FY 2012 budget Presentation
for DOE’s Office of Science

March 7, 2011

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Director, Office of Science
U.S. Department of Energy
www.science.doe.gov
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
“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.”
The Office of Science commands an arsenal of basic science capabilities—major scientific user facilities, national laboratories, and university 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.
Applications of 21\textsuperscript{st} century science to long-standing barriers in energy technologies: employing nanotechnology, biotechnology, and modeling and simulation

Examples:

- **Materials by design**: Using nanoscale structures, simulation and syntheses of materials for carbon capture; radiation-resistant and self-healing materials for the nuclear reactor industry; highly efficient photovoltaics; and white-light emitting LEDs and other energy applications.

- **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).
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 O₂ 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

- 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

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.
### Office of Science FY 2012 Budget Request to Congress

(dollars in thousands)

<table>
<thead>
<tr>
<th></th>
<th>FY 2010 Current Approp.</th>
<th>FY 2011 President's Request</th>
<th>FY 2011 Full Year CR</th>
<th>FY 2012 President's Request</th>
<th>FY 2012 vs. FY 2010</th>
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<tr>
<td>Advanced Scientific Computing Research</td>
<td>383,199</td>
<td>426,000</td>
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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.
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.
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
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.

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

Basic Science
- Discovered new composite structures for stable, high-capacity cathodes
- Nanoparticle TiO₂ anode/C coating
- Tailored electrode-electrolyte interface using nanotechnology

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

Discovered new composite structures for stable, high-capacity cathodes

\[ \text{LixC}_6 \] (Anode)

\[ x\text{Li}_2\text{MnO}_3(1-x)\text{LiMO}_2 \] (Cathode)

\[ \text{Li}^+ \]

\[ \text{e}^- \]

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

Nanoparticle TiO₂ anode/C coating

Tailored electrode-electrolyte interface using nanotechnology

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\[ \text{Li}^+ \]

\[ \text{e}^- \]
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.
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.
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
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.
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.
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?

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

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.
Production Sites of the Isotope Program

Richland:
- Sr-90 – Y-90 gen for cancer therapy

Idaho – ATR:
- Co-60 – Sterilization of surgical equipment and blood

Columbia – MURR:
- Collaborative supplier for research isotopes (e.g. As-72)

Savannah River – Tritium Facility:
- He-3 – Neutron detection
- Fuel source for fusion reactors
- Lung testing

Oak Ridge – HFIR:
- Se-75 - Industrial NDA; Protein studies
- Cf-252 - Industrial source
- W-188 - Cancer therapy

Stable Isotopes Inventory:
Top 10 stable isotopes sold over the last 5 years:
- Ca-48, Ga-69, Rb-87, Cl-37, Pt-195, Nd-146, Sm-149, Ru-99, Zr-96

Inventory:
- Ac-225 - Cancer therapy

UC Davis/McClellan:
- Collaborative supplier for research isotopes (e.g. At-211)

Washington Univ:
- Collaborative supplier for research isotopes (e.g. Cu-64)

NIH - Cyclotrons:
- Collaborative supplier for research isotopes (e.g. Br-76)

Brookhaven – BLIP:
- Ge-68 – Calibration sources for PET equipment; Antibody labeling
- Sr-82 – Rb-82 gen used in cardiac imaging
- Cu-67 – Antibody label for targeted cancer therapy

Los Alamos – LANSCE/IPF:
- Ge-68 – Calibration sources for PET equipment; Antibody labeling
- Sr-82 – Rb-82 gen used in cardiac imaging
- As-73 – Biomedical tracer

Columbia – MURR:
- Collaborative supplier for research isotopes (e.g. Cu-64)

20% Science Research

20% Industry

60% Medical: Clinical Diagnostic, & Research

20% Medical: Clinical Diagnostic, & Research

20% Industry

60% Medical: Clinical Diagnostic, & Research

Medical: Clinical Diagnostic, & Research

Science Research

Industry
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
**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.

**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.

**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.

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 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.
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.

<table>
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<th>Neutrino production target</th>
<th>Near detector</th>
<th>In transit</th>
<th>Far detector</th>
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<tbody>
<tr>
<td>No neutrinos have transformed</td>
<td>neutrinos begin to transform</td>
<td>many neutrinos have transformed</td>
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</tr>
</tbody>
</table>

- Tau neutrino $\nu_\tau$
- Electron neutrino $\nu_e$
- Muon neutrino $\nu_\mu$
**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.

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

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.

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.

DOE SCGF Cohort 2010 at the SCGF Annual Meeting at Argonne National Laboratory.
Section 103:

Establishes a working group under the National Science and Technology Council to coordinate Federal science agency research and policies related to the dissemination and long-term stewardship of the results of unclassified research, including digital data and peer reviewed scholarly publications, supported wholly, or in part, by funding from the Federal science agencies.