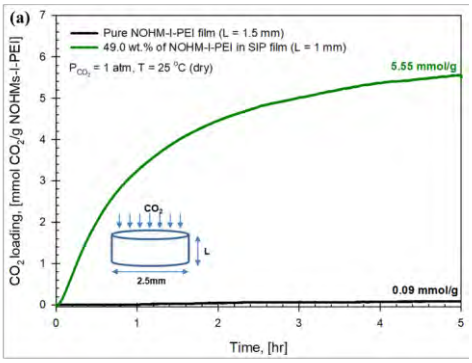
Phys. Chem. Chem. Phys. 2011, 13, 18115-18122

Encapsulation of NOHMs

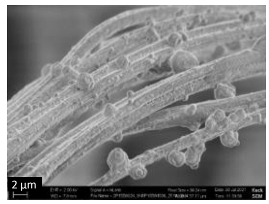
Add NOHMs to a UV-curable resin, emulsify, and cure







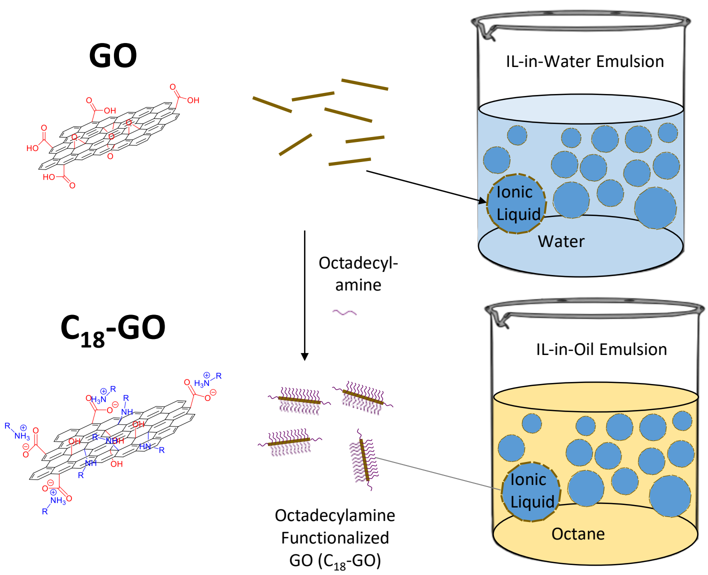
Accelerated CO_2 sorption kinetics due to increased interfacial area and enhanced oxidative thermal stability



Electrospinning NOHMs with polyimides gives coaxial fibers

Adv. Funct. Mater. 2021, 31, 20199947

Soft Template Approach to Encapsulating ILs

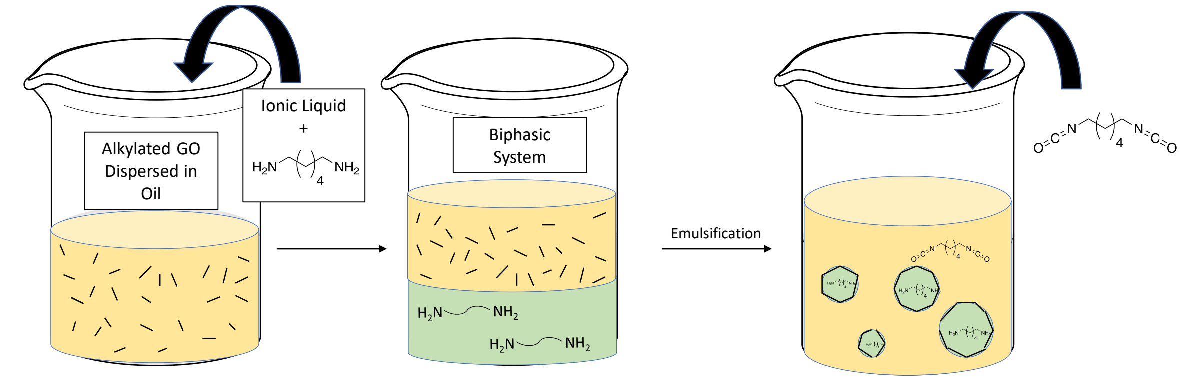


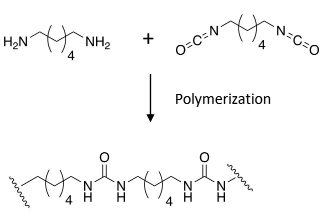
Graphene oxide (GO) nanosheets stabilize droplets of IL in water

Alkylated graphene oxide (GO) nanosheets stabilize droplets of IL in oil

Langmuir, 2018, 34, 10114.

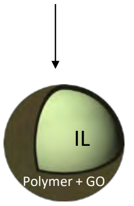
Encapsulation of IL by Interfacial Polymerization



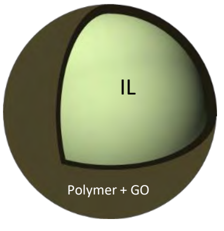


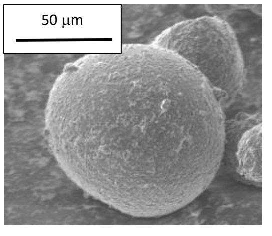
GO as particle surfactant provides access to IL-in-water (or oil) emulsion

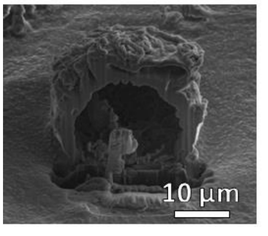
Interfacial polymerization produces capsules with core of IL and shell of polymer/GO

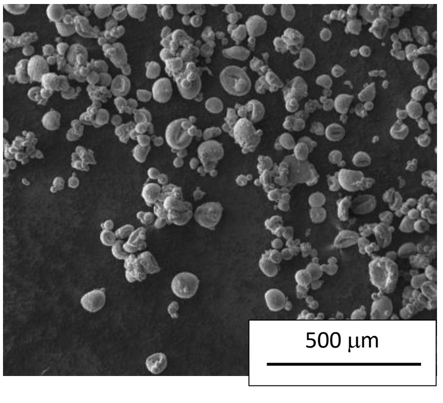


Powders of IL Capsules









Powders of distinct, individual capsules are isolated by gravity filtration

IL remains inside and powders can easily be transferred without leakage

Cutting capsule reveals hollow core

IL-Filled Capsules with Shell of Polymer/GO

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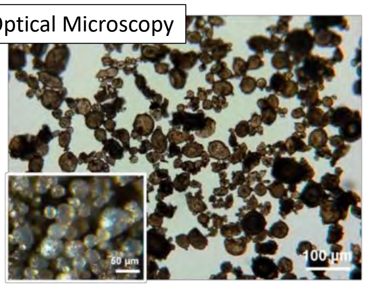
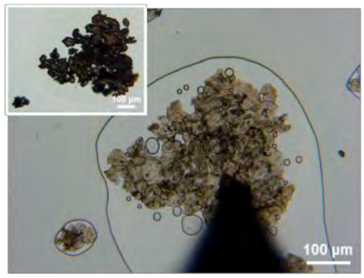
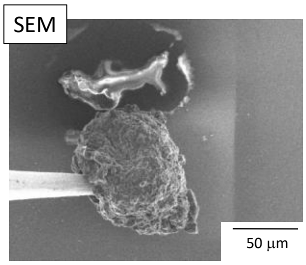
Optical Microscopy



Pressing →



SEM



50 µm

Compression of capsules with top glass slide or Omniprobe in SEM leads to leakage of the encapsulated IL

Composition of IL Capsules

28

FTIR

Raman

Extraction with acetone-d_6 and internal standard shows particles are 80 wt% IL

DSC

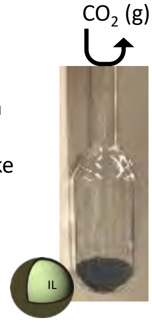
TGA

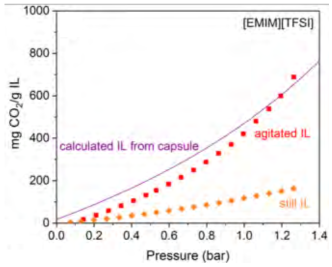
- **FTIR**: presence of IL and polyurea
- **Raman**: presence of GO
- **DSC**: thermal transitions of IL core
- **TGA**: slight decrease in thermal stability of IL

Application of Encapsulated IL: CO_2 Uptake

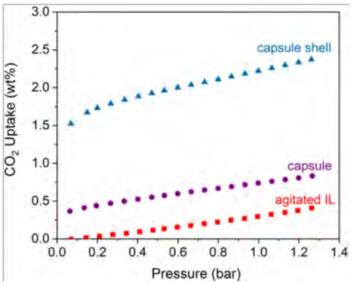
Increased surface area can overcome kinetic limitations of CO_2 uptake

Compare unagitated capsules to stirred IL

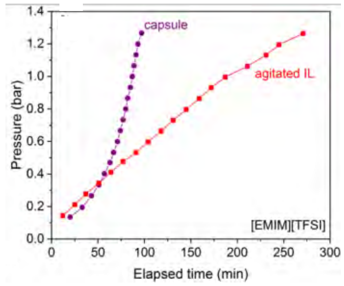




Contribution of IL to CO_2 uptake is consisted with agitated IL and superior to still IL



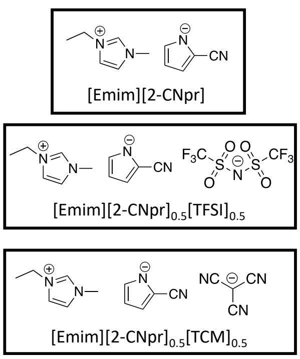
Shell contributes to CO_2 uptake, likely by favorable interaction of gas and polyurea

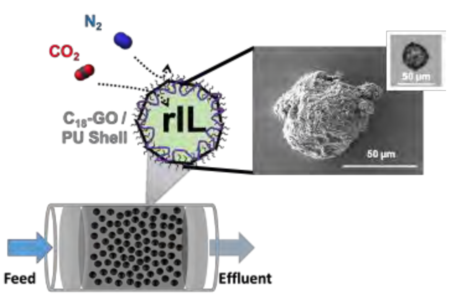


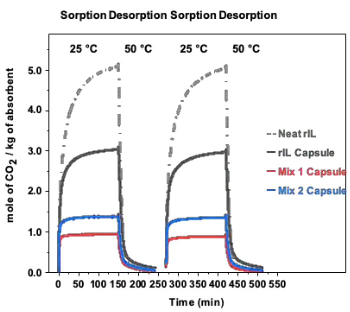
Encapsulated IL requires less time to reach equilibrium compared to agitated IL

Huang, Luo, Wang, Pentzer, Gurkan, Ind. & Chem. Res. Eng., 2019, 58, 10503.

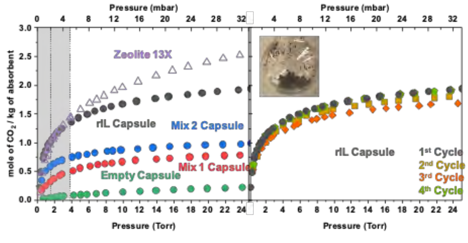
Capsules of Task Specific IL







Emulsion platform at alkylated GO used to encapsulate ILs in which the anions reversible react with CO_2



Capsules are:

- Stable to multiple CO_2 uptake-release cycles
- Outperform zeolites at low pressures
- Stable under humid conditions

Lee, Edgehouse, Pentzer, Gurkan, ACS Appl. Mat. & Int., 2020, 19184.

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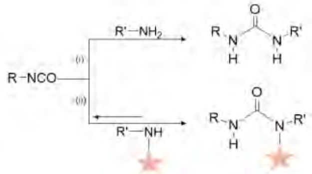
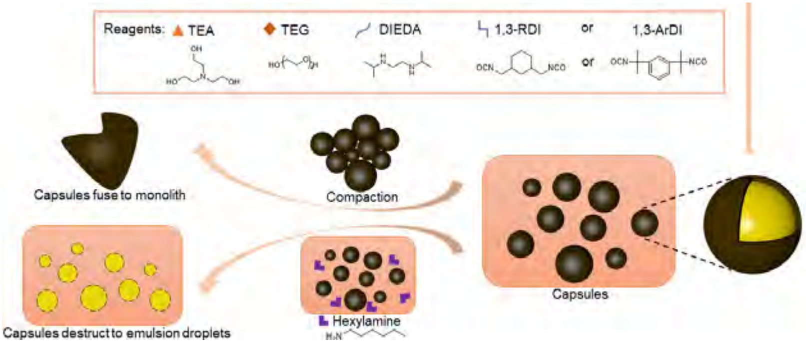
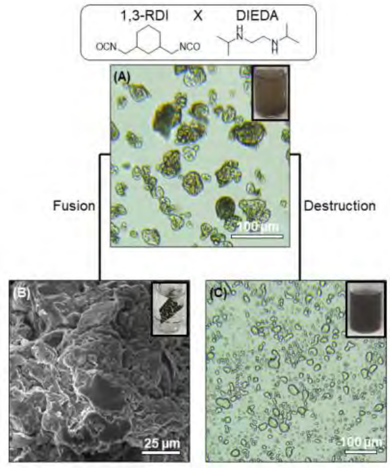
Fusing Capsule Shells



Unlike ureas prepared from primary amines, when a secondary amine is used urea is reversible
Dynamic covalent bonds enable reactive shells





Hindered urea bonds enable fusion of capsules into monoliths or destruction of capsule shells

Wang, Y.; Quevedo, K.; Pentzer, E. Polymer Chemistry, 2021, *12*, 2695.
In preparation

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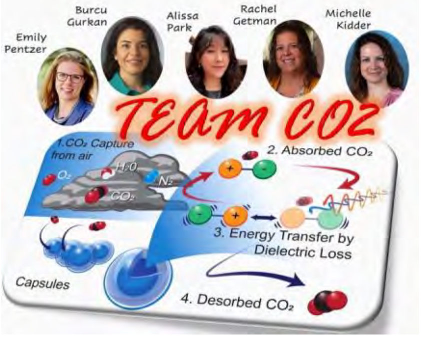
Pentzer Lab October 2021

Pentzer lab
Polymers
Particles
Printing

Current Group Members:
PhD Students: Maria Escamilla, Katelynn Edgehouse, Sarah Lak, Ciera Cipriani, Yifei Wang, Randi Pulukkody, Huaixuan Cao, Cameron Taylor, Evan van Pelt, Krista Schoonover, Evan Fox, Nicholas Starvaggi, Gianni Spencer, Chia-Min Hseiu
MS Student: Greeshma Chathamkandath
Post Docs: Dr. Peiran Wei, Dr. Niradha Sachinthani
Undergrads: Kortney Tooker, Jordan Price, Joseph Duran, Ethan Hammond

Funding



Collaborators: Burcu Gurkan (CWRU), Alissa Park (Columbia), Michelle Kidder (ORNL), Rachel Getman (Clemson)
Micah Green (TAMU), Jodie Lutkenhaus (TAMU), Mark Shifflett (Kansas), Ed Maginn (Notre Dame), Patrick Shamberger (TAMU), Dave Bergbreiter (TAMU), Alp Sehirlioglu (CWRU), Stuart Thickett (Tasmania)

- ✓ **Introduction into the CO_2 problem**
- **Geological storage of CO_2**
- **Sealing systems**

1. Portland-based API Class well cements
2. Calcium aluminate phosphate cement
3. Epoxy resins & mechanical barriers

- **Summary and conclusion**

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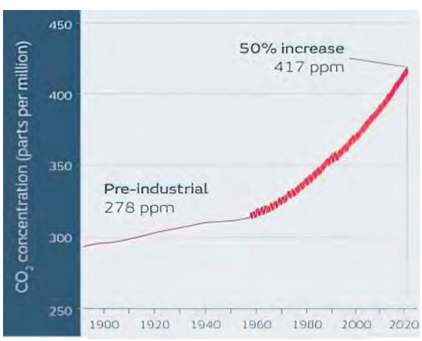
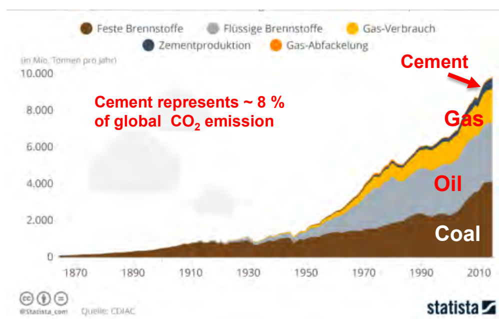
CO_2 and Greenhouse Gas Effect

Atmospheric CO_2 content



Major contributors for CO_2 emission



➡ The Industrial Revolution has triggered global warming

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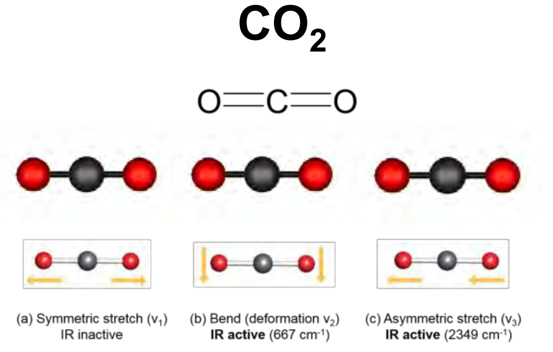
Greenhouse Gase Effect of CO_2

Dr. S. Arrhenius

1895 Arrhenius for the first time describes the greenhouse effect of CO_2 gas

1903 Arrhenius received nobel prize in physical chemistry



CO_2 Released into Atmosphere - 2020

Total anthropogenic emission: ~ 41 billion tons/yr

– CO_2 adsorbed by biosphere: ~ 13 billion tons/yr

– CO_2 adsorbed by oceans: ~ 10 billion tons/yr

Total CO_2 remaining in atmosphere: ~ 18 billion tons/yr

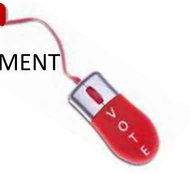
Greenhouse gases and their Global Warming Potential (GWP):

CO_2	1
CH_4	21
H_2O	310
N_2O	265
SF_6	22,000

Source: Global Carbon Budget 2020, Earth Syst. Sci. Data, 12, 3269–3340, https://doi.org/10.5194/essd-12-3269-2020, 2020.

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



Which sector contributes most to CO_2 emission?

- Traffic & Transportation
- Industry
- Buildings & Construction
- Agriculture
- Other (Lets us know more in the chat!)

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Sources of Greenhouse Gas Emissions - Europe

40 % Construction, heating & cooling of buildings

25 % Industry

17 % Agriculture

15 % Transportation & traffic

13 % Miscellaneous

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Global CO_2 Emission - 2019

China	**27.9 %**	Japan	3.0 %	Saudi-Arabia	1.6 %
USA	**14.5 %**	Iran	2.1 %	Canada	1.6 %
EU	**10.0 %**	Germany	1.9 %	South Africa	1.3 %
India	**7.2 %**	Indonesia	1.7 %	Brasil	1.3 %
Russia	4.6 %	S. Korea	1.7 %	Mexico	1.2 %

https://de.statista.com/statistik/daten/studie/179260/umfrage/die-zehn-groessten-c02-emittenten-weltweit/

Main CO_2 Emission Sources in China:

- Coal power plants
- Steel and cement plants (less)

US Strategy:

- Replace coal with natural gas
- increase use of solar and wind energy

EU Strategy:

- Wind, solar, geothermal energy
- Germany: shut down coal power plants by 2038

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✓ Introduction into the CO_2 problem

✓ **Geological storage of CO_2**

- **Sealing systems**

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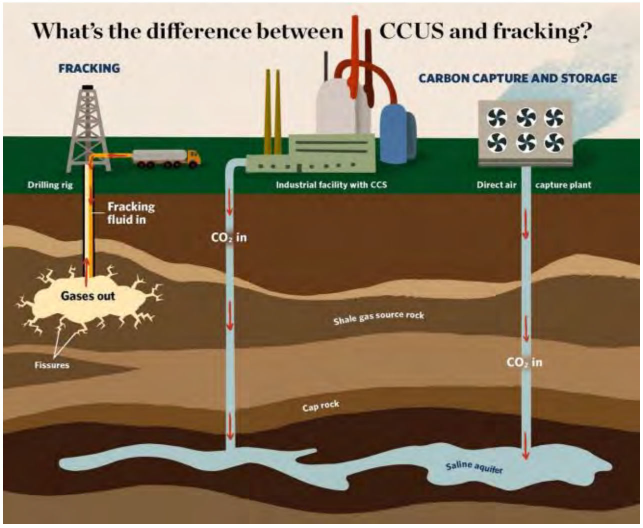
CCS, CCUS and CCU

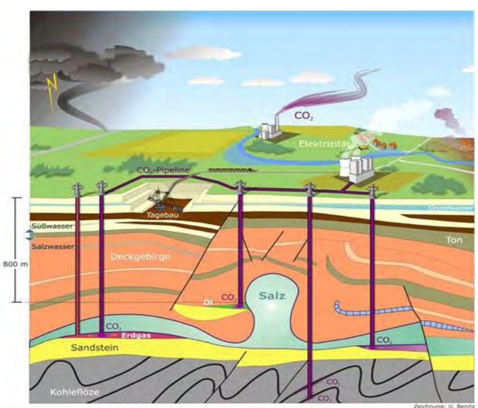


Source: https://www.nature.org/en-us/what-we-do/our-insights/perspectives/carbon-capture-utilization-storage-albritton/

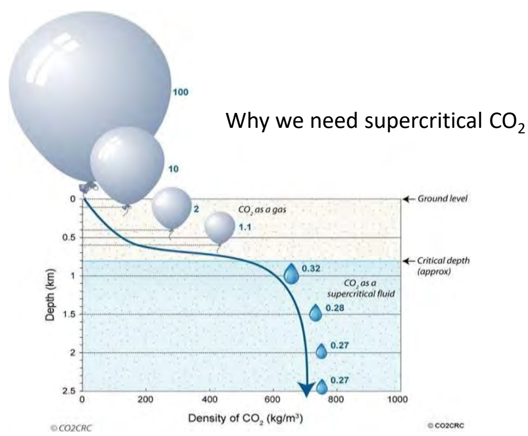
- **CCS: Carbon capture and storage of CO_2**
- **CCUS: Carbon capture and underground storage**
- **CCU: Carbon capture and utilization**

CCS – Carbon Capture & Storage

Geological storage of CO_2 in depleted oil and gas reservoirs (first proposed by C. Marchetti in 1977*)



Source: http://www.unisolar-potsdam.de/?p=1576

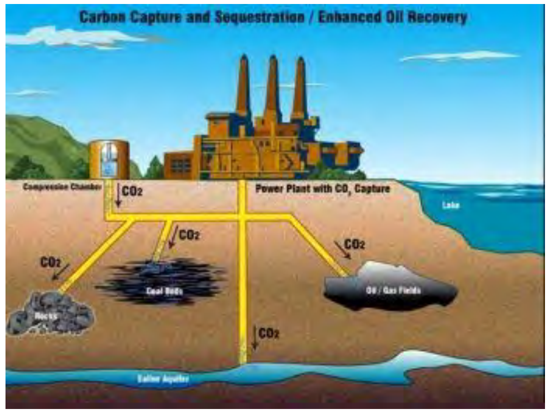


Source: CO2CRC (http://www.co2crc.com.au/imagelibrary)

* C. Marchetti "On geoengineering and the CO_2 problem", *Climate change*, 1 (**1977**) 59 - 68.

Carbon Capture and (Underground) **Storage** (CCS)

- **Capture of CO_2 with amines from the exhaust gas stream**
- **Compression of CO_2 to supercritical fluid**
- **Transport and injection into underground formations (e.g. depleted oil fields, saline aquifers, unmineable coal beds)**



Source: https://www.greentechmedia.com/articles/read/how-to-make-money-in-carbon-capture#disqus_thread

Global CCS Projects

- **Currently ~ 200 CCS projects in operation**
- **40+ CCS projects under construction**
- **CO_2 captured from gas stream of coal power plants, cement & steel industry**
- **Most active countries: Norway, U.K., Canada**
- **Major oil companies involved: Shell, BP, Equinor**

Norway:

- **Re-injects 20 million tons CO_2/yr**
- **About 2/3 of its total CO_2 emission**

"Northern Lights" CCS Project

Source: https://www.visitnorway.de/listings/northern-lights-tour-at-the-cable-car/208036/

Transport of CO_2 to CCS Wells

- Using existing pipelines
- Via railway or ship (LNG)
- Safety aspects:

  leakages or accidents

California Oil Spill October 2021:

Leakage from pipeline

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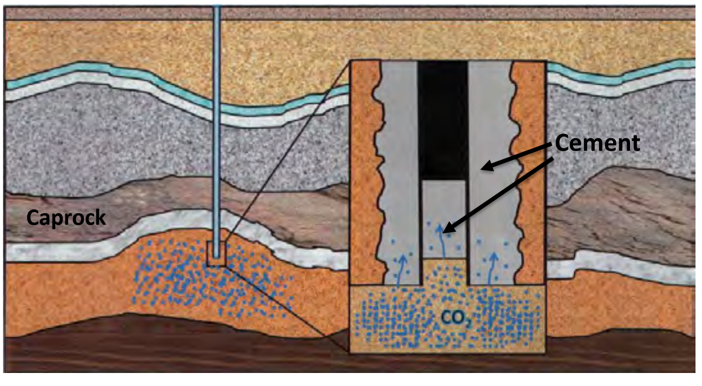
CO_2 Leakage from CCS Wells



Source: J. Plank et al., Resistance of cementing systems under the conditions of permanent geological storage of CO_2 (CCS technology), *ZKG* **2013**, *5*, 28-35

- CO_2 can penetrate cement and potentially destroy it
- Migration to the surface poses a safety risk for population
- Example: CO_2 eruption from lake Nyos, Cameroon killed 1,760 people in 1986

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Main Constituents of OPC and Its Hydrates

Cement Particle

C_3S	**$Ca_3O(SiO_4)$**	**~ 55%**	**C_3A**	**$Ca_9(Al_6O_{18})$**	**~ 3%**
C_2S	**$Ca_2(SiO_4)$**	**~ 22%**	**C_4AF**	**$Ca_4Al_2Fe_2O_{10}$**	**~ 20%**

Main Hydration Reactions:

- $C_3A + H_2O + CaSO_4 \longrightarrow [Ca_3Al(OH)_6]_2 \cdot (SO_4)_3 \cdot 26\ H_2O$ (ettringite)
- $C_3S, C_2S + H_2O \longrightarrow$ C-S-H + $Ca(OH)_2$ (Portlandite)

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Carbonation Reactions of Portland Cement

Reactions of cement hydrates with H_2CO_3 (wet CO_2):

$$Ca(OH)_2 + H_2CO_3 \longrightarrow CaCO_3\,(s) + 2\,H_2O$$

$$C\text{-}S\text{-}H + H_2CO_3 \longrightarrow CaCO_3\,(s) + SiO_2 \cdot n\,H_2O$$

silica gel

$$[Ca_3Al(OH)_6]_2 \cdot (SO_4)_3 \cdot 26\,H_2O + 3\,CO_2 \longrightarrow 3\,CaCO_3 + 3\,CaSO_4 \cdot 2\,H_2O + 2\,Al(OH)_3 + 27\,H_2O$$

Formation of water soluble calcium hydrogen carbonate:

$$CaCO_3 + H_2CO_3 \longrightarrow Ca(HCO_3)_2$$

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Early Studies on CO_2 Stability of Cement

References:

- Onan, D.D., Effects of Supercritical Carbon Dioxide on Well Cements. *Permian Basin Oil & Gas Recovery Conference* **1984**, SPE-12593.
- Bruckdorfer, R.A., Carbon Dioxide in Oilwell Cements. **1986**, SPE-15176.
- Milestone, N.B.; Sugama, T.; Kukacka, L.E.; Carciello, N., Carbonation of Geothermal Grouts – Part 1: CO_2 Attack at 150°C. *Cem. Concr. Res.* **1986**, *16*, 941-950.
- Milestone, N.B.; Aldridge, L.P., Corrosion of Cement Grouts in Aggressive Geothermal Fluids. *Trans. Geo. Res. Council* **1990**, *14* (1), 423-429.
- Rashad, A.M.; Bai, Y.; Basheer, P.A.M.; Collier, N.C.; Milestone, N.B., Chemical and mechanical stability of sodium sulfate activated slag after exposure to elevated temperature. *Cem. Concr. Res.* **2012**, *42* (2), 333-343.
- Barlet-Gouédard, V.; Rimmelé, G.; Goffé, B.; Porcherie, O., Well Technologies for CO_2 Geological Storage: CO_2-Resistant Cement. *Oil & Gas Science and Technology* **2007**, *62* (3), 325-334.

Conclusions:

- Portland cement thermodynamically unstable against CO_2
- Initial $CaCO_3$ formation densifies cement
- Subsequent leaching of $CaCO_3$ as $Ca(HCO_3)_2$ increases permeability

⇨ Carbonation proceeds more rapidly

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Lab Study on Modified Portland Cement Samples

1 Month Storage: at 90° C and 400 bar CO_2 pressure no major effect of $scCO_2$ on the specimens

6 Months Storage:
- System A: rough surface like sandstone
- System B: no effect of $scCO_2$
- System C and D show severe crack formation (direct pathway for CO_2 leakage!)

CO_2-resistent particles

fly ash cement

latex cement

reference cement

6 months storage

Cement Porosity & Crack Formation

According to *Fabbri et al.*, low porosity (w/c ratio) generally leads to increased crack formation

- **$CaCO_3$ crystals need expansion space for their growth**
- **If expansion space is not available, crystallization pressure will destroy the cementitious matrix**
  ⟶ crack formation

Low porosities of cementing systems C and D explain the crack formation after $scCO_2$ exposure

High porosity (w/c ratio) promotes the leaching of $CaCO_3$

Fabbri, A., Jecquemet, N., Seyedi , D. M.,
"A chemo-poromechanical model of oilwell cement carbonation under CO_2 geological storage conditions"*Cem. Concr. Res.*, 42 (**2012**) 8 – 19.

Field Experience from CO_2 Injection Wells

Natural CO_2 producing well in Dakota sandstone formation (30 years):

- **Sample from direct proximity to reservoir (~ 6 m) showed almost complete conversion of portlandite to calcium carbonate**
- **Increase in porosity and permeability**
- **Samples recovered at further distance from reservoir (~ 50 m) and at top of the caprock carbonated only slightly**

W. Crow, D.B. Williams, J.W. Carey, M. Celia, S. Gasda *"Wellbore integrity analysis of a natural CO_2 producer"* Energy Procedia 1 (2009) 3561–3569

CO_2 injection well in the Permian basin of West Texas (30 years):

- **Only minor carbonation of cement sample collected ~ 3.5 m above the reservoir**
- **Minor increase in porosity and permeability**

J.W. Carey, M. Wigand, S.J. Chipera, G. Woldegabriel, R. Pawar, P.C. Lichtner, S.C. Wehner, M.A. Raines, G.D. Guthrie *"Analysis and performance of oil well cement with 30 years of CO_2 exposure from the SACROC Unit, West Texas, USA"* Int. J. Greenhouse Gas Control 1 (2007) 75–85.

Contradicting reports from the field !

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- ✓ Introduction into the CO_2 problem
- ✓ Geological storage of CO_2
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Calcium Aluminate Phosphate Cement

- **Invented by T. Sugama for geothermal wells**
- **Extremely corrosive environment (H_2SO_4, H_2S, CO_2)**
- **Temperatures up to 320 °C, pH = 2**
- **Massive corrosion problems**

Source: https://www.portonews.com/2020/laporan-utama/semburan-uap-di-sumur-ijen-6-1/attachment/937749ec-ba7a-4e7d-a86c-cbc36edf9651/

Main Hydration Reactions in CAPC

(1) **Hydrothermal Reactions:** $CaHPO_4 \cdot 2\,H_2O + Ca_4O(PO_4)_2 \longrightarrow Ca_5(PO_4)_3(OH) + 2\,H_2O$
hydroxy apatite

(2) $5\,CA + 3\,NaPO_3 + 7\,H_2O \longrightarrow Ca_5(PO_4)_3OH + 10\,AlO(OH) + 3\,NaOH$
CA phase, polyphosphate, hydroxy apatite, boehmite

(3) $5\,CA + 3\,Al_6O_9 \cdot Si_2O_4 + 3\,NaPO_3 + 11.5\,H_2O \longrightarrow 3\,NaAlSi_2O_6 \cdot H_2O + Ca_5(PO_4)_3OH + 16\,AlO(OH)$
mullite, analcim, apatite, boehmite

(4) $5\,CA + 5\,Al_6O_9 \cdot Si_2O_4 + 6\,NaPO_3 + 24\,H_2O \longrightarrow 2\,Na_3Al_3Si_5O_{16} \cdot 6\,H_2O + 2\,Ca_5(PO_4)_3OH + 34\,AlO(OH)$
NaP zeolite, apatite, boehmite

no $CaCO_3$ is formed !

Laboratory Testing of CAPC

60 % calcium aluminate cement (CAC)

40 % ASTM Class F Fly Ash

20 % sodium polyphosphate solution

- **Stored in 4 % Na_2CO_3 solution**
- **Exposure over 1 month**
- **Temperature 300 ^oC**

T. Sugama,

"Advanced Cements for Geothermal Wells"

Brookhaven National Library, BNL-77901-2007-IR

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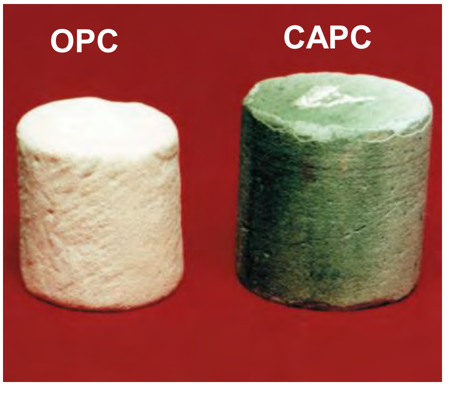
Results – Carbonate Stability of CAPC

- excellent carbonate resistance
- no cracks, no deterioration
- low permeability
- some strength reduction



Source: K. Agapiou, S. Charpiot "Cement and Wellbore Integrity" International Cement Review, August 2013, p. 113 - 116

➡ **currently by far the best field tested cementing system for CO_2 wells**

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CAPC – Issues and Open Questions

- **CAPC causes flash set when in contact with OPC !**
  ⟶ **use of dedicated equipment**

- **CAPC requires special additives** (retarder, dispersant etc.)

- **So far no lab results from storage in $scCO_2$**

- **CAPC is not alkaline ⟶ corrosion protection of casing?**

Sugama, T.; Weber, L.; Brothers, L.E.,
Sodium-polyphosphate-modified fly ash/calcium aluminate blend cement: durability in wet, harsh geothermal environments.
Mater. Lett. **2000**, *44* (1), 45-53.

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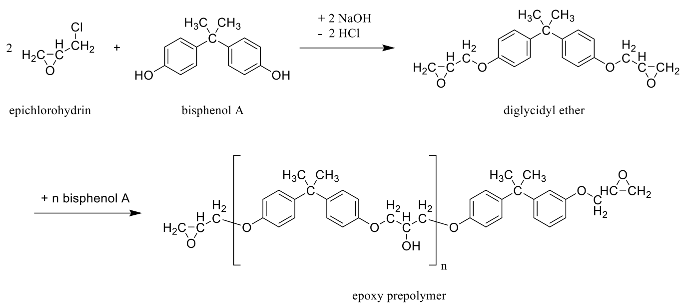
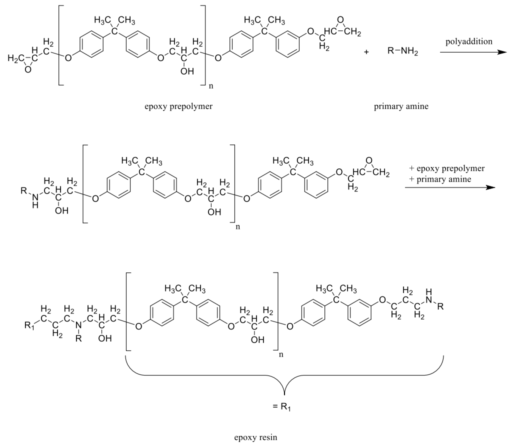
Epoxy Resin Cement

- **2 component system:** **epoxy prepolymer + amine hardener**

chemical reactions occurring in epoxy resin formation:



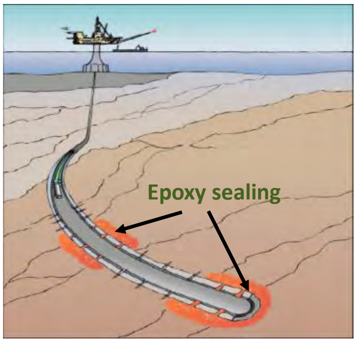


Epoxy well-known organic binder, extremely resistant against acids and solvents; widespread use in construction

Lab Results – CO_2 Exposure of Epoxy

- **Samples stored up to 1 year in brine**
- **500 bar CO_2 pressure, 100 °C**

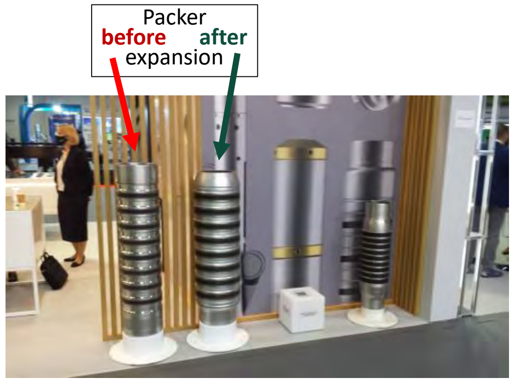
- **No visual deterioration**
- **Stable weight**
- **No change in permeability**
- **Decrease of strength**



Epoxy resin cement appears to exhibit high CO_2 tolerance

Mechanical Barrier Against CO_2

Expandable packers as mechanical seal for CO_2



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Cementing Systems Suitable for CCS

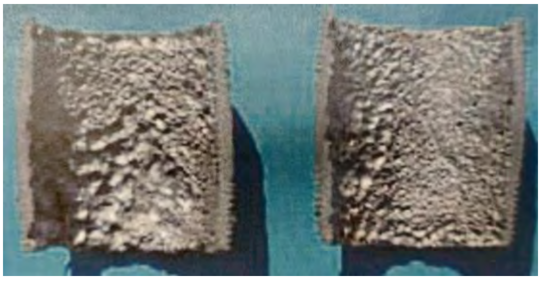
Criteria: Borehole integrity over 500 – 1,000 years

At present only those potential candidates:

- **Calcium aluminate phosphate cement**
- **Epoxy resin cement**

Open question:

Corrosion protection for casing!



Source: Reinicke, K.M. et al., CO_2 Lagerung in Geogrund: Integrität von Tiefbohrungen unter Einfluss von CO_2. DGMK/ÖGEW-Frühjahrstagung **2007**.

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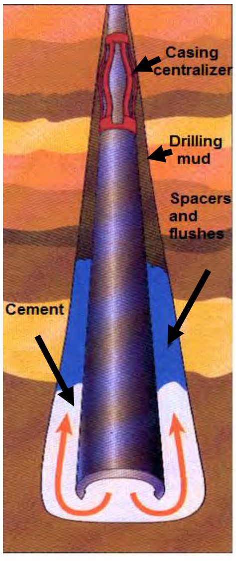
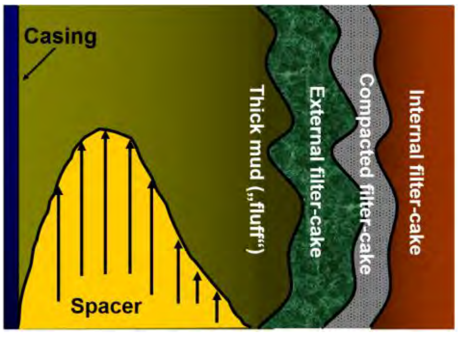
Critical Importance of Mud Displacement For Sealing Off CCS Wells



Use of best practice:

- Centralizers
- Scratchers
- Pipe rotation

Mud displacement by spacer fluid:



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Summary and Conclusion

- Safe sealing of CCS presents a challenge for cementing technology
- Portland cement-based systems do not provide century-long resistance against CO_2, modification can improve their stability
- CAPC presents a much more stable alternative, however field application is more complicated
- Organic binder systems and mechanical barriers present an alternative
- Dual containment strategy appears to work best and guarantees maximum safety

Plank, J. "Cements For Carbon Capture Wells", in: Boul, P. (ed.), "Perspectives in Energy and Materials Sustainability: Addressing Climate Change and the Cyclic Economy", *ACS eBooks*, Washington **2021,** under review

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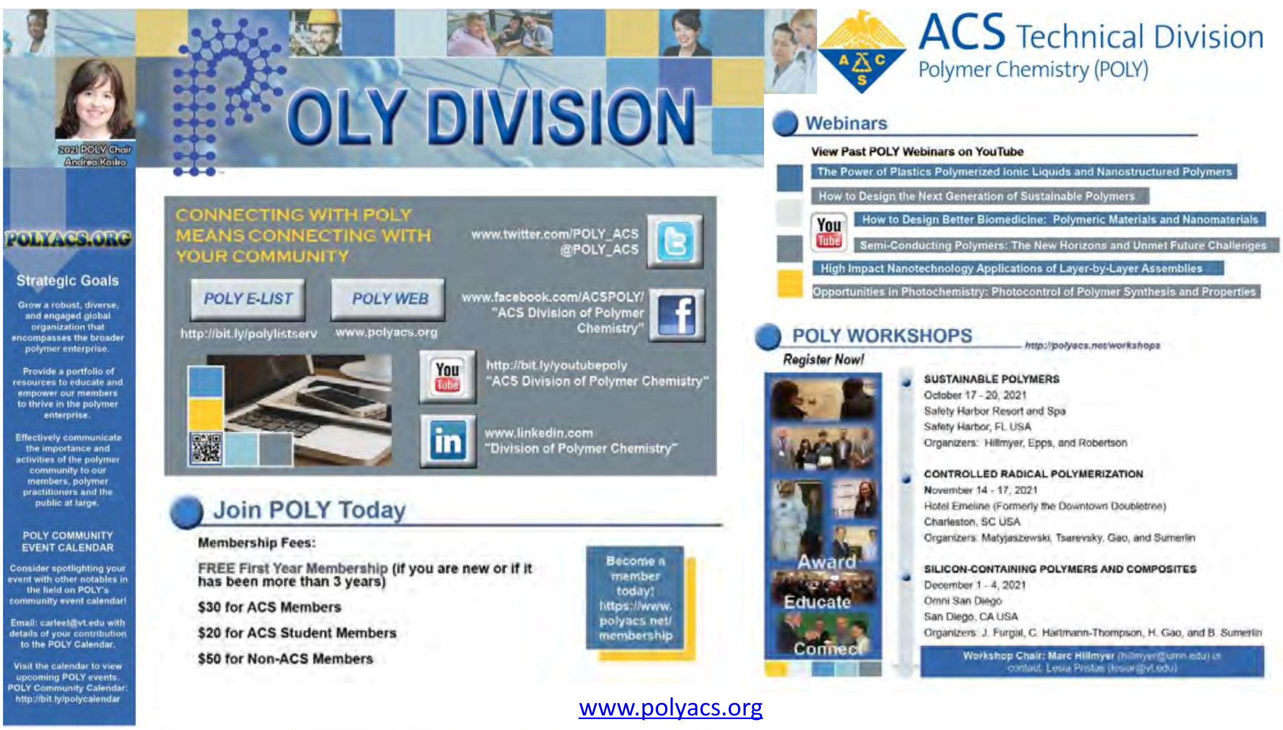

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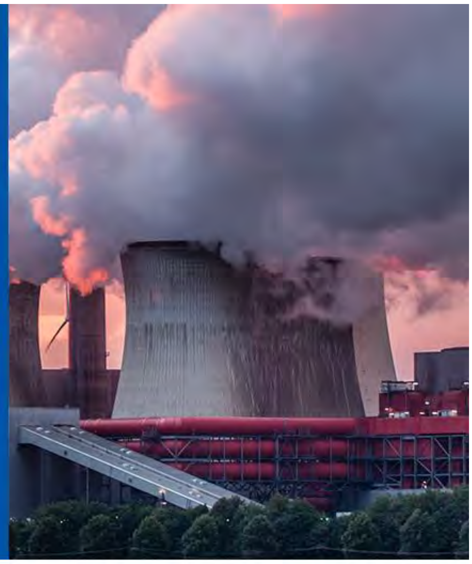

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Director of Science and Technology, Polymer Chemistry Innovations

EMILY PENTZER
Associate Professor, Department of Chemistry and the Department of Materials Science and Engineering, Texas A&M University

JOHANN PLANK
Chair for Construction Chemistry and Full Professor, Department of Chemistry, Technical University of Munich

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