



CO₂ capture using amines bound to silica

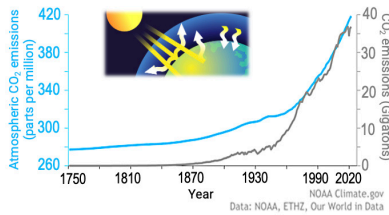
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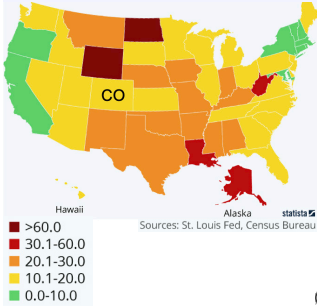
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Why CO₂ capture ?

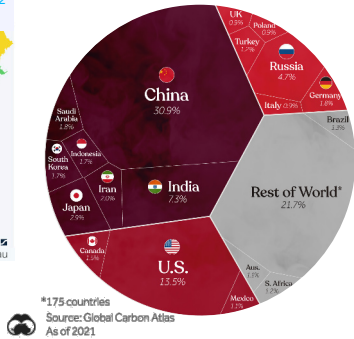
- Carbon dioxide (CO₂) is a major greenhouse gas
- 13% increase in atmospheric CO₂ from 2000 to present^[1]
- U.S. is the 2nd highest CO₂ emitter globally



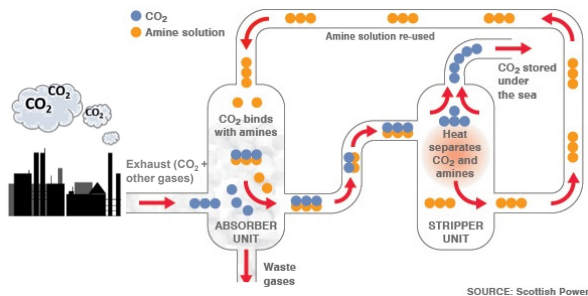
US States Producing the Most CO₂ Per Capita in 2017 (in tons)



World's top CO₂ polluters in 2021



Solvent based industrial CO₂ capture



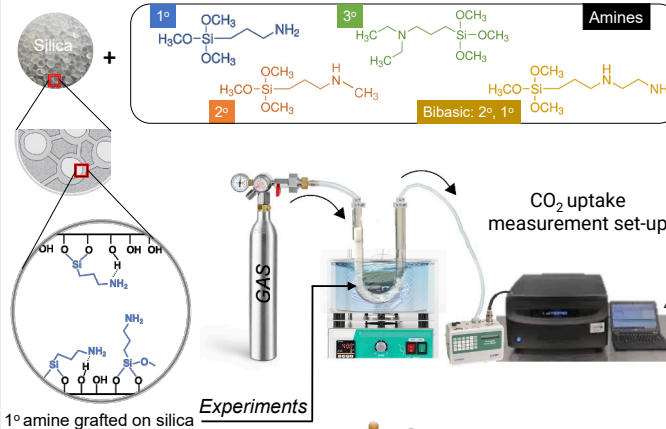
- × Solvent induced reactor corrosion
- × High regeneration energy for repeated cycling
- × Amine degradation, not stable for thousands of cycles

What is our research about?

Goal: Develop descriptors for CO₂ capture capacity and stability against oxygen-induced degradation to guide the design of amines bound to siliceous supports

Advantages of supported-amine CO₂ sorbents

- ✓ Low regeneration energy for repeated cycling
- ✓ Stable for thousands of cycle and tolerant to moisture



Molecular scale computations

Lab-scale measurements

- Amine loading on silica, CO₂ uptake under varying gases
- C/N ratio and product characterization to know amine v/s CO₂ loss

Molecular scale simulations

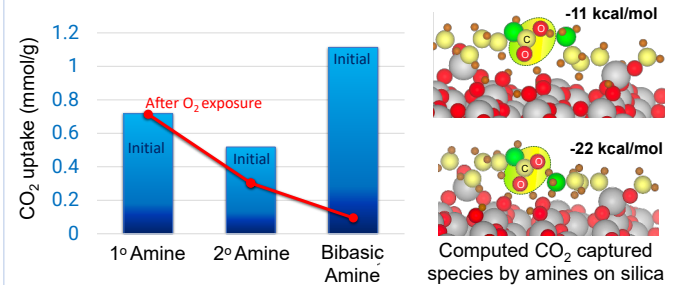
- Obtain energies and stable atomistic structures of amine on silica and CO₂ bound on amines
- Quantum chemistry calculations on high performance computers

References:

- NASA Global Climate Change, *Vital Signs* <https://climate.nasa.gov/vital-signs/carbon-dioxide/>
- Cho, M. et al. *Phys. Chem. Chem. Phys.*, 2018, 20, 12149-12156
- <https://drive.google.com/file/d/1TyxokixCOLFd6CaUKZzeqgKqEIHmJdqt/view>
- Li-Cor Odyssey CLx Imaging System (<https://www.thelabworldgroup.com/product/>)

Results

- Bibasic amine has highest initial CO₂ uptake followed by 1° and 2°
- But bibasic amine shows the most decrease in CO₂ uptake after exposure to O₂ at 150°C under zero-air
- Computations show exothermic CO₂ capture in agreement with experiments²
- Factors influencing CO₂ adsorption capacity of amines on silica
 - Nature of amine groups
 - Spacing between the amino silanes
 - Resistance to oxidative degradation

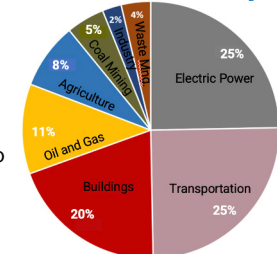


Experiments by Wilson McNeary and Gabrielle Kliegle

Broader Impact

- CO₂ capture can assist in keeping global warming under a 1.5 °C consensus
- Government gives tax credits for each ton of emitted carbon removed
- A shed-size machine for direct air carbon capture built by Global Thermostat in Brighton, CO
- Xcel energy to close 4 coal-fired units to reduce carbon emissions in Colorado 85% from 2005 levels by 2030 and get 80% renewable electricity using solar and wind energy

Colorado's Largest Sources of Carbon Emissions in 2020: 126 MMTCO₂e



Source: Colorado Department of Public Health and Environment³

Source: The Colorado Sun (<https://coloradosun.com/>)