



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Role of Office of Basic Energy Sciences for Subsurface Science

**SubTER Panel
2015 Carbon Storage RD Project Review Meeting
Pittsburgh, PA**

August 19, 2015

P. Thiyagarajan (Thiyaga)
Materials Sciences and Engineering Division



U.S. DEPARTMENT OF ENERGY

Secretary
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Deputy Secretary
Elizabeth Sherwood-Randall

Under Secretary for Nuclear Security
Frank G. Klotz

Under Secretary for Science & Energy
Franklin Orr

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David Klaus (A)

- Defense Nuclear Nonproliferation
- Defense Programs
- Naval Reactors
- Counter-terrorism
- Defense Nuclear Security
- Emergency Operations

Office of Science
Vacant
Patricia Dehmer (A)

Basic Energy Sciences
Harriet Kung

High Energy Physics
James Siegrist

Advanced Scientific Computing Research
Steve Binkley

Nuclear Physics
Tim Hallman

Biological & Environmental Research
Sharlene Weatherwax

Fusion Energy Sciences
Ed Synakowski

SBIR/STTR
Manny Oliver

Workforce Develop. for Teachers & Scientists
Pat Dehmer

Advanced Research Projects Agency – Energy
Ellen Williams

- Energy Efficiency & Renewable Energy**
David Danielson
- Fossil Energy**
Christopher Smith
- Nuclear Energy**
Pete Lyons
- Electricity Delivery & Energy Reliability**
Pat Hoffman

Office of Basic Energy Sciences

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Wanda Smith, Administrative Specialist

BES Budget and Planning

Katherine Chen, Financial Management
Donetta Herbert, Financial Management
Thomas Russell, Senior Technical Advisor

BES Operations

Kerry Hochberger, Program Support Specialist
Robin Hayes, Program Manager
Natalia Melcer, Program Manager
Katie Runkles, Program Analyst / BESAC*
Andy Schwartz, Senior Technical Advisor for EFRCs*

* Basic Energy Sciences Advisory Committee
* Energy Frontier Research Centers

Materials Sciences and Engineering Division

Linda Horton, Director

Teresa Crockett, Program Analyst
Vacant, Program Assistant
Ashley Dyke, Intern

Scientific User Facilities Division

James Murphy, Director

Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant

Chemical Sciences, Geosciences, and Biosciences Division

Tanja Pietraß, Director

Diane Marceau, Program Analyst
Vacant, Program Assistant
Joshua Haines, Intern

Materials Discovery, Design, and Synthesis

Arvind Kini
Vacant, P.A.

Condensed Matter and Materials Physics

Jim Horwitz
Marsophia Agnant, P.A.

Scattering and Instrumentation Sciences

Helen Kerch
Cheryl Howard, P.A.

Materials Chemistry

Craig Henderson
Michael Sennett
◆ Kelly Perry

Experimental Condensed Matter Physics

Michael Pechan

X-ray Scattering

Lane Wilson

Biomolecular Materials

Mike Markowitz

Theoretical Condensed Matter Physics

Jim Davenport
Matthias Graf

Neutron Scattering

Thiyaga P. Thiyagarajan

Synthesis and Processing Science

Bonnie Gersten

Physical Behavior of Materials

Refik Kortan
◆ Kelly Perry

Electron and Scanning Probe Microscopies

Jane Zhu
◆ Kelly Perry

Batteries and Energy Storage Hub; Technology Coordination

Craig Henderson
John Vetrano

Mechanical Behavior and Radiation Effects

John Vetrano

Experimental Program to Stimulate Competitive Research (DOE EPSCoR)

Tim Fitzsimmons

Operations

X-ray and Neutron Scattering Facilities

Peter Lee
Jim Rhyne

NSRCs **

George Maracas
★ Tof Carim

Accelerator and Detector Research

Eliane Lessner

Facilities Coordination; Metrics; Assessment

Van Nguyen

Construction

National Synchrotron Light Source-II

Phil Kraushaar

Facilities Upgrades and MIE*** Projects

Phil Kraushaar
Ed Stevens
Vacant

*** Major Items of Equipment

Fundamental Interactions

Jeff Krause
M. Kyler-Leon, P.A.

Atomic, Molecular, and Optical Sciences

Tom Settersten

Gas Phase Chemical Physics

Wade Sisk

Condensed Phase and Interfacial Molecular Science

Gregory Fiechtner

Computational and Theoretical Chemistry

Mark Pederson

Photochemistry and Biochemistry

Gail McLean
Vacant, P.A.

Solar Photochemistry

Mark Spitzer
Christopher Fecko
◆ Nada Dimitrijevic, ANL

Photosynthetic Systems

Stephen Herbert

Physical Biosciences

Robert Stack

Fuels from Sunlight Energy Innovation Hub

Christopher Fecko

Chemical Transformations

Vacant, Team Lead
Vacant, P.A.

Catalysis Science

Raul Miranda
Viviane Schwartz
▲ Chuck Peden

Separations and Analysis

Larry Rahn

Heavy Element Chemistry

Philip Wilk

Geosciences

Larry Rahn
Vacant

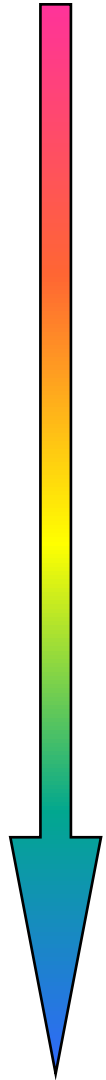
LEGEND

- ★ On detail to OSTP
- ◆ Detailee from DOE Laboratory
- ▲ IPA from BM/PNNL
- ✦ On detail to BES from FES
- P.A. Program Assistant

** Nanoscale Science Research Centers

BES Research Activities

Increasing scope and size



- **Core Research (>1,300 projects)**

Single investigators (\$150K/year) and small groups (\$500K-\$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing.

- **Energy Frontier Research Centers (32)**

\$2-4 million/year research centers for 4 year award terms; focus on fundamental research described in the Grand Challenge and Basic Research Needs Workshop reports.

- **Energy Innovation Hubs (2)**

Research centers, established in 2010 (\$15-25 million/year), engage in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an FOA. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.



BES Role for Subsurface Tech and Engineering RD&D

Activities across BES divisions relevant to subsurface science:

- Geosciences - CSGB
- Nanoscience – MSE, CSGB
- High Performance Computation – MSE, CSGB
- EFRCs – CSGB and MSE
- Advanced Tools for scattering and Imaging - SUF

Discovery Research

Use-inspired Basic Research

Applied Research

Technology Maturation & Deployment

- ◆ Microscopic basis of macroscopic complexity - scaling
- ◆ Highly reactive subsurface materials and environments
- ◆ Thermodynamics of the solute-to-solid continuum
- ◆ Computational geochemistry of complex moving fluids within porous solids
- ◆ Integrated analysis, modeling and monitoring of geologic systems
- ◆ Simulation of multi-scale systems for ultra-long times

- ◆ Mineral-fluid interface complexity and dynamics
- ◆ Nanoparticulate and colloid chemistry and physics
- ◆ Dynamic imaging of flow and transport
- ◆ Transport properties and *in situ* characterization of fluid trapping, isolation and immobilization
- ◆ Fluid-induced rock deformation
- ◆ Biogeochemistry in extreme subsurface environments

- ◆ Develop and test methods for assessing storage capacity and for monitoring containment of CO₂ storage
- ◆ Develop remediation methods to ensure permanent storage
- ◆ Demonstrate procedures for characterizing storage reservoirs and seals
- ◆ Integrated models for waste performance prediction and confirmation
- ◆ Radionuclide partitioning in repository environments.
- ◆ Waste form stability and release models.
- ◆ Incorporate new conceptual models into uncertainty assessments.

- ◆ Develop site selection criteria
- ◆ Develop storage and operating engineering approaches
- ◆ Storage demonstrations
- ◆ Apply assessment protocols and technologies for the lifecycle of projects
- ◆ Evaluate release of radionuclide inventory from the repository
- ◆ Assess corrosion/alteration of engineered materials
- ◆ Long-term safety/risk assessment for emplacement of energy system by-products.



BES-Geosciences Program (Annual Budget ~ \$20M)

Rock Physics

Electrical properties
Nonlinear elasticity
Fracturing and imaging
Signatures of fluids
Attenuation and scattering
Time-lapse imaging
Imaging porosity and permeability

Flow and Transport

Channelization
Porous and fractured media flow
Permeability evolution
Particle transport
Reactive transport
Thermal-chemical-mechanical feedbacks

Fundamental Understanding of Natural Systems – processes and rates

Natural Paradigms – for technological needs

Analytical Geochemistry

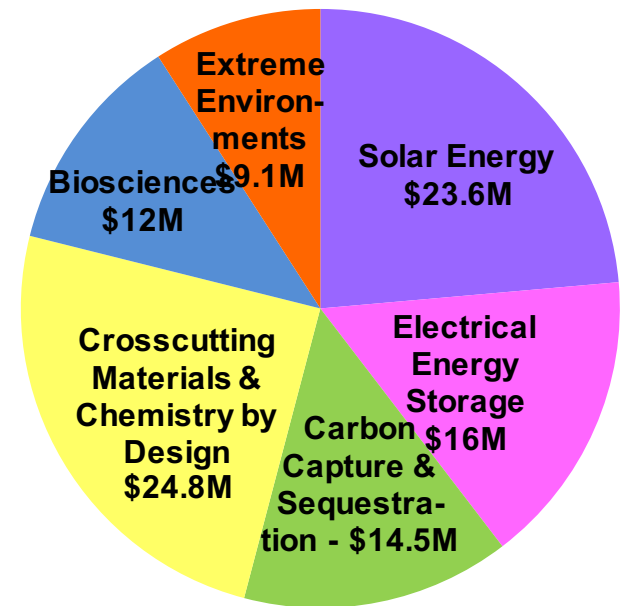
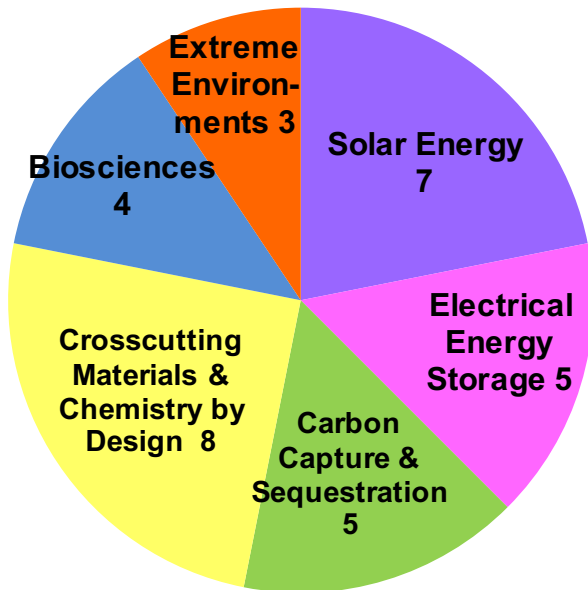
Synchrotron science
Mass spectrometry
Isotope geochemistry
Neutron science

Theoretical & Experimental Geochemistry

Computational modeling
Thermodynamics
Surface geochemistry and reactivity
Microbe-mineral interactions
Chemical imaging
Nanogeosciences

EFRCs with a Major Focus on Carbon Separation and Carbon Sequestration

- **Carbon Sequestration**
 - Lawrence Berkeley National Lab (Don DePaolo)
 - University of Texas/Sandia National Lab (Larry Lake)
 - Illinois State Geological Society at University of Illinois (Scott Frailey)
- **CO₂ Separations**
 - UC-Berkeley (Long)
 - GeorgiaTech (Walton)



BES Round Table on Foundational Research / SubTER

Purpose: In 2015 Convene National Lab, University and Industry experts in the Geosciences to brainstorm basic research area that underpin the goals of the broader SubTER technology Team efforts, and are currently underrepresented in the BES research portfolio.

- **Roundtable took place on May 22, 2015**

Grand challenge

- Imaging subsurface stress distributions and geochemical processes

Priority Research Directions

- Nanoporous geomaterials – reactivity, flow and mechanics
- Chemical-mechanical coupling in stressed rocks
- Reactive Multiphase Flow in Fractured Systems

Crosscutting themes and approaches

- Advanced computational methods for heterogeneous time dependent geologic systems
- Architected geomaterials to address heterogeneity and scaling

