



Lawrence Berkeley  
National Laboratory



# **The Carbon Cycle 2.0 Initiative at LBNL: organizing with labs and industry to meet the demands society will have from science**

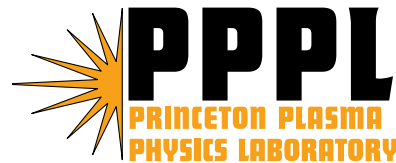
Paul Alivisatos  
Director, Lawrence Berkeley National Laboratory

January 31, 2012

# A two minute primer on the DOE National Labs



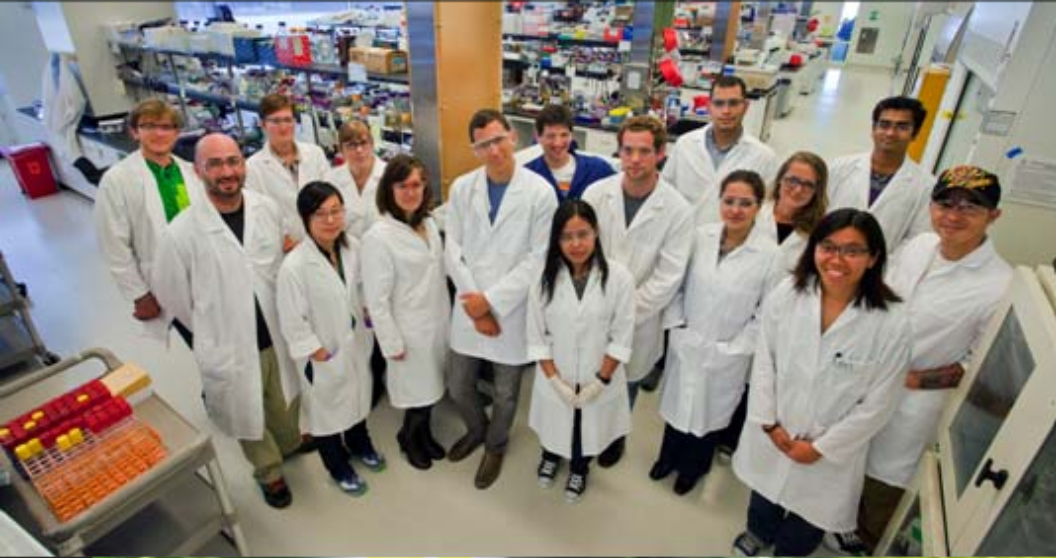
Proudly Operated by **Battelle** Since 1965





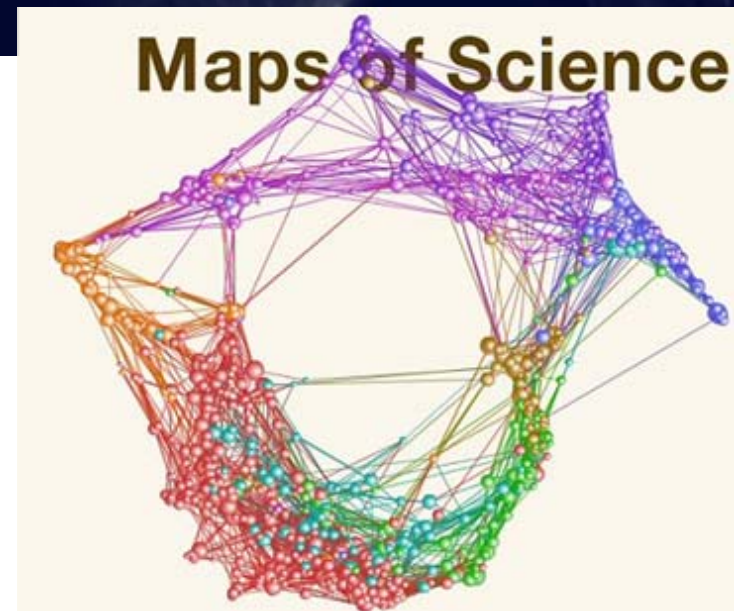
Lawrence's Big Team Science in 1931

# DOE National Labs Today: Special Teams, Unique Facilities

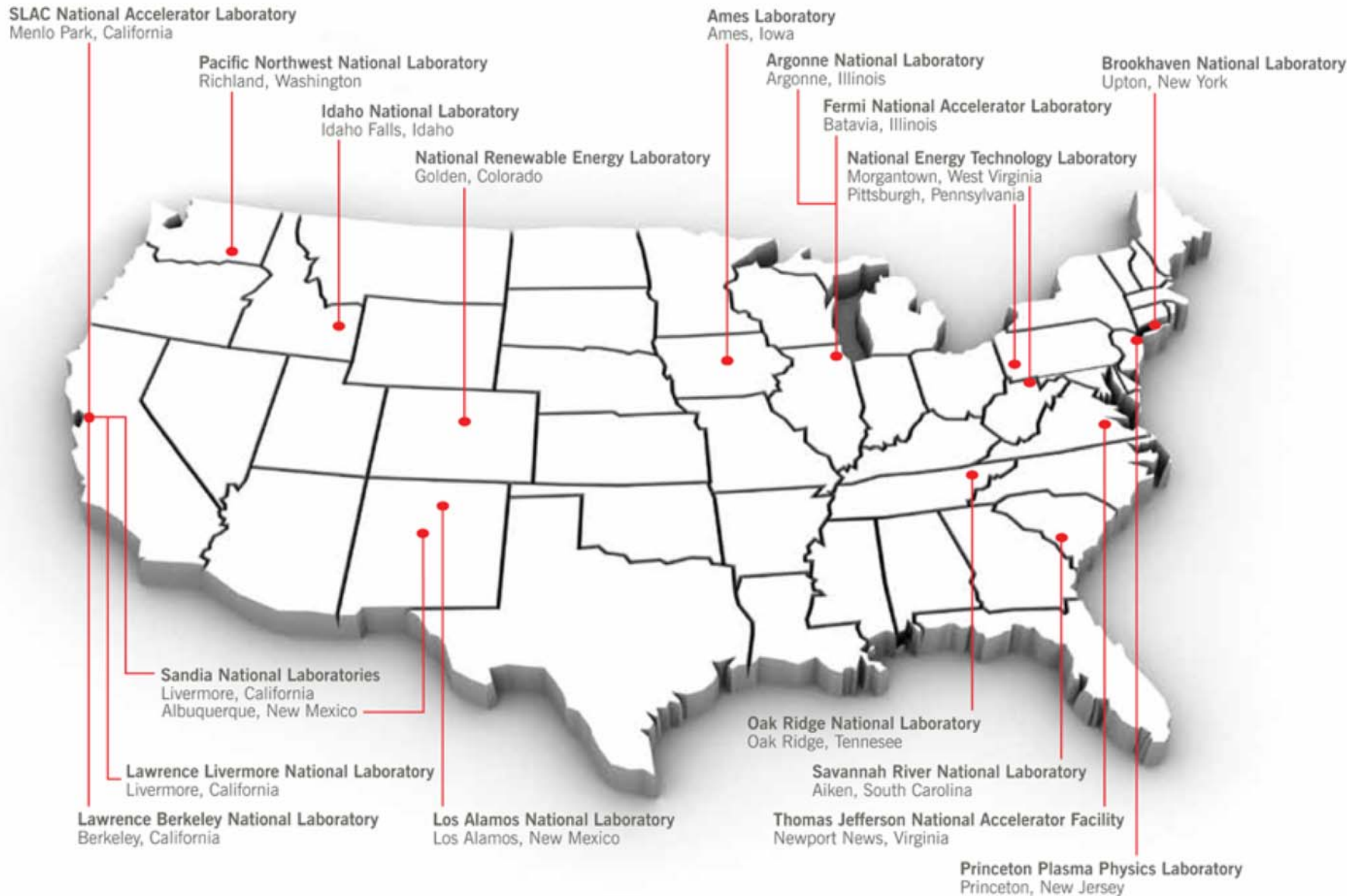


# Today Science teams connect the world

- Cutting edge science *requires* teams working across multiple disciplines
- *International* teams are now the norm
- Global connectivity enhances cooperation and gives competitive advantage to those who embrace it
- Society is more dependent upon science
- More industry partnerships with public research institutions could accelerate innovation in the U.S.



# The DOE National Labs

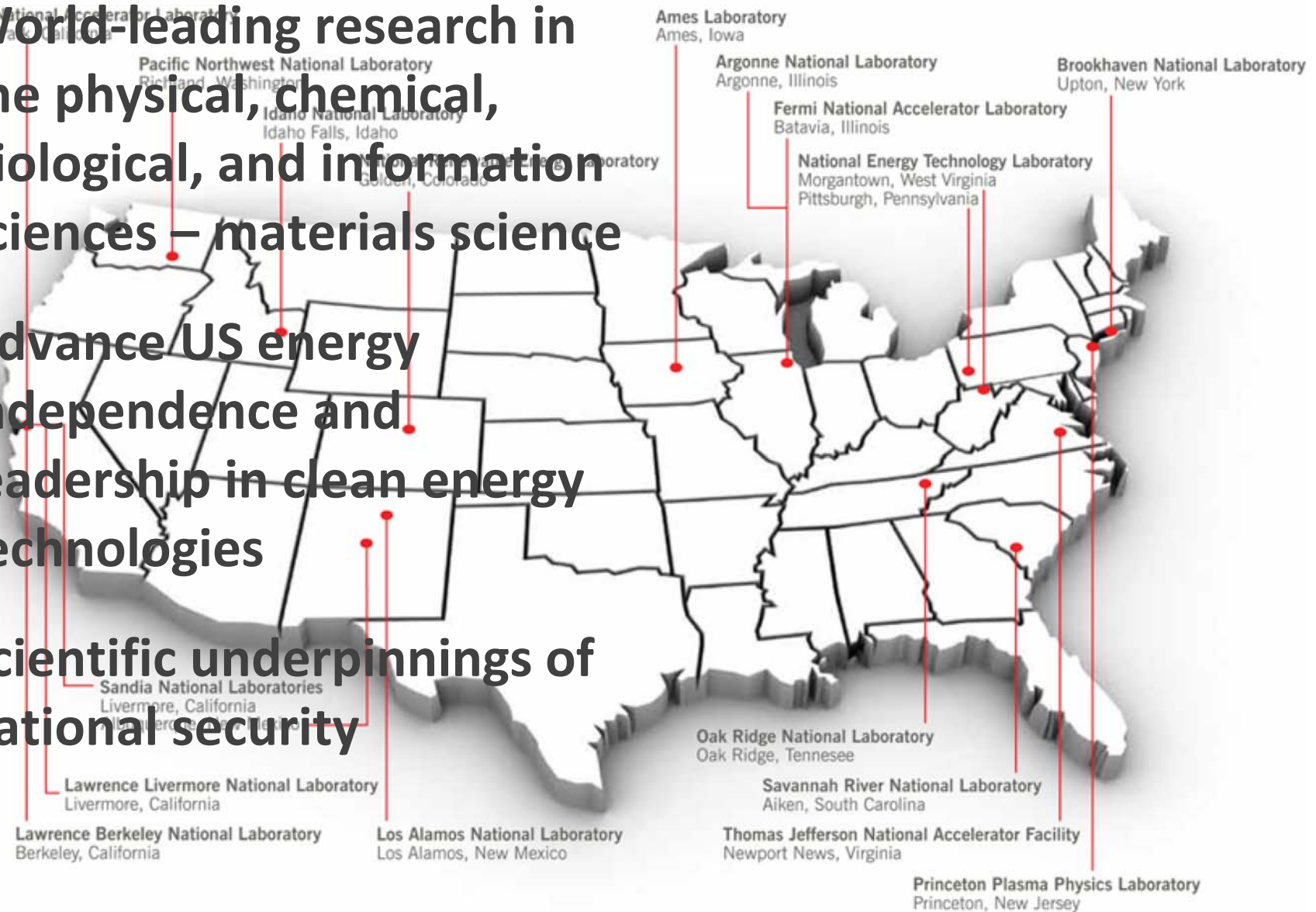


# The National Labs: Strategic Portfolio for DOE Missions

- World-leading research in the physical, chemical, biological, and information sciences – materials science

- Advance US energy independence and leadership in clean energy technologies

- Scientific underpinnings of national security



# World class user facilities at the National Labs

## Lawrence Berkeley National Laboratory

- Advanced Light Source
- Molecular Foundry
- National Center for Electron Microscopy



## Argonne National Laboratory

- Advanced Photon Source
- Center for Nanoscale Materials
- Electron Microscopy Center



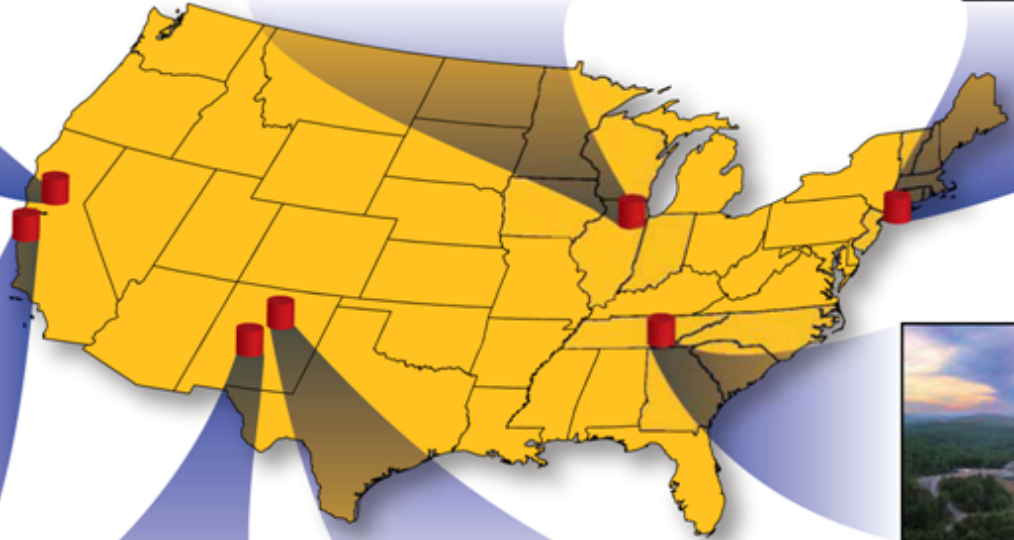
## Brookhaven National Laboratory

- Center for Functional Nanomaterials
- National Synchrotron Light Source
- National Synchrotron Light Source II



## SLAC National Accelerator Laboratory

- Linac Coherent Light Source
- Stanford Synchrotron Radiation Lightsource



## Oak Ridge National Laboratory

- Center for Nanophase Materials Sciences
- High Flux Isotope Reactor
- Shared Research Equipment Facility
- Spallation Neutron Source



## Sandia National Laboratory

- Core Facility for Center for Integrated Nanotechnologies



## Los Alamos National Laboratory

- Gateway Facility for Center for Integrated Nanotechnologies
- Manuel Lujan Jr. Neutron Scattering Center





# Synchrotron Light Sources

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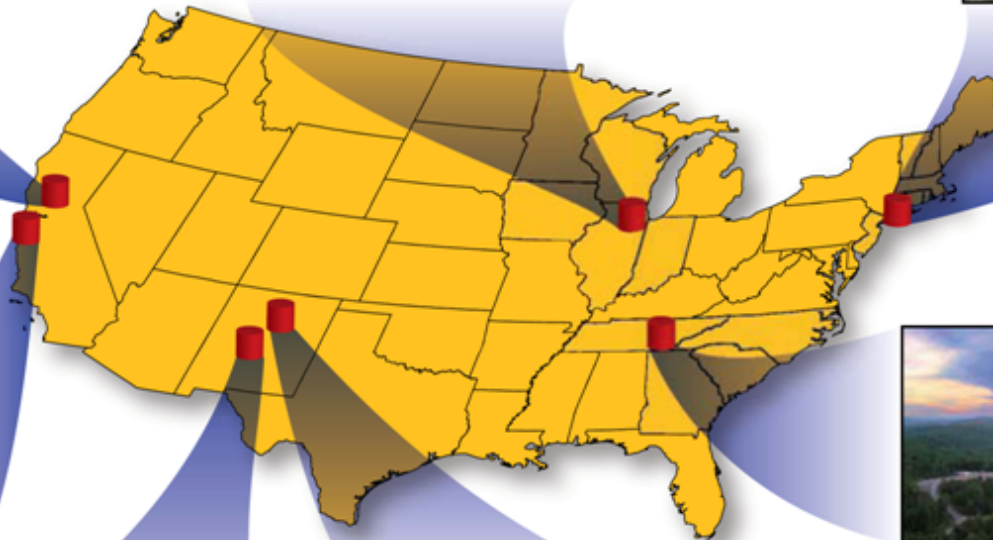
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# Nanoscience Facilities

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# High-performance computing and networking



# Powerful new means of harnessing nature's most sophisticated systems in plants and microbes for practical applications



- Developed modified switchgrass that enable a 30% improvement in the yield of ethanol

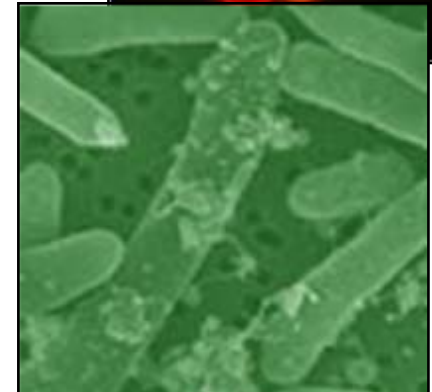
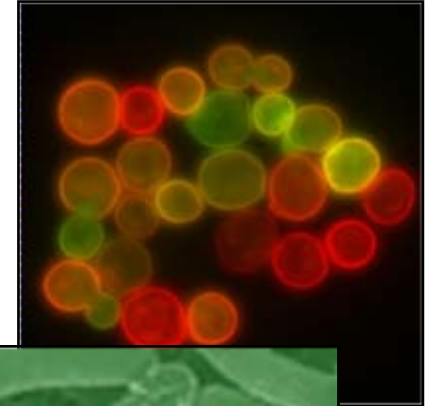


- Used synthetic biology toolkit to construct the first microbes to produce an advanced biofuel (biodiesel) directly from biomass.



- Characterized impacts of biomass crop agriculture on marginal lands, studying shifts in microbial community and potential for changes in greenhouse gas emissions.

In the first three years of operations, the BRCs together had 66 inventions in various stages of the patent process, from disclosure to formal patent application, and over 400 peer-reviewed publications.

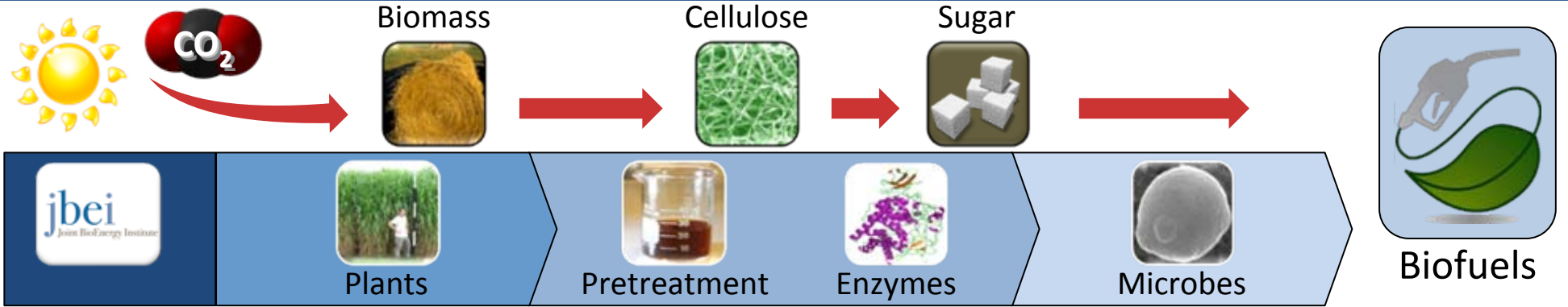


# The JBEI Model



- **Mission:** Provide scientific basis for converting plants into renewable liquid transportation fuels that are compatible with existing and proposed engines and current fuel-distribution infrastructure.
- **Structure:** Partnership of 4 national labs, 3 academic institutions

- **History:** JBEI is one of three DOE Bioenergy Research Centers created in response to the Energy Independence and Security Act of 2007.
- **Budget:** \$134M over 5 years by DOE's Office of Biological and Environmental Research (200 staff)



Mission & Science Achievements	Engineered Plants to Control Lignin Production	New Pretreatment Process to Completely	Microbes Produce Fuels Directly From Biomass	Tools for the Biofuels Research Community
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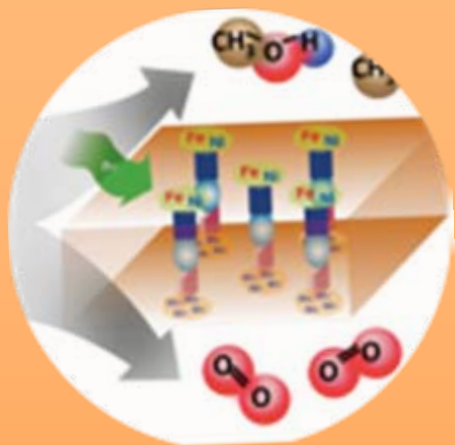
Commercial Achievements	<p><b>88</b> Invention Disclosures</p> <p>Twice national average compared to other research institutes*</p>	<p><b>29 (of 45)</b> Patent Applications in Licensing Negotiations</p> <p>Exceeds national academic standard*</p>	<p><b>1</b> Patent</p> <p><b>4</b> Licenses/Options</p> <p><b>4</b> Startups Originating from JBEI</p>	<p>*Source: Association of University Technology Managers FY2009 survey of academic institutions, calculated per funding dollar</p>
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# The Carbon Cycle 2.0 Initiative at Berkeley Lab

- What are key trends in the evolution of science as we move to 2030?
- How do we fit into the DOE National Lab system and work with industry?
- How can we organize to meet the demands society will have from science?



# Societal needs for technical solutions to energy and environment problems will intensify



Nanoscience  
will create advanced  
materials and designed  
systems



The biology revolution  
will deepen and impact other  
disciplines



Reliance on computation  
will expand while massive  
data sets will challenge

Physics

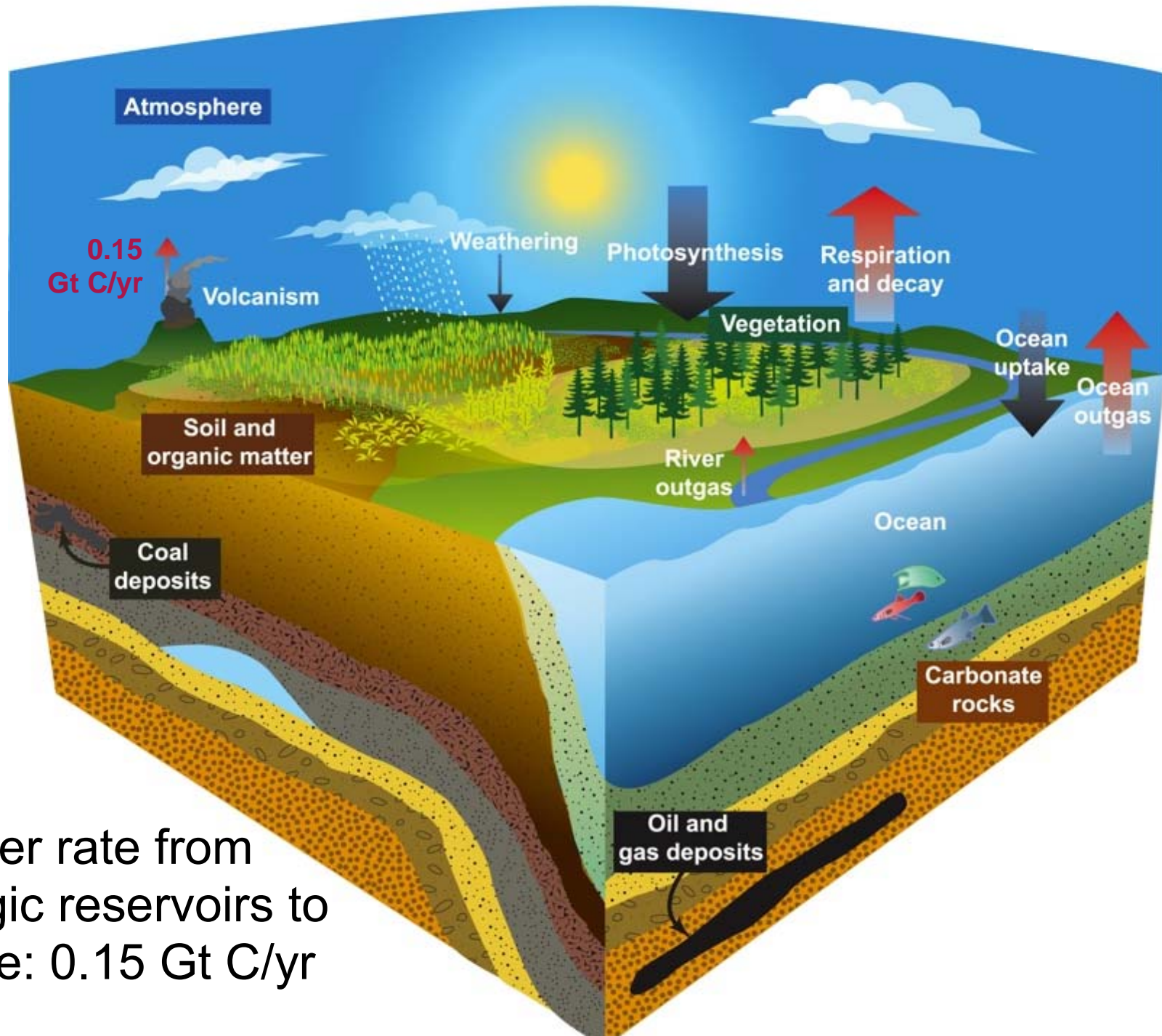
Chemical Sciences

Materials Science

Mathematics

## A Foundation of Basic Science

# Carbon Cycle 1.0: Natural Carbon Cycle



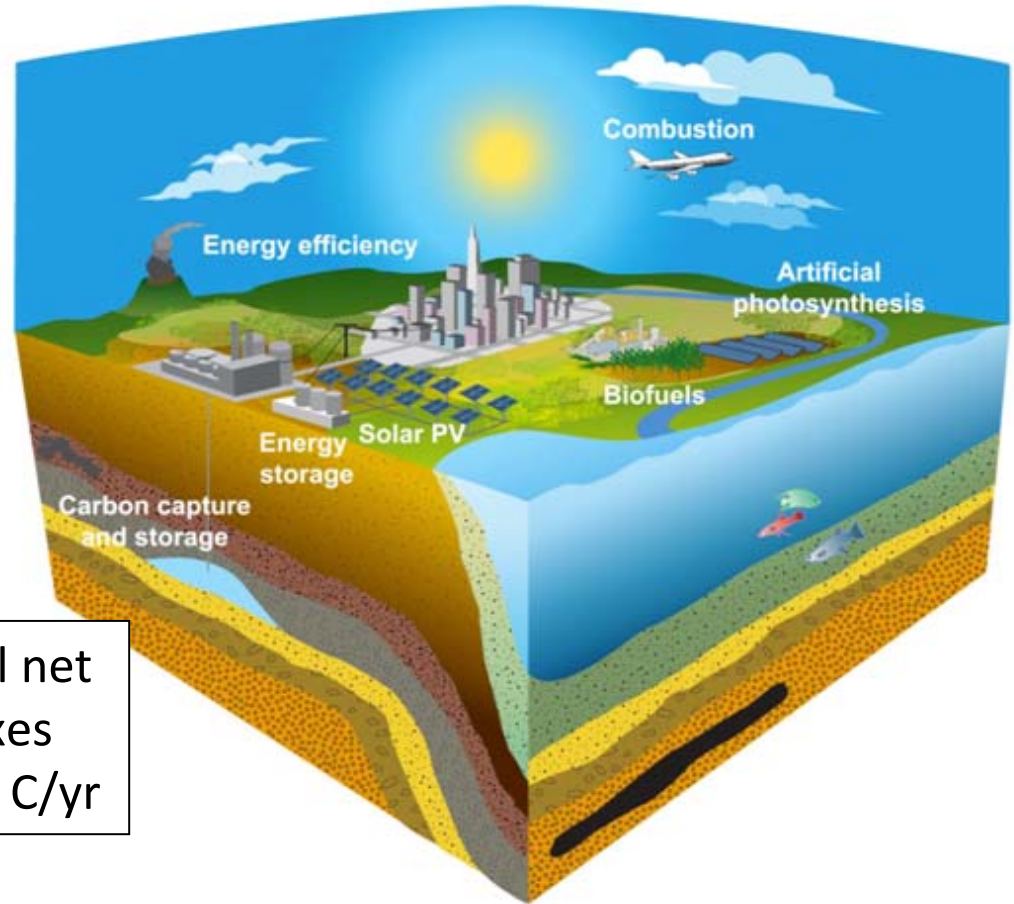
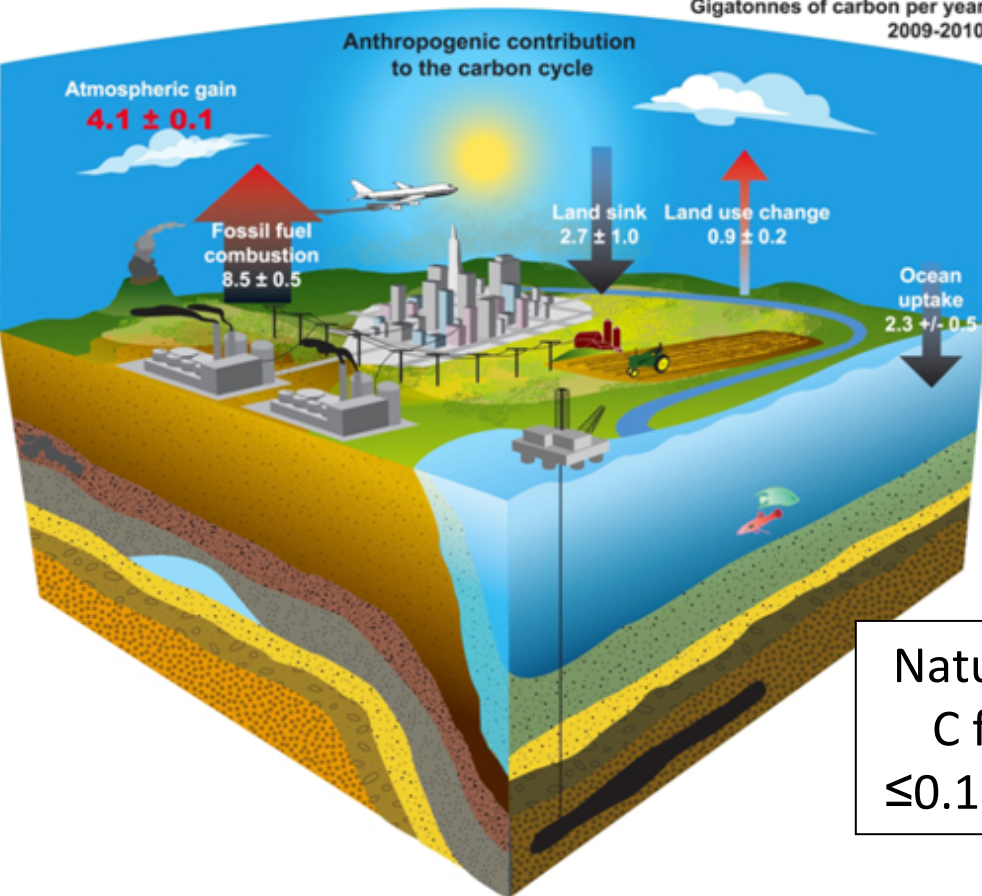
Transfer rate from geologic reservoirs to surface: 0.15 Gt C/yr



Current open-ended C cycle  
Carbon Cycle 1.x (2010 AD)

Future balanced C cycle  
Carbon Cycle 2.0 (2100 AD?)

Gigatonnes of carbon per year  
2009-2010



Natural net  
C fluxes  
 $\leq 0.1$  Gt C/yr

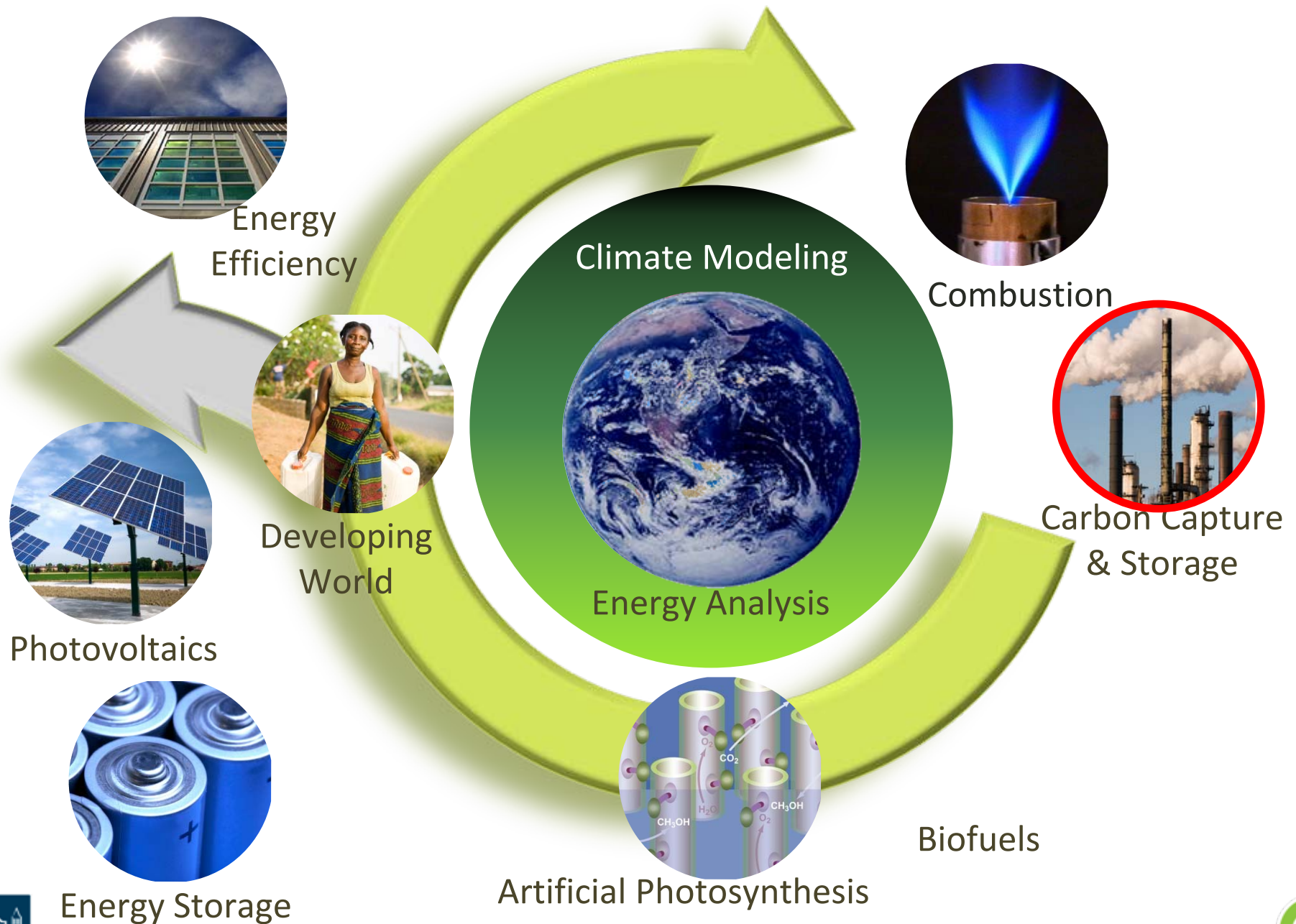
140 PWh/yr energy production  
8.5 Gt/yr carbon emissions

400 PWh/yr energy production  
 $\leq 3$  Gt/yr carbon emissions

60 Mt C / PWh

7.5 Mt C / PWh

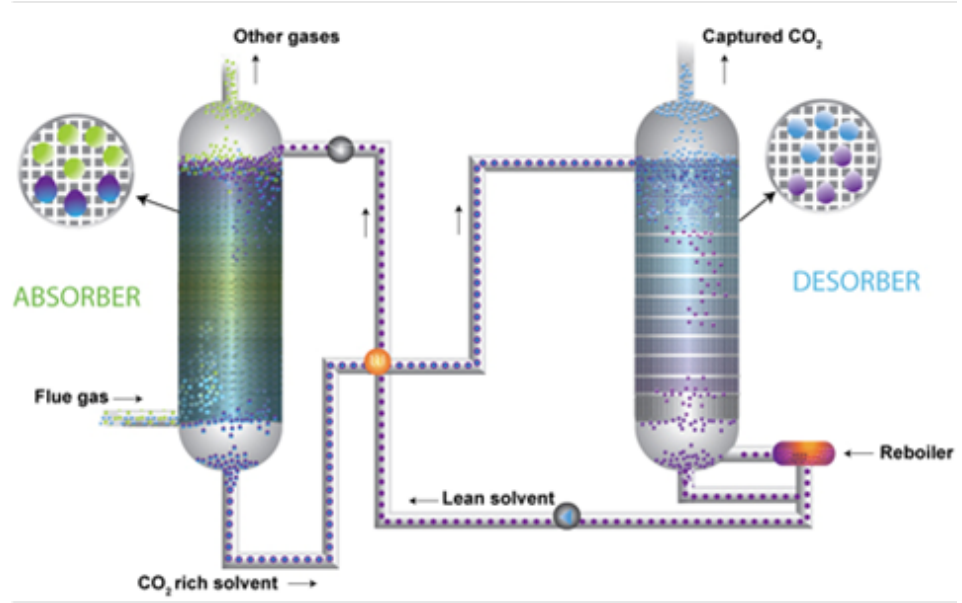
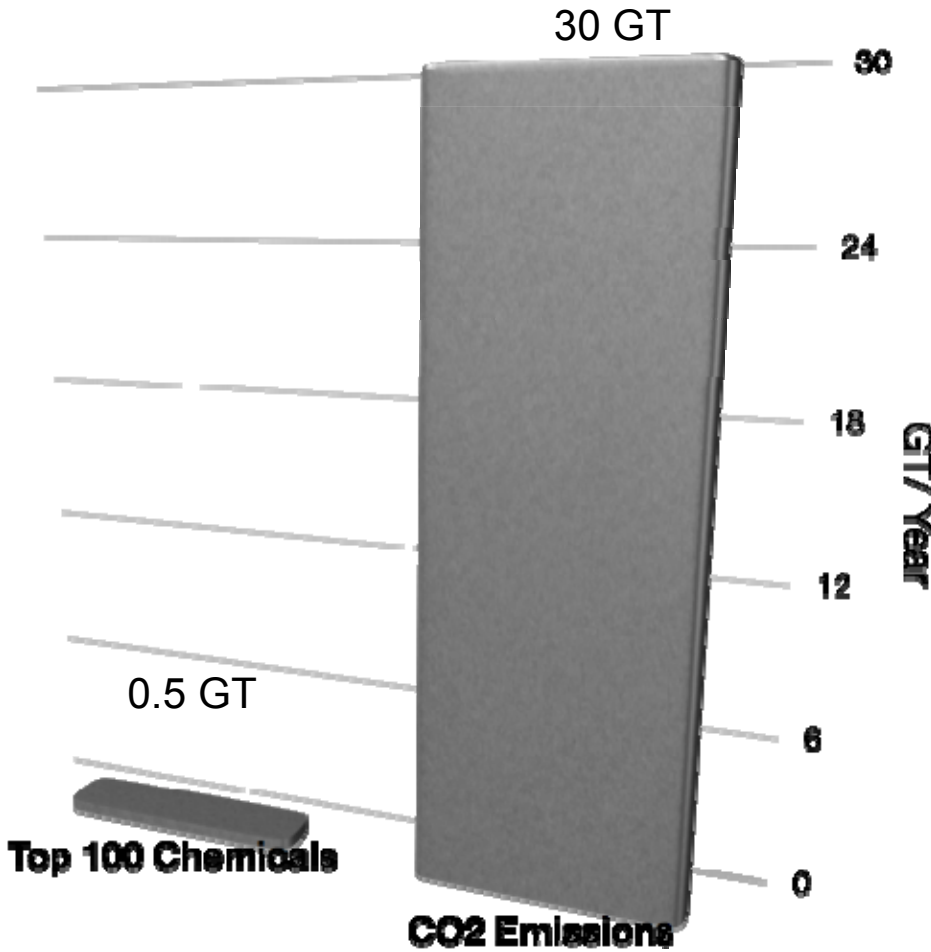
# Carbon Cycle 2.0 at Berkeley Lab





# Carbon Capture and Sequestration

## - scale and scope of the problem

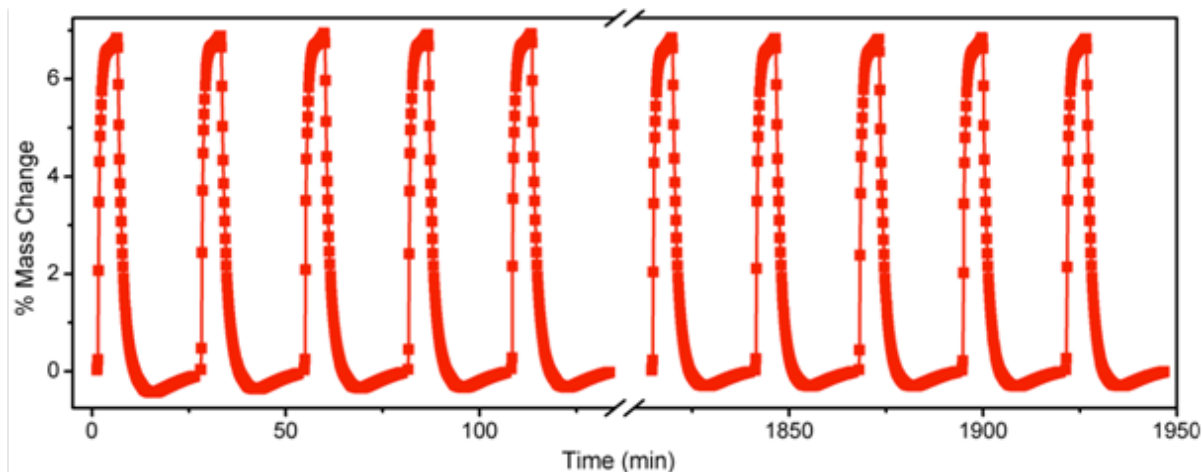
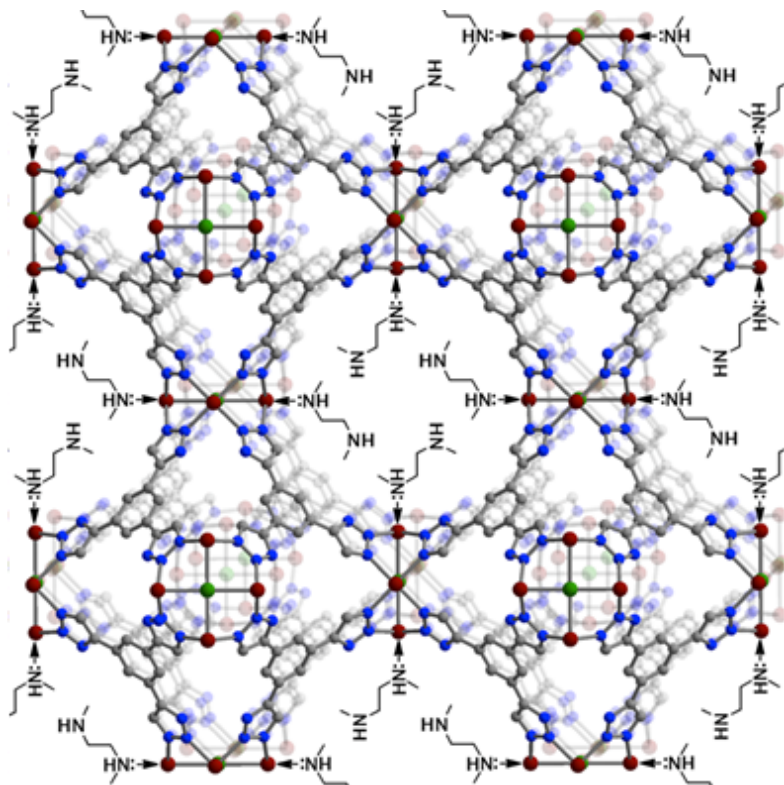


Current amine process energy intensive  
~25% of the power of a plant required  
~8¢/KWh

# Carbon Capture - New materials



The challenge: develop a material that can capture and release vast quantities of CO<sub>2</sub> at 1/3<sup>rd</sup> today's cost of ~8¢/KWh



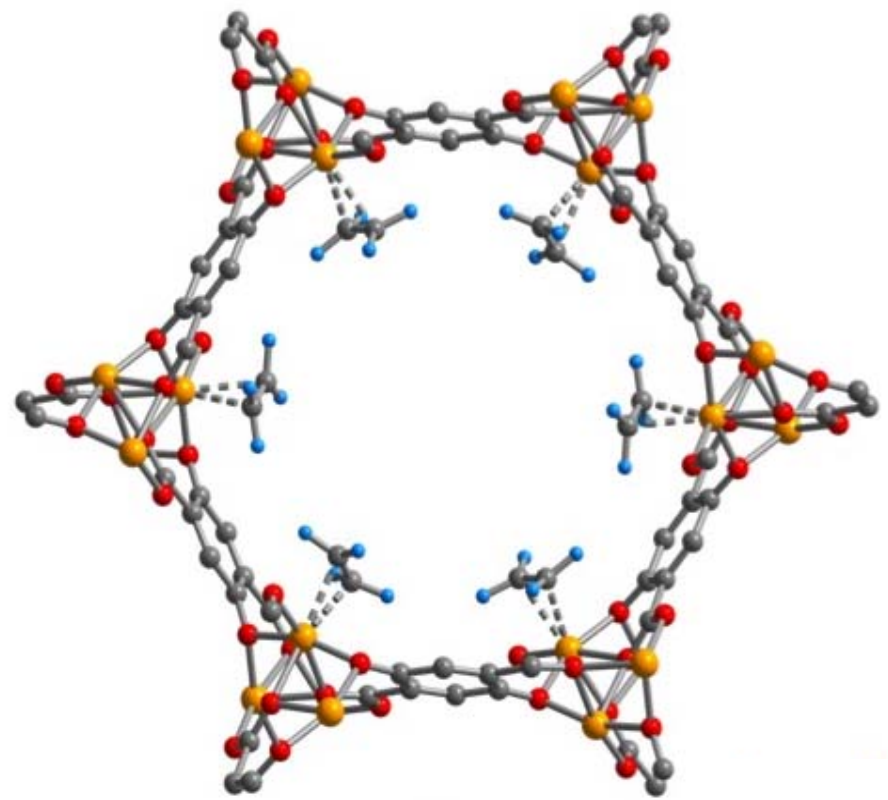
## Metal Organic Frameworks

capture CO<sub>2</sub> w/ secondary alkylamines

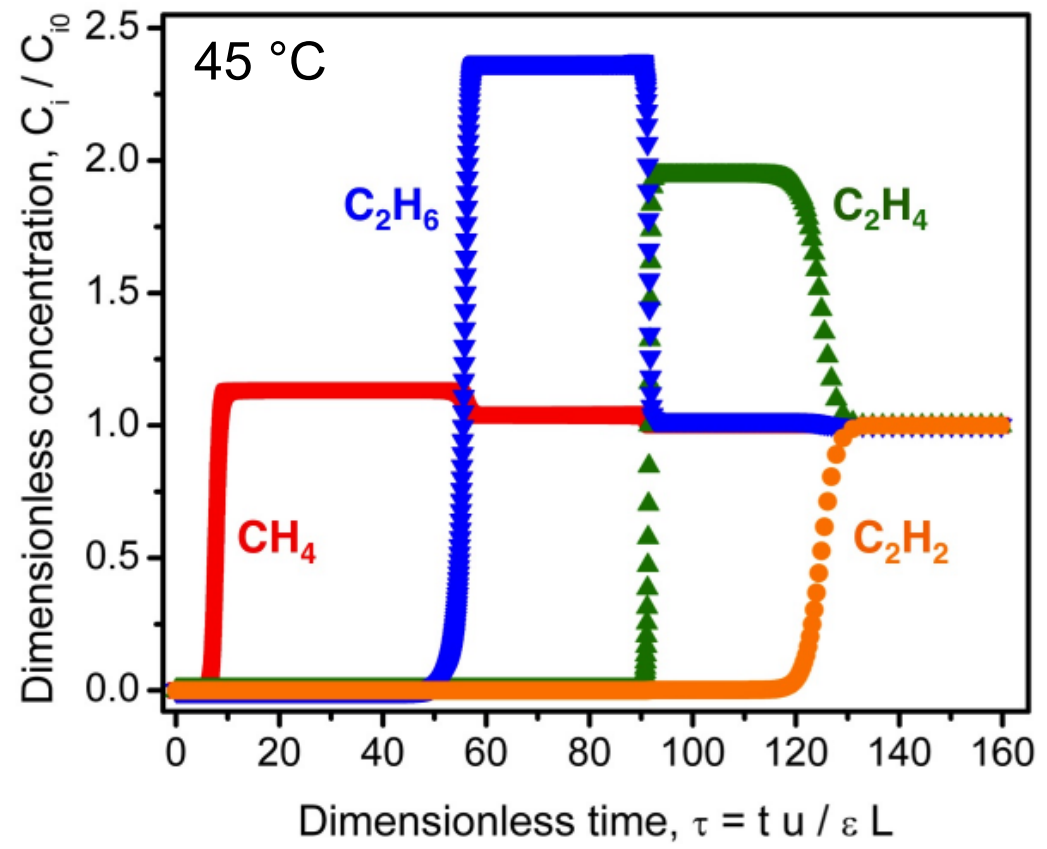
- 6.9 wt % cycling capacity for dry flue gas
  - Feed gas is 15% CO<sub>2</sub> in N<sub>2</sub>
  - Adsorption within 5 minutes at 25 °C
  - Desorption within 5 minutes at 60 °C
- Per kg of CO<sub>2</sub> captured, regeneration energy is approximately one third of the energy required for 30% MEA<sub>(aq)</sub> solutions



# Nanoscience will enable the design of new MOFs impacting a wide range of energy technologies

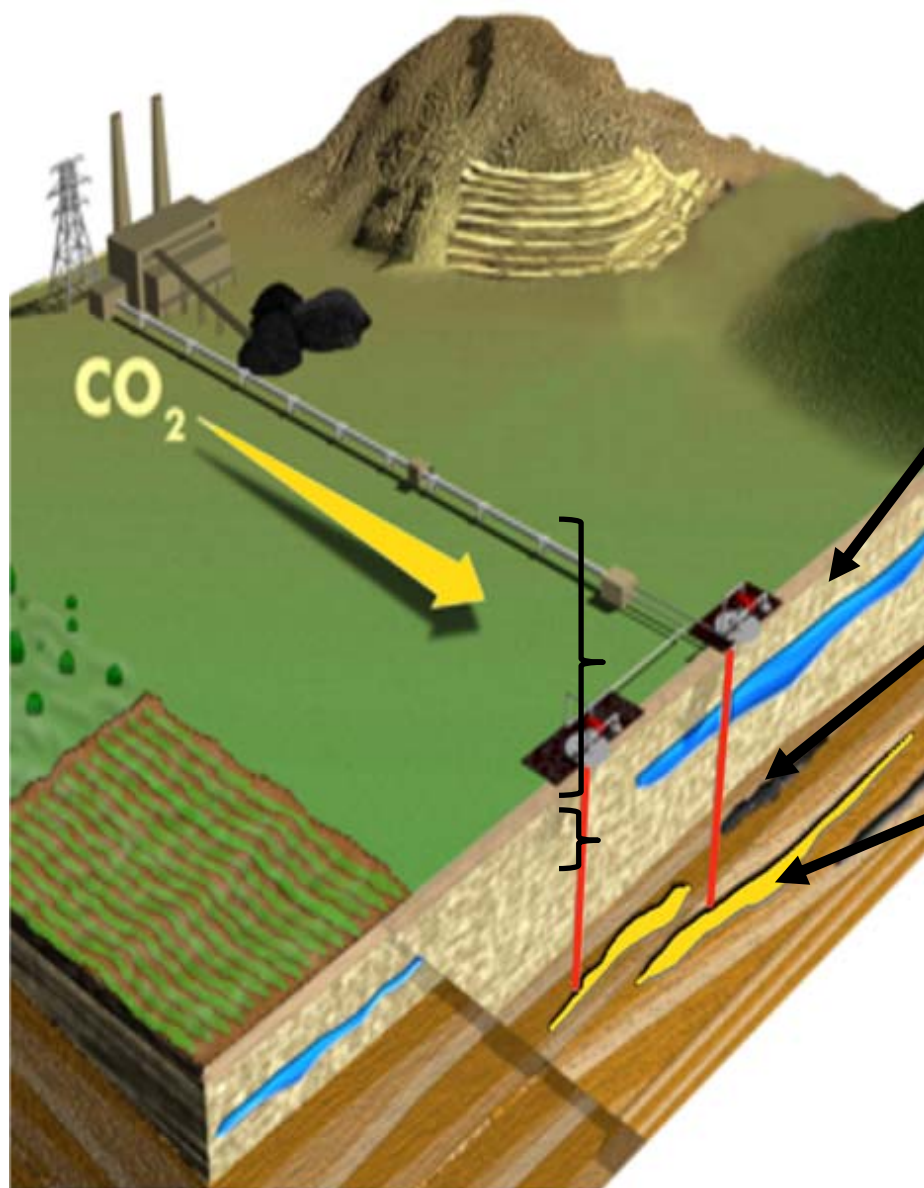


**Fe<sub>2</sub>(dobdc)-2C<sub>2</sub>H<sub>4</sub>**



- A single MOF can be used to fractionate a mixture of CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>2</sub>
- Ethylene/ethane normally separated cryogenically...

# Carbon Sequestration - understand risks



*Monitoring outside of the Reservoir*

*Seal must be robust*

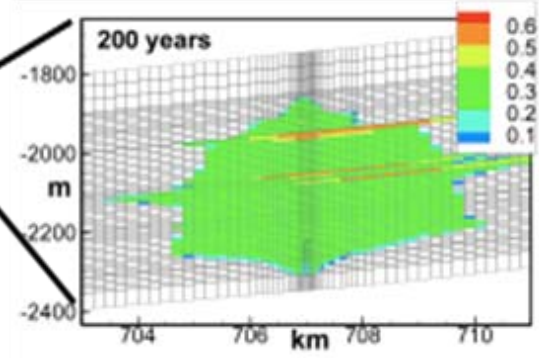
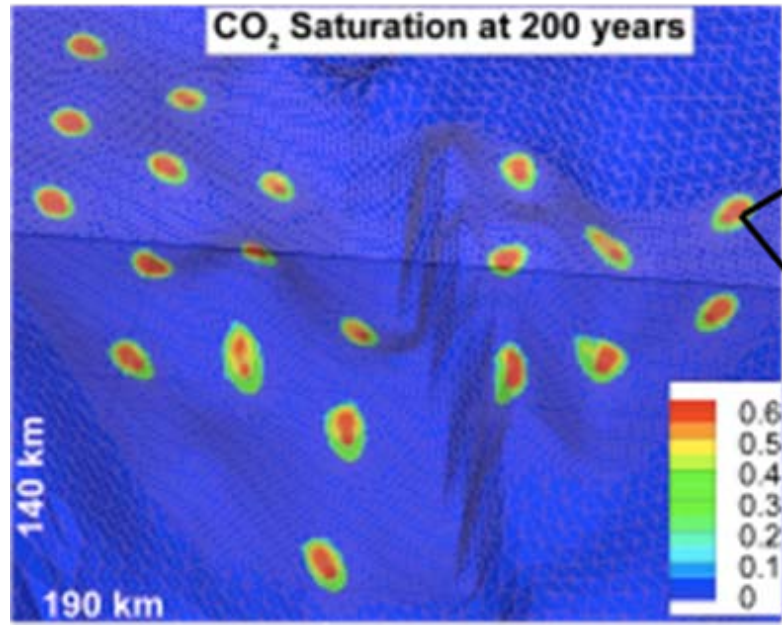
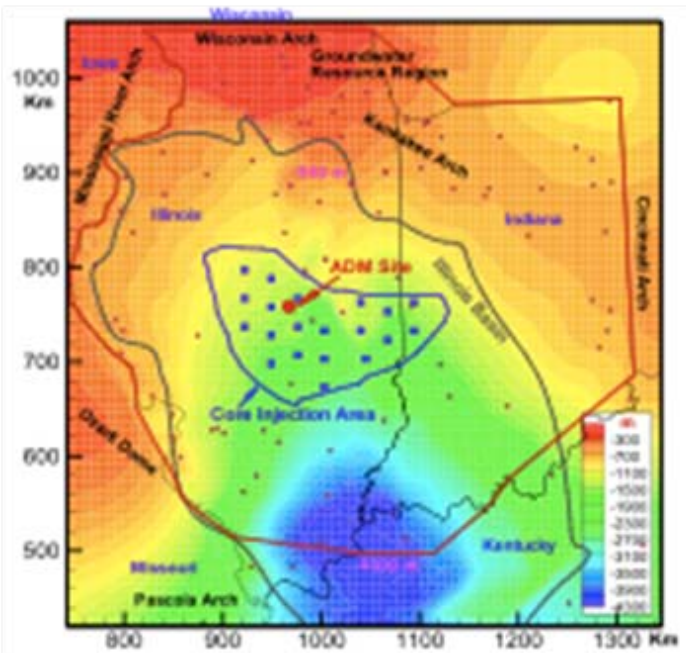
*Reservoir*

- Plume movement in reservoir (CO<sub>2</sub>, brine, pressure front)
- Impacts from introducing CO<sub>2</sub> into the reservoir

The challenge: simulate long term fate of CO<sub>2</sub> injected underground ***from nanometers to kilometers***



# Carbon Sequestration - simulations

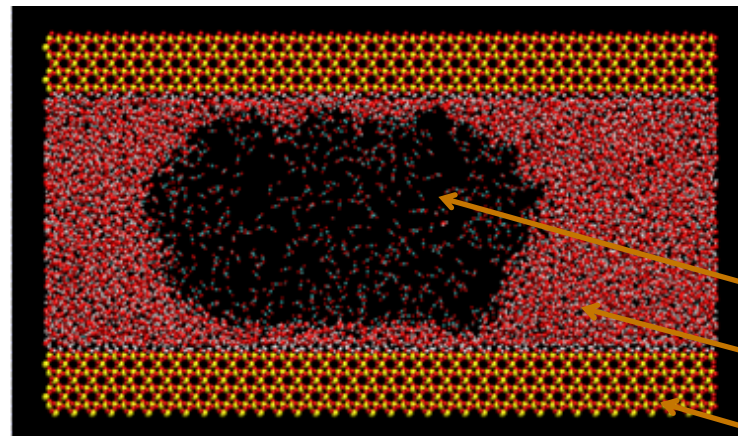


Simulated injection 5 Gt CO<sub>2</sub>,  
Over 50 years at 20 sites

No transport between sites,  
gases move down

Peak pressure rise 30 bar  
dissipates over time - *brine*

Zhou and Birkholzer GHGST, 2011



MD simulation  
snapshot of a 7  
nm-wide pore  
(31,000 atoms)  
at 373 K

H<sub>2</sub>O

Quartz



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# Carbon Sequestration - lifecycle analysis

Analysis of water, energy, and carbon intensities of brine management from CCS:

- Sequestering CO<sub>2</sub> in saline aquifers may require brine extraction
- Extracted brine can be either a waste product or a resource
- Optimal management options will vary with brine characteristics and location

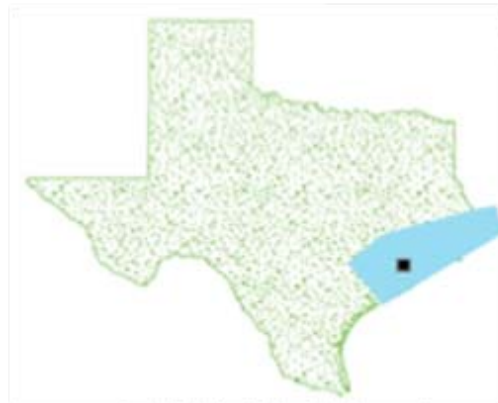
Cost analysis of brine mineral recovery for three disparate saline aquifers  
based on CCS for 10 1GW coal-fired power plants

**Southern San Joaquin**  
evaporation ponds: 100 km<sup>2</sup>



\$2.42/tCO<sub>2</sub> Salt value  
(\$3.90)/tCO<sub>2</sub> Salt recovery  
**(\$1.48)/tCO<sub>2</sub>**

**Jasper Interval**  
evaporation ponds: 1400 km<sup>2</sup>



\$7.90/tCO<sub>2</sub> Salt value  
(\$4.63)/tCO<sub>2</sub> Salt recovery  
**\$3.27/tCO<sub>2</sub>**

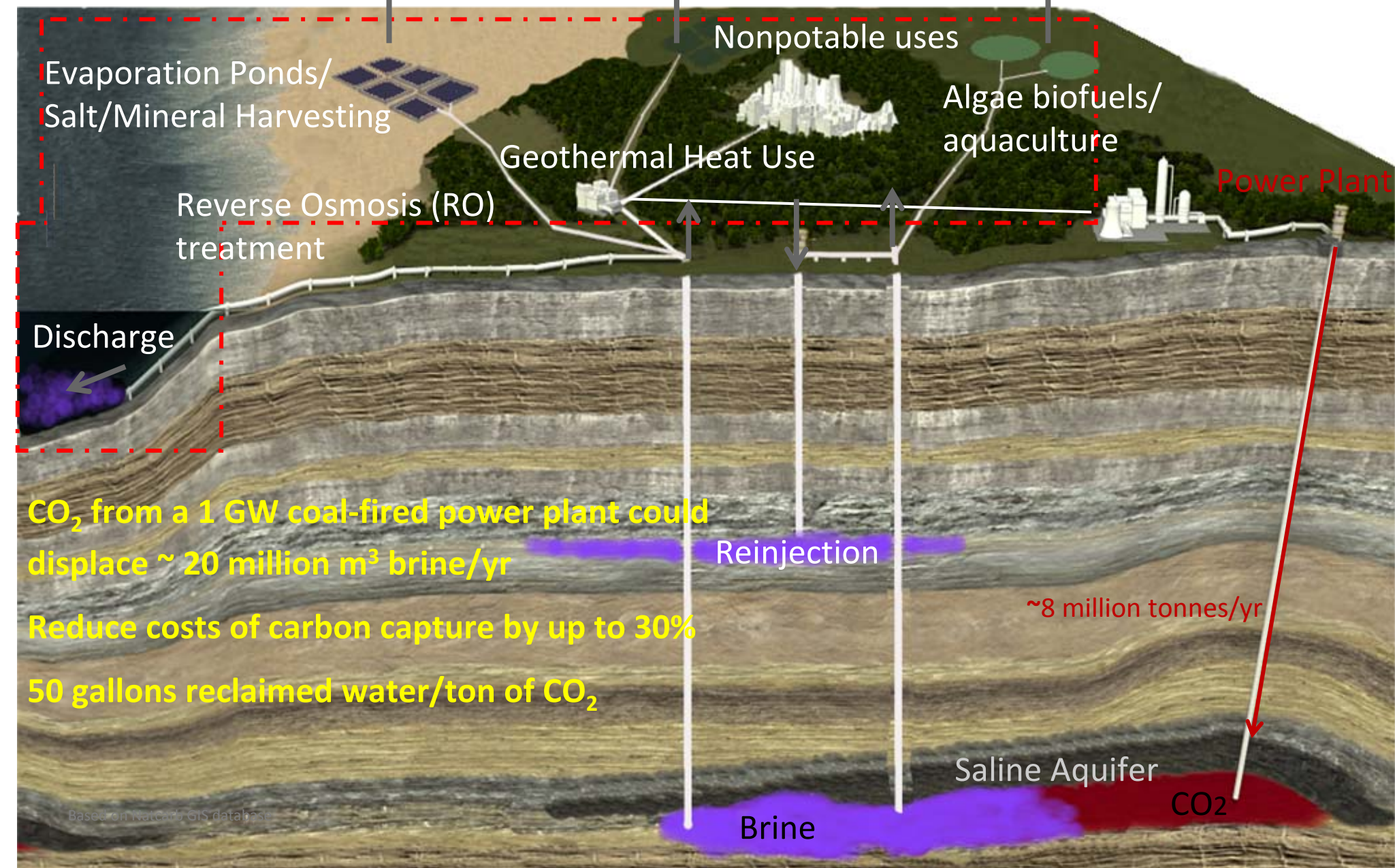
**Mt. Simon Sandstone**  
evaporation ponds: 350 km<sup>2</sup>



\$21.16/tCO<sub>2</sub> Salt value  
(\$4.21)/tCO<sub>2</sub> Salt recovery  
**\$16.94/tCO<sub>2</sub>**



# Lifecycle Analysis – capture value from the brine and water



# Carbon Cycle 2.0 at Berkeley Lab

