National Institute of Standards and Technology
U.S. Department of Commerce

# DIRECT AIR CAPTURE OF $CO_2$ and Carbon Removal


Materials Measurements Lab - Pam Chu, Andrew Allen
Center for Neutron Research - Craig Brown, Dan Neumann
Engineering lab - Aron Newman

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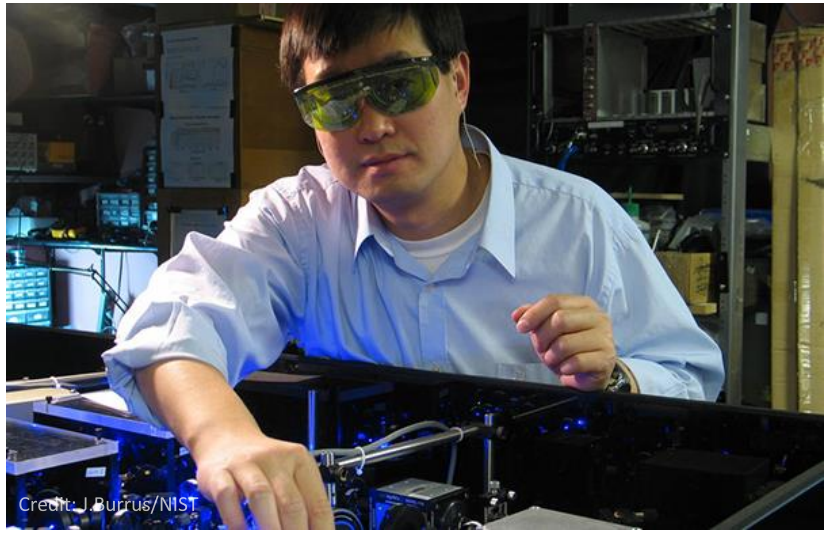
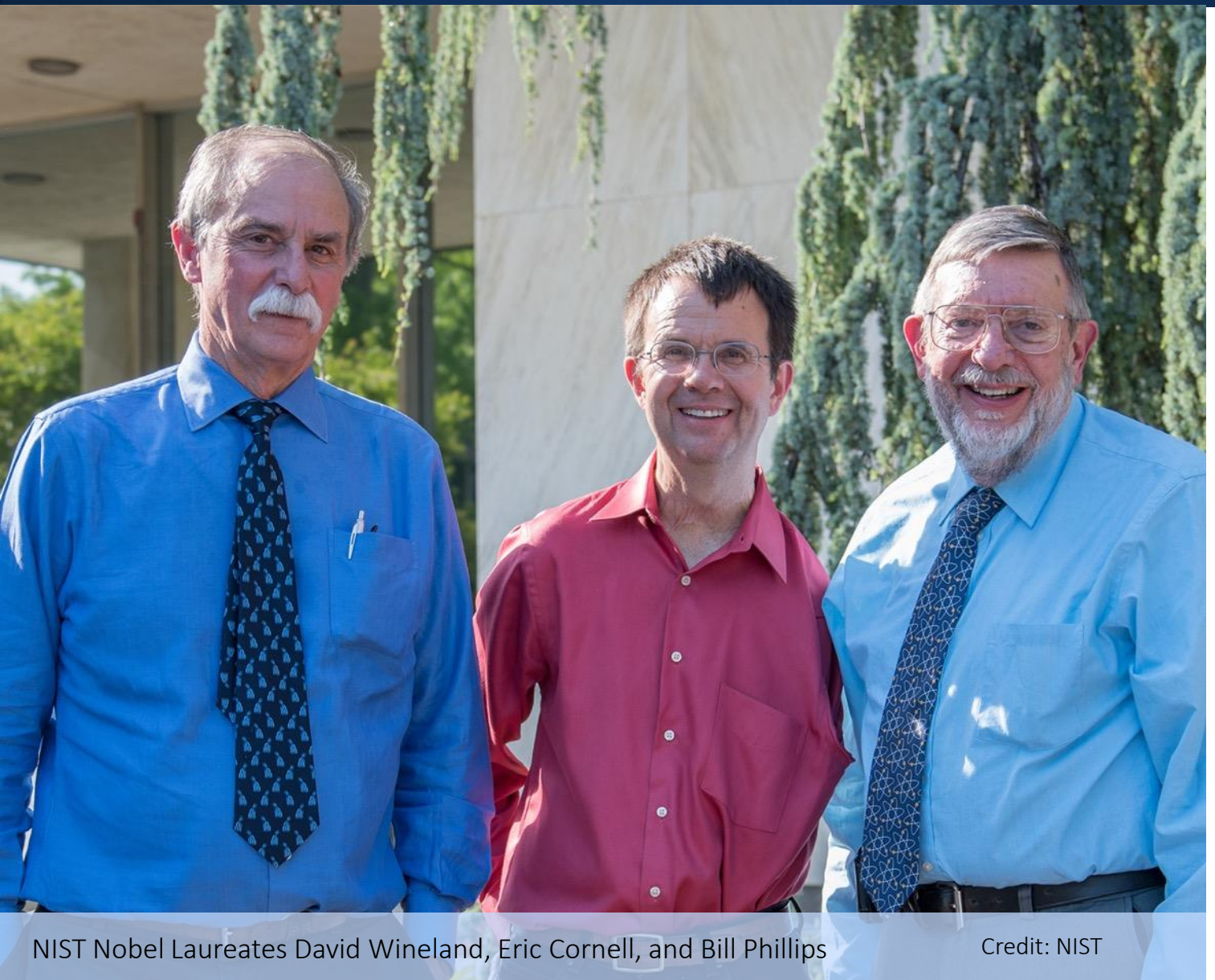
August 2021

# NIST Mission

To promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life


# NIST's Biggest Strength: Our Reputation

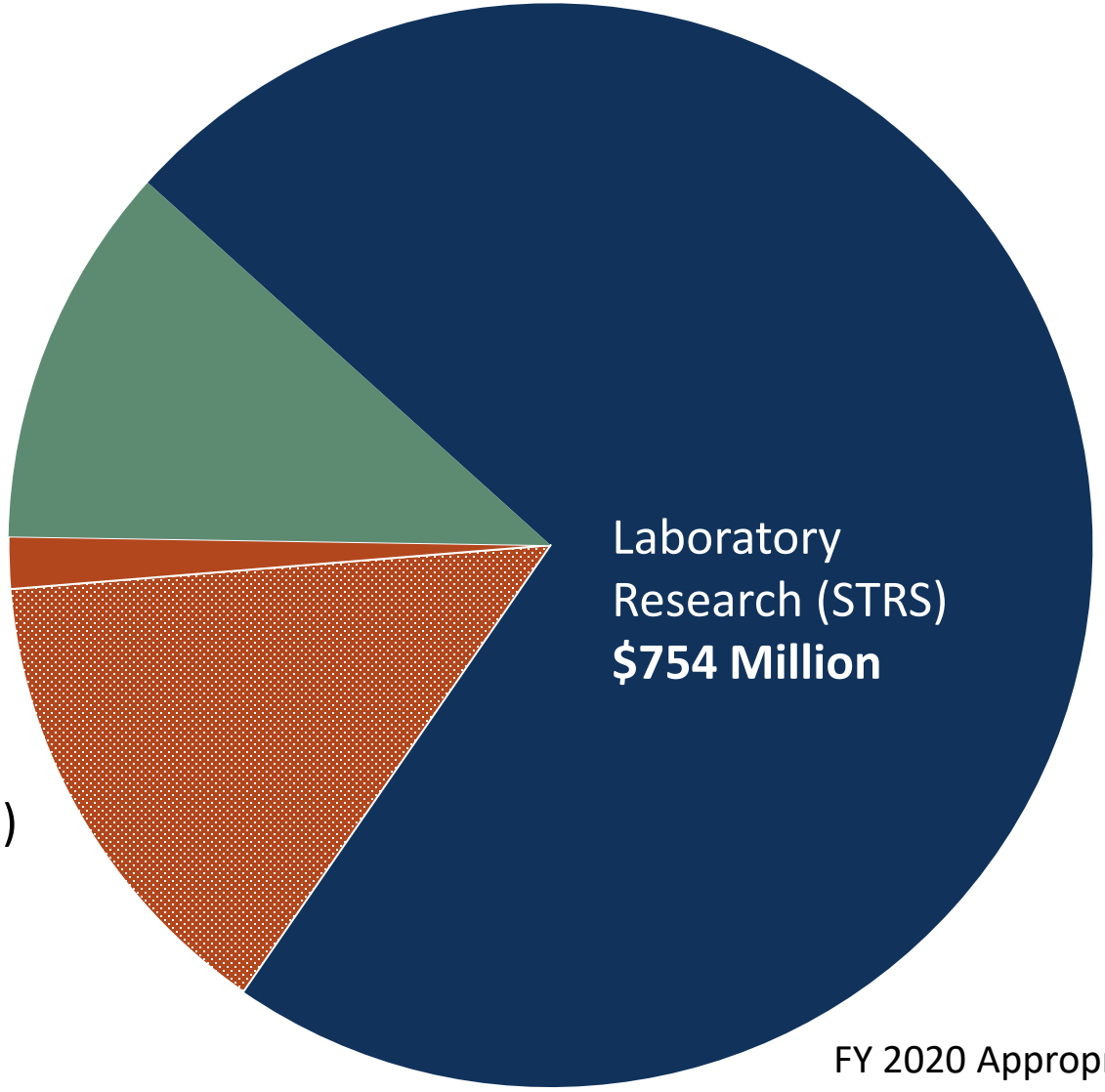


NIST Nobel Laureates David Wineland, Eric Cornell, and Bill Phillips

Credit: NIST

- Technical excellence
- Integrity
- Uncompromising
- Rigorous
- Unbiased
- Industry focused
- Non-regulatory

# NIST FY 2020 Budget : $1.034 B




FY 2020 Appropriated Budget

# NIST AT A GLANCE

## Industry's National Laboratory

**3,400+**
FEDERAL EMPLOYEES

**5**
NOBEL PRIZES

**2 CAMPUSES**
GAITHERSBURG, MD [HQ]
BOULDER, CO

**3,500+**
ASSOCIATES

**10**
COLLABORATIVE INSTITUTES

**400+**
BUSINESSES USING NIST FACILITIES

ManufacturingUSA

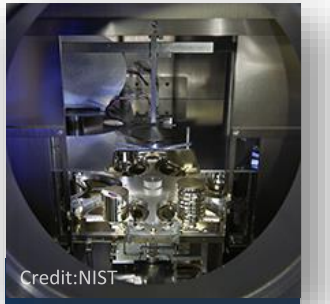
**14**
NATL OFFICE FOR MANUFACTURING INSTITUTES

**51**
MANUFACTURING EXTENSION PARTNERSHIP CENTERS

U.S. BALDRIGE PERFORMANCE EXCELLENCE PROGRAM

# NIST Laboratory Programs


**Material Measurement Laboratory**




**Physical Measurement Laboratory**


**Engineering Laboratory**


**Information Technology Laboratory**


**Communication Technology Laboratory**


**NIST Center for Neutron Research**

# Unique NIST Products and Services

Million-Pound Deadweight Machine

Credit: NIST

**1,200** Standard Reference Material (SRM) products

**100** Standard Reference Data (SRD) products

**600** measurement services

**Every year:**

**32,000** SRM units sold

**13,000** calibrations and tests

**800** accreditations of testing and calibrations laboratories

# Reference Materials


## Important Role e.g.

- **14** cements

  numerous geological materials
- Building/infrastructure materials
- SRM zeolites etc.

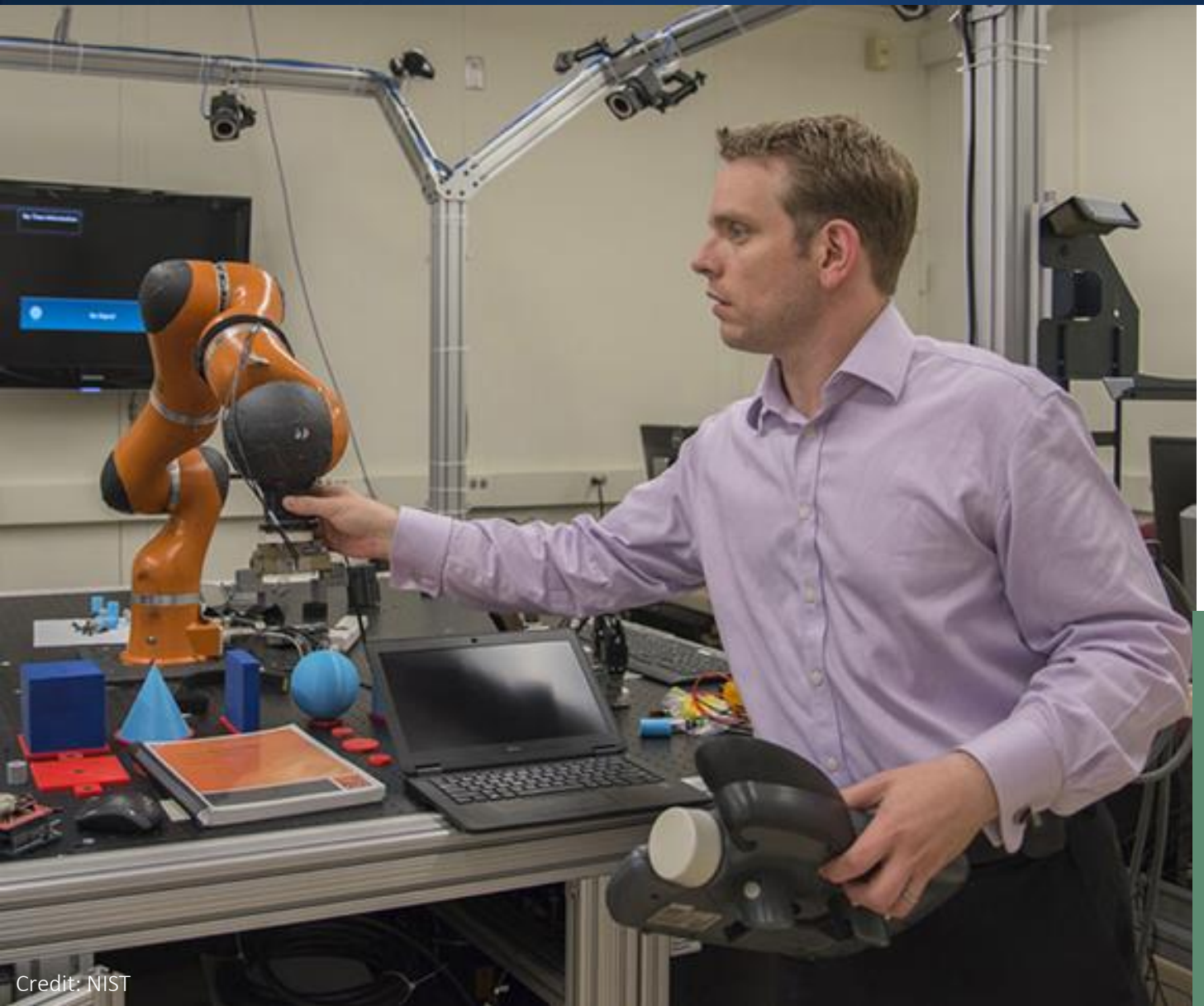
NIST's technical expertise results in improved RM's and development of new materials that are fit-for-purpose

# Calibrated Equipment is Essential

Boeing force measurements are traceable to the SI

Photo Courtesy of Boeing

# Documentary Standards



Credit: NIST

## Important Role

- **400+** NIST technical staff in **100+** standard committees
- Leadership in **international standards** bodies

NIST's technical expertise results in improved standards and U.S. competitiveness

# FY21 NIST appropriation language

IB
Union Calendar No. 366

116TH CONGRESS
2D SESSION

**H. R. 7667**

**[Report No. 116–455]**

IN THE HOUSE OF REPRESENTATIVES

July 16, 2020

Mr. Serrano, from the Committee on Appropriations, reported the following bill; which was committed to the Committee of the Whole House on the State of the Union and ordered to be printed

**A BILL**

laking appropriations for the Departments of Commerce and Justice, Science, and Related Agencies for the fiscal year ending September 30, 2021, and for other purposes.

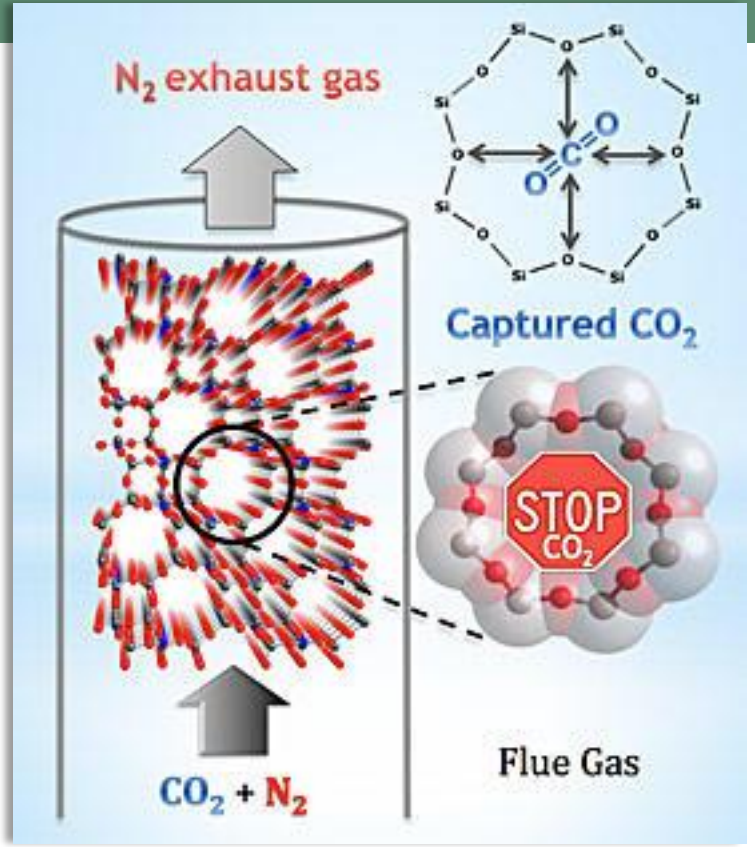
PER H.R. 7667 AND ENACTED IN THE CONSOLIDATED APPROPRIATIONS ACT, 2021, NIST IS CHARGED TO SUPPORT THE NATION'S EFFORT

| | 2020 | 2021 | 2022 |
|---|---|---|---|
| Office of Fossil Energy CCUS | $218M | $228M | |
| DOE<br>DAC/ negative emissions | $50M | $72.5M | |
| **NIST** | | **$3M** | |

"*FOR **DIRECT AIR CAPTURE AND CARBON DIOXIDE REMOVAL RESEARCH**,* SPECIFICALLY TO ***INCREASE WORK ON DEVELOPING STANDARD REFERENCE MATERIALS AND TEST PROCEDURES FOR DIRECT AIR CAPTURE*** AS WELL AS TO *INCREASE SUPPORT FOR **CARBONATE MATERIALS DEVELOPMENT, TESTING, AND CERTIFICATION** FOR CONSTRUCTION MARKETS*."

# VISION (DAC FOCUSED)

## SUPPORT AND VALIDATE SOLUTIONS TO ACHIEVE NET ZERO AND NET NEGATIVE EMISSIONS SYSTEMS




M.R. Hudson, W.L. Queen, J.A. Mason, D.W. Fickel, R.F. Lobo and C.M. Brown. Unconventional, highly selective CO2 adsorption in zeolite SSZ-13. Journal of the American Chemical Society 10.1021/ja210580b

- Identify how NIST can augment the nation-wide R&D effort through stakeholder engagement and partnerships
- Foster NIST-wide connections and collaborations
- 3 Internal discussion groups
  (each ~45 participants, 15 projects proposed)
- 3 Mini-workshops with external stakeholders
- Identified FY21/22 projects

# External discussion groups

## Considerations for Solid sorbents

**What Materials ?**

- Hybrid/MOF-based
- Porous inorganic-based
- Porous polymers

  **w/incorporated amines…**

**What Conditions ?**

- 100 ppm to 450 ppm $CO_2$ (0.045%) isotherms
- Atmospheric composition preferred
- Enthalpy of adsorption
- Energy of regeneration
- Stability, cyclability, lifetime
- …

- What are the critical measurement and metrology needs (both fundamental and applied) that need to be addressed for successful DAC deployment?
- Needs for reference measurements, SRM, SRD?
- Needs for validation of computational simulations, reference data, database development?

# External discussion groups

**Solid sorbents** 5/6 – Craig Brown

- **D. Hancu - NETL- DoE**
- **T. McDonald - Mosaic Materials**
- **P. Llewellyn - Total**

**Membranes/Composites** 6/10 – Chris Soles and Chris Stafford

- **YuanQiao Rao - Core R&D, Dow Chemical**
- **Chunqing Liu, - Membranes R&D Group, Honeywell**
- **William J Koros - Georgia Institute of Technology**

**Mineralization/ Industrial Products**

5/20 – Aron Newman and Andrew Allen

- **G. Sant - Carbon Built & UCLA**
- **R. Aines - LLNL**
- **V. Atakan – Solidia**
- **M. Blondes, USGS**

# Main outcomes: Sorbents

[1] **Lack** of good techniques/procedures in the community

[2] **Need** at least one 'well understood' material (PEI loaded oxides; MOF, … )
standard recipe; attrition rates, lifetime, decomposition mechanisms, …

[3] **Must** include $H_2O$ and $O_2$; consider atmospheric 'impurities' later

[4] **Differentiate** between bulk and engineered contactor

[5] **Need** enthalpies; kinetics for uptakes; thermodynamics for desorption

[6] **Need** to understand material lifetime, loss of capacity

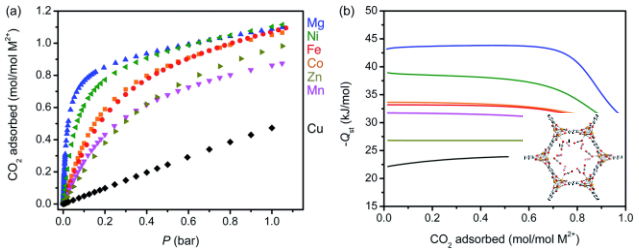
**$CO_2$ adsorption**

$$2\ R{-}NH_2 + CO_2 \rightarrow R{-}NH_3^+ + R{-}NH{-}COO^-$$

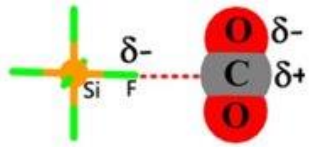
**Regeneration**

$$R{-}NH{-}COO^- + R{-}NH_3^+ \xrightarrow{HEAT} CO_2 + 2\ R{-}NH_2$$

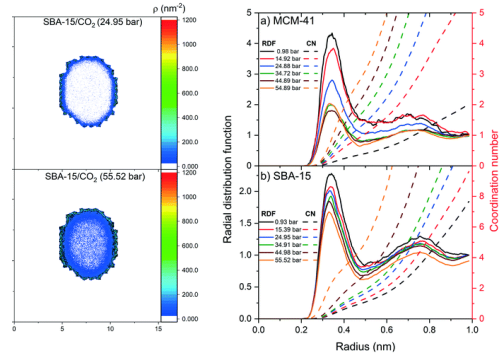
## Solid Sorbents




$CO_2$ adsorption Mg-MOF74
10.1039/C4SC02064B




$CO_2$ adsorption SIFSIX MOF
10.1021/acsami.8b03358




Organization of $CO_2$ confined in silica nanopores
10.1039/D0EN01282C

# Main outcomes: Membrane/Composites

*Part of the materials problem, perhaps not a solution in itself*

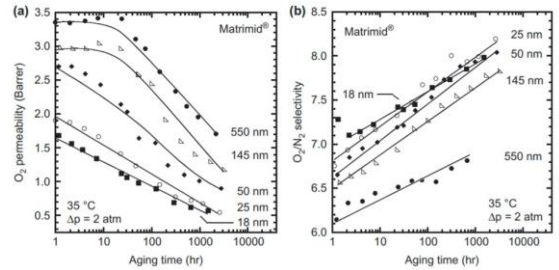
[1] **Need** to monitor chemical and physical changes to materials as a function of contaminants ($O_3$ and $H_2O$, NOx, SOx, organics, and particulates), T, t…

[2] **Need** to establishing general both chemical and physical structure-property relationships (primary material design to final morphologies of devices)

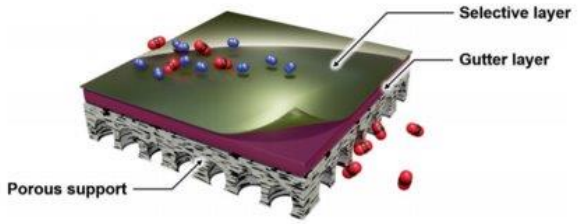
[3] **Need** to ensure candidate materials are scalable and engineerable for devices (e.g. hollow fiber mat morphology) and range of post-capture utilization tech

[4] **Need** to ensure key measurements are applicable to wide range of materials and gaseous compositions: low uncertainty

## Membranes



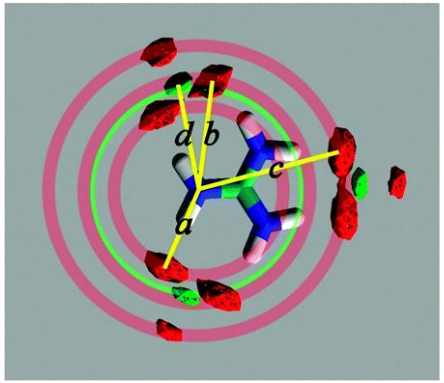

https://doi.org/10.1016/j.polymer.2010.06.004




$CO_2$ sorption in Ultrathin PEI films
10.1038/s41428-020-00429-z

structure of aqueous guanidinium carbonate

https://doi.org/10.1021/jp0572028



# Main outcomes: DAC mineralization through carbonation

[1] **Need** to know carbonate loadings with respect to known history

[2] **Need** to know accessible porosity and surface area with respect to known history

[3] **Need** to know spatial variability in permeability and transport properties

[4] **Need** to Differentiate between bulk powders, bulk monoliths, slices

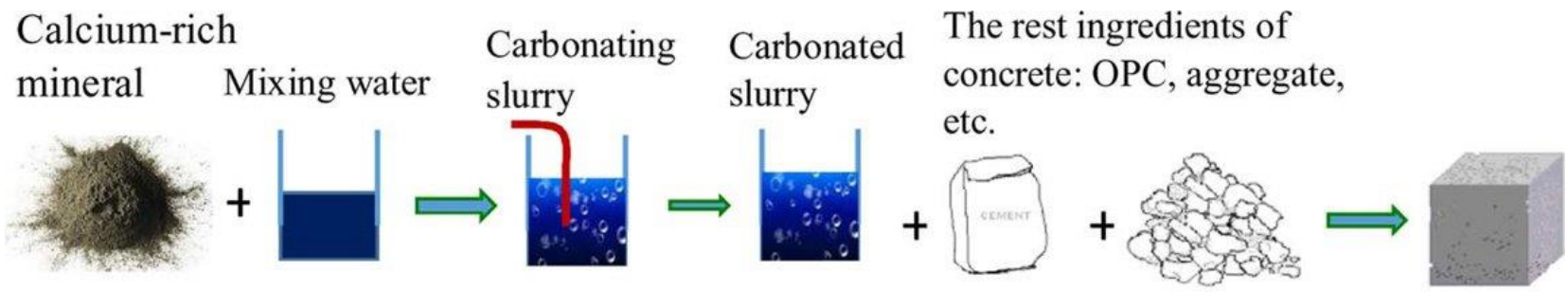
[5] **Must** consider different environmental conditions – temperature, pressure, humidity

[6] **Need** to understand material lifetime, loss of capacity, leaching…

[7] **Need** to develop reference methods and materials for process kinetics

Includes:

- carbonates in available ultramafic rock formations, mine tailings, industrial waste products such as fly ash, slag, etc.
- Industrial products such as cement and concrete used in construction
  (carbonation-modified cement hydration processes may be exception)




Quian et al., *J. CO2 Util.,* **25**, 31-38 (2018).

# NIST Major Capabilities

- Neutron Scattering, Synchrotron techniques
- Facility for Adsorbent Characterization & Testing
- Positron Annihilation Lifetime Spectroscopy
- Nanocalorimetry
- IR-VASE (variable angle spectroscopic ellipsometry)
- Combined Cross-sectional Raman Microscopy with ATR-FTIR and Confocal Microscopy
- HRTEM-STEM/EELS/EDXS: Sub-nm Porosity & Composition
- High-throughput measurement modalities: enabling AI/ML
- Polymers
- Metrology and standards for carbon dioxide systems
- Carbon – combustion analysis, TGA, chemical titration, classical methods, coulometry, HPLC, GCMS, NMR (P,T),
- Digital Holographic Microscopy
- DFT, MD, GCMC, Multiphase Transport, Phase Separation, Wetting/Nonwetting fluids. Diffusive Transport, Sorption/Desorption, Lattice Boltzmann methods,
- Using AI to discover new solid sorbent materials for Direct Air Capture

# NIST's DAC-CCUS Future?

- Flue gas capture – (different requirements compared to DAC)
- $CO_2$ transformation to high value chemicals
- $CO_2$ pipeline transport
- Measurements and standards to monitor and manage ocean carbon systems and support direct ocean capture (DOC)
- Development of metrology and standards to support carbon accounting
- Measurement and standards to manage and accelerate geological storage
- Augmentation of projects to facilitate carbon mineralization in building materials