U.S. DEPARTMENT OF ENERGY | Office of Science

FY 2015 President's Request
Basic Energy Sciences

ASEE Budget Briefing

March 17, 2014

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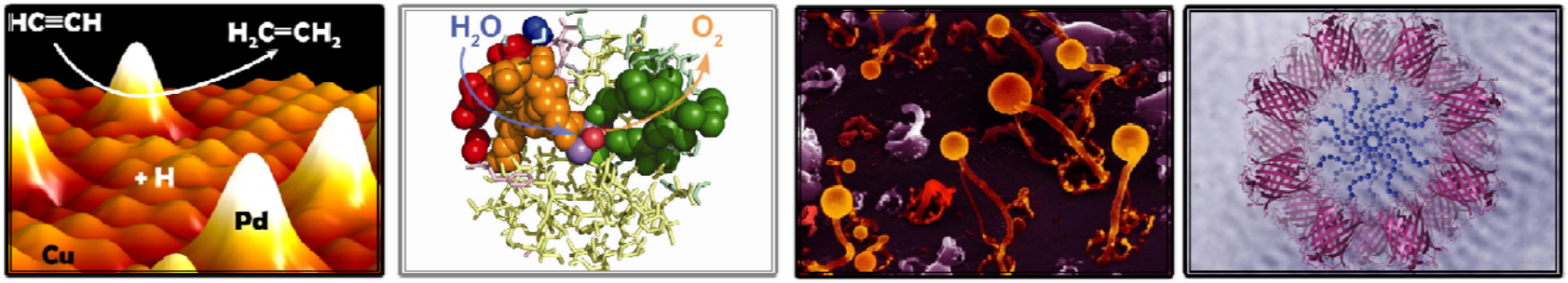
Office of Science, U.S. Department of Energy

Basic Energy Sciences

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels

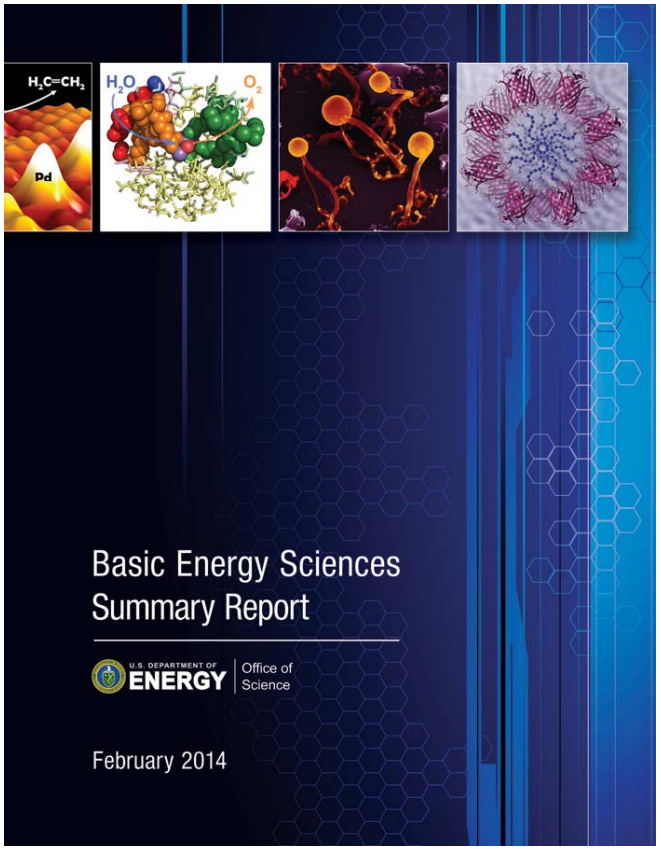
FY 2015 Budget Highlights:

- New **computational materials research** will develop codes for design of functional materials.
- **Energy Frontier Research Centers** (EFRCs) continue at the FY 2014 level.
- Two **Energy Innovation Hubs** continue:
  - Joint Center for Artificial Photosynthesis (JCAP) will be in its fifth project year.
  - Joint Center for Energy Storage Research (JCESR) will be in its third year.
- **National Synchrotron Light Source-II** (NSLS-II) transitions to operations; NSLS ceases operations.
- **Linac Coherent Light Source-II** (LCLS-II) construction continues.
- BES **user facilities** operate at optimum levels.
- Two **major items of equipment**: NSLS-II Experimental Tools (NEXT) and Advanced Photon Source Upgrade (APS-U).
- **Lujan Neutron Scattering Center** ceases operations.



Information on BES-supported Activities

- **BES 2014 Summary Report**
  - Update to the 2011 Summary Report
  - Overview of BES
  - How BES does business
  - Descriptions of all three BES divisions, EFRCs, and Hubs
  - Representative research highlights from the BES divisions, EFRCs, and Hubs



- **BES Core Research Activities (CRAs)**
  - Updated to reflect current portfolio descriptions, accomplishments, and challenges

http://science.energy.gov/bes/research/

FY 2015 BES Budget Request

Research programs

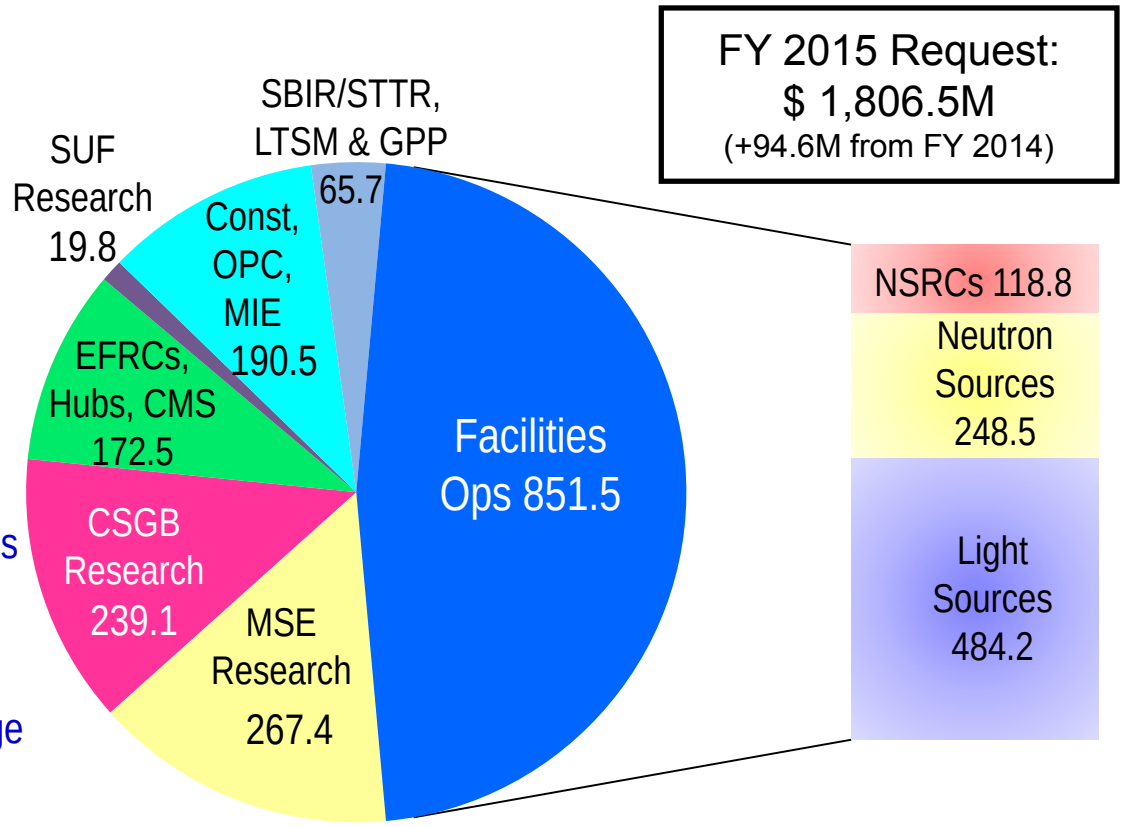
- Energy Innovation Hubs & Energy Frontier Research Centers are funded at FY 2014 levels
- Core Research approximately flat with FY 2014
- Computational Materials Sciences ($24.2M)

Scientific user facilities

- All full operating facilities at optimal operations
- NSLS-II transition to full operations ($115M)
- NSLS & Lujan cease operations; funding requested to transition facilities to safe storage

Construction and instrumentation

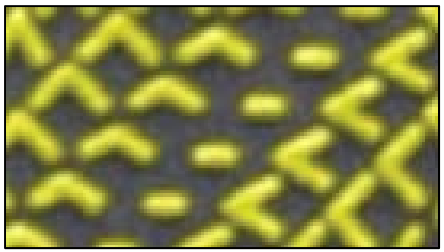
- NSLS-II instrumentation (NEXT) ($22.5M)
- Advanced Photon Source upgrade ($20M)
- Linac Coherent Light Source-II ($138.7M + $9.3M OPC)



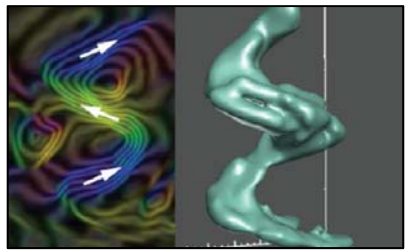
Computational Materials Sciences
Accelerating Materials Discovery and Development

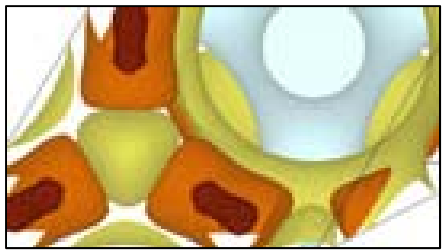
Deliverable: Open-source community codes and software packages that incorporate multiple length and time scales for discovery and prediction of materials functionality

- Deliver research codes and data for design of functional materials to the materials sciences communities in academia, labs, and industry
- Use integrated teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication
- Use facilities and tools for materials synthesis, characterization, simulation, and computation, relying especially on the SC scientific user facilities
- Support will begin in FY 2015 for up to 4 teams for multi-year awards

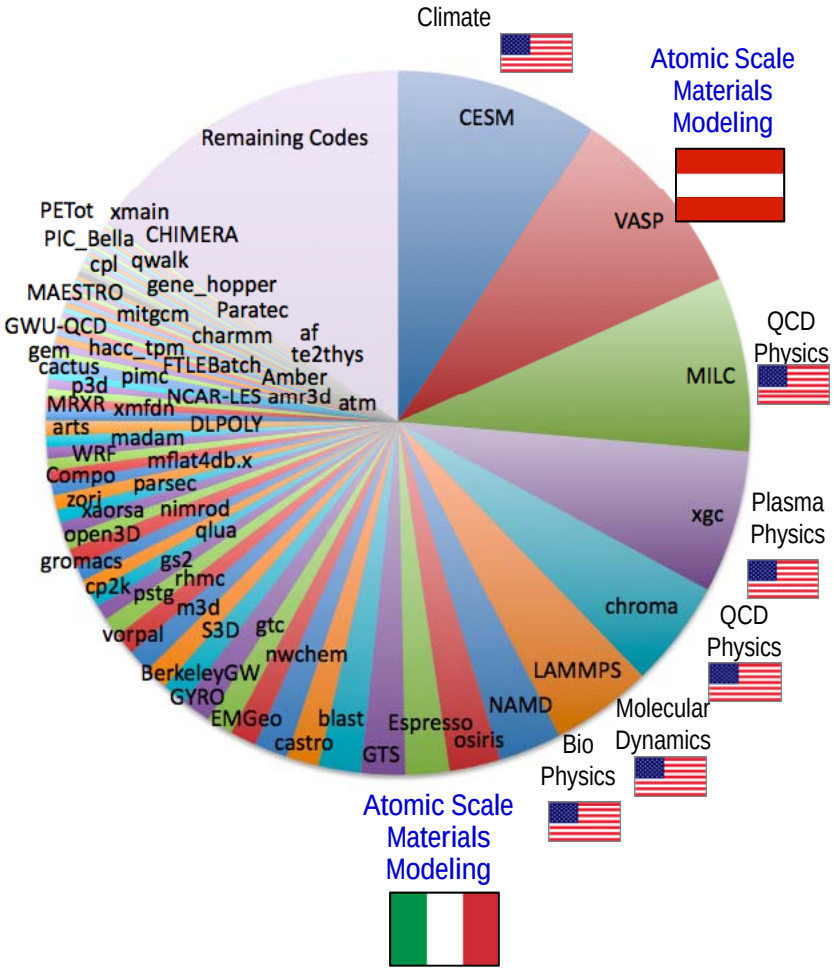

Tailored Surfaces for Advanced Electronics


Novel Thermal Transport


Next Generation Magnets


Enhanced Light Absorption

Software is key to US Leadership in Materials Sciences



2012 Top Application Codes at NERSC

Today – US trails Europe in computational codes for materials discovery and engineering

- For materials users at NERSC, the most used code is VASP
  - Atomic scale materials modeling
  - Commercial code (users have to have their own purchased license) from Austria
- Espresso, a popular materials modeling code, was developed by Italy.
- Top codes for other fields used at NERSC were developed in the U.S. and are all free, community codes.
- Another materials software package in wide use in over 70 countries to calculate thermodynamic data, largely in metals, is Thermo-Calc
  - From Sweden, commercially available for 25 years

Future – US-developed materials sciences software can inform future development of high performance computing, including the path to exascale

Computational Materials Sciences
What is Different?

- Will move theory and computation from research-use by experts to more general use by the community --- then industry
- Will fund teams of theorists and experimentalists with the express purpose of accelerating the development of multiscale, validated computational software
  - Fill in theoretical and scientific knowledge gaps
    - Current codes fail for strategic functional materials – magnets, thermal materials, superconductors, advanced semiconductors
  - Open source software, maintained for broad-use
    - Enhance speed and complexity by taking full advantage of super computers at the petascale and beyond
- Builds on the current portfolio of theory research and experimental characterization facilities, including user facilities
  - Seamlessly integrate codes with databases of validated information from both theory and experiments
- Will provide U.S. computational software for materials discovery – restoring the U.S. as a leader in the field

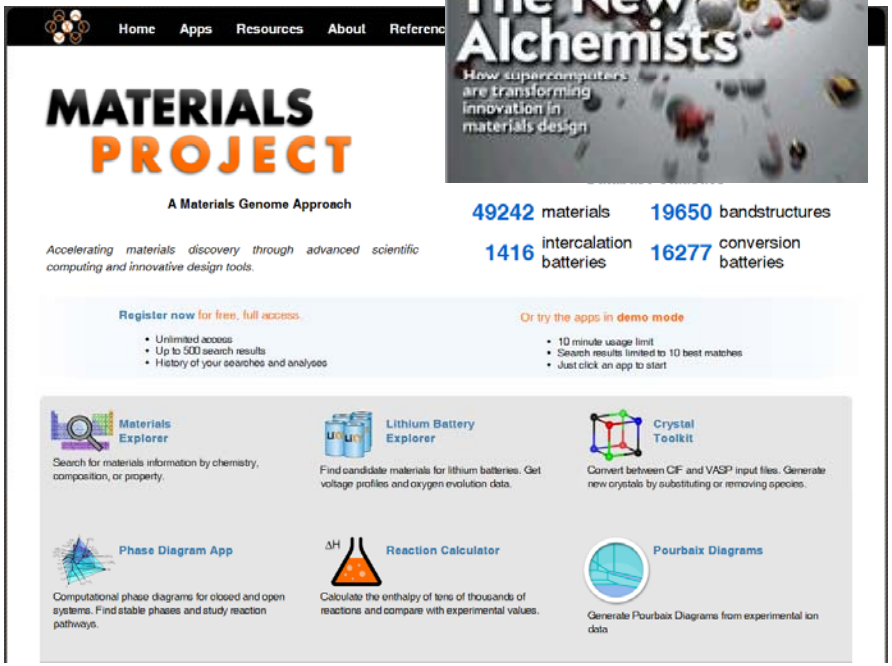
Management of BES Research Software

- Transparency & 'Open Source'
  - The goal is to enable broad availability and access to software and the associated databases developed under BES funding
  - Transparency is required for verification & validation, uncertainty quantification

- Possible Modes of Implementation:
  - Freely distributed software via the web
  - Open Source Software available under GNU or other public license
  - Available through DOE's Energy Science and Technology Software Center (ESTSC) using DOE standard software licenses
  - Commercial licensing may be an option pending additional DOE review and approval

Computational Materials Sciences: Example of Early Success – The Materials Project

- The Materials Project, a current BES supported research activity, is leading the discovery of new oxides and materials for batteries
  - Free resource for the community
  - Performs calculations for new compounds
  - Mines existing data through comprehensive collections of calculated and experimental data
  - Utilizes NERSC and the VASP code
- Opportunity for Computational Materials Sciences to replace the VASP code with better community code
- Capabilities are expanding with the JCESR Hub
  - Developing an “electrolyte genome”
  - Data from characterization and theory-modeling-computation



Joint Center for Energy Storage Research

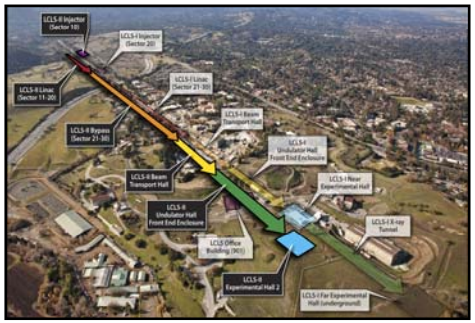
An Energy Innovation Hub led by Argonne National Laboratory

Maintaining World Leadership in Light Sources

Upgrades and Instrumentation Ensure that the Facilities Remain at the Top

National Synchrotron Light Source-II (NSLS-II)

- No construction funding request in FY 2015. CD-4 in 1Q FY2015. Start operations with six project beamlines.
- NSLS-II instrument MIE (NEXT) FY 2015 request $22.5M. CD-3 expected April 2014. Deliver 5-6 beamlines by FY 2017.
- NSLS Facility operation ceases in FY 2014 and will transition to safe storage in FY 2015. NSLS-II FY 2014 early operations $56M. FY 2015 request $115M for operations.



Linac Coherent Light Source-II (LCLS-II)

- High repetition rate, ultra-bright, transform limited x-ray pulses with expanded energy range (200eV – 5keV), polarization control, and control pulse length down to ~1 femtosecond.
- New 4 GeV superconducting linac feeding two new independently tunable undulators and enhanced experimental stations.
- FY 2014 $85.7M; FY 2015 request $148M for R&D, design, prototyping, long lead procurement, and construction of technical systems.

Advanced Photon Source Upgrade (APS-U)

- Currently implementing recommendations from the July 2013 BESAC Report through initial design and component prototyping for installation of a Multi-Bend Achromat magnetic lattice.
- FY 2014 $20M; FY 2015 Request $20M for R&D, design, and limited prototyping.

Architectural Design of Graphene Electrodes: From Theory to New Materials and Technology

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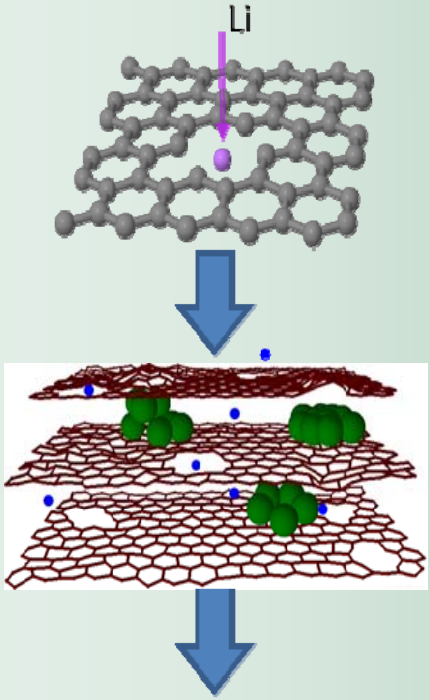
Energy Frontier Research Center



Theory inspired the development of a 'holey' graphene composite where vacancy defects enable facile Li diffusion in electrodes.

Predicted behavior was realized with the encapsulation of silicon nanoparticles (green spheres) in graphene papers leading to near-theoretical capacity with excellent rate capabilities and improved cycling.
Zhao, et al. *ACS Nano*, 2011, 5(11), 8739.

Technology shown to be compatible in a full cell configuration of a Li ion battery (coin cell-sized anode material shown)

Center for Electrical Energy Storage (CEES)

Argonne NATIONAL LABORATORY · ILLINOIS · NORTHWESTERN UNIVERSITY

Manufacturing/ Commercialization

SiNode SYSTEMS

EFRC student-led start up
(Cary Hayner is Chief Technology Officer)

- Won >$1M in start up capital
- Winner of the 2013 DOE National Clean Energy Business Plan Competition
- Winner of the 2013 Rice Business Plan Competition

http://www.youtube.com/watch?v=OnMKuXjkj2o

Field-Structured Composites for Chemical Sensors

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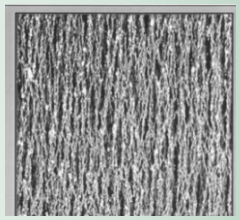
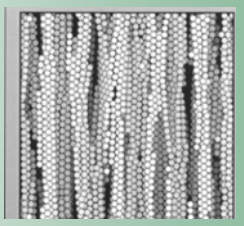
Magnetic fields reproducibly create a network of conducting magnetic particles in an insulating polymer that is acutely sensitive to volume changes of the resulting composite.

Network of chains formed by a uniform uniaxial magnetic field

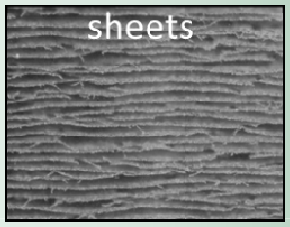
Experimental images

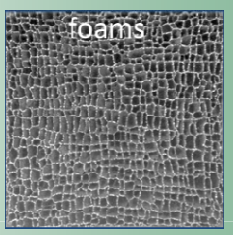




Simulation images

Views normal to the applied field

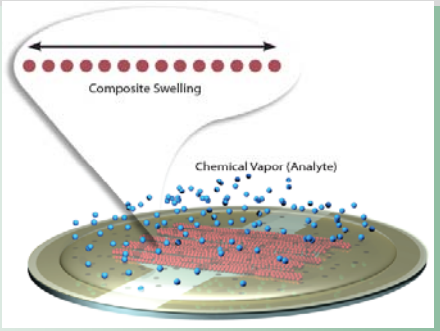




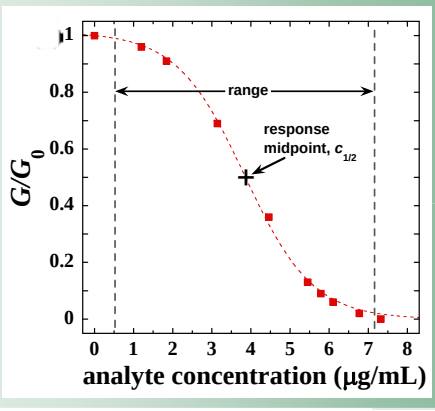
Other complex structures formed by biaxial and triaxial magnetic fields

Applied R&D

Chemical vapors were found to swell the polymer, disrupting the electrical contacts and effecting a conductor-to-insulator transition. This chemically induced switching can be used as a chemical sensor.



Normalized conductance curve



Manufacturing/ Commercialization

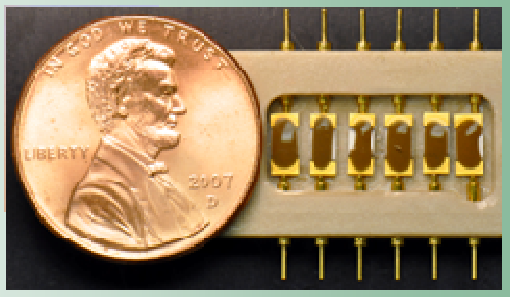
This research established a new class of composite materials and led to numerous patents and collaborations with companies licensing the technology.

Patents

8 Patents/Applications (four issued)

Patent Licensing Activity

Patents licensed by Smiths Detection and EmNet LLC for sensor applications. Two more companies are in license negotiations (names proprietary).



Sandia National Laboratories

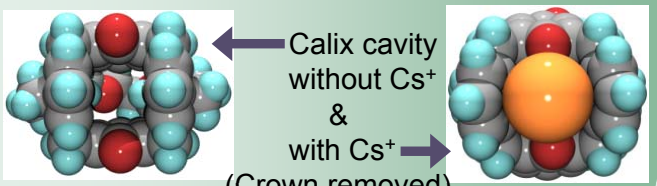
Science Speeds Nuclear Waste Clean-up
From Chemistry Nobel Prize to $Billions Saved

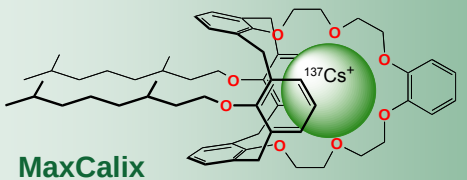
Basic Science

Sustained BES support in separations science

1987 Noble Prize in Chemistry
Host-guest molecular complexes by design
CJ Pederson, JM Lehn, DJ Cram

Basic research in synthesis, thermodynamics, binding & extraction leads to molecular host-guest approaches for cesium (Cs^+) extraction





MaxCalix

Applied R&D

DOE Environmental Management supports DOE Labs, industry, and academia

Caustic-Side Solvent Extraction (CSSX) developed using calix host for radioactive Cs^+ waste

Validation of CSSX in hot cell

Further improvements with Next Generation Caustic-Side Solvent Extraction (NGS)

Since January 2014, NGS successfully processed over 20,000 gallons of radioactive cesium waste

Enables processing of 1M gal/yr

Manufacturing/ Commercialization

Modular CSSX Unit at the Savannah River Site (SRS) currently using NGS

$1.6B SRS Salt Waste Processing Facility (SWPF) operational in 2016

NGS in SWPF will enable:

- faster waste processing
- improved Cs^+ removal efficiency
- reduced life-cycle costs for >30M gal.

➢ **$Billions Saved**

PARSONS

Catalytic Exhaust After-Treatment

From Molecular-Level Understanding to Emissions Reductions

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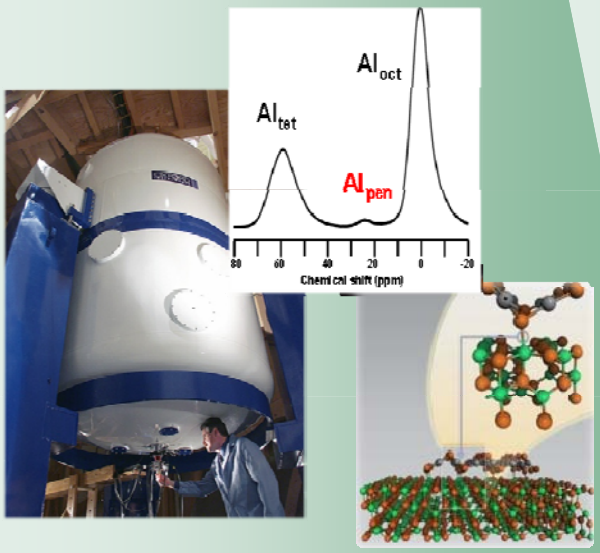
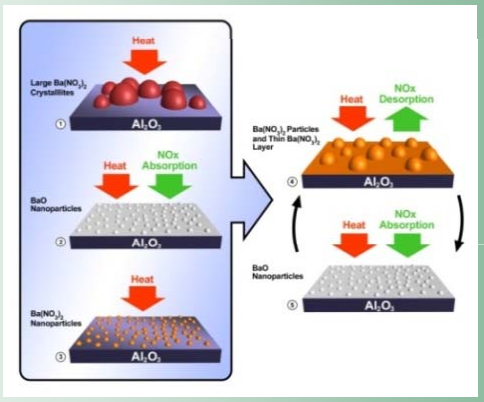


Ultra-high field magnetic resonance spectroscopy enabled fundamental research on trapping nitrogen oxide (NOx) pollutants using a lean NOx trap catalyst made with barium and platinum supported by aluminum oxide.

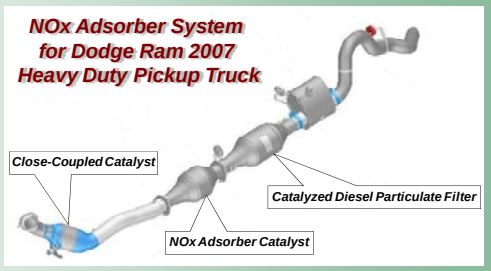
Applied R&D EERE



Issues of long-term structural stability were identified and resolved in collaboration with industrial partners.

Emission Control CRADAs with:
Ford, GM, Dow, GE, Cummins, Johnson Matthey, Caterpiller, PACCAR

Commercialization Cummins & Johnson Matthey



The lean NOx trap technology used as an after-treatment on Cummins ISB diesel engine on Dodge Ram pickup in 2007 met 2010 emissions standards 3 years early.

More than 200,000 sold.