Research Opportunities in the Office of Basic Energy Sciences at the Department of Energy

Jim Horwitz
Division of Materials Sciences and Engineering
Office of Basic Energy Sciences
U.S. Department of Energy

LPC Workshop
Jefferson Labs
March 10, 2004
Office of Science

Director
Raymond L. Orbach
Principal Deputy Director
James F. Decker
Deputy Director for Operations
Milton D. Johnson
Chief of Staff
Jeff Salmon

Office of Basic Energy Sciences
Associate Director
Patricia M. Dehmer

Office of Information Technology Management
Director
William J. Valdez

Office of Information Technology Management
Senior Information Management Executive
C. Edward Oliver (Acting)

Office of Laboratory Policy
Director
Antionette Joseph

Office of Laboratory Operations and ES&H
Associate Director
G. Leah Dever (Acting)

Chicago Operations Office
Manager
Marvin E. Gunn, Jr.

Oak Ridge Operations Office
Manager
James A. Turi (Acting)

Berkeley Site Office
Director
Richard H. Nolan

Stanford Site Office
Director
John S. Muhlestein

Office of Resource Management
Associate Director
John Rodney Clark

Office of Planning and Analysis
Director
William J. Valdez

Office of Laboratory Policy
Director
Antionette Joseph

Office of Laboratory Operations and ES&H
Associate Director
G. Leah Dever (Acting)

Chicago Operations Office
Manager
Marvin E. Gunn, Jr.

Oak Ridge Operations Office
Manager
James A. Turi (Acting)

Berkeley Site Office
Director
Richard H. Nolan

Stanford Site Office
Director
John S. Muhlestein

Office of Information Technology Management
Senior Information Management Executive
C. Edward Oliver (Acting)

Office of Laboratory Policy
Director
Antionette Joseph

Office of Laboratory Operations and ES&H
Associate Director
G. Leah Dever (Acting)

Chicago Operations Office
Manager
Marvin E. Gunn, Jr.

Oak Ridge Operations Office
Manager
James A. Turi (Acting)

Berkeley Site Office
Director
Richard H. Nolan

Stanford Site Office
Director
John S. Muhlestein

NOTE: Director of Science equivalent to Assistant Secretary position and filled by Presidential Appointment (Senate confirmed); Principal Deputy Director equivalent to Principal Deputy Assistant Secretary; Associate Directors equivalent to Deputy Assistant Secretaries.
The Basic Energy Sciences Program ...

☑ ... is one of the Nation's largest sponsors of basic research.

☑ ... supports research in more than 150 academic institutions and 13 DOE laboratories.

☑ ... supports world-class scientific user facilities.

☑ ... is uniquely responsible in the Federal government for supporting research in materials sciences, chemistry, geosciences, and aspects of biosciences related to energy resources, production, conversion, efficiency, and use – all in an environmentally conscientious manner.
### FY 2004 President’s Request

<table>
<thead>
<tr>
<th>FY 2002 Comparable</th>
<th>FY 2003 Budget</th>
<th>FY 2004 Budget</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approp.*</td>
<td>Request</td>
<td>Request</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1 Materials Sciences and Engineering</th>
<th>223,701</th>
<th>251,422</th>
<th>253,759</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 Research</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 MIE, SSRL SPEAR3 Upgrade (SLAC)</td>
<td>8,300</td>
<td>9,300</td>
<td>0</td>
</tr>
<tr>
<td>4 MIE, ANL Nanoscale Research Center</td>
<td>0</td>
<td>0</td>
<td>10,000</td>
</tr>
<tr>
<td>5 Facility Operations</td>
<td>268,032</td>
<td>274,118</td>
<td>290,004</td>
</tr>
<tr>
<td>6 SBIR/STTR</td>
<td>0</td>
<td>12,737</td>
<td>13,948</td>
</tr>
<tr>
<td>7 Total, Materials Sciences and Engineering</td>
<td>500,033</td>
<td>547,577</td>
<td>567,711</td>
</tr>
<tr>
<td>8 Chemical Sciences, Geosciences, and Energy Biosciences</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9 Research</td>
<td>194,150</td>
<td>208,488</td>
<td>209,597</td>
</tr>
<tr>
<td>10 MIE, SSRL SPEAR3 Upgrade (SLAC)</td>
<td>700</td>
<td>700</td>
<td>0</td>
</tr>
<tr>
<td>11 Facility Operations</td>
<td>5,377</td>
<td>5,805</td>
<td>5,967</td>
</tr>
<tr>
<td>12 SBIR/STTR</td>
<td>0</td>
<td>5,022</td>
<td>5,350</td>
</tr>
<tr>
<td>13 Total, Chemical Sciences, Geosciences and Energy Biosciences</td>
<td>200,227</td>
<td>220,015</td>
<td>220,914</td>
</tr>
<tr>
<td>14 <strong>Construction</strong></td>
<td>276,300</td>
<td>210,571</td>
<td>124,600</td>
</tr>
<tr>
<td>15 Spallation Neutron Source (ORNL)</td>
<td>3,000</td>
<td>11,000</td>
<td>3,000</td>
</tr>
<tr>
<td>16 PED, Nanoscale Science Research Centers</td>
<td>0</td>
<td>24,000</td>
<td>20,000</td>
</tr>
<tr>
<td>17 Center for Nanophase Materials Sciences (ORNL)</td>
<td>0</td>
<td>24,000</td>
<td>20,000</td>
</tr>
<tr>
<td>18 The Molecular Foundry (LBNL)</td>
<td>0</td>
<td>0</td>
<td>35,000</td>
</tr>
<tr>
<td>19 Center for Integrated Nanotechnologies (SNL, LANL)</td>
<td>0</td>
<td>0</td>
<td>29,850</td>
</tr>
<tr>
<td>20 PED, Linac Coherent Linac Source (SLAC)</td>
<td>0</td>
<td>6,000</td>
<td>7,500</td>
</tr>
<tr>
<td>21 Total Construction</td>
<td>279,300</td>
<td>251,571</td>
<td>219,950</td>
</tr>
<tr>
<td>22 <strong>Total, Basic Energy Sciences</strong></td>
<td>979,560</td>
<td>1,019,163</td>
<td>1,008,575</td>
</tr>
<tr>
<td>23 * Excludes $16,612,000 that was transferred to the SBIR and STTR programs.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**BES FY 2005 President’s Budget Request**

**CONSTRUCTION**
(Spallation Neutron Source, Nanoscale Science Research Centers, & Linac Coherent Light Source)

**Research (Universities*)**

**Research (Laboratories)**

**User Facilities (Operating)**

**Capital Equipment**

**GPP**

**SBIR/STTR**

**FACILITY OPERATIONS**
(X-ray and Neutron Scattering Facilities & the Combustion Research Center)

**B/A in millions of dollars**
$1,063.5

*Includes the funding for not-for-profits, other agencies, and private institutions.*
NSRCs ( ) and the BES User Facilities

- Advanced Photon Source
- Electron Microscopy Center for Materials Research
- Advanced Photon Source
- Center for Microanalysis of Materials
- National Synchrotron Light Source
- Center for Functional Nanomaterials
- Spallation Neutron Source
- Center for Nanophase Materials Sciences
- Shared Research Equipment Program
- High-Flux Isotope Reactor
- Materials Preparation Center
- Pulse Radiolysis Facility
- Center for Functional Nanomaterials
- Center for Microanalysis of Materials
- Special Purpose Centers
- 4 Nanoscale Science Research Centers

- Under construction
- In design/engineering

- 4 Synchrotron Radiation Light Sources
- Linac Coherent Light Source (CD0 approved)
- 4 High-Flux Neutron Sources (SNS under construction)
- 4 Electron Beam Microcharacterization Centers
- 4 Special Purpose Centers
- 5 Nanoscale Science Research Centers
Nanoscale Science Research Centers (NSRCs)

- Research facilities for synthesis, processing, and fabrication of nanoscale materials
- Co-located with existing user facilities (synchrotron radiation light sources, neutron scattering facilities, other specialized facilities) to provide characterization and analysis capabilities
- Operated as user facilities; available to all researchers; access determined by peer review of proposals
- Provide specialized equipment and support staff not readily available to the research community
- Conceived with broad input from university and industry user communities to define equipment scope
- Extensively reviewed by external peers, by the Basic Energy Sciences Advisory Committee, and by the Office of Science construction project management division
Experimental Condensed Matter Physics

Condensed Matter Physics and Materials Chemistry Team
Materials Sciences and Engineering Division
Strategic Themes in Condensed Matter and Materials Physics

√ Understanding magnetism and superconductivity
√ Materials synthesis, processing and nanofabrication
√ Structure and properties of materials at reduced dimensionality
√ Controlling electrons and photons in solids on the atomic scale
√ Properties of materials under extreme conditions
√ Quantum mechanics of large, interacting systems
√ Nonequilibrium processes and the relationship between molecular and mesoscopic properties
√ Materials with increasing complexity in composition, structure and function
Portfolio

- Fundamental research program in experimental condensed matter and materials physics
  - Provide the understanding of the physical phenomena and processes underlying the properties and behavior of advanced materials
- Development of advanced experimental techniques, instrumentation and methodology
- Provide the knowledge base for energy technologies
Major Historical Impacts

- **Thermoacoustic refrigeration:** Discovered, developed and expanded the field of thermoacoustic refrigeration, having applied the scientific discoveries to the development of cryocoolers, a stirling cycle thermoacoustic refrigerator, and a thermoacoustic natural gas-fired gas liquifier. Numerous publications, several patents, licensing agreements and practical devices have resulted. The technology won a R&D 100 award in 1999.

- **Z-contrast microscopy:** Invention and perfection of a high resolution scanning transmission electron microscopy capable of both atomic resolution and chemical element identification. This microscopy has had major impact on the study of materials structure. A sub-Angstrom resolution microscope is now under development. The technology won a R&D 100 award in 1990.

- **Photonic Band Gap Materials:** The predictive design, and the fabrication and characterization of photonic band gap materials, regular array structures which transmit, reflect or guide photons of specific frequencies. These materials offer great promise for the development of antennas, resonant filters, detectors and optical signal handling systems.

- **Ion channeling/lon implantation:** Discovered, initially by computer simulations, verified and developed the phenomenon of ion channeling-one of the first materials physics discoveries using computers. The effect has been expanded into such diverse and important applications as Rutherford Back Scattering, ion implantation and ion beam modification of materials.
Challenges

- Materials Synthesis and Crystal Growth
  - Superconductors
  - Complex oxides
  - Carbon species
  - Magnetic materials
- Low Temperature Physics
  - Superconductivity
  - 2-D electron systems
- Very High Magnetic Field Research Program
  - 60 and 100T magnets at LANL
  - Support novel quantum phenomena research
Challenges Continued

- **Correlated Electron Systems**
  - Mechanisms of magnetism and superconductivity
  - Low dimensional electron systems
  - Novel quantum effects, e.g. Bose-Einstein
  - Condensation, fractional quantum hall effect

- **Nanoscale Systems**
  - Electronic properties of nanoscale materials and structures
  - Doping of clusters and nanocrystals
  - Quantum effects in nanocrystals and nanoscale arrays

- **Underway**
  - Laser/Material Interactions
  - Casimir Force
**Interactions**

- **BES**
  - Joint funding with EPSCoR
  - Key participant in two Center of Excellence in Synthesis and Processing thrusts

- **DOE**
  - EE - Photovoltaics; superconductivity; materials
  - DP - Photoemission characterization of actinides; laser crystals; positron spectroscopy
  - EM, FE - Granular materials; fluids; thermoacoustics

- **National**
  - Joint funding with several agencies of the Solid State Sciences Committee of the National Academy of Sciences
  - Periodic joint funding with the National Science Foundation
## Funding Summary

### Dollars in Thousands

<table>
<thead>
<tr>
<th>Performer</th>
<th>Funding Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Laboratories</td>
<td>77%</td>
</tr>
<tr>
<td>Universities</td>
<td>23%</td>
</tr>
</tbody>
</table>

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.
FY 2003 -2004 Highlights


◆ First observation of superconductivity in a magnetically doped semiconductor (PtSb$_2$/1% Yb) , M. Aronson, Univ. of Michigan

◆ Phase Separations under Pressure, D. J. Buttrey, U. Delaware
Stoichiometry-controlled layered perovskites of nickel show very complex oxygen-content phase diagrams exhibiting multiple phase separations. Under hydrostatic pressure, phase separations can be made to appear or disappear as oxygen defects migrate between coexisting phases or generate new phases

◆ Josephson Plasmon Microscopy, D.N. Basov UCSD A novel technique: Josephson plasmon microscopy has been proposed to investigate spatial non-uniformities of superconducting condensate within the CuO$_2$ planes in high-Tc superconductors. This approach enables experimental access to phase segregation of the superfluid density on the length scales of the order of 200-300 Å.
FY 2003 -2004 Highlights

◆ The catalytic activity of nanogold, S. Pennycook ONRL, Sub-nanometer gold rafts found in highly active nanogold. First-principles theory shows rafts bind both O2 and CO - Franceschetti, Lupini, et al., to be submitted to Science.

◆ Vibrational Dynamics of Hydrogen and Deuterium in Crystalline and Amorphous Silicon, N. H. Tolk and L. C. Feldman, Vanderbilt University, and G. Lupke, College of William and Mary. Significant progress in reaching this goal has been accomplished in recent landmark studies exploring the excitation and dynamics of vibrational states associated with hydrogen in crystalline and amorphous silicon. The lifetime of the Si-H stretch mode, is found to be extremely dependent on the local solid-state structure, ranging from picoseconds to several nanoseconds. Such large variations in lifetime (transition probability) are extraordinarily rare in solid-state science.

◆ Tunneling and Transport in Nanowires, A. M. Goldman, University of Minnesota- Twin Cities. A scanning tunneling microscope system has been developed which permits the low temperature study of the properties of one-dimensional wires of metallic atoms grown in situ. For sufficiently small wires, conventional Fermi liquid theory will fail, and the tunneling density of states should be a power law in voltage. This is a signature of Luttinger liquid behavior. One dimensional structures such as those being studied may emerge as interconnects in electronic device systems as very small feature sizes are realized.
FY 2003 - 2004 Highlights

- **Time-reversal symmetry breaking in high-TC superconductors:** Angle resolved photoelectron spectroscopy revealed the existence of time-reversal symmetry breaking in the pseudogap phase of underdoped Bi2212 superconductors (Kaminski, Ames Laboratory).

- **Development of the Thermal Spin Valve** – PRL 86, 1 (2001); PRL 88, 9 (2002); PRL 91, 14 (2003). In many layered antiferromagnets the thermal conductivity can be dramatically increased with application of a modest magnetic field. This is analogous to a conventional spin valve, in which the electrical conductivity can be increased with application of magnetic field. (Mandurs, ORNL)

- **Crystal Growth and Characterization of Layered Cobaltate Metals and Superconductors** – PRL 91, 217001 (2003). Layered cobaltates are exotic “21st century” materials in which charge, spin, and structural degrees of freedom couple in new ways to produce new phenomena. Theoretically, these materials have attracted interest because in Na0.3CoO2·1.4H2O the intercalation of water produces an anomalous superconductor on a triangular lattice of Co ions. Practically, the extraordinarily high thermopower of some metallic cobaltates makes these materials attractive for potential power generation applications. (Mandurs, ORNL)
Basic Research Needs to Assure a Secure Energy Future
A Basic Energy Sciences Advisory Committee Study

The Charge:

What are the 21st century fundamental scientific challenges that BES must consider in addressing the DOE missions in energy efficiency, renewable energy resources, improved use of fossil fuels, safe and publicly acceptable nuclear energy, future energy sources, science-based stockpile stewardship, and reduced environmental impacts of energy production and use?

Dr. John Stringer, EPRI, Chair
Dr. Linda Horton, ORNL, Co-Chair
Workshop: October 21 – 25, 2002
Basic Research for a Secure Energy Future
Supply, End Use, and Carbon Management

Global Climate Change Science

Policy

Fossil Carbon Energy Sources
- Coal
- Petroleum
- Natural Gas
- Oil shale, tar sands, hydrates,...

Non-Carbon Energy Sources
- Nuclear Fission
- Nuclear Fusion
- Hydrogen
- Geothermal
- Hydroelectric
- Solar
- Wind

Carbon Recycle
- Natural
- Synthetic

Energy Consumption
- Transportation
- Buildings
- Industrial

CO₂ Sequestration
- Geologic
- Terrestrial
- Ocean

Conservation and Efficiency

BES basic research activities address these areas
The Products of the BESAC Workshop

- A set of 37 Proposed Research Directions (PRDs)
  - Fossil Energy
  - Nuclear Fission Energy
  - Fusion Energy
  - Renewable and Solar Energy
  - Distributed Energy, Fuel Cells, and Hydrogen
  - Transportation Research
  - Residential, Commercial, and Industrial Energy
  - Energy Biosciences Research
  - Cross Cutting Research and Education

- Supporting statements for each PRD in the form of a one-page Executive Summary and three pages of detailed information

- A set of 10 General Research Areas derived from the 37 PRDs

- A “Factual Document” summarizing the status of energy supply and use.

- Web address: [http://www.science.doe.gov/bes/BESAC/reports.html](http://www.science.doe.gov/bes/BESAC/reports.html)

- No single solution to secure energy future

- Required research areas are highly interdisciplinary

- Basic science has to be accompanied by applications
“Tonight I'm proposing $1.2 billion in research funding so that America can lead the world in developing clean, hydrogen-powered automobiles... With a new national commitment, our scientists and engineers will overcome obstacles to taking these cars from laboratory to showroom, so that the first car driven by a child born today could be powered by hydrogen, and pollution-free.”

President Bush
State-of the-Union Address
January 28, 2003
Basic Research for Hydrogen Production, Storage, and Use
May 13-15, 2003

Workshop Chair: Millie Dresselhaus (MIT)
Associate Chairs: George Crabtree (ANL)
Michelle Buchanan (ORNL)

Breakout Sessions:
Hydrogen Production
Tom Mallouk, PSU & Laurie Mets, U. Chicago
Hydrogen Storage and Distribution
Kathy Taylor, GM (retired) & Puru Jena, VCU
Fuel Cells and Novel Fuel Cell Materials
Frank DiSalvo, Cornell & Tom Zawodzinski, CWRU

Pre-Workshop Briefings by EERE:
<table>
<thead>
<tr>
<th>Hydrogen Storage</th>
<th>JoAnn Milliken</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Cells</td>
<td>Nancy Garland</td>
</tr>
<tr>
<td>Hydrogen Production</td>
<td>Mark Paster</td>
</tr>
</tbody>
</table>

Workshop Plenary Session Speakers:
Steve Chalk (DOE-EERE) -- overview
George Thomas (SNL-CA) -- storage
Scott Jorgensen (GM) -- storage
Jae Edmonds (PNNL) -- environmental
Jay Keller (SNL-CA) – hydrogen safety

Charge: To identify fundamental research needs and opportunities in hydrogen production, storage, and use, with a focus on new, emerging and scientifically challenging areas that have the potential to have significant impact in science and technologies. Highlighted areas will include improved and new materials and processes for hydrogen generation and storage, and for future generations of fuel cells for effective energy conversion.
There exists an enormous gap between present state-of-the-art capabilities and requirements that will allow hydrogen to be competitive with today’s energy technologies:

- Production: 9M tons ⇒ 40M tons (vehicles)
- Storage: 4.4 MJ/L (10K psi gas) ⇒ 9.72 MJ/L
- Fuel cells: $3,000/kW ⇒ $35/kW (gasoline engine)

Major R&D efforts will be required:
- Simple improvements of today’s technologies will not meet requirements
- Technical barriers can be overcome only with high risk/high payoff basic research

Research is highly interdisciplinary, requiring chemistry, materials science, physics, biology, engineering, nanoscience, computational science.

Basic and applied research should couple seamlessly.
Priority Research Areas in Hydrogen Production

**Fossil Fuel Reforming**
Molecular level understanding of catalytic mechanisms, nanoscale catalyst design, high temperature gas separation

**Solar Photoelectrochemistry/Photocatalysis**
Light harvesting, charge transport, chemical assemblies, bandgap engineering, interfacial chemistry, catalysis and photocatalysis, organic semiconductors, theory and modeling, and stability

**Bio- and Bio-inspired H₂ Production**
Microbes & component redox enzymes, nanostructured 2D & 3D hydrogen/oxygen catalysis, sensing, and energy transduction, engineer robust biological and biomimetic H₂ production systems

**Nuclear and Solar Thermal Hydrogen**
Thermodynamic data and modeling for thermochemical cycle (TC), high temperature materials: membranes, TC heat exchanger materials, gas separation, improved catalysts
Priority Research Areas in Hydrogen Storage

**Metal Hydrides and Complex Hydrides**
Degradation, thermophysical properties, effects of surfaces, processing, dopants, and catalysts in improving kinetics, nanostructured composites

**Nanoscale/Novel Materials**
Finite size, shape, and curvature effects on electronic states, thermodynamics, and bonding, heterogeneous compositions and structures, catalyzed dissociation and interior storage phase

**Theory and Modeling**
Model systems for benchmarking against calculations at all length scales, integrating disparate time & length scales, first principles methods applicable to condensed phases
**Priority Research Areas in Fuel Cells**

**Electrocatalysts and Membranes**
Oxygen reduction cathodes, minimize rare metal usage in cathodes and anodes, synthesis and processing of designed triple percolation electrodes

**Low Temperature Fuel Cells**
‘Higher’ temperature proton conducting membranes, degradation mechanisms, functionalizing materials with tailored nano-structures

**Solid Oxide Fuel Cells**
Theory, modeling and simulation, validated by experiment, for electrochemical materials and processes, new materials—all components, novel synthesis routes for optimized architectures, advanced in-situ analytical tools
HYDROGEN FUEL INITIATIVE

Research and Development Funding in the President's 2005 Budget

The Hydrogen Fuel Initiative (HFI), announced in the President’s 2003 State of the Union address, seeks to help industry develop practical and cost-effective technologies for using hydrogen to power automobiles by 2015. HFI focuses primarily on development of technologies for the production, storage, and delivery of hydrogen, and on development of fuel cell technologies that can be used to power automobiles with virtually no emissions of air pollutants or greenhouse gases. Widespread use of fuel-cell vehicles would make the United States much less dependent on foreign sources of energy. The 2005 Budget for HFI is $228 million, 43% larger than the amount just enacted for FY 2004.

Hydrogen Fuel Initiative Budget ($ million)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy / Energy Efficiency and Renewable Energy</td>
<td>73</td>
<td>147</td>
<td>173</td>
<td>100</td>
<td>137</td>
</tr>
<tr>
<td>Energy / Fossil Energy (coal)</td>
<td>0</td>
<td>5</td>
<td>16</td>
<td>16</td>
<td>-</td>
</tr>
<tr>
<td>Energy / Nuclear Energy</td>
<td>0</td>
<td>6</td>
<td>9</td>
<td>9</td>
<td>-</td>
</tr>
<tr>
<td>Energy / Basic Energy Sciences</td>
<td>0***</td>
<td>0***</td>
<td>29</td>
<td>29</td>
<td>-</td>
</tr>
<tr>
<td>Transportation</td>
<td>0</td>
<td>0.6</td>
<td>0.8</td>
<td>0.8</td>
<td>-</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>73</strong></td>
<td><strong>159</strong></td>
<td><strong>228</strong></td>
<td><strong>155</strong></td>
<td><strong>212</strong></td>
</tr>
</tbody>
</table>

* Reflects funding for baseline activities that HFI augments and/or redirects. 2004 was the first year for the HFI.

** Reflects rescissions, general reductions, and other adjustments included in relevant 2004 appropriations.

*** Base funding for hydrogen-related activities in Basic Energy Sciences was roughly $8 million in 2001 and 2004. These activities have been reoriented and expanded to support the goals of the President’s HFI in 2005.
Approximately $21.5 million will be awarded in FY 2005, pending appropriations.

A solicitation will request pre-applications for **innovative basic research** proposals to establish the scientific basis that underpins the physical, chemical, and biological processes governing the interaction of hydrogen with materials. We seek to support **outstanding fundamental research** programs to ensure that discoveries and related conceptual breakthroughs from basic research will provide a solid foundation for the innovative design of materials and processes to usher in hydrogen as the clean and sustainable fuel of the future.

Five high-priority research directions, encompassing both short-term showstoppers and long-term grand challenges, will be the focus of the solicitation. They are:

- Novel Materials for Hydrogen Storage
- Membranes for Separation, Purification, and Ion Transport
- Design of Catalysts at the Nanoscale
- Solar Hydrogen Production
- Bio-Inspired Materials and Processes
These five focus areas will be described in greater detail in the solicitation.

**PREAPPLICATIONS ARE REQUIRED. No applications will be accepted without a preapplication followed by a BES response encouraging a full application.**

Preapplications must be submitted electronically as specified in the call.

Each FFRDC is limited to the submission of up to six preapplications as leading institution. For FFRDCs, BES reserves the right to encourage, in whole or in part, any, all, or none of the preapplications submitted, and BES may issue further guidance on the scope of full proposal submissions of those encouraged.

The solicitation will be silent on issues of project size, number of PIs, number of institutions, interdisciplinary or multidisciplinary nature of the work, etc.

It is anticipated that up to $12 million annually will be available for multiple awards for each of the following: universities and FFRDCs. Initial awards will be in Fiscal Year 2005, and applications may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs.

BES will coordinate with all appropriate groups both inside and outside of DOE, particularly EERE.
BES Plans for a Solicitation for Research in Support of the President’s Hydrogen Fuel Initiative – III

**Important Dates**

- **February 23, 2004**  Discussion at BESAC
- **May 15, 2004**  Call for preapplications published
- **July 15, 2004**  Preapplications due
- **September 1, 2004**  Decisions on preapplications sent to PIs
- **January 1, 2005**  Full proposals due
- **June – July 2005**  Awards made
Materials Sciences and Engineering

Information Sheet for Grant Applicants is Available

Some information that may be of interest to grant applicants

Please note that many of the suggestions and procedures below are specific to the Division of Materials Sciences and Engineering, and pertain only to applications submitted under our “core” research program - not to special initiatives or other announced program opportunities.

Fundamental science is the primary concern in the work that our Division supports. Studies that are directed primarily towards engineering, demonstration, or development goals, such as producing specific devices or identifying optimal processing for a particular application, are less likely to compete successfully. However, our portfolio does include scientific instrument development that enables fundamental materials research.

Practical details:

Electronic Submission: Please note that the Office of Science is moving over to a secure, web-enabled proposal submission system. Effective June 1, 2002, applications should be submitted in PDF format through this system at http://e-center.doe.gov. Paper applications will continue to be accepted until September 30, 2002. Further information is available at DOE’s Grants and Contracts web site: http://www.sc.doe.gov/production/grants/grants.html.

Pre-proposals (2 pages or less) may be submitted but are not required, and in general (for our core program) they will be used mainly to establish whether the topic area falls within our purview. If you do wish to submit a pre-proposal, electronic submission as an e-mail attachment is preferred. We will respond to them by phone or e-mail.

Proposal handling: Most new proposals are examined by most of the program managers within our Division, with one taking the lead on handling it. Some may be declined without external peer review. On the other hand, we are required to obtain outside peer reviews for any that we intend to fund.

Timing of submissions and awards: Proposals may be submitted at any time, but we recommend that they be sent to us between April 1st and September 30th. This allows sufficient time for completion of the peer review process prior to the annual cut-off date for new award decisions. Proposals that arrive later run the risk of being turned down regardless of the quality of reviews because all funds for the fiscal year may be committed prior to completion of the review process. Decisions on new proposals are usually made early in the following calendar year.

Typical term of support: Usually three or four years for a new proposal and three years for subsequent renewals. Renewal applications should be submitted at least nine months in advance of the scheduled termination date.

Names of reviewers: Within our Division, we do not ask applicants to suggest reviewers, and typically do not use anyone so suggested. We will honor any request to not use a specific reviewer; no reason is needed.

Sabbaticals or other leaves of absence during the grant should be discussed with us in advance.

Conferences, symposia, workshops, and meetings, other than those we initiate, are rarely supported.

Contacts within our Division, including phone and e-mail information, are available on the second web site listed below. The corresponding organization chart can be reached via a click button on this site. For further inquiries, please contact the program manager whose areas of expertise and/or responsibility most closely match the topic area.

Web sites with further information:
http://www.science.doe.gov/bes (Office of Basic Energy Sciences)
http://www.science.doe.gov/bes/dms/dmshome.html (Division of Materials Sciences & Engineering)
http://www.science.doe.gov/production/grants/grants.html (sponsored research details)
http://www.energy.gov/scitech/index.html (science and technology across the Dept. of Energy)
Relevant web sites for DOE-SC-BES programs:

- [http://www.science.doe.gov/bes](http://www.science.doe.gov/bes) (Office of Basic Energy Sciences)
- [http://www.science.doe.gov/bes/besstaff.html](http://www.science.doe.gov/bes/besstaff.html) (BES staff contacts and directory; click to org chart)
- [http://www.science.doe.gov/bes/dms/dmshome.html](http://www.science.doe.gov/bes/dms/dmshome.html) (Division of Materials Sciences & Engineering)
- [http://www.science.doe.gov](http://www.science.doe.gov) (Office of Science)