



U.S. DEPARTMENT OF
ENERGY

Office of
Science

FY 2012 budget Presentation for DOE's Office of Science

March 3, 2011

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www.science.doe.gov

Office of Science

Science to Meet the Nation's Challenges Today and into the 21st Century

The Frontiers of Science

- Supporting research that led to over 100 Nobel Prizes during the past 6 decades—22 in the past decade alone
- Providing 45% of Federal support of basic research in the physical sciences and key components of the Nation's basic research in biology and computing
- Supporting over 27,000 Ph.D.s, graduate students, undergraduates, engineers, and support staff at more than 300 institutions

21st Century Tools of Science

- Providing the world's largest collection of scientific user facilities to over 26,000 users each year

Science, Innovation, and DOE's Office of Science

- Science is the basis of technology and underpins all of the work of DOE.
- Science of the 20th century brought us the high standard of living we now enjoy. Today, we are laying the foundations for the new technologies of the coming decades.
- Progress in science and technology depends on continuing advances in, and replenishment from, basic research, which is the federal government's—and SC's—special role.
- A highly trained work force is required to invent the future—scientists and engineers trained in the most modern science and technologies and with access to the best tools.

Our Generation's Sputnik Moment



Remarks of President Barack Obama
State of the Union Address to the Joint Session of Congress
Tuesday, January 25, 2011

“This is our generation's Sputnik moment. Two years ago, I said that we needed to reach a level of research and development we haven't seen since the height of the Space Race.

...[this] budget to Congress helps us meet that goal. We'll invest in biomedical research, information technology, and especially clean energy technology—an investment that will strengthen our security, protect our planet, and create countless new jobs for our people.”



Office of Science Research Underpins the President's Goals

- The Office of Science commands an arsenal of basic science capabilities—major scientific user facilities, national laboratories, and researchers—that we are using to break down the barriers to new energy technologies.
- We have focused these capabilities on critical national needs, e.g., through the Bioenergy Research Centers, the Energy Frontier Research Centers, and the new Energy Innovation Hub—the Joint Center for Artificial Photosynthesis.

New in FY 2012: Science for Innovation and Clean Energy

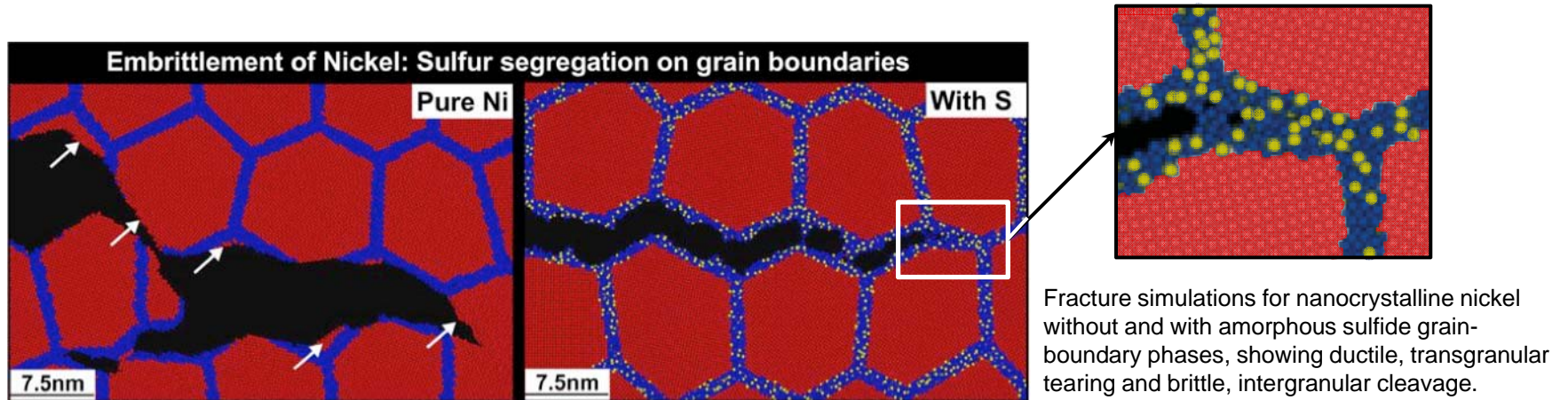
Applications of 21st century science to long-standing barriers in energy technologies: employing nanotechnology, biotechnology, and modeling and simulation

Examples:

- **Materials by design** using nanoscale structures and syntheses for: carbon capture; radiation-resistant and self-healing materials for the nuclear reactor industry; highly efficient photovoltaics; and white-light emitting LEDs.
- **Biosystems by design** combining the development of new molecular toolkits with testbeds for the design and construction of improved biological components or new biohybrid systems and processes for improved biofuels and bioproducts.
- **Modeling and simulation** to facilitate materials and chemistry by design and to address technology challenges such as the optimization of internal combustion engines using advanced transportation fuels (biofuels).

Stress Corrosion Cracking

Molecular Dynamics Simulation Reveals Mechanisms of Nickel Fracture

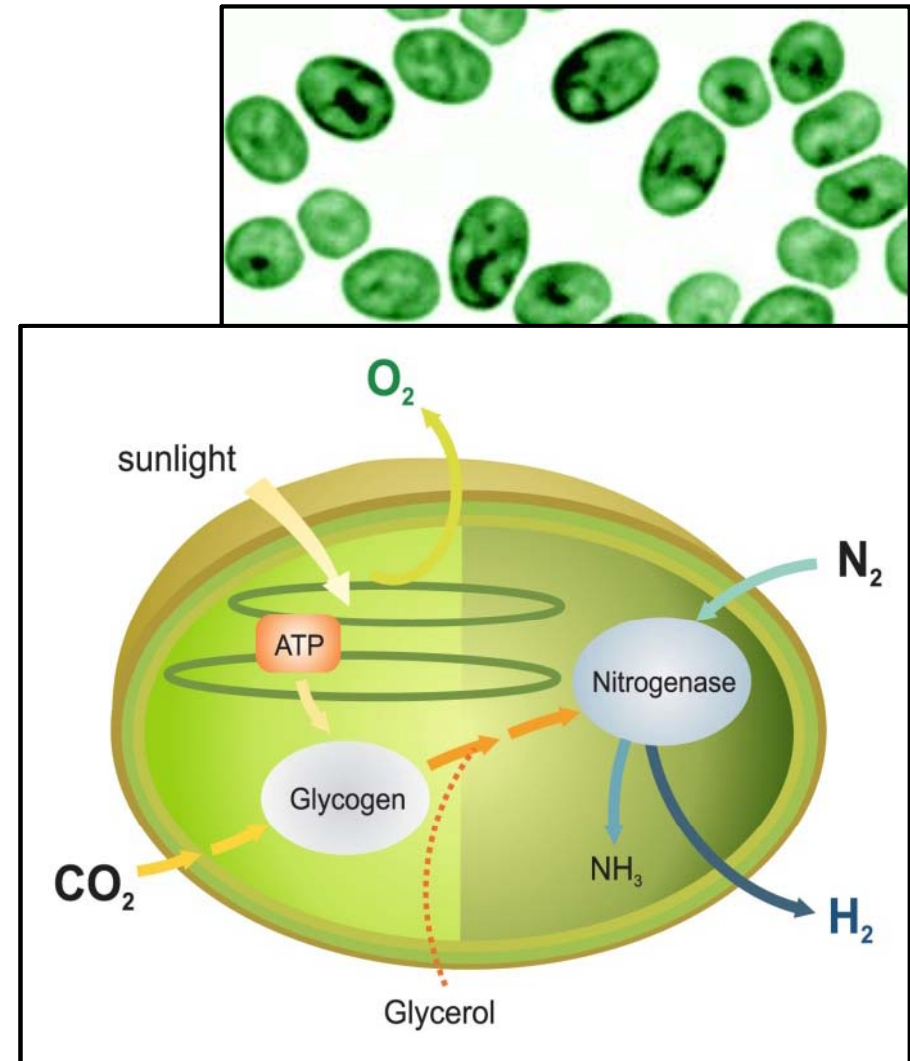


- The performance and lifetime of materials used in nuclear technology and in advanced power generation are severely limited by corrosive environments and extreme conditions.
- Premature failure of materials can result from undetected stress corrosion cracking.
- Annually, corrosion costs about 3% of the U.S. gross domestic product.
- 48-million-atom simulation on Argonne Leadership Computing Facility showed a link between sulfur impurities segregated at grain boundaries of nickel and embrittlement. An order-of-magnitude reduction in grain-boundary shear strength, combined with tensile-strength reduction, allows the crack tip to always find an easy propagation path in this configuration. This mechanism explains an experimentally observed crossover from microscopic fracture to macroscopic cracks due to sulfur impurities.



Systems Biology for Bioenergy Production

- Systems biology techniques were used to dissect how the common microbe *Cyanothece* balances photosynthesis with carbon, nitrogen, and hydrogen metabolism.
- Although oxygen is toxic to the enzymes involved in ammonia and hydrogen production, *Cyanothece* is unique in generating both in the presence of air and while producing O_2 as a byproduct of photosynthesis.
- These results suggest metabolic engineering this microbe for enhanced production of hydrogen, biodiesel, or other biofuels using only water and sunlight and without the need for added fertilizers.



Modeling and Simulation at the Petascale



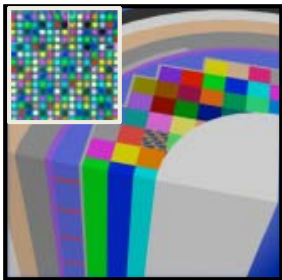
Argonne Leadership Computing Facility



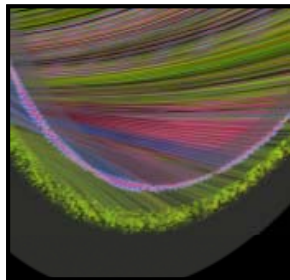
Oak Ridge Leadership Computing Facility

In FY 2012, the Argonne LCF will be upgraded with a 10 petaflop IBM Blue Gene/Q. The Oak Ridge LCF will continue site preparations for a system expected in FY 2013 that will be 5-10 times more capable than the Cray XT-5.

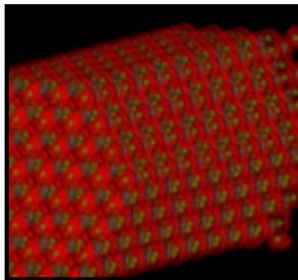
- The Cray XT5 ("Jaguar") at ORNL and the IBM Blue Gene/P ("Intrepid") at ANL will provide ~2.3 billion processor hours in FY12 to address science and engineering problems that defy traditional methods of theory and experiment and that require the most advanced computational power.
- Peer reviewed projects are chosen to advance science, speed innovation, and strengthen industrial competitiveness.
- Demand for these machines has grown each year, requiring upgrades of both.
- Among the topics in FY2011:
 - Advancing materials for lithium air batteries, solar cells, and superconductors
 - Exploring carbon sequestration
 - Improving combustion in fuel-efficient, near-zero-emissions systems
 - Understanding how turbulence affects the efficiency of aircraft and other transportation systems
 - Designing next-generation nuclear reactors and fuels and extending the life of aging reactors
 - Developing fusion energy systems
 - Understanding the roles of ocean, atmosphere, land, and ice in climate change



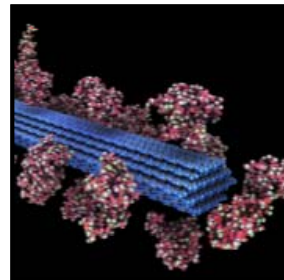
Nuclear Reactor Simulation



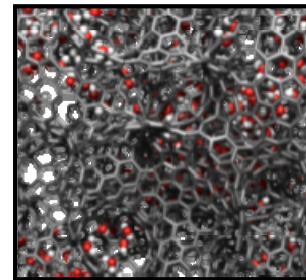
Fusion Plasmas



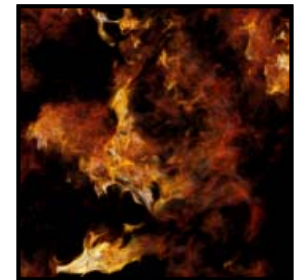
Nanoscale Science



Biofuels



Energy Storage Materials



Turbulence



Office of Science FY 2012 Budget Request to Congress

(dollars in thousands)

	FY 2010 Current Approp.	FY 2011 President's Request	FY 2011 Full Year CR	FY 2012 President's Request	FY 2012 vs. FY 2010	
Advanced Scientific Computing Research	383,199	426,000	394,000	465,600	+82,401	+21.5%
Basic Energy Sciences	1,598,968	1,835,000	1,636,500	1,985,000	+386,032	+24.1%
Biological and Environmental Research	588,031	626,900	604,182	717,900	+129,869	+22.1%
Fusion Energy Sciences	417,650	380,000	426,000	399,700	-17,950	-4.3%
High Energy Physics	790,811	829,000	810,483	797,200	+6,389	+0.8%
Nuclear Physics	522,460	562,000	535,000	605,300	+82,840	+15.9%
Workforce Development for Teachers and Scientists	20,678	35,600	20,678	35,600	+14,922	+72.2%
Science Laboratories Infrastructure	127,600	126,000	127,600	111,800	-15,800	-12.4%
Safeguards and Security	83,000	86,500	83,000	83,900	+900	+1.1%
Science Program Direction	189,377	214,437	189,377	216,863	+27,486	+14.5%
Subtotal, Office of Science	4,721,774	5,121,437	4,826,820	5,418,863	+697,089	+14.8%
Small Business Innovation Research/ Technology Transfer (SBIR/STTR) (SC portion)	107,352	-107,352	-100.0%
Congressionally-directed projects	74,737	-74,737	-100.0%
Undistributed	76,890
Use of prior year balances	-153	-2,749	-2,596	-1,696.7%
Subtotal, Office of Science	4,903,710	5,121,437	4,903,710	5,416,114	+512,404	+10.4%
SBIR/STTR (transfer from other DOE programs)	60,177	-60,177	-100.0%
Total, Office of Science	4,963,887	5,121,437	4,903,710	5,416,114	+452,227	+9.1%

Continuing Resolution (CR) column reflects the current CR (P.L. 111-322), annualized to a full year. Funding amounts reflect the FY 2010 appropriation level prior to the SBIR/STTR transfer. Funding on the undistributed line reflects FY 2010 Congressionally directed project funding prior to the SBIR/STTR transfer.

Science for Clean Energy: Materials by Design

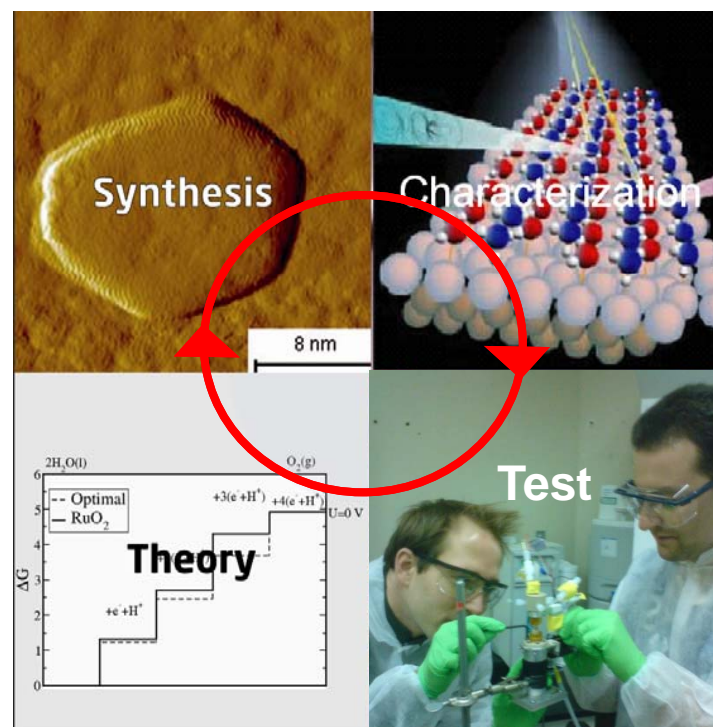
- Research to establish materials design rules to launch an era of predictive modeling, changing the paradigm of materials discovery from serendipity to rational design.
- Discovery of new materials has been the engine driving science frontiers and fueling technology innovations. The U.S. has the world's most powerful suite of tools for materials synthesis, characterization, and computation.

- Research Focus:

Synthesis: Rational molecular-scale design guided by simulation.

Characterization and Testing: Verify & validate computational designs and software, including in situ measurements using x-ray, neutron, microscopy, and nanoscience facilities.

Theory/Simulation: New methods and algorithms for complex, multi-scale systems. Development of software and toolkits through a networked, broad community. Emphasis areas include: catalysis, light-weight materials, and materials for energy applications including radiation-resistant materials, carbon capture, batteries, liquid fuels, and photocatalysis.

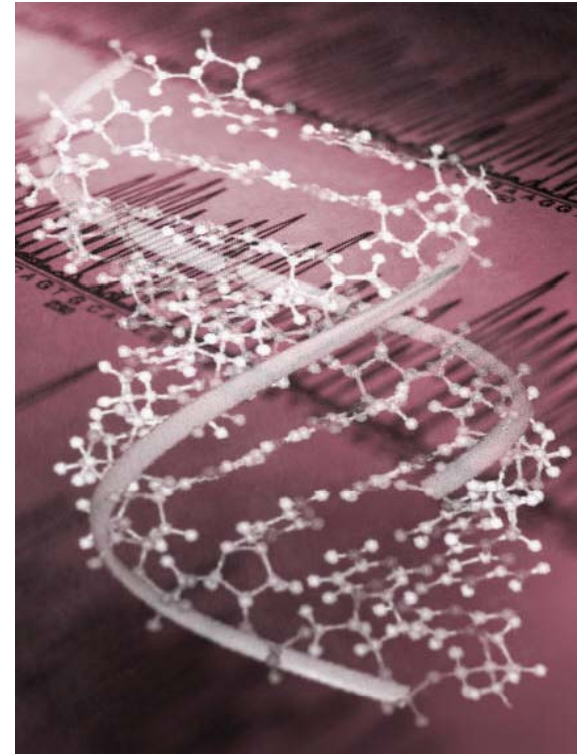


Science for Clean Energy: Biosystems by Design

- Research to establish biological design rules to enable the predictive design of innovative natural and hybrid systems for clean energy production.
- Discovery and synthetic redesign of plant and microbial systems pushes science frontiers and paves the way for sustainable production of advanced biofuels and bioproducts. Leverages strong U.S. resources and leadership in fundamental biological research and industrial biotechnology.
- Research focus:

Synthesis: New methods for high-throughput data acquisition to catalogue components of biological systems. Develop genetic toolkits to measure rates and magnitudes of processes, and identify regulatory control points in metabolic pathways and cellular networks. Apply fundamental biological design rules for predictive integration of components and processes, including potentially new cellular functions.

Characterization & Testing: Verify & validate computer-aided design toolkits for improved genetic manipulation of plants and microbes and design of hybrid biosystems, building on knowledge of the natural world. Develop new testbeds to prototype and validate performance and function.



JCAP Collaborating Energy Frontier Research Centers

Harry Atwater	Light-Material Interactions in Energy Conversion	California Institute of Technology, Pasadena, CA
Friedric B. Prinz	Center on Nanostructuring for Efficient Energy Conversion	Stanford University, Stanford, CA
Berend Smit	Center for Gas Separations Relevant to Clean Energy Technologies	UC Berkeley, Berkeley, CA
John Bowers	Center on Materials for Energy Efficiency Applications	UC Santa Barbara, Santa Barbara, CA
James Spivey	Computational Catalysis and Atomic-Level Synthesis of Materials: Building Effective Catalysts from First Principles	Louisiana State University, Baton Rouge, LA
Thomas Russell	Polymer-Based Materials for Harvesting Solar Energy	University of Massachusetts, Amherst, MA
Peter Green	Solar Energy Conversion in Complex Materials	University of Michigan, Ann Arbor, MI
Victor Klimov	The Center for Advanced Solar Photophysics	Los Alamos National Labs
Hector Abruna	Nanostructured Interfaces for Energy Generation, Conversion, and Storage	Cornell University, Ithaca, NY
Kenneth Reifsnider	Science Based Nano-Structure Design and Synthesis of Heterogeneous Functional Materials for Energy Systems	University of South Carolina, Columbia, SC
Devens Gust	EFRC Center for Bio-Inspired Solar Fuel Production	Arizona State University, Tempe, AZ
Neal R. Armstrong	Center for Interface Science: Hybrid Solar Electric Materials	University of Arizona, Tucson, AZ
Vidvuds, Ozolins	Molecularly Assembled Material Architectures for Solar Energy Production, Storage, and Carbon Capture	UC Los Angeles, Los Angeles, CA
Daniel Dapkus	Emerging Materials for Solar Energy Conversion and Solid State Lighting	University of Southern California, Los Angeles, CA
Alex Zunger	Center for Inverse Design	National Renewable Energy Laboratory, Golden, CO
Michael Thackeray	Center for Electrical Energy Storage: Tailored Interfaces	Argonne Nat'l Labs, Argonne, IL
Michael Wasielewski	Argonne-Northwestern Solar Energy Research Center	Northwestern University, Evanston, IL
Thomas Meyer	Solar Fuels and Next Generation Photovoltaics	University of North Carolina, Chapel Hill, NC
David Wesolowski	Fluid Interface Reactions, Structures and Transport Center	Oak Ridge National Labs, Oak Ridge, TN
Morris Bullock	Center for Molecular Electrocatalysis	Pacific Northwest National Laboratory, Richland, WA

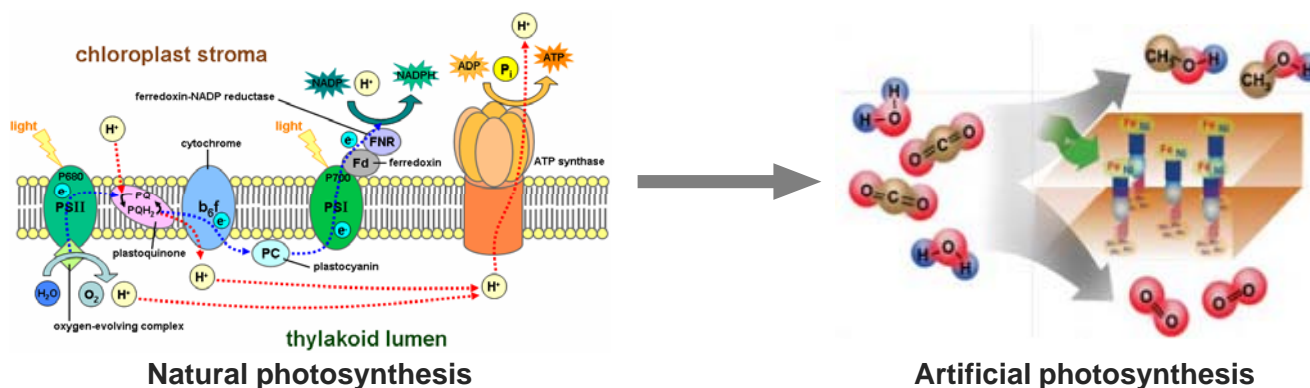


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Fuels from Sunlight Energy Innovation Hub: Joint Center for Artificial Photosynthesis (JCAP)

- The design of highly efficient, non-biological, molecular-level “machines” that generate fuels directly from sunlight, water, and carbon dioxide is the challenge.
- Basic research has provided an understanding of the complex photochemistry of the natural photosynthetic system and the use of inorganic photo-catalytic methods to split water or reduce carbon dioxide – key steps in photosynthesis.
- **JCAP Mission: To demonstrate a scalable, manufacturable solar-fuels generator using Earth-abundant elements, that, with no wires, robustly produces fuel from the sun 10 times more efficiently than (current) crops.**
- JCAP R&D focuses on:
 - Accelerating the rate of catalyst discovery for solar fuel reactions
 - Discovering earth-abundant, robust, inorganic light absorbers with optimal band gap
 - Providing system integration and scale-up
- **Begun in FY 2010, JCAP serves as an integrative focal point for the solar fuels R&D community – formal collaborations have been established with 20 Energy Frontier Research Centers.**



Batteries and Energy Storage Energy Innovation Hub

Transform the Grid and Electrify Transportation

- Improved energy storage is critical for the widespread use of intermittent renewable energy, electric vehicles, and efficient and reliable smart electric grid technologies.
- The Hub, proposed for FY 2012, will develop electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life.
- These are systemic challenges requiring new materials, systems, and knowledge.
- The Hub will address key fundamental questions in energy storage including:
 - Can we approach theoretical energy density?
 - Can we safely increase the rate of energy utilization?
 - Can we create a reversible system with minimal energy loss?
- The Hub will link fundamental science, technology, and end-users, and it will collaborate with relevant Energy Frontier Research Centers, ARPA-E and EERE



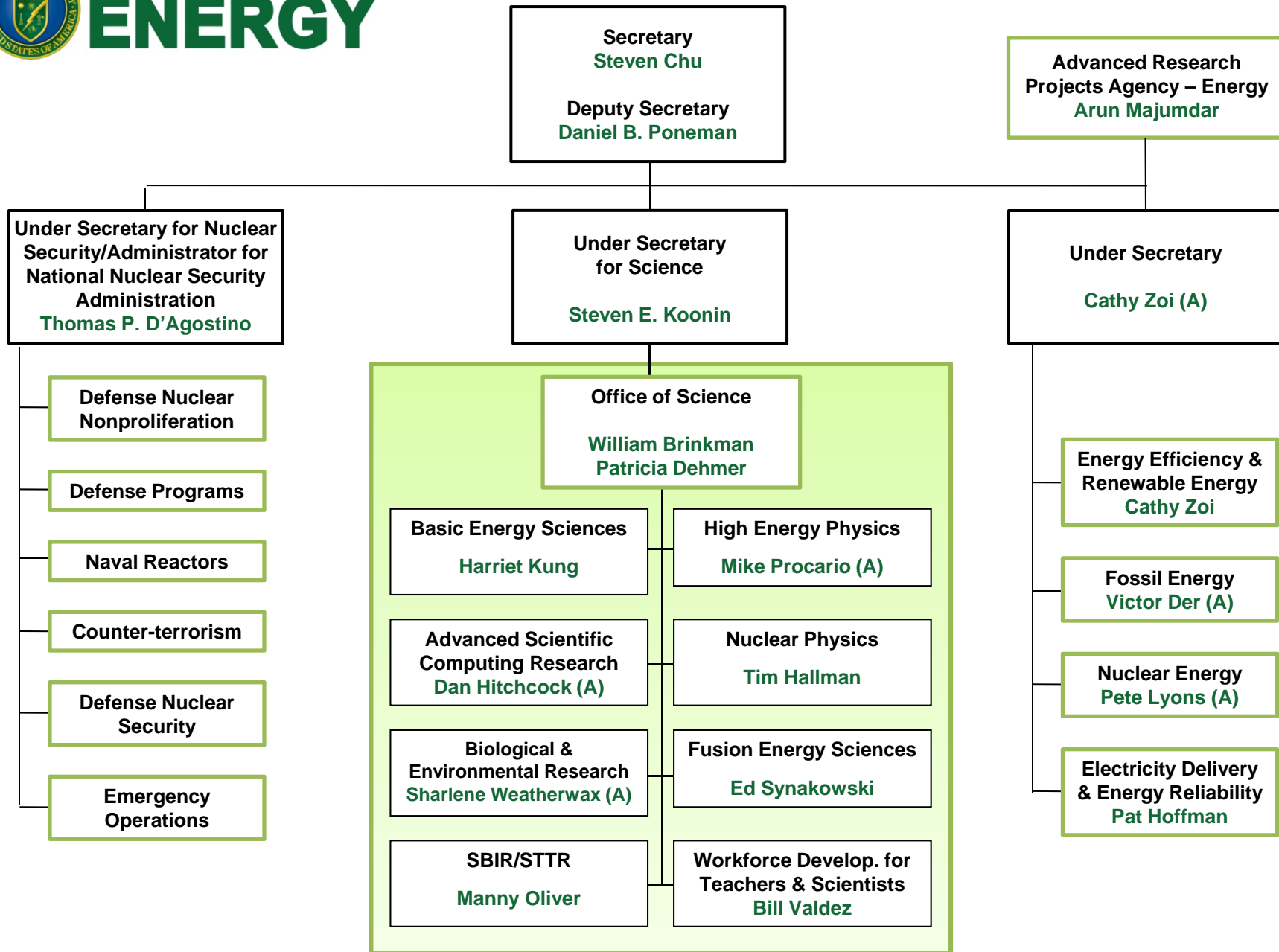
R&D Coordination

- The FY 2012 budget request includes funding for integrated R&D activities across the **Office of Science** and the DOE **technology programs**.
- The **Office of Science** will address topics for which an understanding of fundamental phenomena is required to achieve game-changing discoveries for mid-to-long-term technological innovation.
- The DOE **technology programs** will address topics in applied research, development, and deployment to gain and apply knowledge to achieve identified near-to-mid-term clean energy goals.

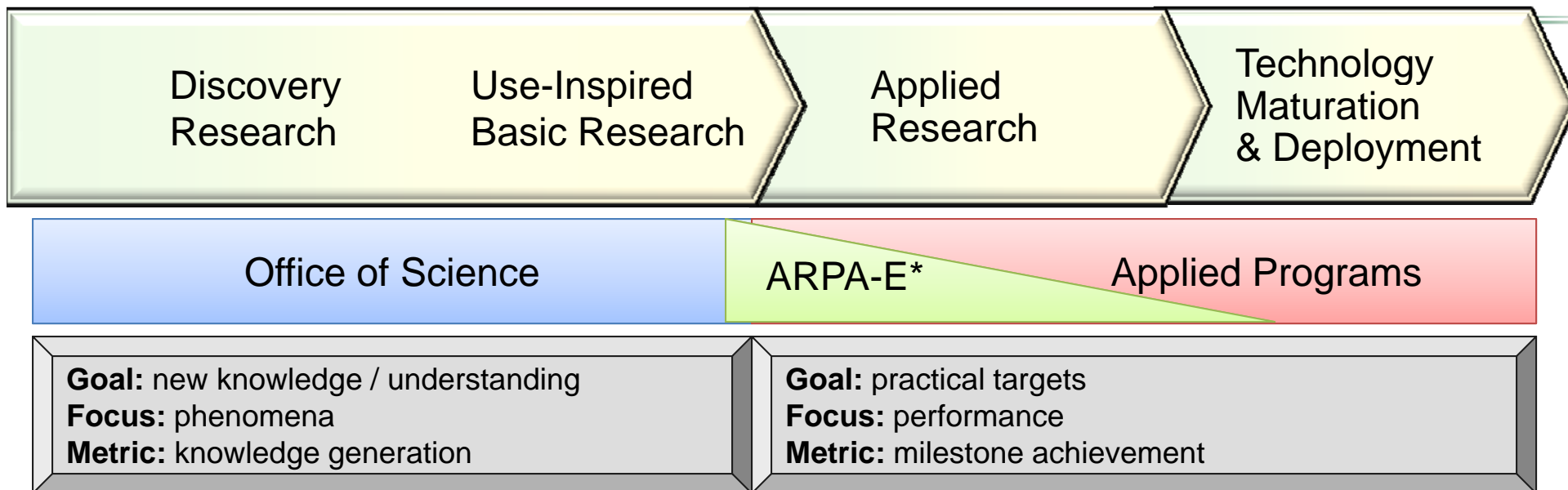




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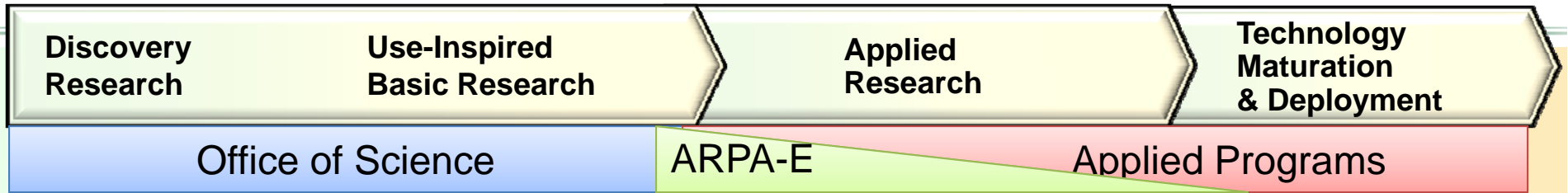
Continuum of Research, Development, and Deployment



- Basic research to address fundamental limitations of current theories and descriptions of matter in the energy range important to everyday life – typically energies up to those required to break chemical bonds.
- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies
- Basic research for fundamental new understanding, usually with the goal of addressing scientific showstoppers on real-world applications in the energy technologies
- Proof of new, higher-risk concepts
- Prototyping of new technology concepts
- Explore feasibility of scale-up of demonstrated technology concepts in a "quick-hit" fashion.
- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Scale-up research
- Small-scale and at-scale demonstration
- Cost reduction
- Manufacturing R&D
- Deployment support, leading to market adoption
- High cost-sharing with industry partners



R&D Continuum for Energy Storage (Batteries/Vehicles)



BES

- Understand and predict interfacial charge transfer and multi-body effects
- Predict and control dynamics of phase transitions
- Control of chemistry and its dynamics at electrified interfaces
- Physicochemical consequences of nano-dimensions
- Fundamentals of solvation dynamics and ionic transport

- Retrosynthetic approaches to high performance new materials
- Design of new materials capable of multi-electron storage per redox center
- Understand design criteria for electrolytes that enable higher voltages
- Tailor nanoscale electrode architectures for optimal transport
- Novel chemistries for scavenging impurities and self-healing
- Generation of knowledge and computational and experimental tools to predict properties, performance evolution, and lifetime of materials

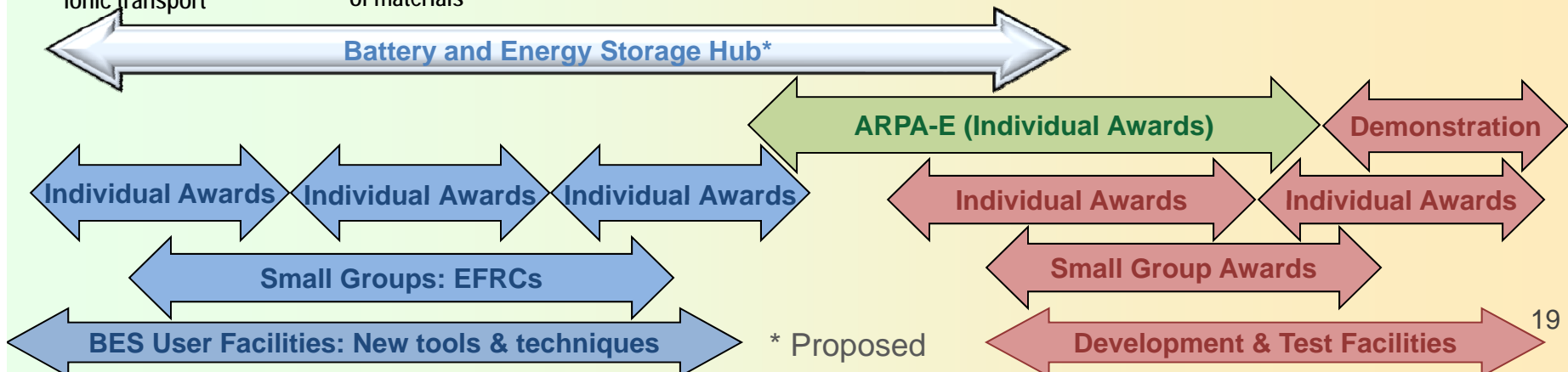
ARPA-E

- Quick scale-up feasibility tests of demonstrated new-generation battery technology concepts
- Rapid development of new technology concepts—demonstration within 1-2 years

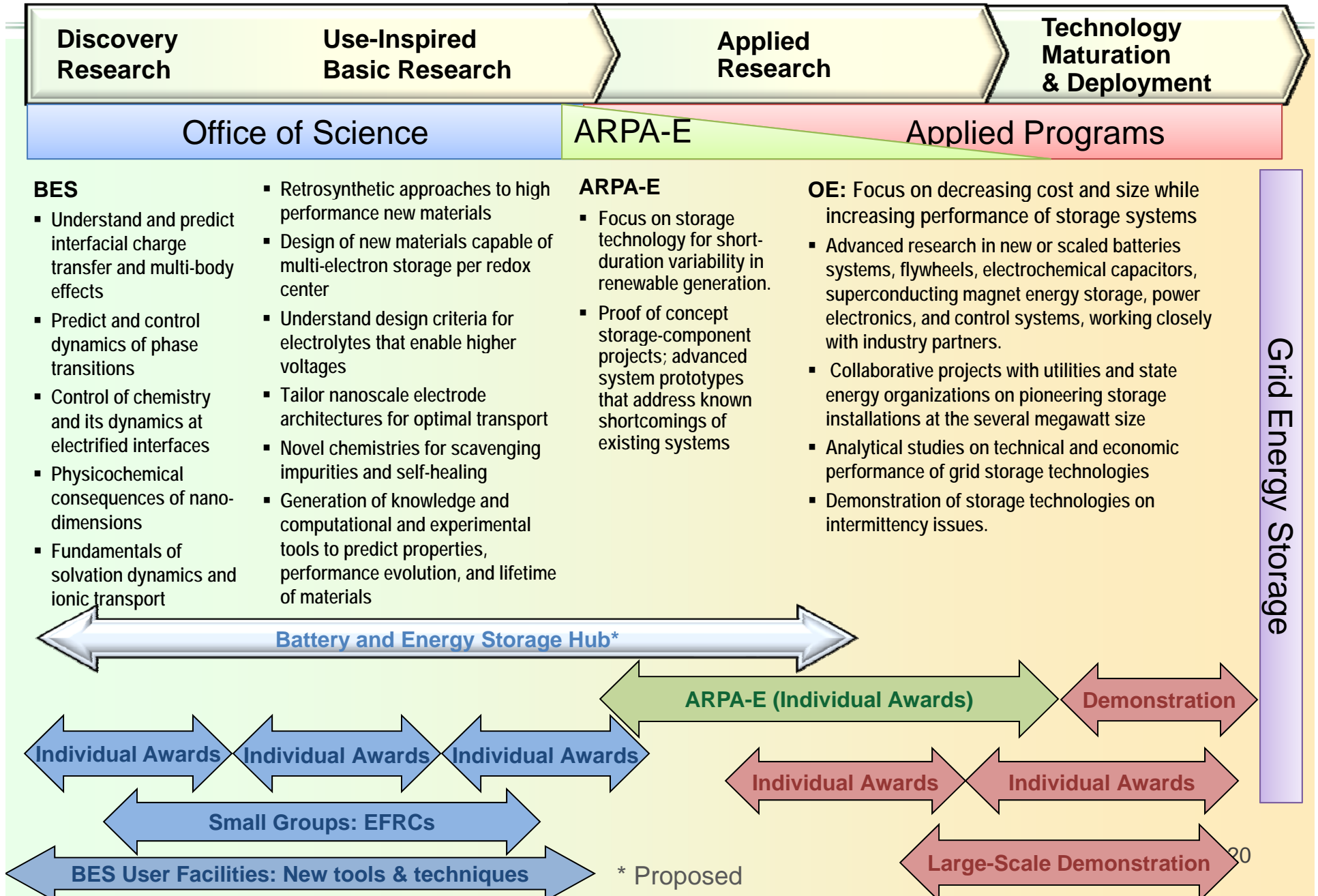
EERE: Significant focus on batteries and capacitors for vehicle applications

- Development of full battery systems and advanced materials for those systems
- Systems analysis which includes thermal analysis and simulation, various simulations to determine battery requirements, life modeling, and recycling studies
- Research, development, and engineering of higher energy advanced materials and cell chemistries that simultaneously address the life, performance, abuse tolerance, and cost issues.
- Research on inherent thermal and overcharge abuse tolerance of different Li-ion cell materials, components, and cell chemistries.

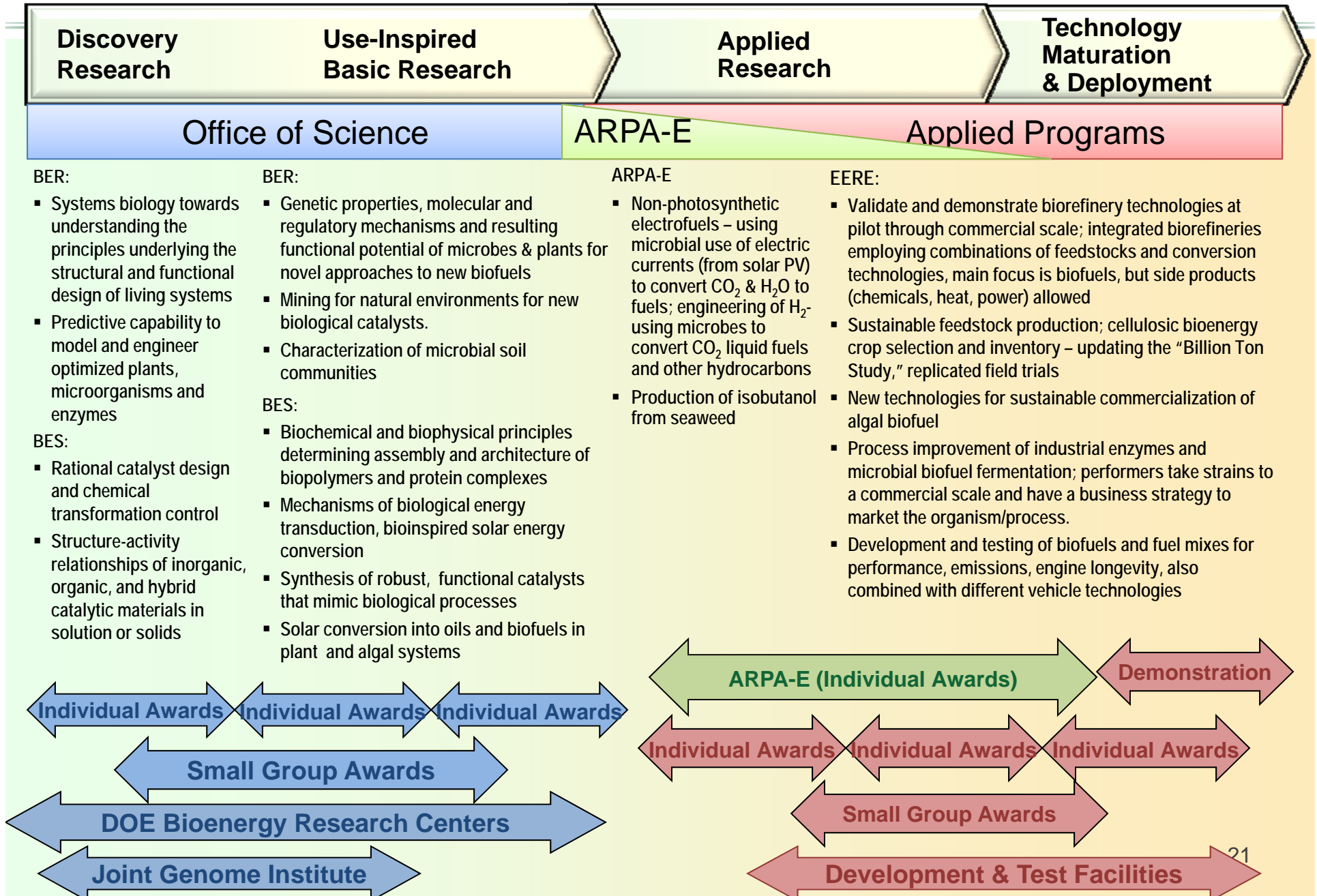
Batteries/ Vehicle Energy Storage



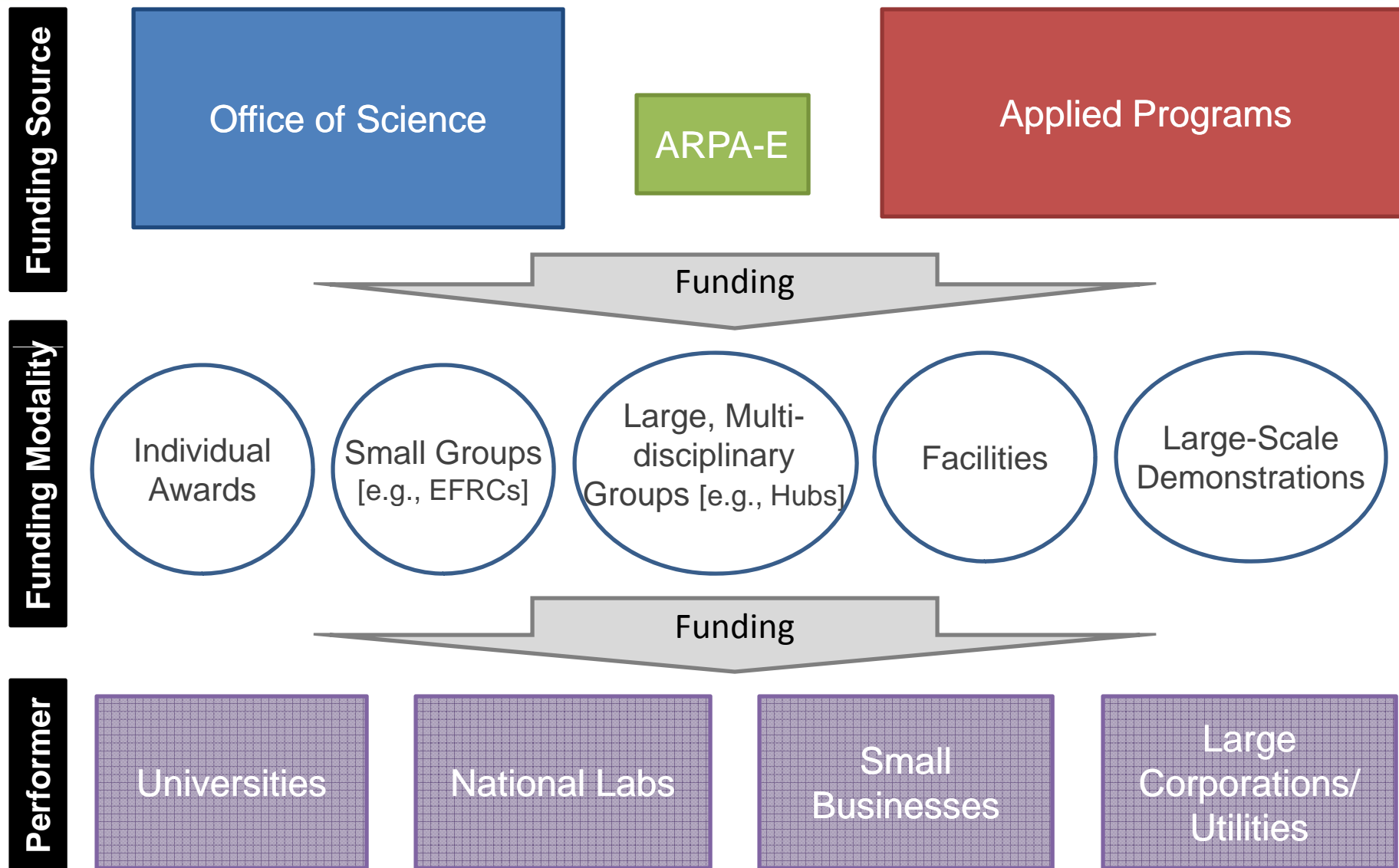
R&D Continuum for Energy Storage (Grid)



R&D Continuum for Biofuels

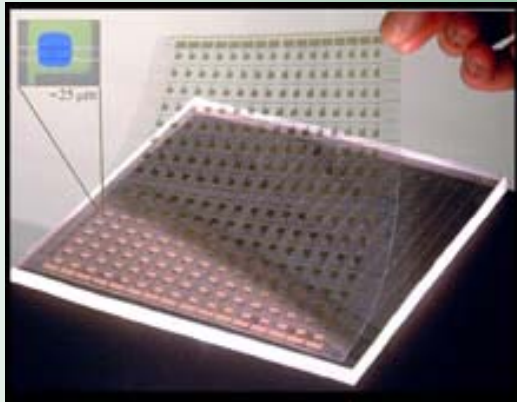


Funding Overview



Low Cost Solar Cells: From Fundamental Research to Commercialization

Basic Science



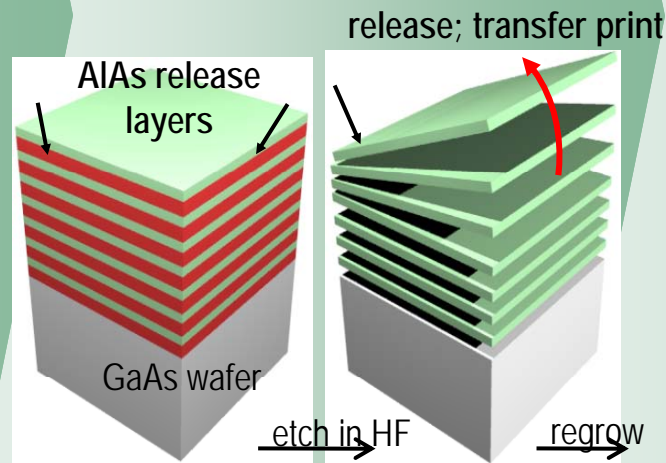
Basic research focused on materials-centric aspects of a micro-transfer printing process for single crystalline silicon and other semiconductors, dielectrics and metals.

Applied R&D

EERE Solar America Initiative:

Established new materials strategies & manufacturing methods for low-cost, high performance photovoltaic modules

GaAs epi-stacks for solar microcells



Manufacturing/ Commercialization



John Rogers, Ralph Nuzzo (co-founders)

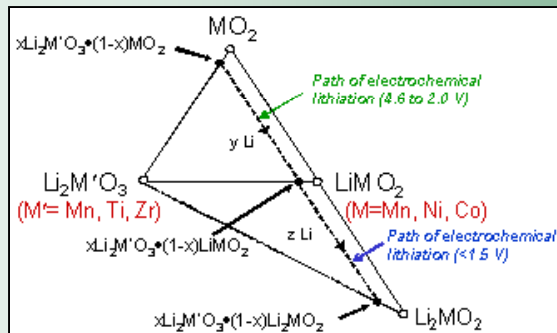
*Micro-Contact Printed
Solar Cells*

Industrial collaborations

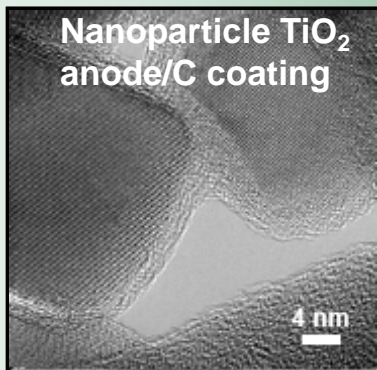


High-Energy Lithium Batteries: From Fundamental Research to Cars on the Road

Basic Science



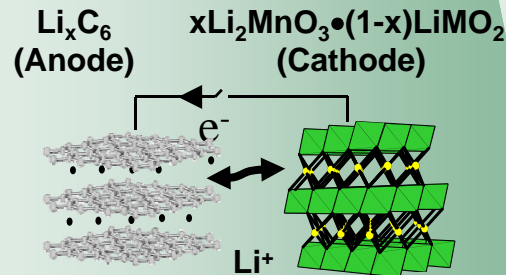
Discovered new composite structures for stable, high-capacity cathodes



Tailored electrode-electrolyte interface using nanotechnology

EFRC research

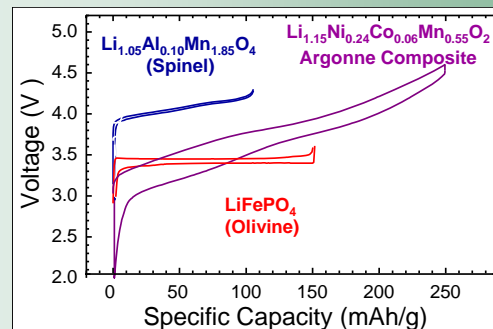
Applied R&D



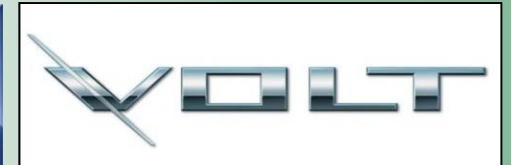
Created high energy Li-ion cells...



...with double cathode capacity, enhanced stability



Manufacturing/ Commercialization



Licenses to materials and cell manufacturers and automobile companies

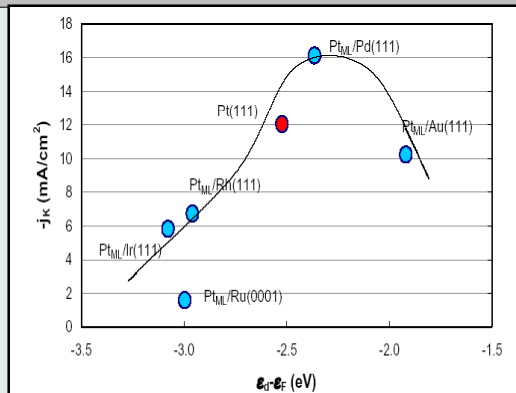
Platinum Monolayer Electro-Catalysts: Stationary and Automotive Fuel Cells

Basic Science

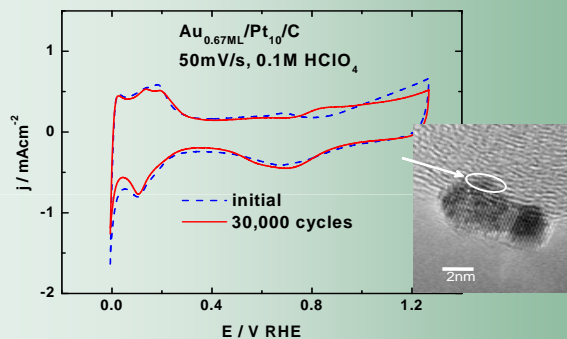
BES

Two research advances

1. Pt Monolayer catalysis – high activity with ultralow Pt mass



2. Pt stabilized against corrosion in voltage cycling by Au clusters



Science 315, 220 (2007)

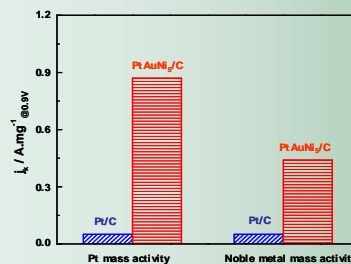
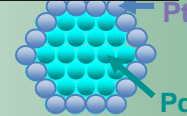
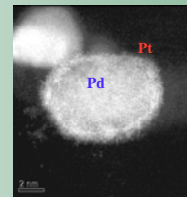
Applied R&D

BES → EERE

Core-Shell Nanocatalysts

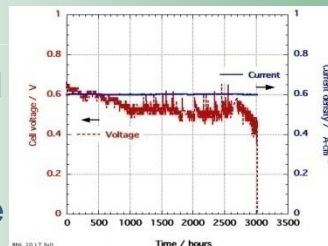
Active Pt ML shell – Metal/alloy core
Core tunes activity & durability of shell

Model and HAADF image of a Pt Monolayer on Pd nanoparticle



Pt-mass weighted activity enhanced 20x

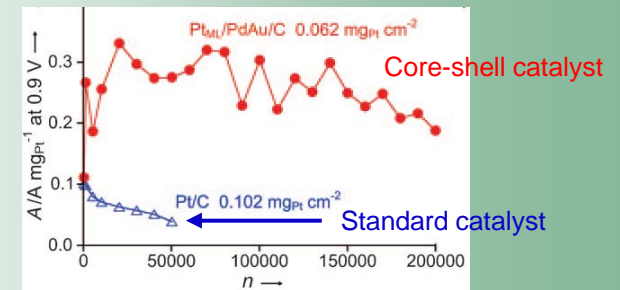
3000 hr Fuel Cell Durability Performance



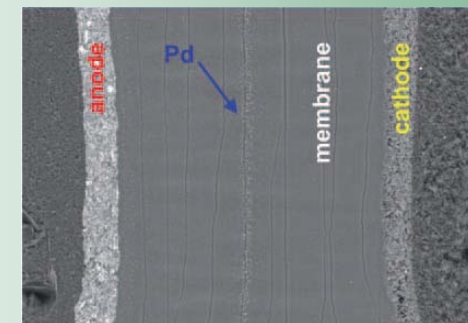
Manufacturing/
Commercialization

BNL-Toyota CRADA

Scale-up synthesis: Pt-ML/Pd₉Au₁/C
Excellent fuel Cell durability 200,000 cycles



Membrane Electrode Assembly >200K cycles
Very small Pt diffusion & small Pd diffusion



Angewandte Chemie 49, 8602 (2010)

Fuel Cell Catalyst readied for automotive application

25



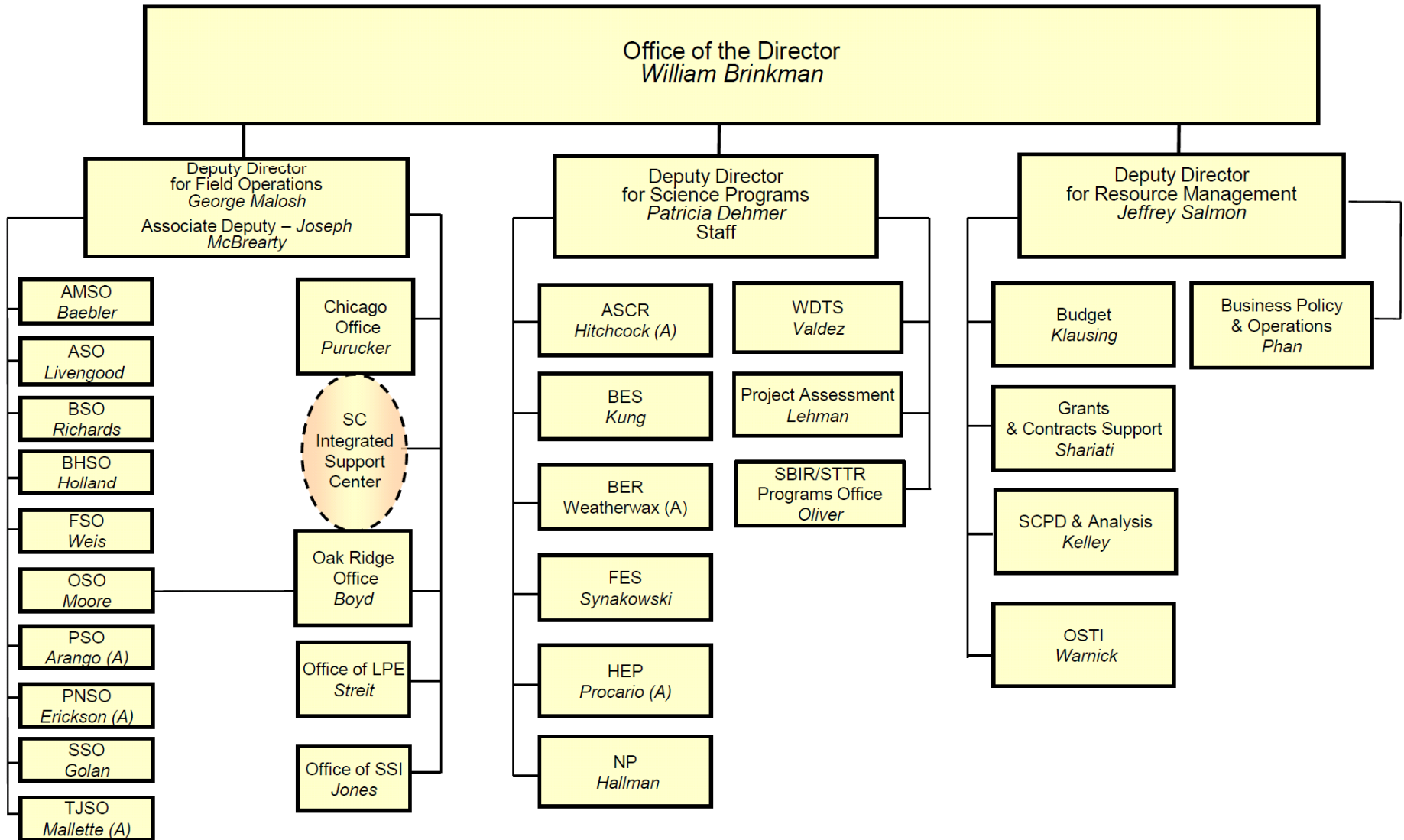
U.S. DEPARTMENT OF
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Office of
Science

Program Details



U.S. DEPARTMENT OF ENERGY



Advanced Scientific Computing Research

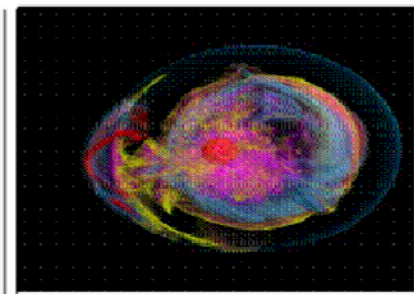
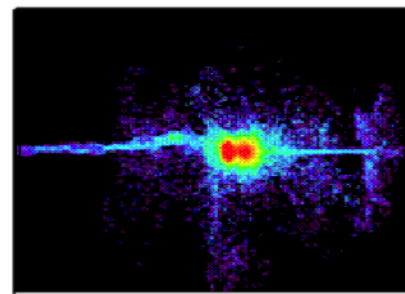
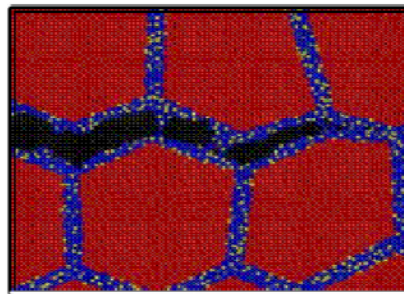
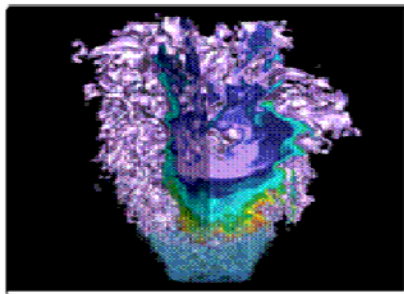
Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

The Scientific Challenges:

- Deliver next-generation scientific applications using today's petascale computers.
- Discover, develop and deploy tomorrow's exascale computing and networking capabilities.
- Develop, in partnership with U.S. industry, next generation computing hardware and tools for science.
- Discover new applied mathematics and computer science for the ultra-low power, multicore-computing future.
- Provide technological innovations for U.S. leadership in Information Technology to advance competitiveness.

FY 2012 Highlights:

- Research in uncertainty quantification for drawing predictive results from simulation
- Co-design centers to deliver next generation scientific applications by coupling application development with formulation of computer hardware architectures and system software.
- Investments in U.S. industry to address critical challenges in hardware and technologies on the path to exascale
- Installation of a 10 petaflop low-power IBM Blue Gene/Q at the Argonne Leadership Computing Facility and a hybrid, multi-core prototype computer at the Oak Ridge Leadership Computing Facility.



Investments for Exascale Computing

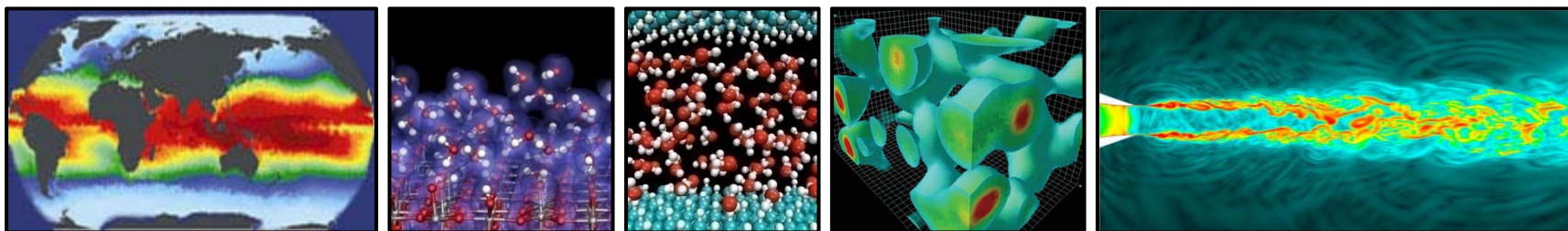
Opportunities to Accelerate the Frontiers of Science through HPC

Why Exascale?

- **SCIENCE:** Computation and simulation advance knowledge in science, energy, and national security; numerous S&T communities and Federal Advisory groups have demonstrated the need for computing power 1,000 times greater than we have today.
- **U.S. LEADERSHIP:** The U.S. has been a leader in high performance computing for decades. U.S. researchers benefit from open access to advanced computing facilities, software, and programming tools.
- **BROAD IMPACT:** Achieving the power efficiency, reliability, and programmability goals for exascale will have dramatic impacts on computing at all scales—from PCs to mid-range computing and beyond.

DOE Activities will:

- Leverage new chip technologies from the private sector to bring exascale capabilities within reach in terms of cost, feasibility, and energy utilization by the end of the decade;
- Support research efforts in applied mathematics and computer science to develop libraries, tools, and software for these new technologies;
- Create close partnerships with computational and computer scientists, applied mathematicians, and vendors to develop exascale platforms and codes cooperatively.



High Performance Computing: SmartTruck/DOE Partnership

Aerodynamic forces account for ~53% of long haul truck fuel use.

- Class 8 semi trucks (300,000 sold annually) have average fuel efficiency of 6.7 MPG
- Used ORNL's Jaguar Cray XT-5 2.3 petaflop computer for complex fluid dynamics analysis – cutting in half the time needed to go from concept to production design
- Outcome: SmartTruck UnderTray add-on accessories predict reduction of drag of 12% and yield EPA-certified 6.9% increase in fuel efficiency.
- If the 1.3 million Class 8 trucks in the U.S. had these components, we would save 1.5 billion gallons of diesel fuel annually (~\$4.4B in costs and 16.4M tons of CO₂)
- Awarded as one of the “Top 20 products of 2010” from *Heavy Duty Trucking* magazine



Con-way Freight Inc. is the first corporation to install the SmartTruck UnderTray system.



Basic Energy Sciences

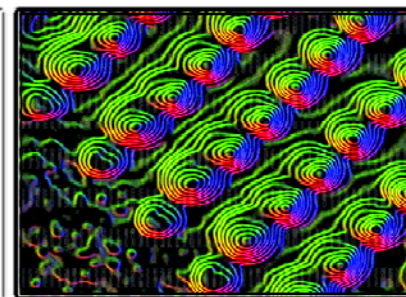
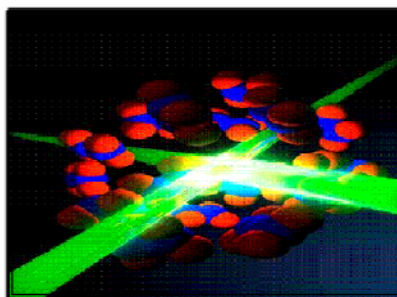
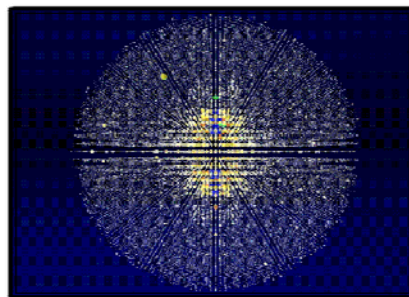
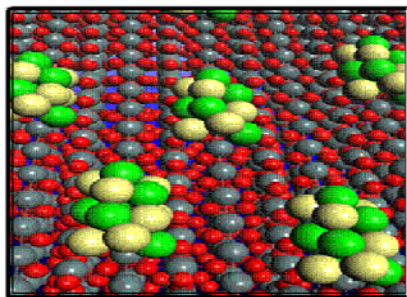
Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels

The Scientific Challenges:

- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

FY 2012 Highlights:

- Science for clean energy
 - Batteries and Energy Storage Hub
 - Interface sciences for high efficiency PV & next-generation nuclear systems; molecular design for carbon capture and sequestration; enabling materials sciences for transmission and energy efficiency; predictive simulation for combustion
- Computational Materials and Chemistry by Design and Nanoelectronics research with inter-agency coordination.
- Enhancements at user facilities:
 - LCLS expansion (LCLS-II); NSLS-II EXperimental Tools (NEXT); APS Upgrade (APS-U); TEAM II (aberration-corrected microscope); upgraded beamlines and instruments at the major facilities



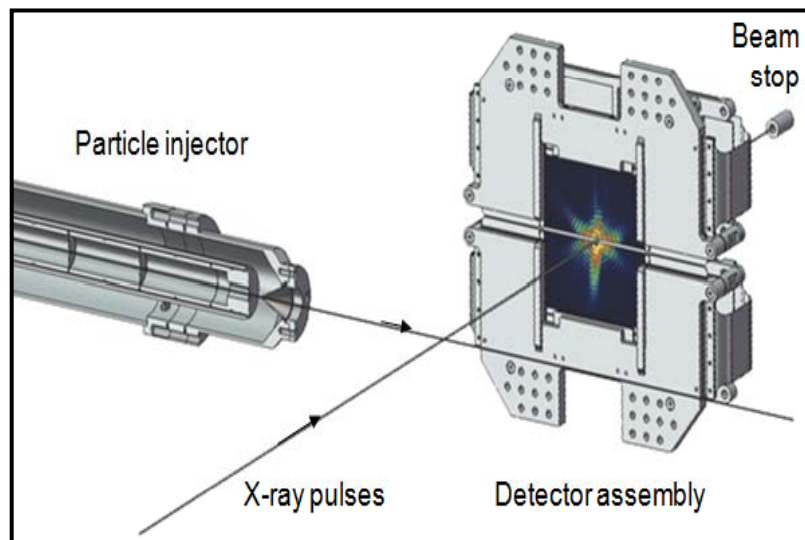
Nature Publishes First Bioimaging Results from the LCLS

The World's First Hard X-ray Laser



Within 6 months of completion, LCLS is being used to study a wide array of science topics, including:

- Hollow atoms
- Magnetic materials
- Structure of biomolecules in nano-crystals
- Single shot images of viruses and whole cells

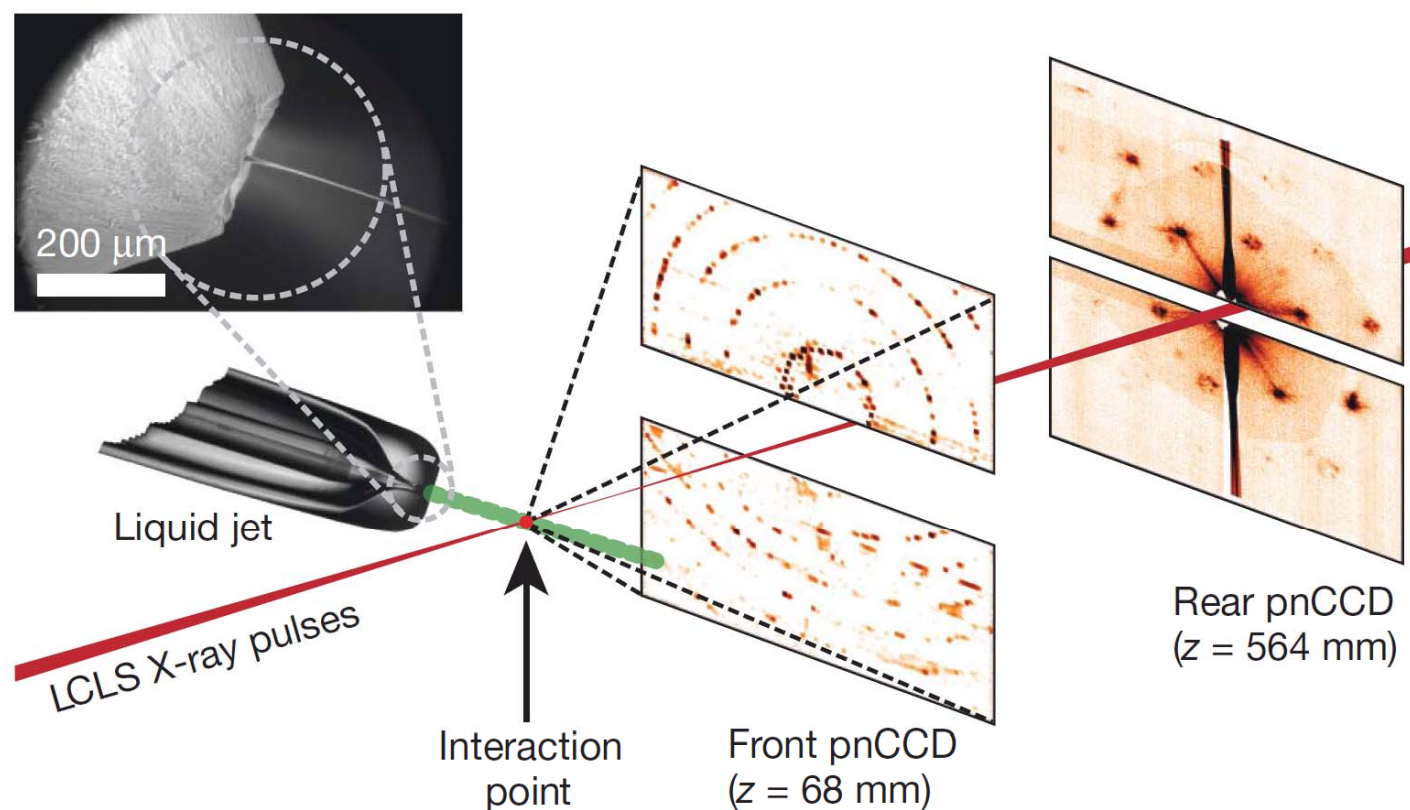


LCLS instruments provide new approach to x-ray bioimaging:

- Liquid or aerosol injection
- Very low noise, high-frame-rate CCD detectors
- Integrated computing infrastructure to manage gigabytes of data per day



Femtosecond X-ray Protein Nanocrystallography

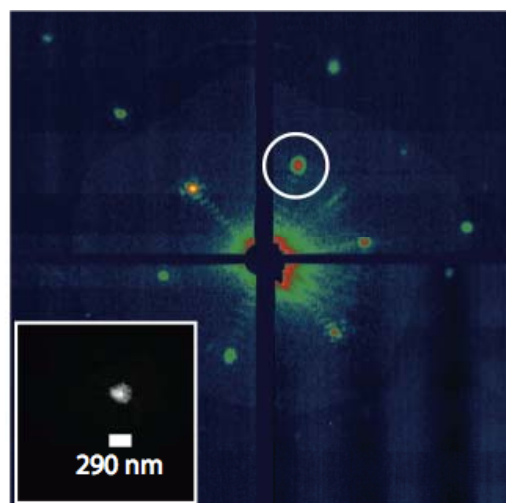


Nanocrystals flow in their buffer solution in a gas-focused, 4-μm-diameter jet at a velocity of 10m/sec perpendicular to the pulsed X-ray FEL beam that is focused on the jet.

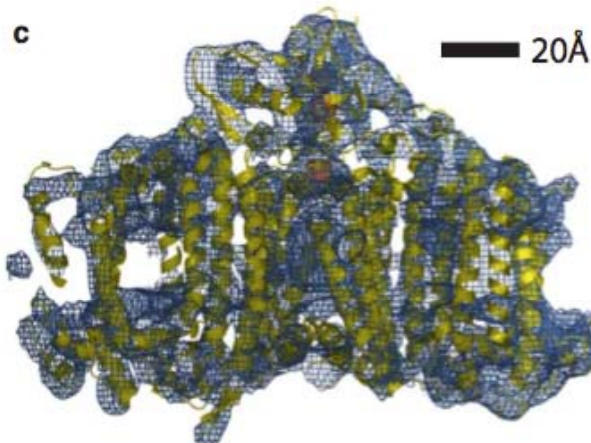
Chapman, H. N., et al. **Nature**, Feb 3rd, 2011.



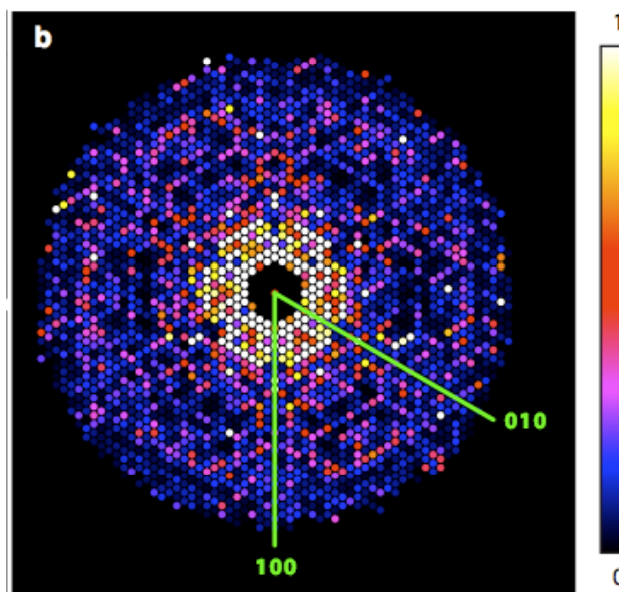
Femtosecond X-ray Protein Nanocrystallography



Single shot diffraction pattern



Reconstructed 3-D Structure



Combined 3D diffraction pattern

- Photosystem I plays key role in photosynthesis.
- Difficult to crystallize and use standard x-ray crystallography to obtain structure.
- Single shot images from LCLS of nanocrystals used to build up full 3-D diffraction pattern.
- Low resolution (~ 9 Å) shows structural details (e.g., helix density).

Chapman, H. N., et al. **Nature**, Feb 3rd, 2011.

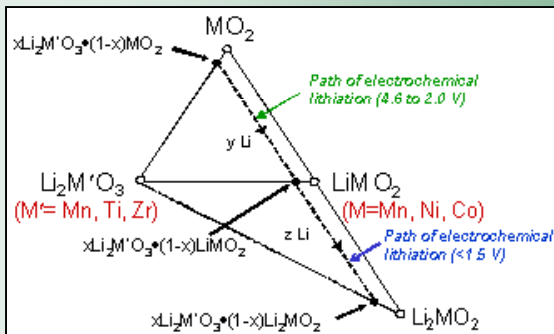


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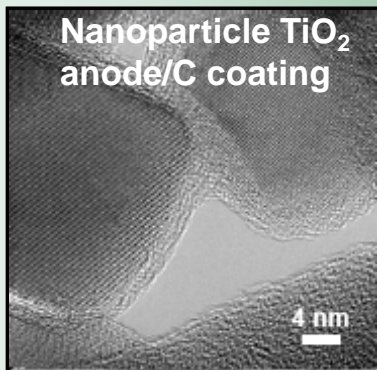
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High-Energy Lithium Batteries: From Fundamental Research to Cars on the Road

Basic Science



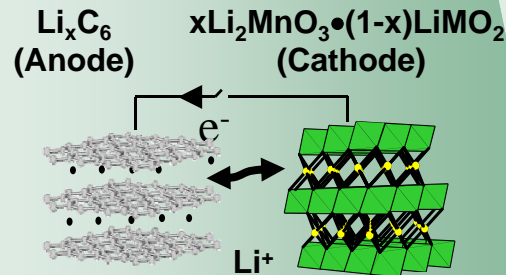
Discovered new composite structures for stable, high-capacity cathodes



Tailored electrode-electrolyte interface using nanotechnology

EFRC research

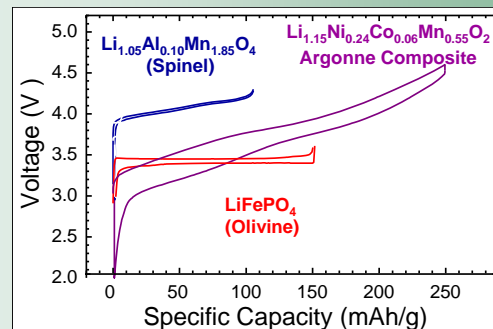
Applied R&D



Created high energy Li-ion cells...



...with double cathode capacity, enhanced stability

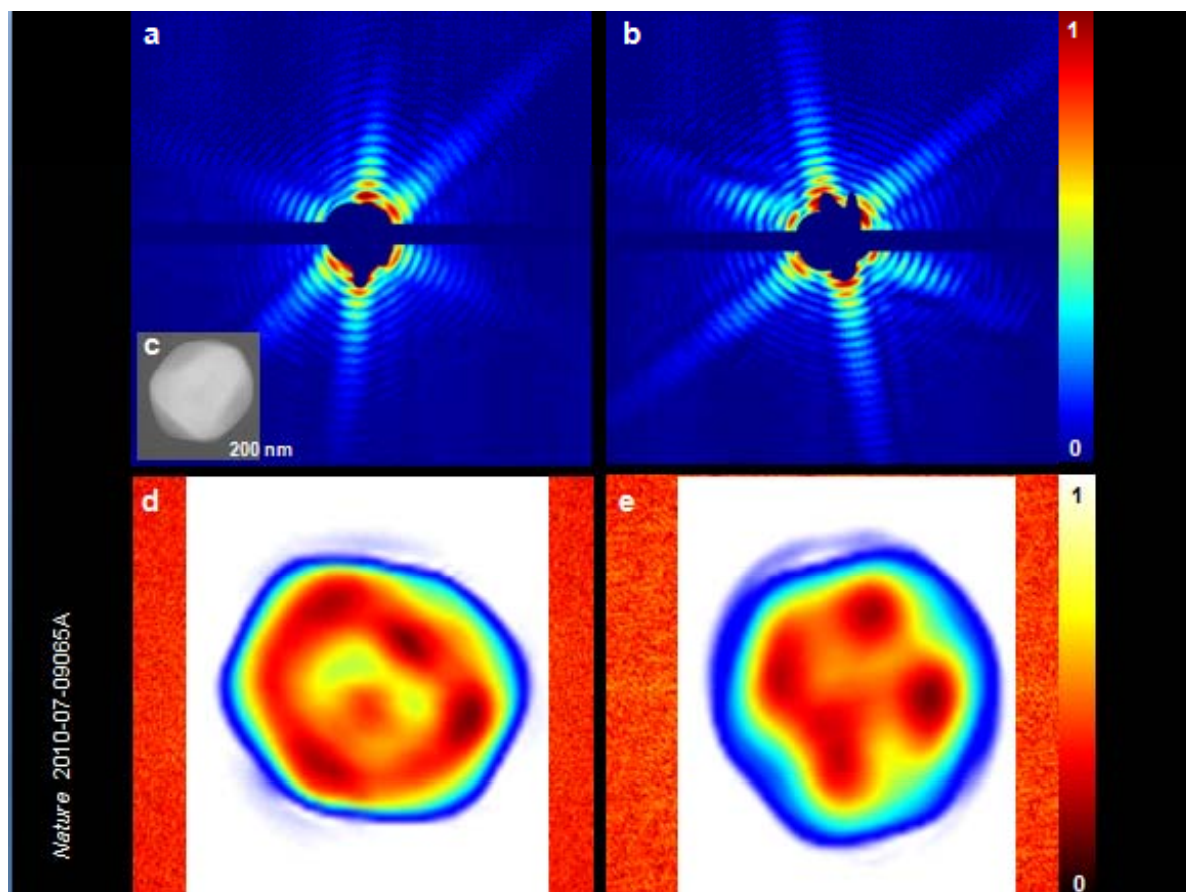


Manufacturing/ Commercialization



Licenses to materials and cell manufacturers and automobile companies

Single Mimi Virus Particles Intercepted and Imaged



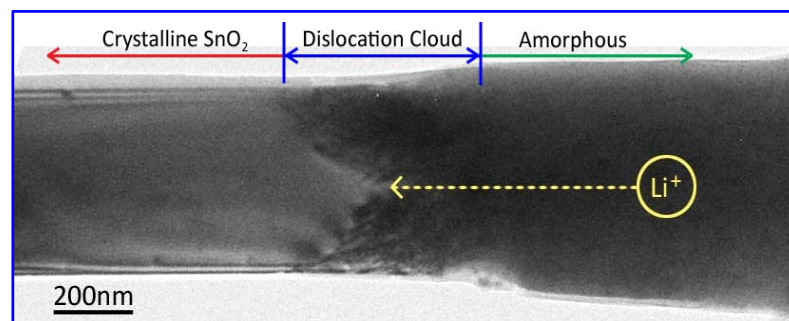
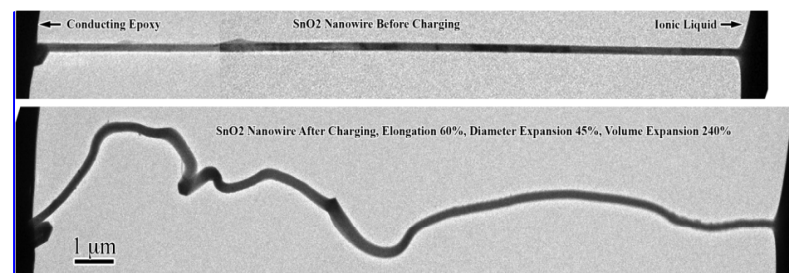
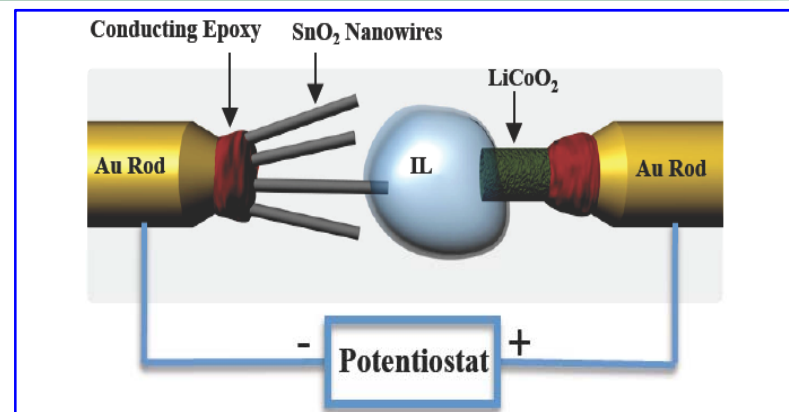
Single shot scattering patterns (above) and reconstructed images (below)

- Mimi virus is the largest known virus. Its size is comparable to the size of the smallest living cells – 45 μ m.
- Cannot be crystallized or imaged by conventional techniques.
- Reconstructions of single shot images from LCLS (32 nm resolution) reveal inhomogeneous interior structure of virion.
- Future enhancements will improve resolution and enable visualization of contents of living cells.

Seibert, M. M., et al. **Nature**, Feb 3rd, 2011

Advancing Energy Technologies through Energy Frontier Research Centers

- World's smallest battery placed inside an electron microscope yields images of electrochemistry at atomic scales
- New insight into electrochemical processes at the nanoscale:
 - Nanowires can sustain large stresses (>10 GPa) caused by Li^+ transport without breaking—good candidate for battery
 - Elongation and twisting of nanowires during charging may lead to a short circuit and failure of the battery, a key factor to consider during design

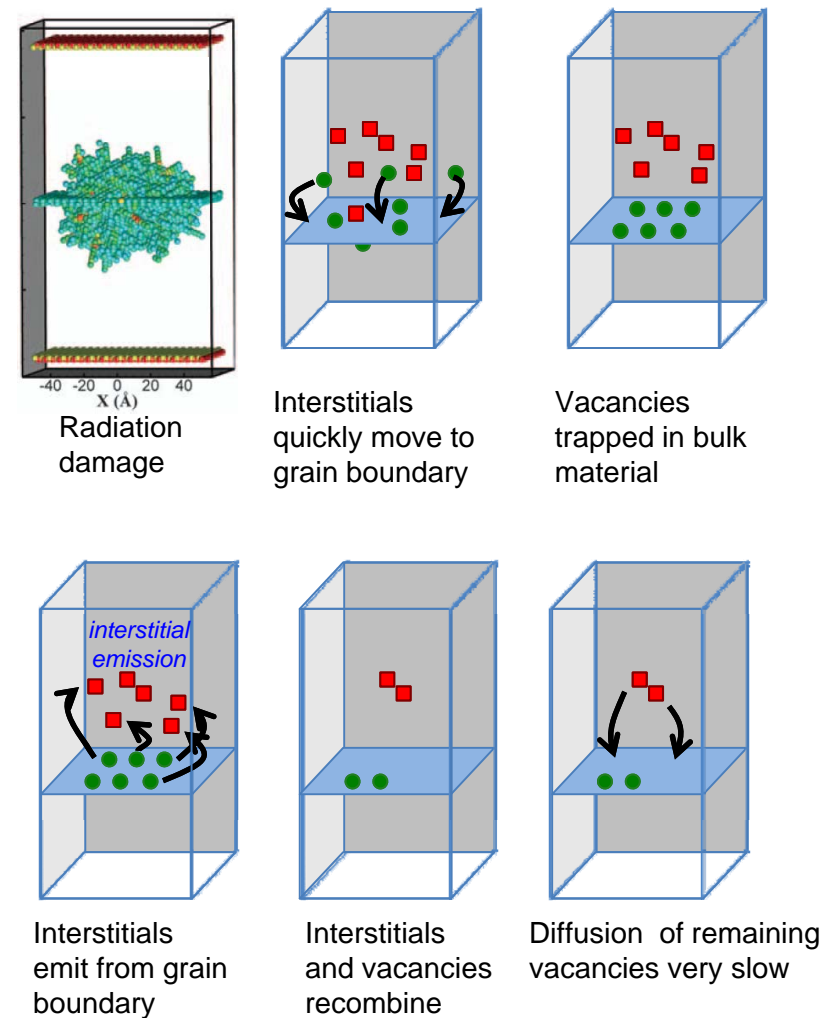


Research at SNL supported by the *Center for Science of Precision Multifunctional Nanostructures for Electrical Energy Storage* (an EFRC led by University of Maryland) and in collaboration with PNNL and university contributors

Jian Yu Huang, et al., *Science* 330, 1515 (2010)

EFRC Research Predicts Radiation Damage Resistant Materials

- Simulations reveal why nanostructured materials with a large number of grain boundaries exhibit increased tolerance to radiation damage
- New interstitial emission and vacancy recombination mechanism critical to self-healing of radiation damaged material
 - At very short times, interstitial atoms are concentrated on the grain boundary, but at longer times they re-emit and annihilate trapped vacancies many atomic distances away
 - Grain boundaries loaded with interstitials reduce the barrier for vacancy diffusion and promote defect recombination
 - Designed nanostructured grain boundaries could slow down the accumulation of radiation damage



Research supported by the *Center for Materials at Irradiation and Mechanical Extremes* (an EFRC led by Los Alamos National Laboratory)

Xian-Ming Bai et al. *Science*, 327, 1631 (2010)

Biological and Environmental Research

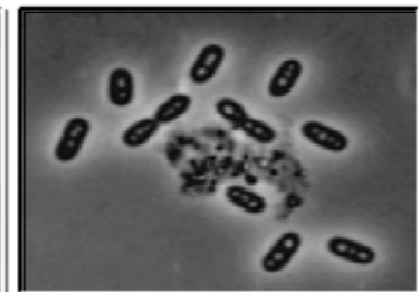
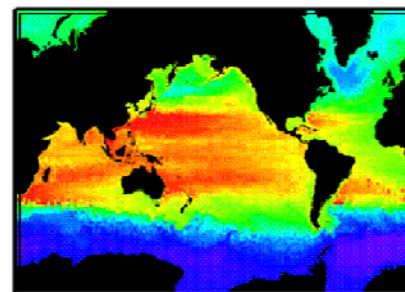
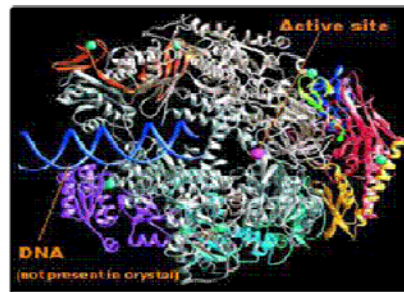
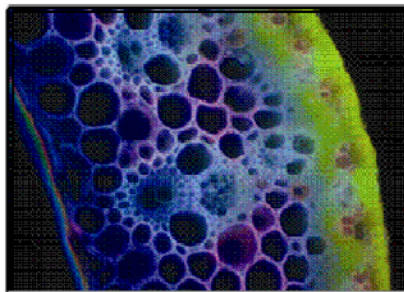
Understanding complex biological, climatic, and environmental systems across vast spatial and temporal scales

The Scientific Challenges:

- Understand how genomic information is translated with confidence to redesign microbes, plants or ecosystems for improved carbon storage, contaminant remediation, and sustainable biofuel production
- Understand the roles of Earth's biogeochemical systems (atmosphere, land, oceans, sea ice, subsurface) in determining climate so we can predict climate decades or centuries into the future, information needed to plan for future energy and resource needs.

FY 2012 Highlights:

- Clean energy biodesign on plant and microbial systems through development of new molecular toolkits for systems and synthetic biology research.
- Research and new capabilities to develop a comprehensive Arctic environmental system model needed to predict the impacts of rapid climate change.
- Continue support for the three DOE Bioenergy Research Centers, and operations of the Joint Genome Institute, the Environmental Molecular Sciences Laboratory, and the Atmospheric Radiation Measurement Climate Research Facility.

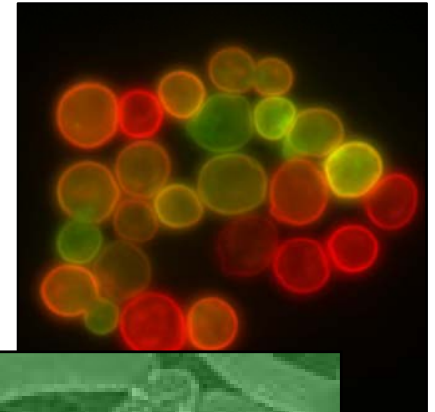


Advancing Energy Technologies through Bioenergy Research Centers

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.



- 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.

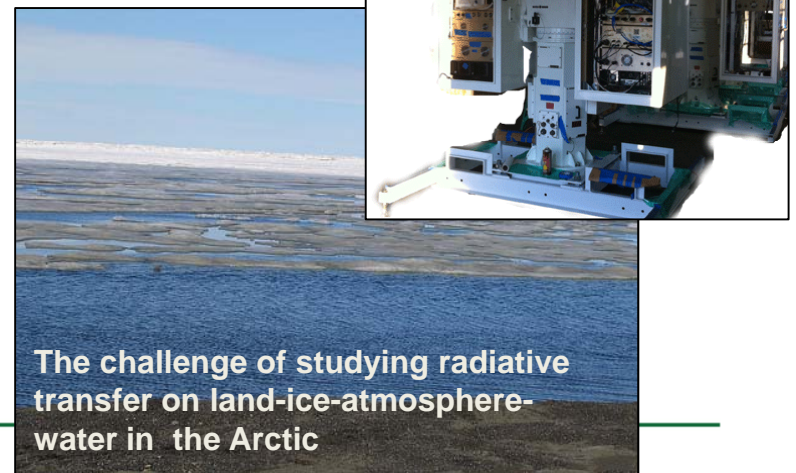
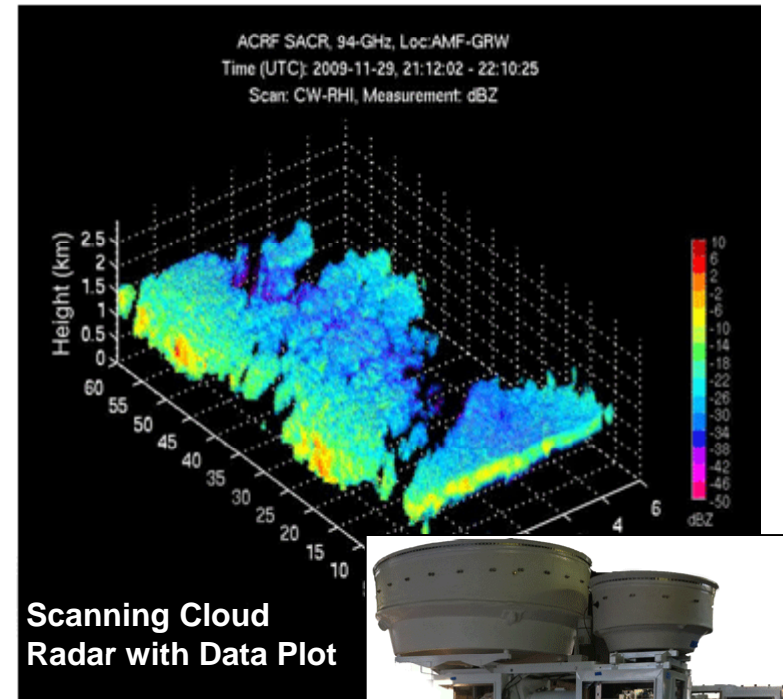


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Tackling Major Climate Uncertainties: The Atmospheric Radiation Measurement Climate Research Facility (ACRF)

- The ACRF provides the world's most comprehensive 24/7 observational capabilities for obtaining atmospheric data for climate change research.
- ARM data have transformed our understanding of aerosol-cloud interactions and built the most advanced parameterizations of atmospheric radiative transfer.
- The ARM Facility operates highly instrumented ground stations worldwide to study cloud formation and aerosol processes and their influence on radiative transfer.
- In FY 2012, ARM will deploy its new suite of measurement capabilities to regions of high scientific interest, e.g., the Azores (marine clouds) and Alaska (Arctic clouds and aerosols over land, sea, and ice).



Fusion Energy Sciences

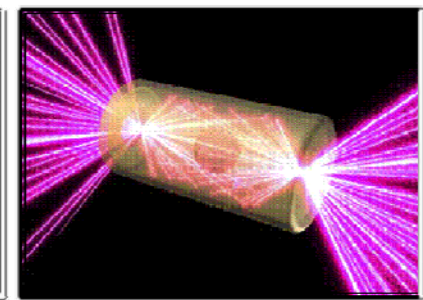
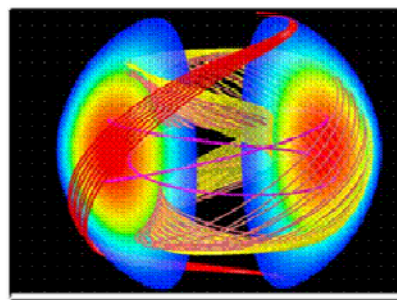
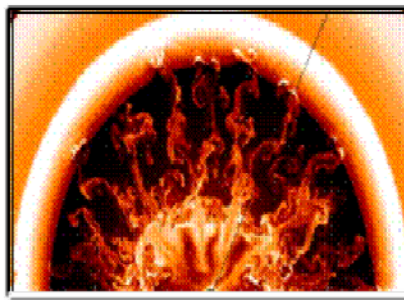
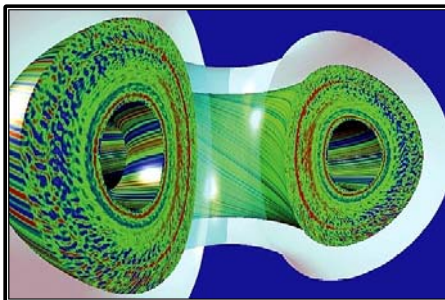
Understanding matter at very high temperatures and densities and building the scientific foundations for a fusion energy source

The Scientific Challenges:

- Control a burning plasma state to form the basis for fusion energy
- Develop materials that can withstand the harsh heat and neutron irradiation in fusion facilities
- Manipulate and control intense transient flows of energy and particles
- Control the interaction of matter under extreme conditions for enabling practical inertial fusion energy

FY 2012 Highlights:

- ITER construction is supported
- DIII-D, Alcator C-Mod, and NSTX operate and investigate predictive science for ITER
- HEDLP investments continue in basic research on fast ignition, laser-plasma interaction, magnetized high energy density plasmas, and warm dense matter
- International activities are increased
- SciDAC expands to include fusion materials
- The Fusion Simulation Program pauses to assess now-completed planning activities

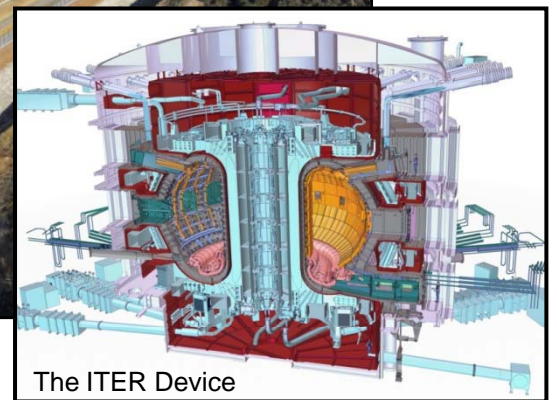


Progress on the ITER Project

- ITER's goal: first demonstration of high-gain fusion energy production—fusion power 10 times greater than that used to heat the plasma.
 - The U.S. is a member to the ITER partnership, formed by seven governments representing more than half the world's population. It is a 10-year construction activity in France.
- This past year, the U.S. led initiatives to put in place a world-leading management team for the construction phase of ITER and to establish the cost and schedule baselines.



Site construction is underway in Cadarache, France

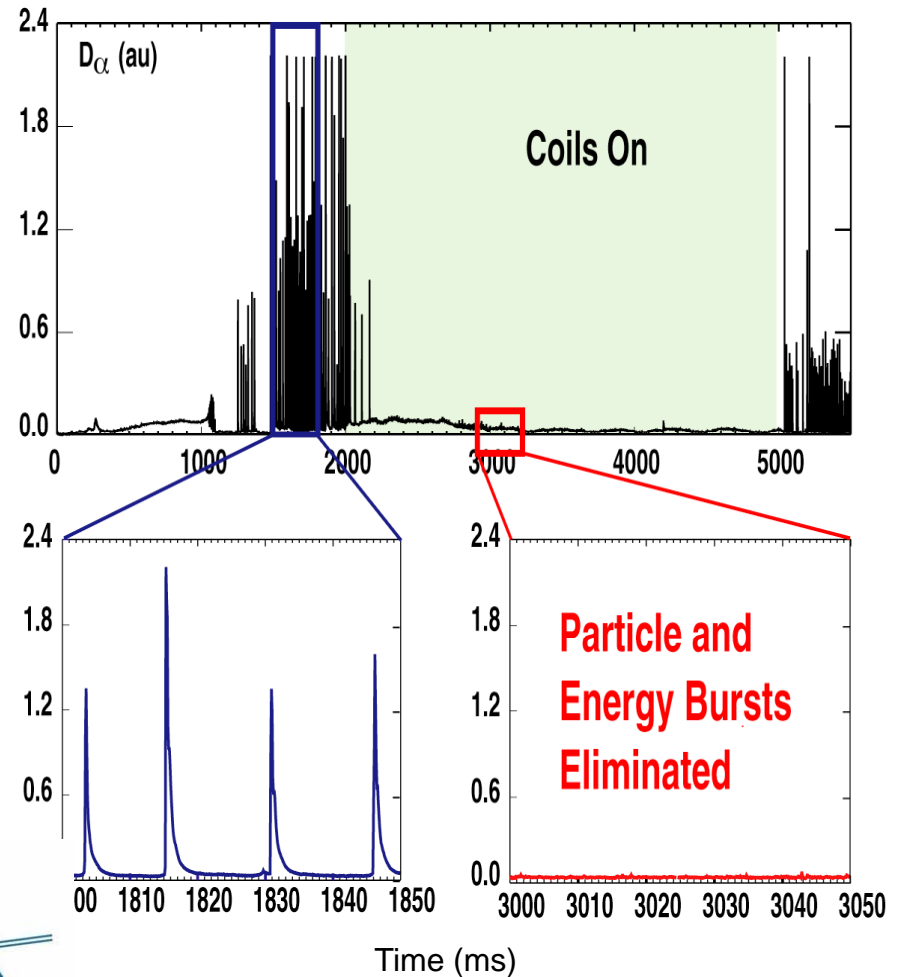
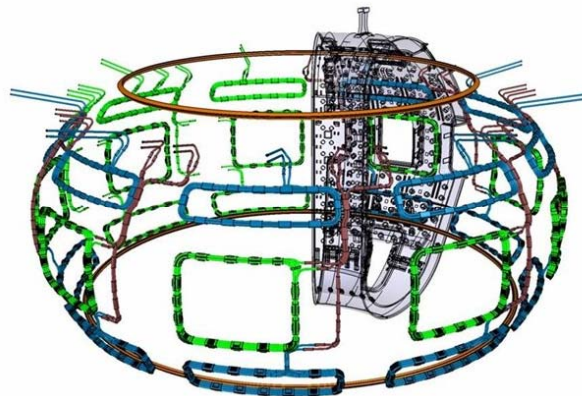
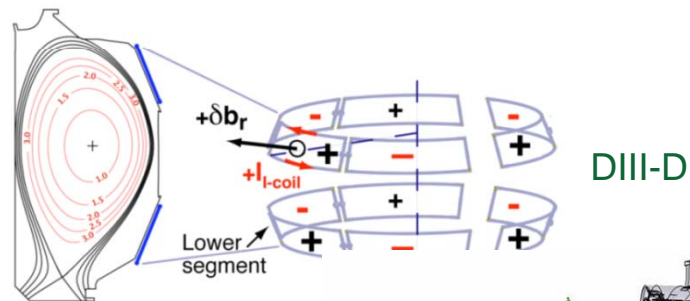


The ITER Device



Stabilization of High-Temperature Plasmas

- U.S. researchers at the DIII-D tokamak invented a new method for mitigating potentially damaging transient heat fluxes (Edge Localized Modes) by precision manipulation of the magnetic field.
- This can have an enormous positive impact for ITER if the results can be verified.
- Researchers at the Max Planck Institute (Garching, Germany) recently made major modifications to the ASDEX-U tokamak and reproduced these results.



ITER: ELM coil design

Nuclear Physics

Discovering, exploring, and understanding all forms of nuclear matter

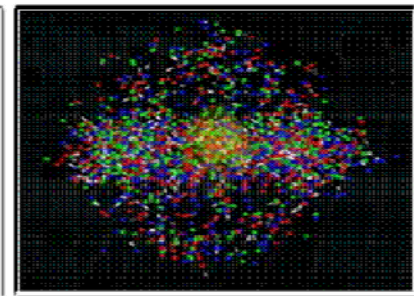
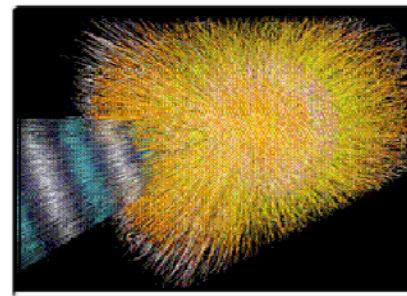
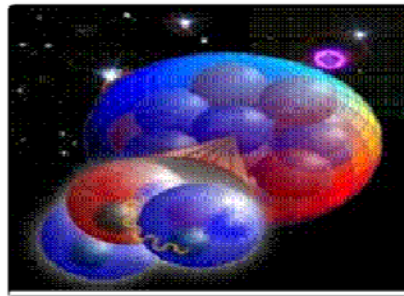
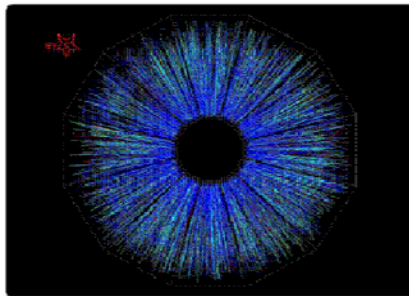
The Scientific Challenges:

Understand:

- The existence and properties of nuclear matter under extreme conditions, including that which existed at the beginning of the universe
- The exotic and excited bound states of quarks and gluons, including new tests of the Standard Model
- The ultimate limits of existence of bound systems of protons and neutrons
- Nuclear processes that power stars and supernovae, and synthesize the elements
- The nature and fundamental properties of neutrinos and neutrons and their role in the matter-antimatter asymmetry of the universe

FY 2012 Highlights:

- 12 GeV CEBAF Upgrade to study exotic and excited bound systems of quarks and gluons and for illuminating the force that binds them into protons and neutrons.
- Design of the Facility for Rare Isotope Beams to study the limits of nuclear existence.
- Operation of three nuclear science user facilities (RHIC, CEBAF, ATLAS); closure of the Holifield Radioactive Ion Beam Facility at ORNL.
- Research, development, and production of stable and radioactive isotopes for science, medicine, industry, and national security.



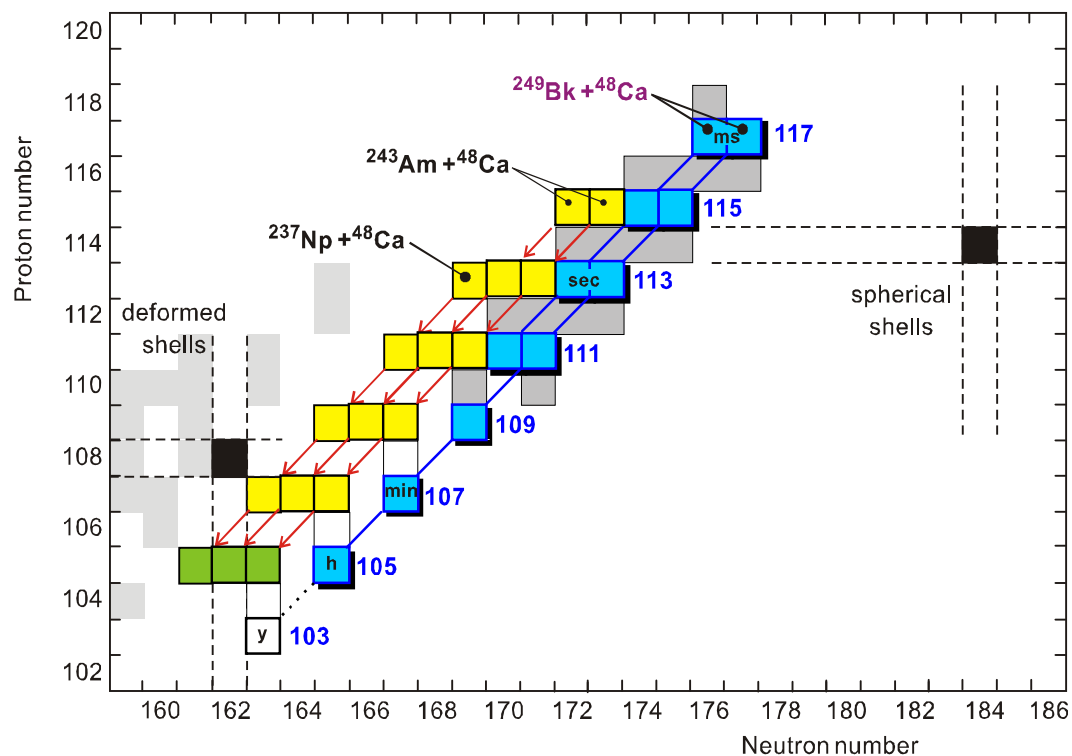
Discovery of Element 117

A new super heavy element (SHE) with atomic number 117 was discovered by a Russian-U.S. team with the bombardment of a Berkelium target by 48-Ca. The existence and properties of SHEs address fundamental questions in physics and chemistry:

- How big can a nucleus be?
- Is there a “island of stability” of yet undiscovered long-lived heavy nuclei?
- Does relativity cause the periodic table to break down for the heaviest elements?



Rare short-lived 248-Bk was produced at HFIR and processed in Isotope Program hot cell facilities at ORNL to purify the 22 mg of target material used for the discovery of element 117.



- Experiment conducted at the Dubna Cyclotron (Russia) with an intense 48-Ca beam
- Berkelium target material produced and processed by the Isotopes Program at ORNL
- Detector and electronics provided by U.S. collaborators were used with the Dubna Gas-Filled Recoil Separator



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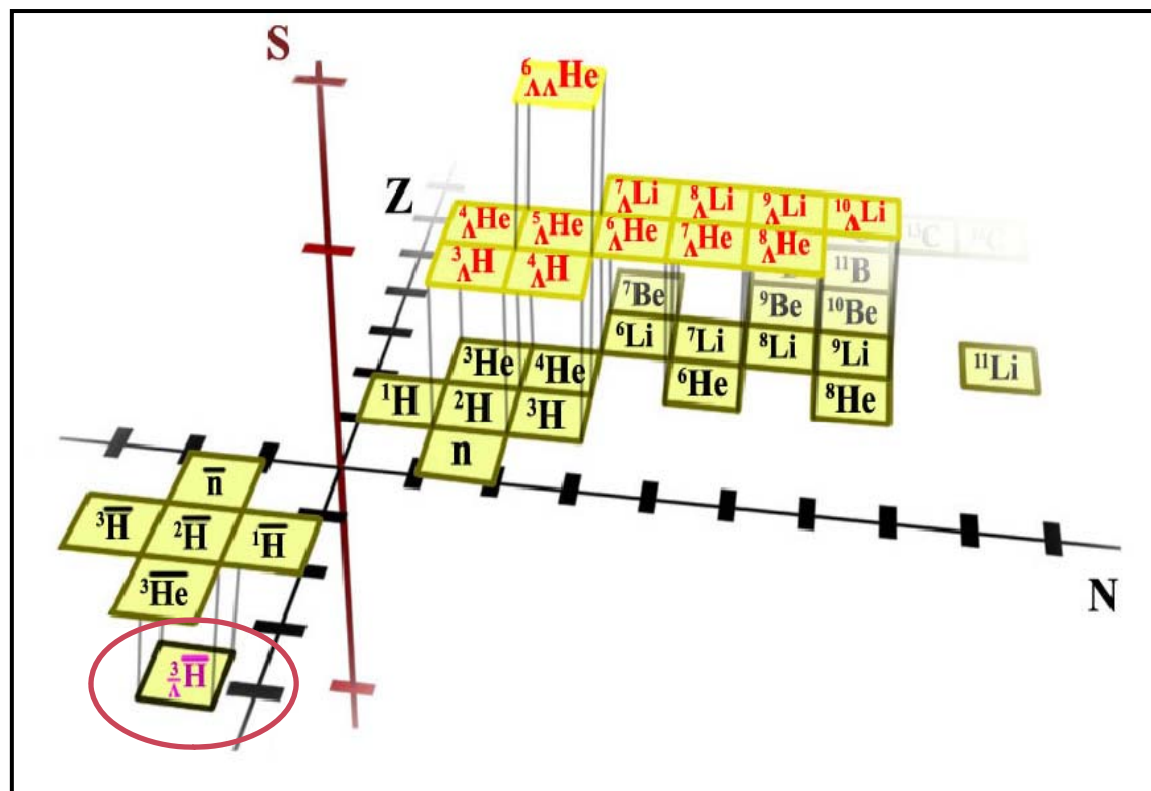
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New Antimatter Detected at RHIC's STAR Detector

Discovery of the heaviest known antinucleus and first antinucleus with an anti-strange quark, from gold nuclei collisions at RHIC.

- Opens further exploration of fundamental symmetries and understanding the dominance of matter over antimatter in the universe
- Has implications for our understanding of the structure of collapsed stars
- Discovery extends 3-D chart of the nuclides and suggests even heavier antinuclei exist.

Results highlighted at the American Physical Society Meeting, Feb 13-16, 2010; Over 500 related news articles published worldwide.



The STAR collaboration observed the first antimatter hypernucleus: antihypertriton. This nucleus contains an antiproton, an antineutron, and an antilambda hyperon, which is made up of an up quark, a down quark, and a strange quark. The discovery extends our knowledge of the nuclear terrain, represented by a three-dimensional graph with axes Z, the number of protons in a nucleus; N, the number of neutrons; and S, the degree of strangeness. Each axis has positive and negative sections, representing particles and antiparticles. This latest result extends the nuclear terrain below the N-Z plane for the first time.



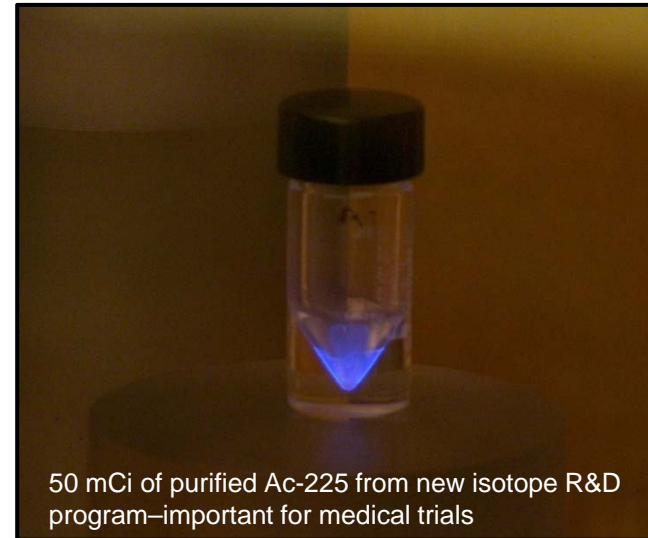
Isotope Development and Production Program

Making hundreds of isotopes available to the community for science, medicine, industry and national security.

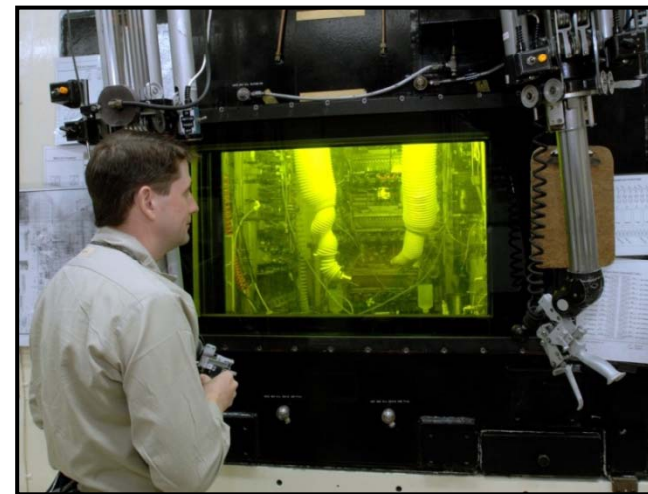
- Decision-making guided by strategic planning with federal agencies, community, and peer review mechanisms
- Coordinating with other federal agencies on addressing shortages of critical isotopes such as He-3 and Mo.
- Broadening the suite of isotope production facilities to include university facilities and other laboratory facilities.



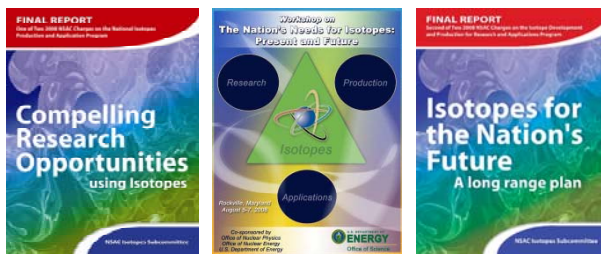
Production of Ni-63 for trace explosives detection systems



50 mCi of purified Ac-225 from new isotope R&D program—important for medical trials



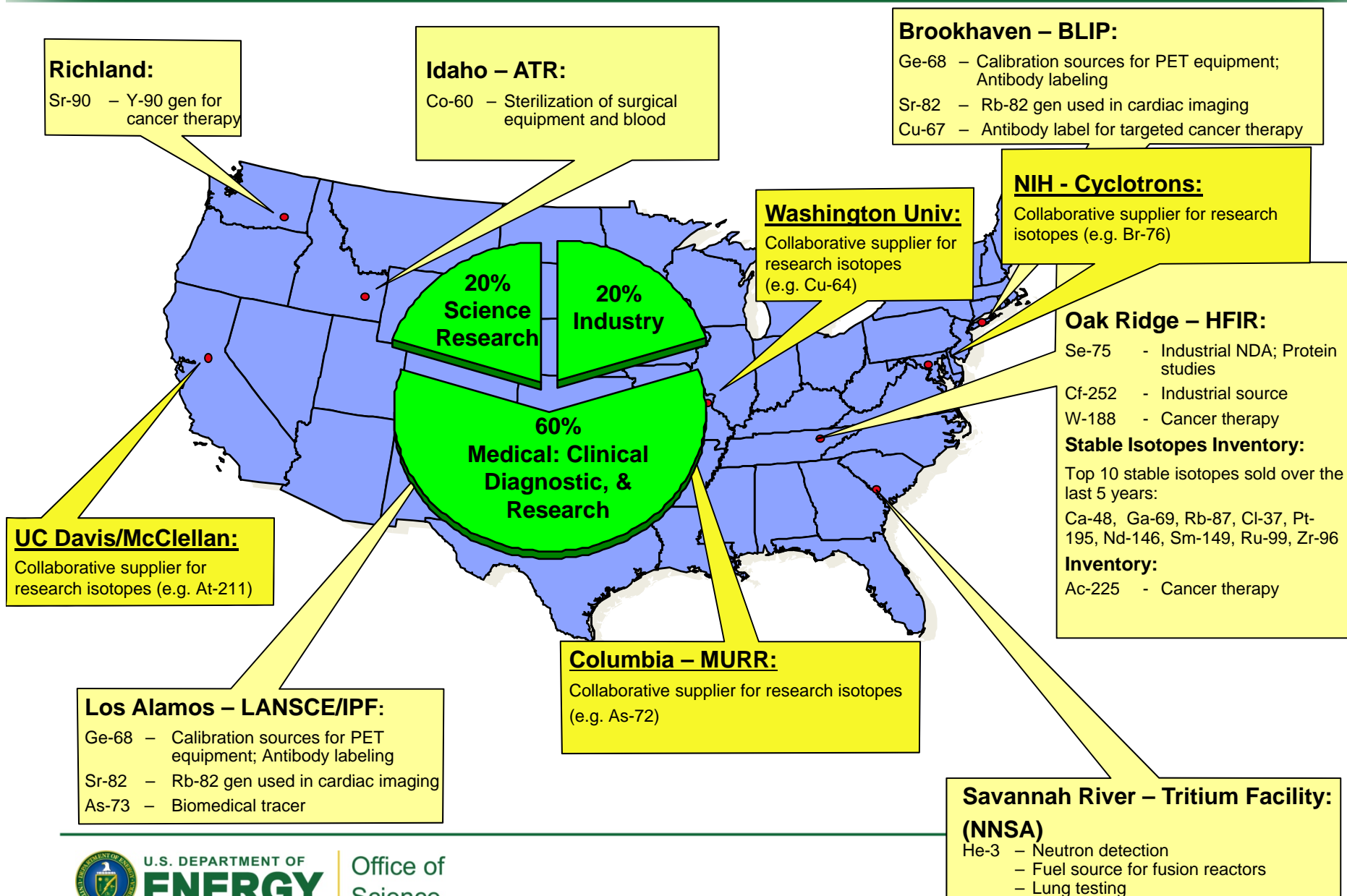
Cf-252 production for well logging and research



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Production Sites of the Isotope Program



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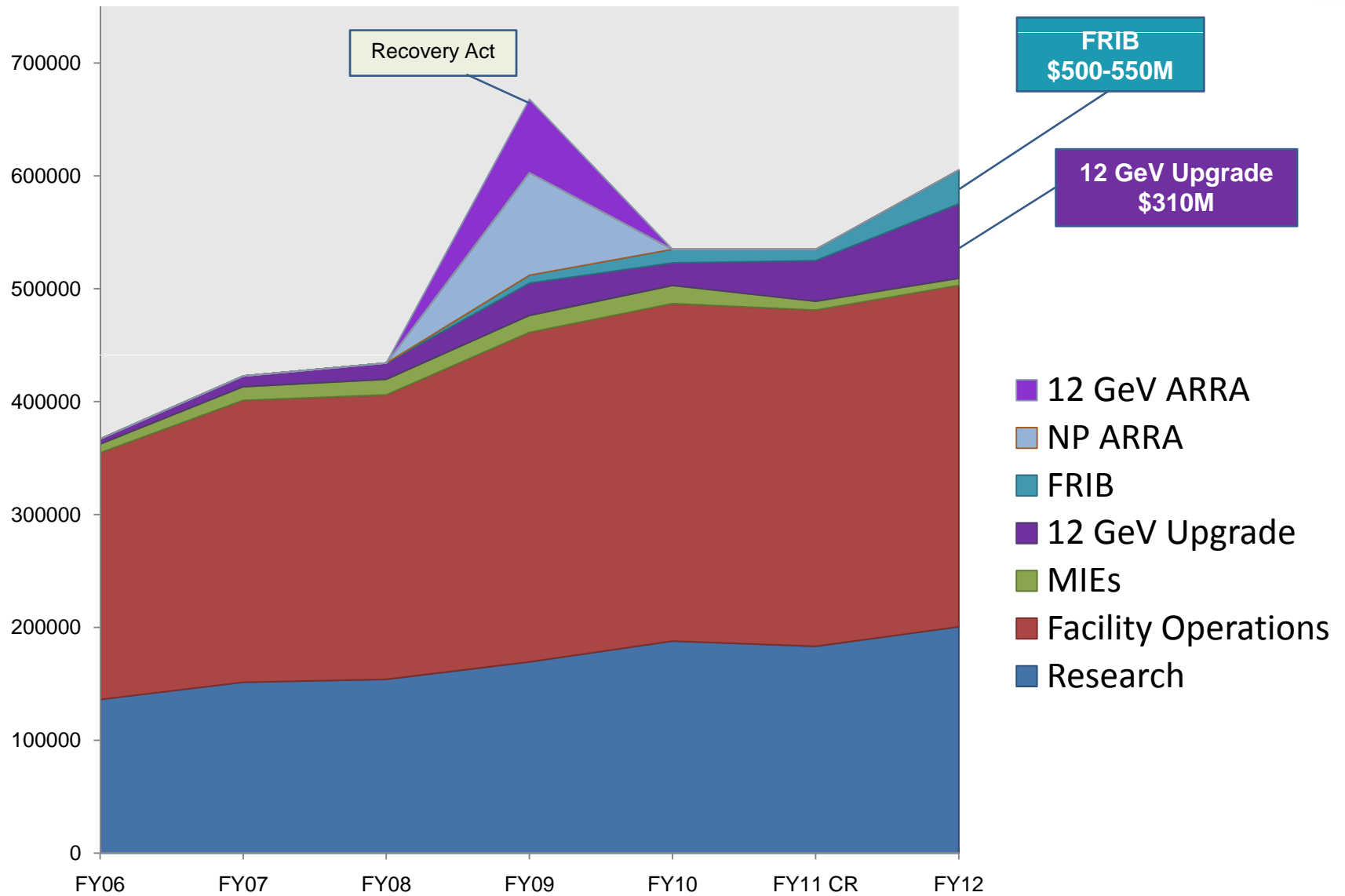
Office of
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Decision to close HRIBF

- We are facing a tight budget for the next years
- The nuclear community has two major projects to support and unlikely prospects for getting large increases

Nuclear Physics FY 2012 Request

Significant Increase to build 12 GeV and FRIB



High Energy Physics

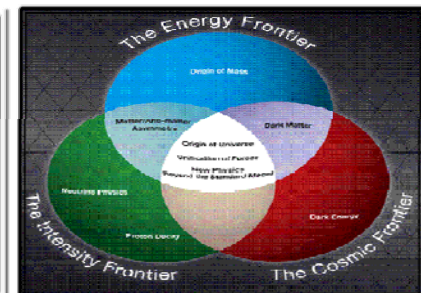
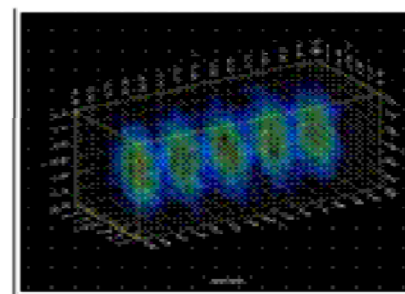
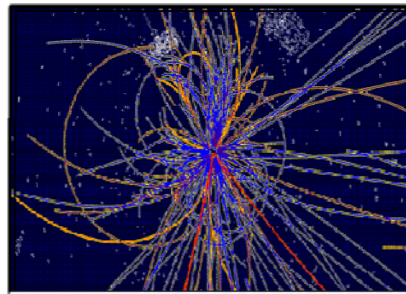
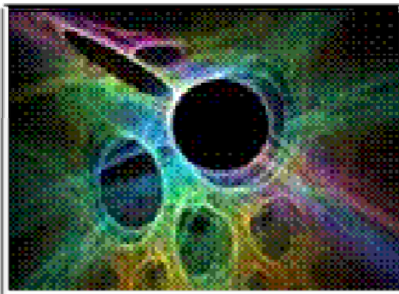
Understanding how the universe works at its most fundamental level

The Scientific Challenges:

- Determine the origins of mass in terms of the fundamental particles and their properties
- Exploit the unique properties of neutrinos to discover new ways to explain the diversity of particles
- Discover new principles of nature, such as new symmetries, new physical laws, or unseen extra dimensions of space-time
- Explore the “dark” sector that is 95% of the Universe (Dark Matter and Dark Energy)
- Invent better and cheaper accelerator and detector technologies to extend the frontiers of science and benefit society

FY 2012 Highlights:

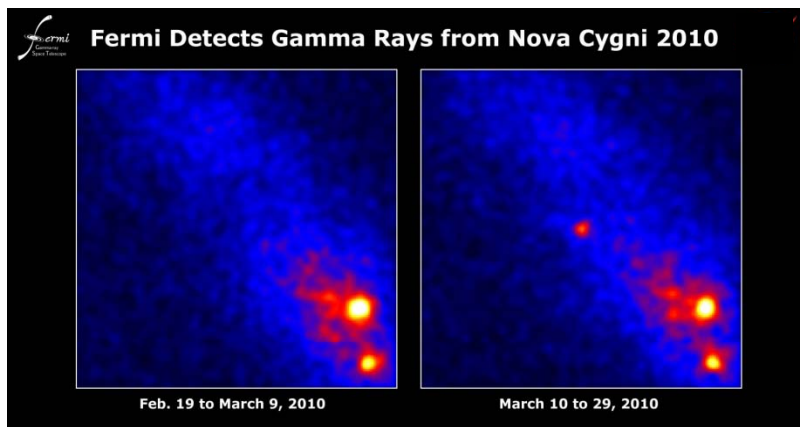
- Support for U.S. researchers at the LHC
- Research, design, and construction for NOvA, LBNE, and Mu2e experiments as part of a program of high energy physics at the intensity frontier
- Research in accelerator technologies including superconducting radio frequency and plasma wakefield acceleration.
- U.S. participation in international collaborations pursuing dark matter, dark energy and neutrino physics; the Reactor Neutrino Experiment in China and the Dark Energy Survey in Chile begin operations in FY 2012



Fermi Gamma-Ray Space Telescope (FGST)

Many Unexpected Findings about the Gamma-ray Sky

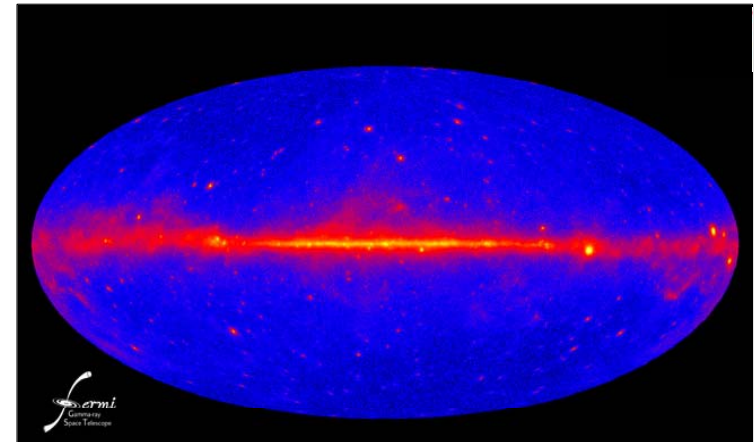
March 2010: Results show that less than 1/3 of gamma-ray emission arises from black-hole-powered jets in active galaxies. Particle acceleration occurring in normal star-forming galaxies or gamma-ray production from dark matter particle interactions may be the cause.



August 2010: The Fermi LAT detected gamma-rays from a nova for the first time overturning the long-held assumption that novae explosions lack the power to emit such high-energy radiation.



DOE partnered with NASA on the fabrication of the Large Area Telescope (LAT), with contributions from France, Japan, Italy and Sweden. The LAT is the primary instrument on NASA's FGST, launched in June 2008. SLAC managed the fabrication and now hosts the LAT Instrument Science Operations center.

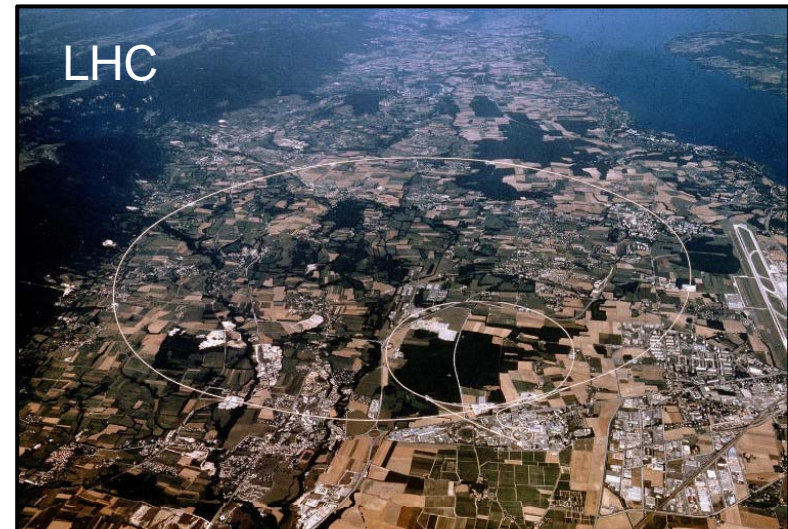


October 2009: 1 year map of the gamma-ray sky, showing the rate at which the LAT detects gamma-rays above 300 MeV. Brighter colors represent higher rates. Blue denotes the extragalactic gamma-ray background.

The 2011 Bruno Rossi Prize in Astrophysics is being awarded to Bill Atwood (SLAC) and Peter Michelson (Stanford) and the FGST/LAT team for enabling, through the development of the LAT, new insights into variety of high energy cosmic phenomena.

The Energy Frontier: Tevatron (FNAL) and the LHC

- The Tevatron at FNAL has been running extremely well.
 - Experiments now significantly limit the allowed values of the Standard Model (SM) Higgs Boson. These limits will continue to improve, ruling out a larger range of SM Higgs masses.
- The LHC is also running extremely well.
 - LHC is expected to discover or rule out the Higgs Boson across the entire SM mass range by the end of 2012.
- An extended Tevatron run was considered
 - Though shutdown was planned after FY 2011, the High Energy Physics Advisory Panel (HEPAP) was asked to advise the Office of Science on extension of running. In light of potential impacts on the rest of the HEP program, particularly the Intensity Frontier activities, HEPAP recommended that the Tevatron run be extended for three years only if additional funds could be secured.
- The FY 2012 President's Request does not include running the Tevatron beyond 2011.



The Intensity Frontier: Neutrinos and Rare Processes

- The Intensity Frontier uses intense particle beams to uncover properties of neutrinos and observe rare processes that point to new paradigms of physics.
- The U.S. is poised to make significant advances at the Intensity Frontier.
- The FY 2012 budget request builds on unique capabilities at Fermilab and supports associated research in Intensity Frontier physics.

Neutrino Physics

- **Mixing:** Experimental evidence that neutrinos can switch (“mix”) from one type to another proved that these elementary particles have non-zero mass, which violates the predictions of the Standard Model of particle physics.
- More detailed measurements of mixing in neutrinos and other elementary particles could reveal differences between matter and antimatter and discover new physics.

Rare Processes

- The Mu2e experiment will search for the conversion of a muon to an electron in the field of a nucleus.
- This is expected to be a very rare event, and an intense source of muons and a large detector will be required.
- This experiment searches for fundamentally new symmetries in the laws of nature.



The Neutrino Physics Program

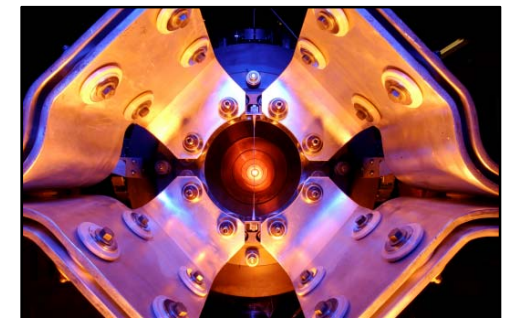
- Neutrinos from the Main Injector (NuMI) is the most intense neutrino beamline in the world.
- Experiments using this beamline use a detector near the neutrino source at Fermilab and also a far detector, hundreds of kilometers away.
- Experiments seek to quantify neutrino mixing; measure the neutrino masses; and detect the effects of matter on neutrinos as they pass through the earth.

Summary of key experiments:

- **MINOS** – This experiment has produced the most precise measurement of one of the neutrino mass differences. Operations continue to collect data for initial measurements of neutrino and antineutrino behavior.
- **NuMI Off-Axis Electron Neutrino Experiment (NOvA)** – Results from MINOS and other experiments worldwide helped determine the design specifications for this experiment. NOvA will provide precision measurements of neutrino mixing and will determine the relative masses of neutrinos. Funds are requested to continue construction in FY 2012. Operations are planned to begin in 2013.
- **Long Baseline Neutrino Experiment (LBNE)** – Like NOvA, the specific design will be determined by the results of currently active experiments. LBNE should be sensitive to differences between neutrinos and antineutrinos to test our assumptions about the symmetries between matter and antimatter and will deliver more precise measurements of neutrino mixing.



The trajectory of the NuMI beam and far detectors

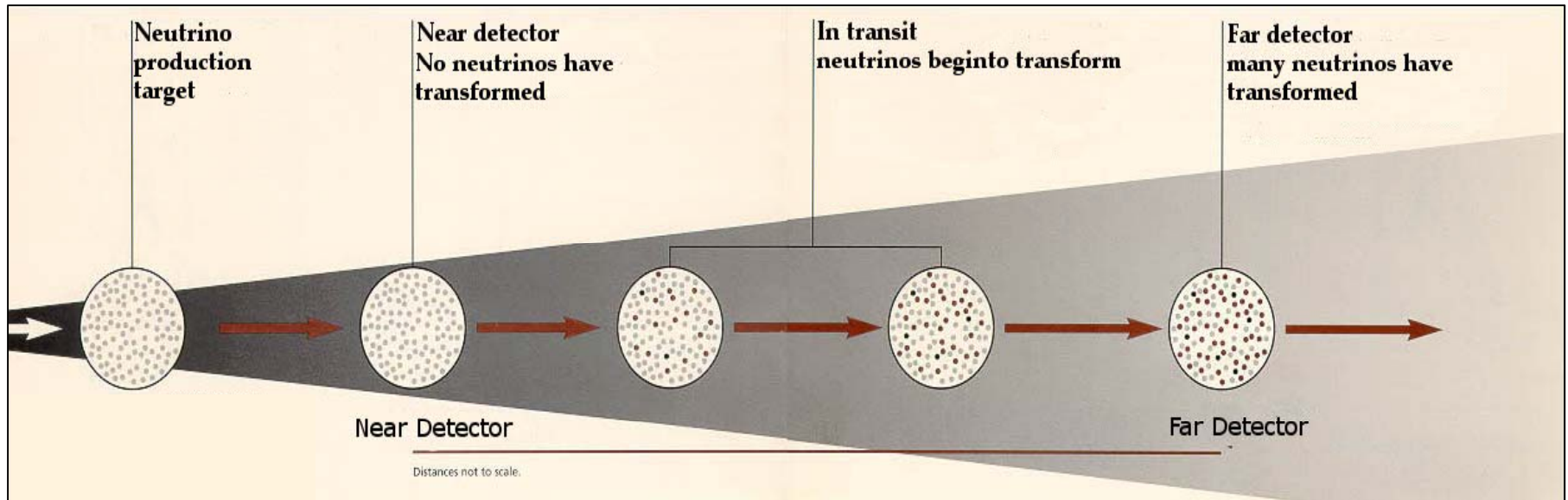


The NuMI horn, part of the neutrino sources

Long Baseline Neutrino Experiment (LBNE)

A high priority experiment at the intensity frontier

- LBNE will explore the interactions and transformations of neutrinos from the world's highest intensity neutrino beam at FNAL.
- Precision measurements from LBNE could explain why there is more matter than antimatter in the Universe and bring us closer to a Grand Unified Theory of the fundamental forces of nature.



- Tau neutrino ν_{τ}
- Electron neutrino ν_e
- Muon neutrino ν_{μ}



Deep Underground Science and Engineering Laboratory (DUSEL)

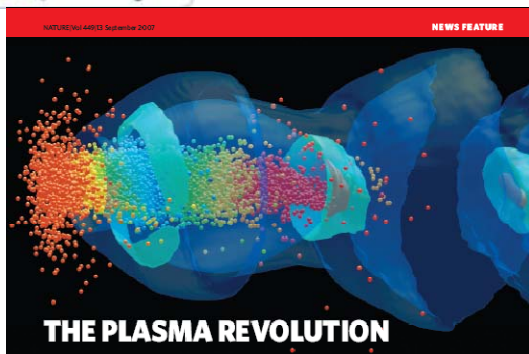
- The FY2012 Request includes \$15 M (\$10 M in HEP and \$5M in NP) to maintain the viability of DUSEL, including dewatering and maintaining security, while DOE assesses options for an underground research program.
- DOE has plans for Long Baseline Neutrino, Dark Matter, and Double Beta Decay experiments.
- A DOE assessment will identify options to carry out the planned research program in a cost effective way, including an alternatives analysis for the location of individual experiments.
- The DOE assessment will seek input from the DOE, NSF, and the DUSEL stakeholder communities as well as the Sanford Laboratory in Lead, South Dakota.

Accelerator Technologies Developed for Basic Research Have Far-Reaching Benefits

- **Higher field magnets using new superconductors enable new applications**
 - High frequency NMR by Oxford Instruments using materials developed by HEP
 - Compact cyclotrons for making medical isotopes
 - ITER will use new superconducting cables first developed by HEP



- **Higher gradient superconducting RF cavities for new accelerators**
 - HEP R&D led to new US companies producing high performance superconducting RF cavities.



Particle accelerators that use plasma technology promise to shake up the fields of high-energy particle physics and cancer treatment. Challenges remain, but smaller, cheaper machines are within reach. Navroz Patel reports.

Entirely new methods of accelerating particles using plasmas could make Accelerators 10-100x smaller.



U.S. DEPARTMENT OF
ENERGY

Office of
Science

HEP & NP Superconducting Radio Frequency (SRF) Development

The U.S. is now the leader in SRF technology



Superconducting electron gun, developed at BNL by DOE in cooperation with DOD and industry.

World's most advanced superconducting accelerator cavity developed at ANL.



- A large variety of RF cavities are used in particle accelerators. Historically they have been made of copper and operated near room temperature with water cooling. In the past two decades, though, there has been a growing number of accelerator facilities for which SRF cavities were desirable or necessary.
- Several U.S. laboratories have world-leading capabilities in SRF technology: ANL, BNL, FNAL, TJNAF.
- U.S. industries are commercializing SRF: Advanced Energy Systems (Medford, NY) and Niowave, (Lansing, MI)
- Other potential applications include high-power lasers, naval defense, disposal of long-lived nuclear waste, “clean” accelerator-driven-systems nuclear energy



Workforce Development for Teachers and Scientists

Encouraging and supporting the next generation of scientific talent

Program Goals:

- Increase the pipeline of talent pursuing research important to the Office of Science
- Leverage the resources of the DOE national laboratories for education and training
- Increase participation of under-represented students and faculty in STEM programs
- Improve methods of evaluation of effectiveness of programs and impact on STEM workforce

FY 2012 Highlights:

Office of Science Graduate Fellowships—

- 3-year fellowships to pursue advanced degrees in areas of research important to the Office of Science
- 150 Fellowships in FY10 (1st year of the program); 450 in steady state

National Science Bowl (NSB)—

- Regional and national middle school and high school competitions to encourage education and careers in science, with 22,000 students from 1,500 schools

Research Experiences at DOE Labs—

- Science Undergraduate Laboratory Internship
- Community College Institutes
- Academies Creating Teacher Scientists for middle school and high school educators



Supporting and Encouraging Next Generation Scientists

The National Science Bowl Middle School and High School Students

- Begun in 1991, DOE's National Science Bowl® is a nationwide academic competition that tests students' knowledge in all areas of science. High school and middle school students are quizzed in a fast paced question-and-answer format similar to Jeopardy.
- 22,000 students from 1,500 schools; 6000 volunteers



First Lady Michelle Obama and Secretary of Energy Steven Chu congratulate Albuquerque Academy, Albuquerque, NM, First Place winner in the 2010 NSB Middle School competition .

Office of Science Graduate Fellowship Graduate Students

- Begun in 2009 with ARRA funding, the SCGF program provides 3-year fellowship awards totaling \$50,500 annually.
- The awards provide support towards tuition, a stipend for living expenses, and support for expenses such as travel to conferences and to DOE user facilities.



DOE SCGF Cohort 2010 at the SCGF Annual Meeting at Argonne National Laboratory.



Science Laboratory Infrastructure

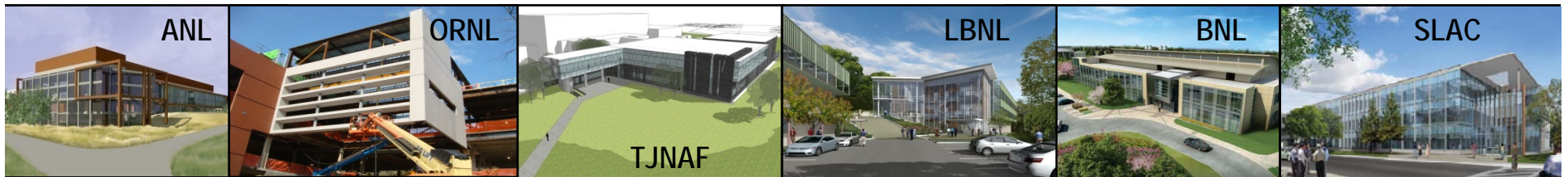
Supporting infrastructure and fostering safe and environmentally responsible operations at the Office of Science laboratories

Program Goals:

- Support scientific and technological innovation at the Office of Science laboratories by providing state-of-the-art research space in modern, safe, and sustainable laboratory facilities.
- Correct longstanding infrastructure deficiencies while ensuring laboratory infrastructure provides a safe and quality work environment.
- Support stewardship responsibilities for the Oak Ridge Reservation and the Federal facilities in the city of Oak Ridge, and provide payments in lieu of taxes to local communities around the Argonne, Brookhaven, and Oak Ridge National Laboratories.

FY 2012 Highlights:

- Continuation of funding for five ongoing line item construction projects at ANL, BNL, LBNL, SLAC and TJNAF
- Supports one new construction start at SLAC for the Science & User Support Building which will bring together many of the laboratory's visitors, users, and administrative services
- Modernization of Laboratory Facilities at ORNL project is scheduled to complete construction in 1QFY12
- Building 74 Renovation at LBNL is scheduled for completion in 1QFY12



Safeguards and Security

Supporting appropriate levels of protection against unauthorized access, theft, or destruction of DOE assets and hostile acts

Program Goals:

- Provide physical and cyber security controls at Office of Science national laboratory facilities to mitigate risks to facilities and laboratory employees to an acceptable level while enabling the mission.
- Assure site security programs result in the secure workplace required to facilitate scientific advances.
- Align accountability for performance through National Standards, rigorous peer review, and Federal oversight through mature contractor assurance systems.
- Protect special, source, and other nuclear materials, radioactive material, and classified and unclassified controlled information at Office of Science laboratories.

FY 2012 Highlights:

- The baseline level of protection to provide mission tailored security
- Full recovery for S&S services to non-DOE customers to reduce pressure on overhead burdens and S&S budgets
- Oversight through mature contractor assurance systems to minimize duplicative audits and assessments.
- Investments in infrastructure and automation technology to reduce reliance on personnel for routine security functions and long-term costs



Program Direction

Supporting a skilled workforce to oversee the Office of Science investments in world-leading scientific research

Program Goals:

- Ensure the recruitment and retention of a highly skilled workforce to provide the planning, execution, oversight, and management of the Office of Science's research programs and world-leading facilities
- Provide an effective modernized business infrastructure to support the scientific mission
- Provide public access to DOE-supported research results
- Support professional development opportunities for the Office of Science workforce

FY 2012 Highlights:

- Supports salaries and benefits of over 1,000 FTEs across the Office of Science complex.
- Supports the development of an improved internal grants management system through best-in-class software development.
- Supports development of an integrated, transparent information technology system between HQ and Field operations looking to cloud computing and other cost efficiency gains.

