U.S. DEPARTMENT OF ENERGY | Office of Science

Post-Combustion CO_2 Capture: Beyond 2020, a BES Perspective

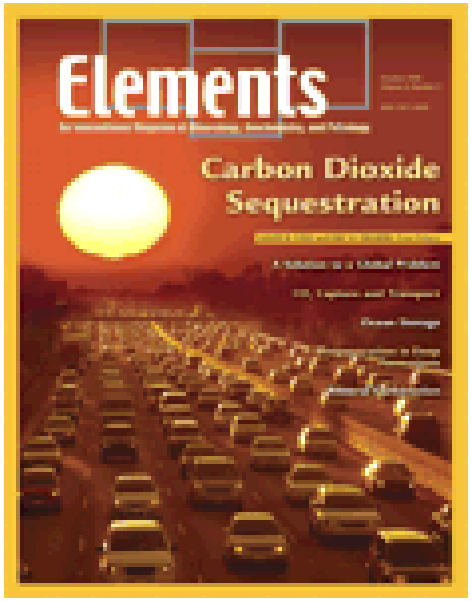
Presented to Office of Science and Fossil Energy

Oct. 5, 2009

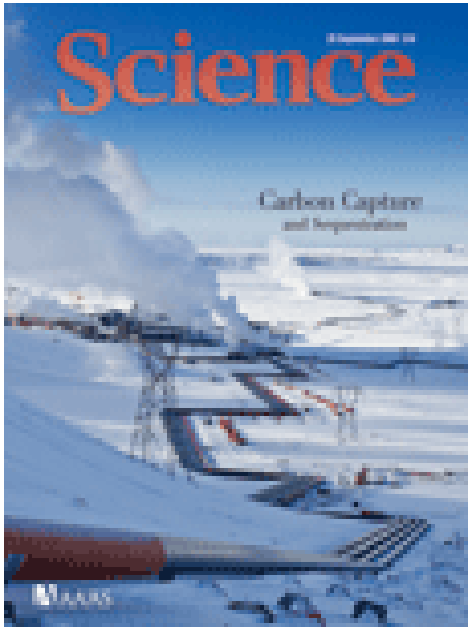
Outline

- Post-combustion Capture: Background and Challenges
- BES Current Portfolio relevant to CO_2 Capture
- Going Forward

Carbon Capture and Sequestration

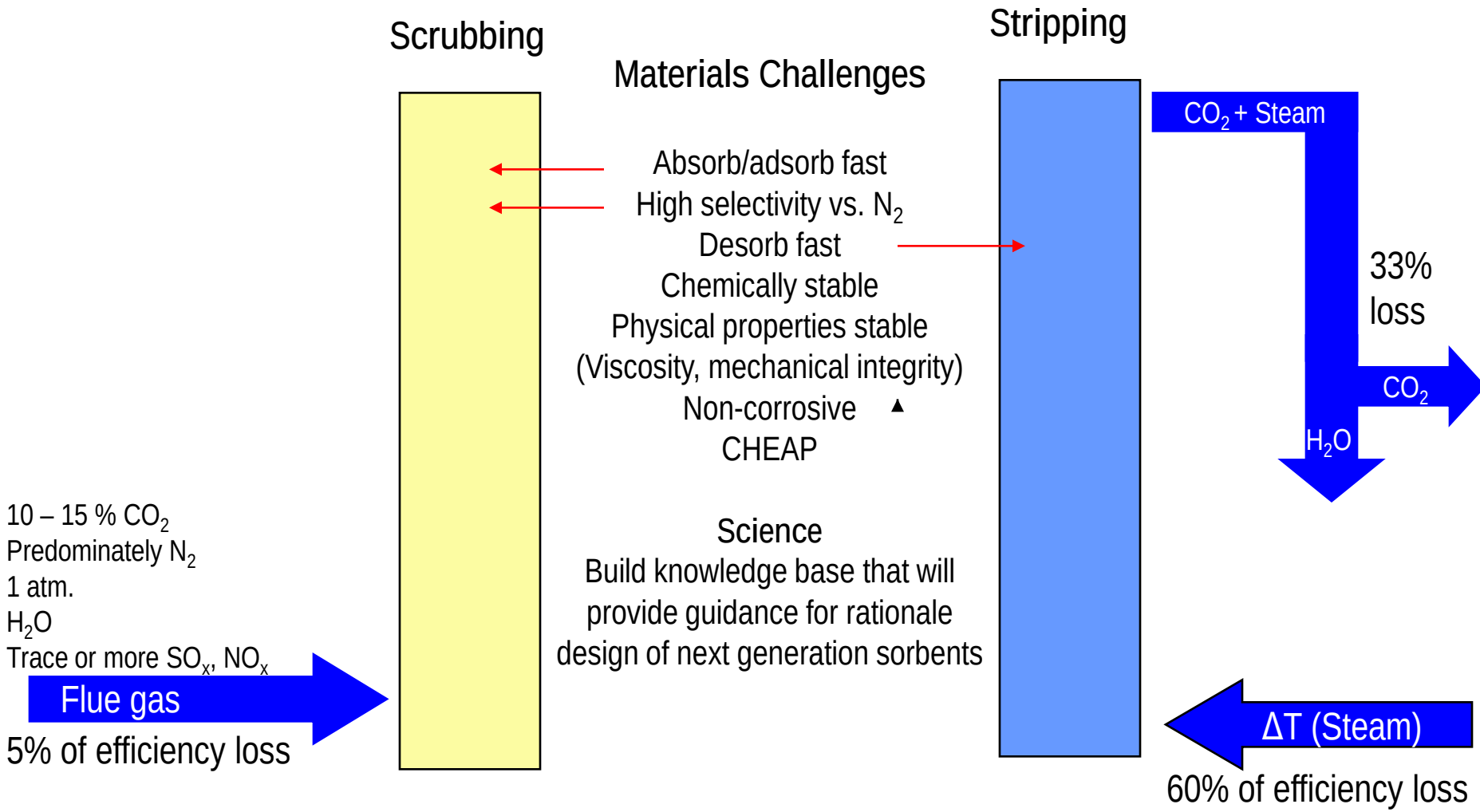


Oct. 2008, Volume 4, Number 5
Perspective by Dr. Steven Koonin, Under Secretary For Science



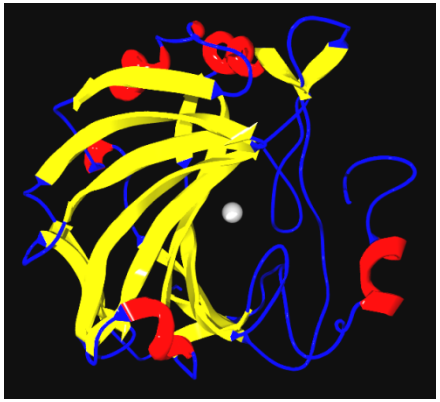
25 September 2009, Vol 325, Issue 5948
Perspective by Dr. Steven Chu, Secretary of Energy

Post-Combustion Capture



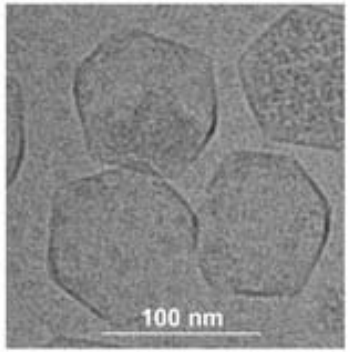
Biology and CO_2

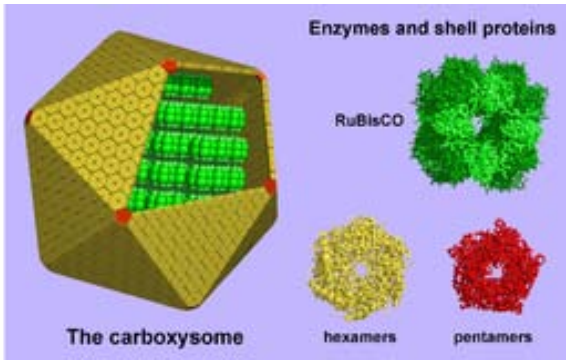
- Nature and CO_2
- Plants
  - Deal with dilute CO_2 (not efficiently)
  - Carbonic Anhydrase - in plants – increases CO_2 concentration
  - RuBisCO – plant enzyme converts CO_2 to sugar – 3 CO_2/sec



Ribbon diagram of human carbonic anhydrase with Zn atom in center

- Bacteria
  - Carboxysome - concentrates CO_2 levels to increase chemical transformation
  - Strategy: Concentrate, isolate and transform



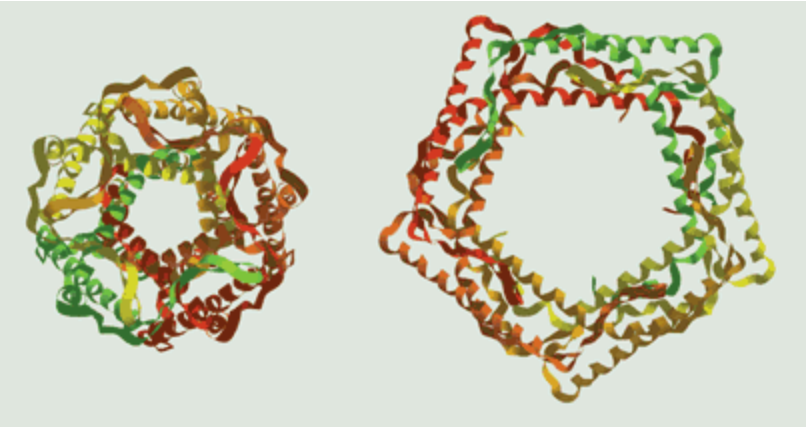


Carboxysomes – protein bacterial organelles on left is electron microscope image, on right is model of structure

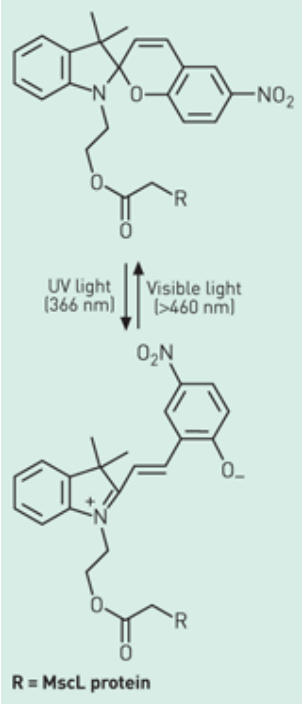
Source: http://en.wikipedia.org/wiki/File:Carbonic_anhydrase.png and http://en.wikipedia.org/wiki/Carboxysome

Nature's Triggers

- While nature does not deal with CO_2 ideally for post-combustion capture – can provide hints for non-thermal triggers
  - Ecoli have a channel protein that opens and shuts with pressure –
    - Has been modified to open and shut with light[1]



Channel proteins modified with spiropyran opens or closes channel with light.



Reversible spiropyran photo-switch.

  - Synapses electrical field triggers release of neurotransmitter

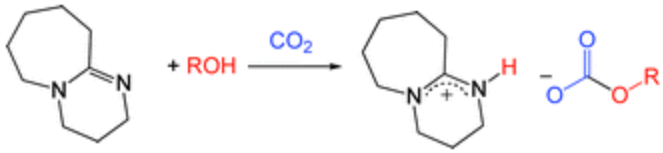
[1]Source – *Science,* 2005, *309*,755, Copied from C&E News report http://pubs.acs.org/cen/news/83/i31/8331notw1.html

Novel Approaches: Base + Alcohol

Alternate science approach may offer a better pathway in the future Heldebrant, PNNL

- Eliminate water and H bonding – reduces energy of stripping
  - Lower specific heat of organic liquids
    - Same strip temperature, considerable energy savings

- Organic amidine or biological guanidine base plus alcohol
  - Binds CO_2 – reversed with heat
  - Higher binding capacity for CO_2 than commercial MEA (monoethanolamine)
    - Design base to minimize hydrogen bonding – more energy savings



- Demonstrated uptake in 50% CO_2/ 50% N_2 , strip 90 to 130 C
- Issue - water form bicarbonate salt of base – strips MEA temperature

Source: Heldebrant et al. *Energy Procedia,* 1 (2009) 1187-1195

Science – Beyond 2020

- CO_2 sorbent that can be stripped with minimal energy
  - Look to Nature for ideas on triggers but unlikely to be a biological solution
  - Electrical, electrochemical, pressure, light, pH, phase change (liquid crystal)*
  - Nanoscale approaches

- Build the knowledge base to facilitate a rationale design of sorbents from first principles
  - Advanced computational modeling and theory - First-principles methods for capture and release of nonpolar molecules
  - Advanced characterization tools, including those supported by BES, to
    - Identify structure of binding sites
    - Understand kinetics and thermodynamics of sorption/desorption in realistic conditions
  - New chemistries for advanced sorbents
    - New sorbents
    - Synthesis

*Source: *Advanced Post-Combustion CO_2 Capture*, prepared for Clean Air Task Force, Howard Herzog, Jerry Meldon and Alan Hatton

Current BES Related Research

- Directly related (EFRC funding) – CO_2 from N_2
  - Zeolitic imidazolate framework (ZIFs) , metal organic frameworks (MOFs), membranes for separation
  - Synthesis, characterization, computation/modeling
- CO_2 Binding/Separation
  - Often from CH_4
  - MOFs, ZIFs
  - Polymer membranes
  - Computation, theory, modeling
- Hydrogen – Binding and Separation
  - H_2 sorbents
  - Inorganic clathrates, MOFs
  - Membranes
- Separation Sciences, Materials, Theory & Computation
  - Membrane synthesis
  - Transport
  - Theory and Computation

CO_2 Related BES Supported EFRCs

- Gas Separations for Clean Energy Technologies: (Smit, Berkeley)
  Focus: New strategies and materials for energy efficient selective capture or separation of CO_2 from gas mixtures based on molecule-specific chemical interactions

- Molecularly Engineered Energy Materials (Ozolins, UCLA) – (1/3 of EFRC)
  Focus: Novel ZIFs for gas separation including CO_2 capture

- Center for Nanoscale Control of Geologic CO_2 (DePaolo, LBNL)
  Focus: Molecular, nano-scale, and pore network scale approaches for controlling flow, dissolution, and precipitation in subsurface rock formations during emplacement of supercritical CO_2; predict long-term performance

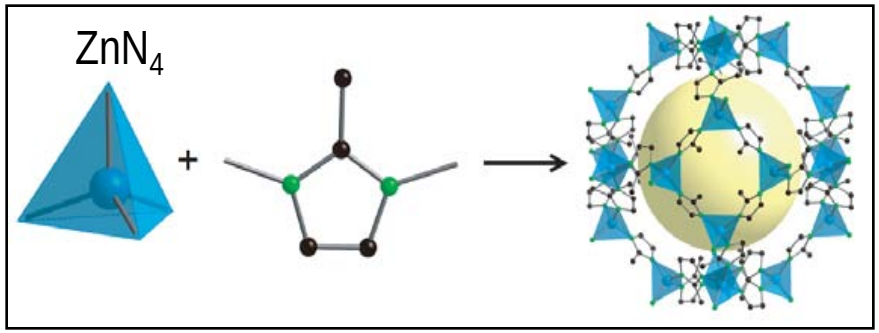
Examples of BES-Supported Projects: Synthesis

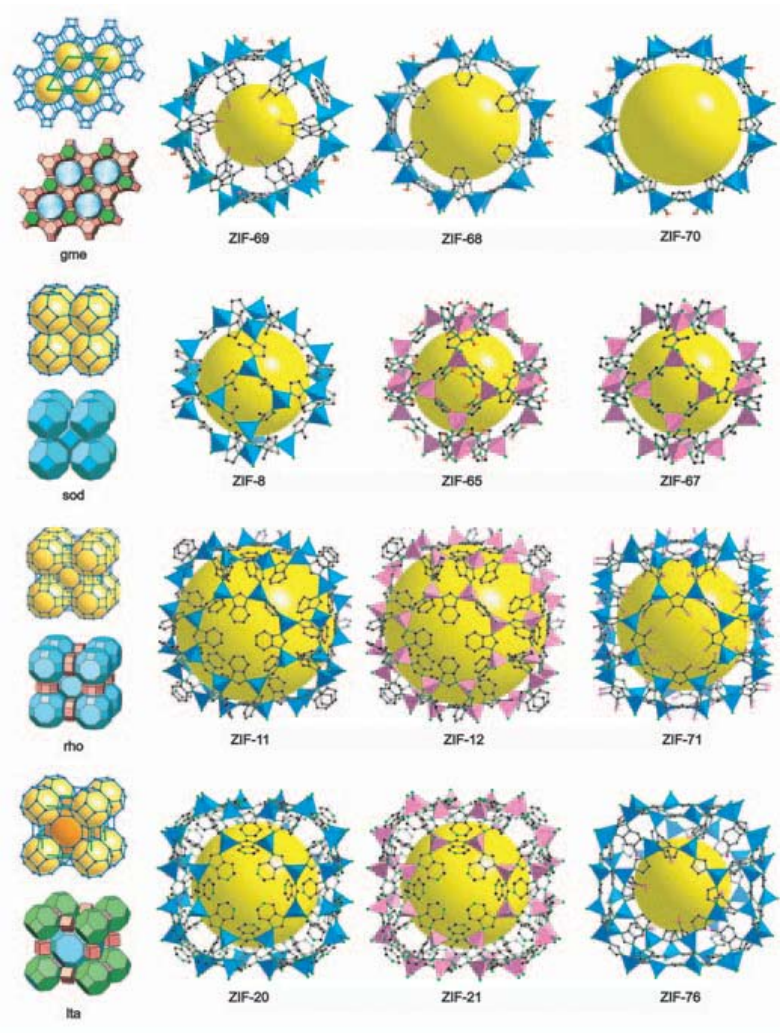
Capture is 1/3 of this EFRC: Novel ZIFs for gas separation including CO_2 capture

Yaghi – Synthesis, characterization

Asta – Electronic structure calculations

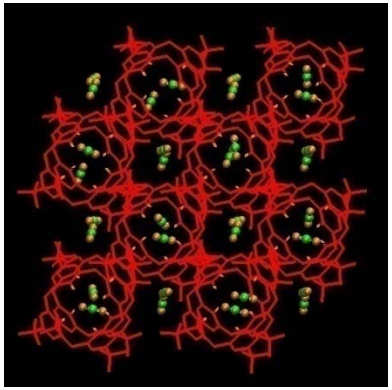
Laird & Houndonougbo – Monte Carlo Simulations





EFRC: Molecularly Engineered Energy Materials (Ozolins, UCLA)

Examples of BES-Supported Projects: Theoretical and Computational Modeling



PNNL: Dang et al

One interpretation: Computer simulations show that at ambient temperatures, CO_2 molecules require ~ 4 times more energy than average to desorb. *Novel Strategies for selective heating may be necessary*.

Computational studies of load dependent guest dynamics and free energies of inclusion for CO_2 in low density p-*tert*-butylcalix[4]arene at loadings up to 2:1.

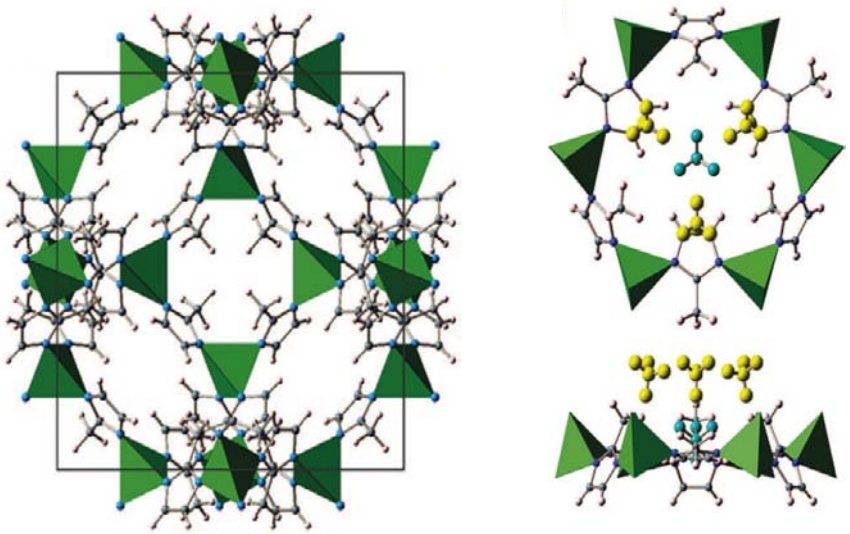
John L. Daschbach, Xiuquan Sun, Tsun-Mei Chang, Praveen. K. Thallapally, B. Peter McGrail, and Liem X. Dang. *J. Phys. Chem. A, Vol. 113, No. 14, 2009*

Theoretical and Computational Chemistry (Start FY09): Modeling CO_2 capture and separation in zeolitic imidazolate frameworks (Wisconsin, Schmidt)

- Molecular Level Mechanism of CO_2 adsorption?
- Specificity of CO_2 over N_2 ?
- Mechanism for CO_2/N_2 Selectivity in ZIFs ?
- Thermal and Solvent Stability?

Example of BES-Supported Projects: Neutron Diffraction

- Studied CD_4 absorption in a ZIF with a deuterated methyl imidazolate linker.



- Structure of ZIF
  - Changes with sorption
  - Changes with temperature
- Identify binding sites
  - Primary and stronger binding site - imidazolate
  - Secondary and weaker site - center

Note: This can be used with CO_2 since the organic linkers in the ZIF can be deuterated

Source: Yildirim - J. Phys. Chem. C, Vol. 113, No. 7, 2009

NIST Center for Neutron Research

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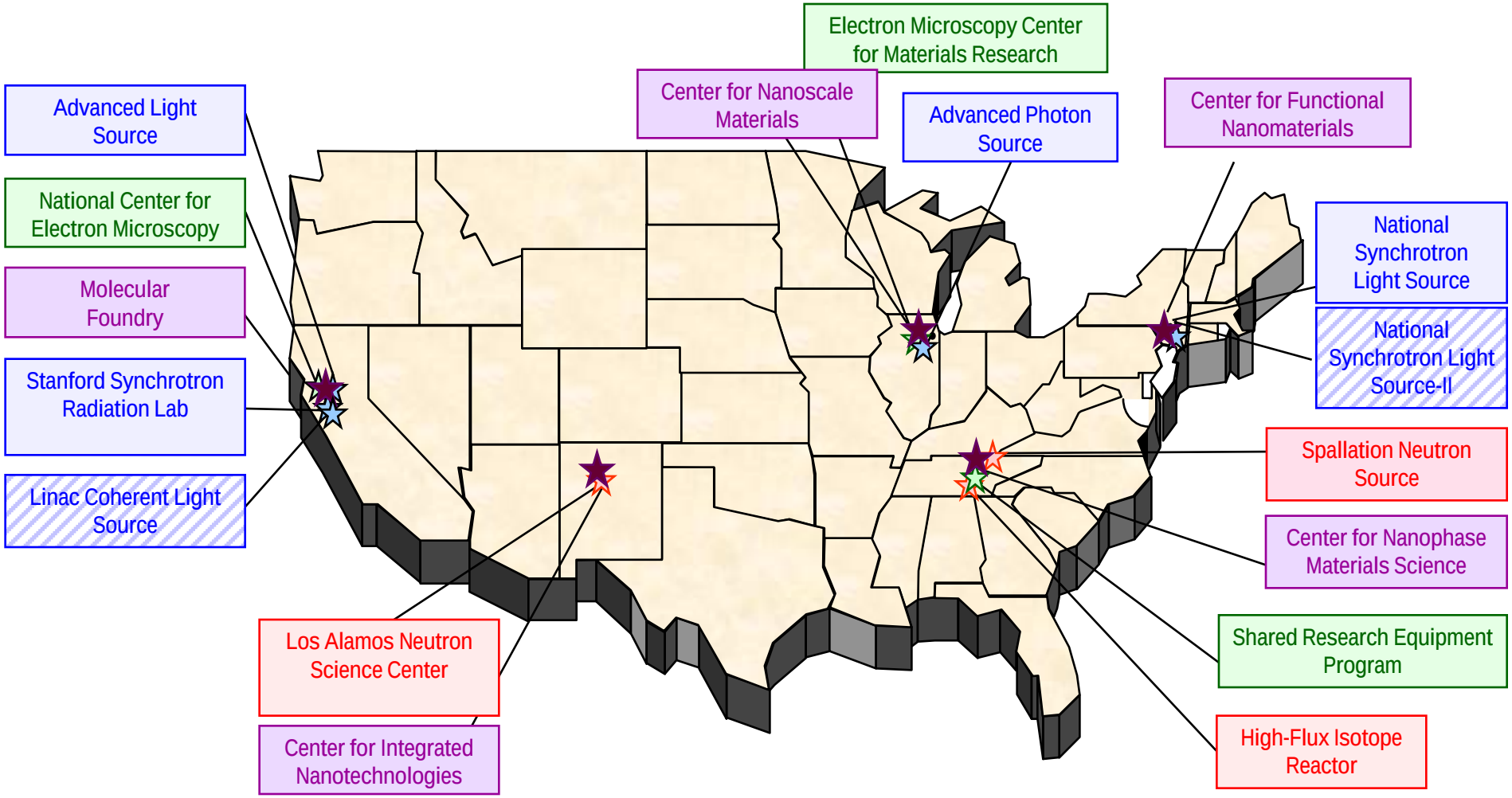
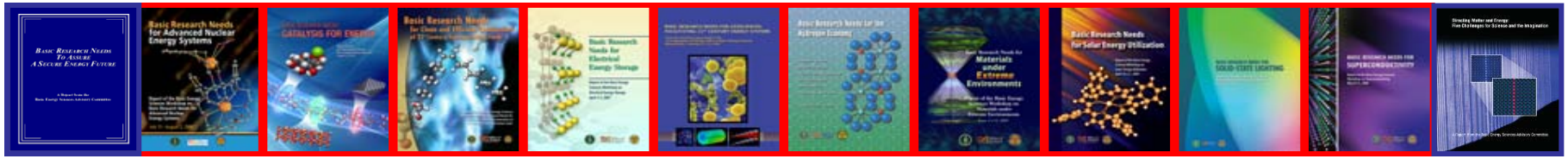
BES Scientific User Facilities



- 4 Synchrotron Radiation Light Sources
- Linac Coherent Light Source (Under construction)
- 3 Neutron Sources
- 3 Electron Beam Microcharacterization Centers
- 5 Nanoscale Science Research Centers

"Basic Research Needs" Style Workshop – Carbon Capture Beyond 2020

- Timing – Early in 2010
- Build on output of Carbon Capture 2020 Workshop
  - **Goal - Identify priority research directions for the challenges beyond 2020**
- Approach (Basic Research Needs style and format)
  - Integration with DOE BES, DOE FE, Academia, National Labs, and Industry
- Workshop format:
  - Plenary talks on technical and scientific challenges
  - Breakout panels focused on development of priority research directions
  - Crosscutting panel focused on identification of grand challenge science themes
  - Dedicated report writers to ensure rapid progress on written report
- Venue in the DC area



- Thank you
- Questions?