Update

Basic Energy Sciences Program

Office of Science, U.S. DOE

Patricia M. Dehmer
Director, Office of Basic Energy Sciences
Office of Science, U.S. Department of Energy
27 April 2007
## The FY 2008 Congressional Budget Request for SC Prior to FY 2007 Approp.

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>Basic Energy Sciences</td>
<td>1,083,616</td>
<td>1,110,148</td>
<td><strong>1,250,250</strong></td>
<td>+310,832 +28.0%</td>
<td>1,498,497</td>
<td>+77,517 +5.5%</td>
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<tr>
<td>Advanced Scientific Computing</td>
<td>226,180</td>
<td>228,382</td>
<td>318,657</td>
<td>-20,272 -39.5%</td>
<td>340,198</td>
<td>+21,544 +6.8%</td>
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<tr>
<td>Research</td>
<td></td>
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<tr>
<td>Biological &amp; Environmental Research</td>
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<tr>
<td>BER Base Program</td>
<td>487,474</td>
<td>435,476</td>
<td>510,263</td>
<td>+72,787 +14.2%</td>
<td>531,897</td>
<td>+21,634 +4.2%</td>
</tr>
<tr>
<td>Congressionally-directed projects</td>
<td>79,123</td>
<td>128,601</td>
<td></td>
<td>-49,478 -60.0%</td>
<td></td>
<td>-21,167 -34.0%</td>
</tr>
<tr>
<td>Total, Biological &amp; Environmental Research</td>
<td>566,597</td>
<td>564,077</td>
<td>510,263</td>
<td>-54,314 -9.5%</td>
<td>531,897</td>
<td>+21,634 +4.2%</td>
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<tr>
<td>High Energy Physics</td>
<td>722,906</td>
<td>698,238</td>
<td>775,099</td>
<td>+76,861 +11.0%</td>
<td>782,238</td>
<td>+7,139 +0.9%</td>
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<tr>
<td>Nuclear Physics</td>
<td>394,549</td>
<td>357,756</td>
<td>454,060</td>
<td>+96,304 +26.9%</td>
<td>471,319</td>
<td>+17,259 +3.8%</td>
</tr>
<tr>
<td>Fusion Energy Sciences</td>
<td>266,947</td>
<td>280,683</td>
<td>318,950</td>
<td>+38,267 +13.6%</td>
<td>427,850</td>
<td>+108,900 +34.1%</td>
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<tr>
<td>Science Laboratories Infrastructure</td>
<td>37,498</td>
<td>41,684</td>
<td>50,888</td>
<td>+9,294 +22.1%</td>
<td>78,956</td>
<td>+28,068 +55.2%</td>
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<tr>
<td>Science Program Direction</td>
<td>154,031</td>
<td>159,118</td>
<td>170,877</td>
<td>+16,759 +7.4%</td>
<td>184,934</td>
<td>+14,057 +8.2%</td>
</tr>
<tr>
<td>Workforce Development for Teachers &amp; Scientists</td>
<td>7,599</td>
<td>7,120</td>
<td>10,952</td>
<td>+3,382 +53.8%</td>
<td>11,000</td>
<td>+48 +0.4%</td>
</tr>
<tr>
<td>S&amp;S</td>
<td>67,168</td>
<td>68,025</td>
<td>70,987</td>
<td>+2,862 +4.4%</td>
<td>70,987</td>
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<td>Use of prior year balances</td>
<td>-5,062</td>
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<td>SBIR/STTR (from SC programs)</td>
<td>77,842</td>
<td>81,160</td>
<td></td>
<td>-3,318 -4.1%</td>
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<tr>
<td>Subtotal, Science</td>
<td>3,599,871</td>
<td>3,596,391</td>
<td>4,101,710</td>
<td>+505,319 +14.1%</td>
<td>4,397,876</td>
<td>+296,166 +7.2%</td>
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<tr>
<td>SBIR/STTR (transferred from other DOE programs)</td>
<td>35,779</td>
<td>35,653</td>
<td></td>
<td>-128 -0.4%</td>
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<tr>
<td>Total, Science</td>
<td>3,635,650</td>
<td>3,632,044</td>
<td>4,101,710</td>
<td>+469,666 +12.9%</td>
<td>4,397,876</td>
<td>+296,166 +7.2%</td>
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</table>

† The FY 2008 President’s Budget Request and the material presented here assume the requested level for FY 2007, as the timing of FY 2007 appropriations did not allow their inclusion.

**††** A portion of Stanford Linear Acceleration Center linac operations transfers from High Energy Physics to Basic Energy Sciences in FY 2007 and FY 2008. Excluding the linac operations funding, the remainder of the High Energy Physics budget increases by 12.6% in the FY 2007 request and a further 3.7% in FY 2008.
FY 2008 President's Request for BES = $1,498,497K

Materials Sciences Research

Chemistry, Biosciences, Geosciences Research

Nanoscale Science Research Centers

Synchrotron Light Source Facilities Operation

Neutron Scattering Facilities Operation

Design and Construction (LCLS, NSLS-II)

Major Items of Equipment
- Electron Beam Centers
- Combustion Research Facility
- GPP, GPE, SBIR/STTR
- 4 Synchrotron Radiation Light Sources
- Linac Coherent Light Source & NSLS-II (PED or construction)
- 4 Neutron Sources
- 3 Electron Beam Microcharacterization Centers
- 5 Nanoscale Science Research Centers (2 complete and 3 nearly complete)
- 1 Special Purpose Center
The Spallation Neutron Source Project is Complete
Ahead of schedule, under budget, meeting all technical milestones
Construction is Complete and Initial Operations are Underway at Four NSRCs

1. Center for Functional Nanomaterials
   (Brookhaven National Laboratory)

2. Molecular Foundry
   (Lawrence Berkeley National Laboratory)

3. Center for Nanoscale Materials
   (Argonne National Laboratory)

4. Center for Nanophase Materials Sciences
   (Oak Ridge National Laboratory)

5. Center for Integrated Nanotechnologies
   (Sandia & Los Alamos National Labs)
Technology, Energy, and Society are Inextricably Intertwined

Today’s Energy Technologies and Infrastructures are Firmly Rooted in the 20th Century

U.S. Energy Consumption by Source

Quadrillion Btu

Wood
Hydroelectric Power
Coal
Petroleum
Natural Gas
Nuclear Electric Power

Incandescent lamp, 1870s
Four-stroke combustion engine, 1870s
Watt Steam Engine, 1782

Watt Steam Engine, 1782

Wind, water, wood, animals, (Mayflower, 1620)
Intercontinental Rail System, mid 1800s
Rural Electrification Act, 1935
Eisenhower Highway System, 1956

Technology, Energy, and Society are Inextricably Intertwined

Today’s Energy Technologies and Infrastructures are Firmly Rooted in the 20th Century
What Will the 21st Century Bring?

21st Century Science and Technology Will Exert Control at the Atomic, Molecular, and Nanoscale Levels

- **Wood**
- **Hydroelectric Power**
- **Coal**
- **Natural Gas**
- **Nuclear Electric Power**

**Graph:**
- Quadrillion Btu on the y-axis
- Years from 1850 to 2000 on the x-axis
- Lines for Wood, Coal, Hydroelectric Power, Natural Gas, and Nuclear Electric Power

**Equation:**

$$2H_2O + 4H^+ + 4e^- \rightarrow 4H_4$$

**Key Points:**
- DOE Formed, 1977
- Bio-inspired nanoscale assemblies - self-repairing and defect-tolerant materials and selective and specific chemical reactivity.

**Additional Images:**
- High Tc superconductors
- Peta-scale computing
- Designer molecules
- Solid-state lighting and many other applications of quantum confinement and low-dimensionality

**Legend:**
- **Mn**
- **O**
- **H**
### The Continuum of Research, Development, and Deployment

<table>
<thead>
<tr>
<th>Grand Challenge Research</th>
<th>Discovery Research</th>
<th>Use-Inspired Basic Research</th>
<th>Applied Research</th>
<th>Technology Maturation &amp; Deployment</th>
</tr>
</thead>
<tbody>
<tr>
<td>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.</td>
<td>Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies</td>
<td>Basic research for fundamental new understanding, usually with the goal of addressing showstoppers on real-world applications in the energy technologies</td>
<td>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</td>
<td>Scale-up research</td>
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<td>At-scale demonstration</td>
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<td>Cost reduction</td>
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<td>Prototyping</td>
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<td>Manufacturing R&amp;D</td>
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<td>Deployment support</td>
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#### Goal: new knowledge / understanding
- Focus: phenomena
- Metric: knowledge generation

#### Goal: practical targets
- Focus: performance
- Metric: milestone achievement
Grand Challenges

Our 20th century theoretical frameworks for condensed matter and materials physics, chemistry, and biology fail as we move to:

- ultrasmall or isolated systems at one extreme and
- complex or interacting systems at the other extreme.

New 21st century frameworks must be created to provide the language to interpret the discoveries of the last quarter of the 20th century: superconductivity, metamaterials, nano-x, chemistry in all its complexities including replication, and more. These frameworks will recognize that the boundaries among condensed matter and materials physics, chemistry, and biology are erased at small scales.

The BESAC Grand Challenges subcommittee has posed five questions:

- **How do electrons move in atoms, molecules and materials?**
  *Creating a new language for electron dynamics to replace the 20th century assumption that electrons move independently from atoms*

- **Can we control the essential architecture of nature?**
  *Designing the placement of atoms in materials using tools of self-assembly, self-repair, self-replication*

- **How do particles cluster?**
  *Understanding primary patterns, emergence, and strong correlations*

- **How do we learn about small things?**
  *Interrogating the nanoscale, and communicating with it*

- **How does matter behave beyond equilibrium?**
  *Formulating the basis for non-equilibrium behavior, which dominates the world around us at both very small and very large scales*
The Continuum of Research, Development, and Deployment

- Grand Challenge Research
- Discovery Research
- Use-Inspired Basic Research
- Applied Research
- Technology Maturation & Deployment

(BESAC) Grand Challenges Panel
(BES) Basic Research Needs Workshops
(BES, BESAC, ...) Tools and Facilities in Support of Research

Technology Office/Industry Roadmaps
Discovery and Use-Inspired Research
The “Basic Research Needs” Workshops

- Basic Research Needs to Assure a Secure Energy Future
  BESAC Workshop, October 21-25, 2002
  The foundation workshop that set the model for the focused workshops that follow.

- Basic Research Needs for the Hydrogen Economy

- Nanoscience Research for Energy Needs
  BES and the National Nanotechnology Initiative, March 16-18, 2004

- Basic Research Needs for Solar Energy Utilization
  BES Workshop, April 18-21, 2005

- Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors
  BES, ASCR, FES, and NE Workshop, March 31-April 2, 2004

- The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycles
  BES, NP, and ASCR Workshop, September 2005

- Basic Research Needs for Superconductivity
  BES Workshop, May 8-10, 2006

- Basic Research Needs for Solid-state Lighting
  BES Workshop, May 22-24, 2006

- Basic Research Needs for Advanced Nuclear Energy Systems
  BES Workshop, July 31-August 3, 2006

- Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels
  BES Workshop, October 30-November 1, 2006

  BES Workshop, February 21-23, 2007

- Basic Research Needs for Electrical Energy Storage
  BES Workshop, April 2-5, 2007

- Basic Research Needs for Materials under Extreme Environments
  BES Workshop, June 10-14, 2007

- Basic Research Needs for Catalysis for Energy
  BES Workshop, August 5-10, 2007

- Basic Research Needs – Final Wrap-up Workshop
  BESAC, TBD
### Example: Solar-to-Electric Conversion

<table>
<thead>
<tr>
<th>Discovery Research</th>
<th>Use-inspired Basic Research</th>
<th>Applied Research</th>
<th>Technology Maturation &amp; Deployment</th>
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</thead>
</table>
| Low-dimensionality, quantum confinement, and the control of the density of states of photons, phonons, electrons | New or nanostructured materials for multiple-junction solar cells | Technology Milestones:  
- Decrease the cost of solar to be competitive with existing sources of electricity in 10 years  
- Deploy 5-10 GW of photovoltaics (PV) capacity by 2015, to power ~2 million homes.  
- Residential: 8-10 ¢/kWhr  
- Commercial: 6-8 ¢/kWhr  
- Utility: 5-7 ¢/kWhr (2005 $s) | Scale-up research |
| Defects, disorder, and tolerance to same of advanced materials | Control and extraction of energy from multiple-exciton generation | Silicon solar cells – single crystal, multicrystal, ribbon, thin-layer; production methods; impurities, defects, and degradation | At-scale demonstration |
| Molecular self-assembly and self-repair | Radiative and non-radiative processes in solar cells | Thin-film solar cells – a-Si, CuInSe, CdTe, Group III-V technologies | Cost reduction |
| Designer interfaces and thin films | Interfacial photochemistry of dye-sensitized nanostructures | High-efficiency solar cells | Prototyping |
| Photon management, including exciton creation and transport | Synthesis and processing science: Thin-film growth, templating, strain relaxation, nucleation and growth | Polymeric and dye-sensitized solar cells | Manufacturing R&D |
| Control of light absorption and scattering | Enhanced coupling of solar radiation to absorber materials, e.g., by periodic dielectric or metallodielectric structures | Assembly and fabrication R&D issues | Deployment support |
| Novel theoretical and experimental tools | Energy transduction in novel molecular, polymeric, or nanoparticle-based photovoltaics | |

**BES**

**EERE**
## Example: Solar-to-Fuels Conversion

<table>
<thead>
<tr>
<th>Discovery Research</th>
<th>Use-inspired Basic Research</th>
<th>Applied Research</th>
<th>Technology Maturation &amp; Deployment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge transfer and separation in natural and bio-inspired photosynthetic systems</td>
<td>Novel photoelectrode materials and molecular configurations for efficient photoelectrolysis</td>
<td>Technology Milestones:</td>
<td>Scale-up research</td>
</tr>
<tr>
<td>Nano-architectures for coupling light-harvesting and catalytic functions</td>
<td>Biomimetic multi-electron catalysts and proton-coupled electron transfer for solar water splitting</td>
<td>2010 to 2012: Laboratory-scale demonstration of solar driven high-temperature thermochemical hydrogen production that projects to a cost $6.00/gge (ultimate target: $7.00/gge delivered)</td>
<td>At-scale demonstration</td>
</tr>
<tr>
<td>Self-organization and controlled-assembly of complex structures</td>
<td>Photocatalytic cycles for CO₂ reduction to alcohol fuels</td>
<td>2015 to 2018: Laboratory-scale photo-electrochemical water splitting system to produce hydrogen at a 10% solar-to-hydrogen efficiency. Laboratory-scale photobiological water splitting system to produce hydrogen with 5% efficiency.</td>
<td>Cost reduction</td>
</tr>
<tr>
<td>Robust, functional catalysts that mimic biological processes</td>
<td>Multi-scale control of reactivity in hybrid molecular materials</td>
<td>Accelerate and expand research on the low-cost solar production of hydrogen:</td>
<td>Prototyping</td>
</tr>
<tr>
<td>Ultrafast imaging of electron dynamics</td>
<td>Defect formation mechanisms and self-repair in solar-to-fuels pathways</td>
<td>- Component development and systems integration to enable electrolyzers to operate from inherently intermittent and variable-quality power derived from solar sources</td>
<td>Manufacturing R&amp;D</td>
</tr>
<tr>
<td>Multi-scale theoretical and computational approaches</td>
<td>Hierarchical organization of molecular constructs for artificial photosynthesis</td>
<td>- Solar-driven high-temperature chemical cycle water splitting</td>
<td>Deployment support</td>
</tr>
</tbody>
</table>

**BES**

**EERE**
A DOE Analysis Looked at the Vertical and the Horizontal Connections

Supply
- Advanced Nuclear
- Zero Emission Fossil Electric Generation
- Renewable Energy
- Fusion Energy
- Alternative Liquid Fuels
- Bioenergy/Chemicals

Distribution
- Electric Grid of the Future
- Hydrogen & Gas Infrastructure
- Fuel Grid of the Future

Use
- Industrial Technologies
- Advanced Building Systems
- Vehicle Technologies

Future Electricity Systems
Future Liquid Fuels Systems
Future Hydrogen & Gaseous Fuels Systems
Cross-cutting / Enabling Science and Technology