

---

# ***Materials Research Directions and Opportunities in the DOE Office of Basic Energy Sciences***

**Materials Research Society Spring Meeting  
April 18, 2017**

**Andy Schwartz  
Senior Technical Advisor  
DOE Office of Basic Energy Sciences**



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



# U.S. DEPARTMENT OF ENERGY

**Secretary**  
**Rick Perry**  
Deputy Secretary



“Our scientists and labs are the envy of the world, and I am a major proponent of maintaining American leadership in the area of scientific inquiry.”

**Under Secretary for Nuclear Security**

**Frank G. Klotz**

**Under Secretary for Science & Energy**

**Patricia Hoffman (A)**

**Under Secretary for Management & Performance**

**Defense Nuclear Nonproliferation**

**Defense Programs**

**Naval Reactors**

**Counter-terrorism**

**Defense Nuclear Security**

**Emergency Operations**

**Office of Science**

**Steve Binkley (A)**

**Basic Energy Sciences**

**Harriet Kung**

**High Energy Physics**

**James Siegrist**

**Advanced Scientific Computing Research**

**Barb Helland**

**Nuclear Physics**

**Tim Hallman**

**Biological & Environmental Research**

**Sharlene Weatherwax**

**Fusion Energy Sciences**

**Ed Synakowski**

**SBIR/STTR**

**Manny Oliver**

**Workforce Develop. for Teachers & Scientists**

**James Glownia**

**Advanced Research Projects Agency – Energy**

**Energy Efficiency & Renewable Energy**

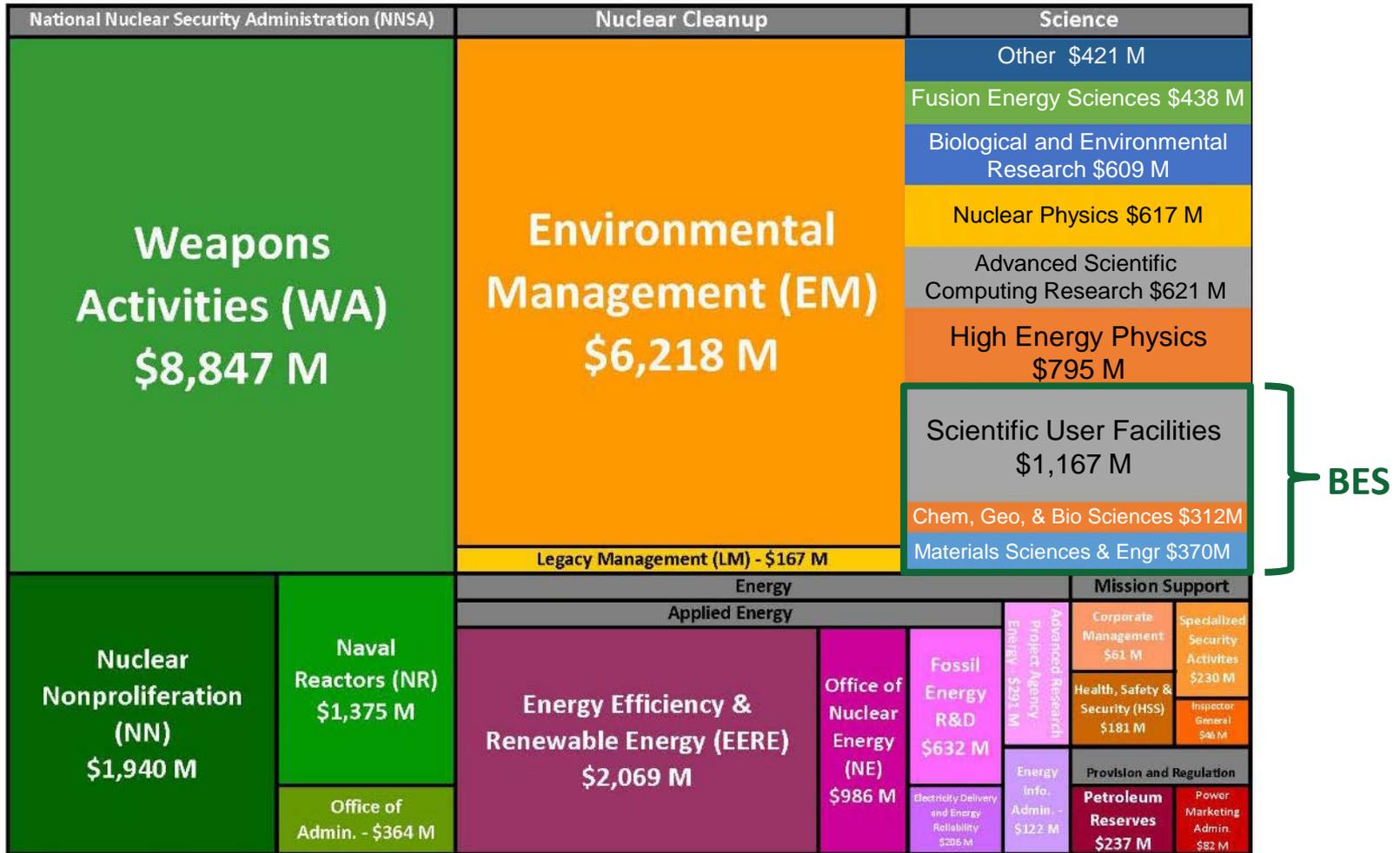
**Fossil Energy**

**Nuclear Energy**

**Electricity Delivery & Energy Reliability**

# The DOE Portfolio (~\$30B Total)

Department of Energy - FY 2016 Enacted - \$29,603 M



\* Representation does not include - \$199 M for All Other DOE

# FY 2016 BES Budget Appropriation

## Research programs

- Energy Frontier Research Centers (\$110M;  $\Delta = +\$10M$ )
- Computational Materials Sciences (\$12M;  $\Delta = +\$4M$ )
- Core Research & Hubs at ~FY 2015 level (\$558.5M)

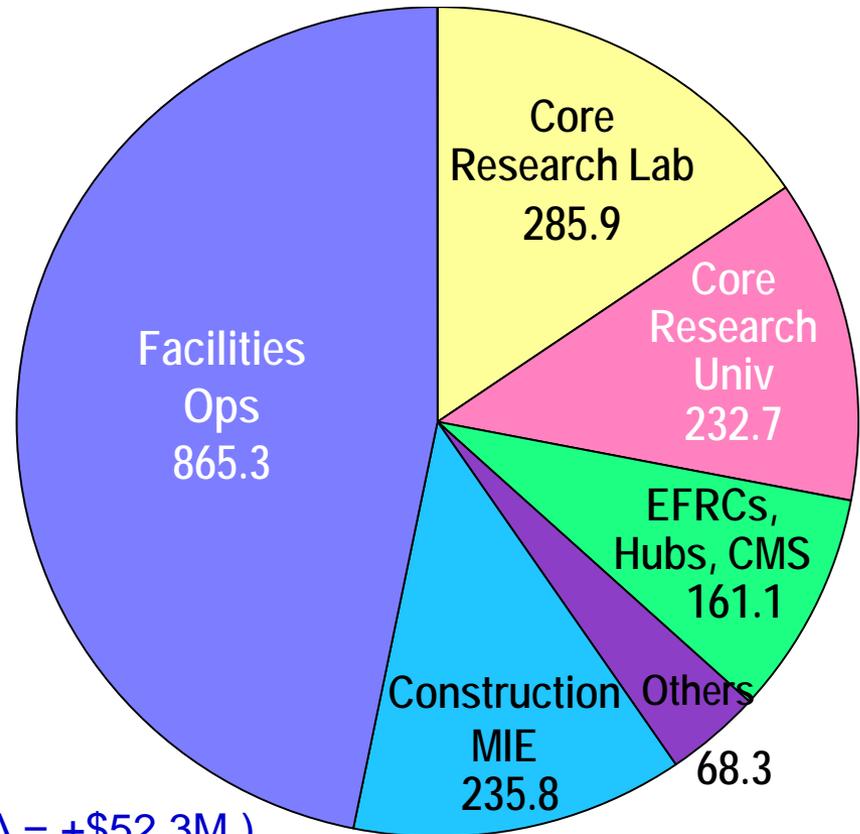
## Scientific user facilities

- All full operating facilities at near optimal operations (\$865.3M)
- NSLS-II 1<sup>st</sup> year of full operations (\$110M)

## Construction and instrumentation

- NSLS-II instrumentation (NEXT) (\$15.5M)
- Advanced Photon Source Upgrade (\$20M)
- Linac Coherent Light Source-II (\$200.3M;  $\Delta = +\$52.3M$ )

**FY 2016 Appropriation:**  
**\$1,849 M**  
**(+\$115.8M from FY 2015)**



# Basic Energy Sciences

**Materials sciences & engineering**—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

**Chemical sciences, geosciences, and energy biosciences**—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

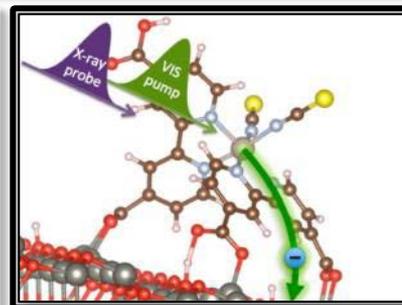
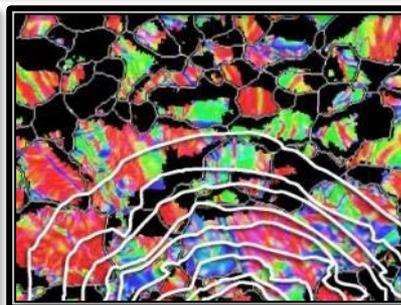
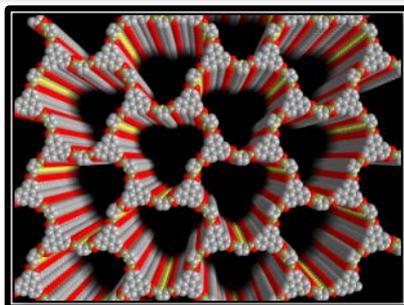
**Scientific User Facilities**—the largest collection of facilities for electron, x-ray, and neutron scattering in the world

In FY 2016, BES supported:

- ~**5,460 Ph.D.** scientists and ~**1,670 students**
- Research at over 150 academic institutions in 46 states and at 17 DOE laboratories.
- Over **1,000** research projects in **25** core research areas
- 36 Energy Frontier Research Centers
- Fuels from Sunlight & Batteries and Energy Storage Hubs
- More than **15,000 users** at 12 BES facilities
- New grant success rates ~**15%**

In FY 2016, BES invested ~**\$680 M** in research and ~**\$870 M** in operations for world-class, open-access scientific user facilities.

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



## Administrative Staff

Marsophia Agnant,  
MaryBeth Luther,  
Teresa Crockett

# Materials Sciences and Engineering Division

Linda Horton, Division Director



## Materials Discovery, Design, and Synthesis Team



Team Lead – Helen Kerch (A)

### Materials Chemistry



Michael Sennett Craig Henderson

### Biomolecular Materials



Mike Markowitz

### Synthesis and Processing Science



Bonnie Gersten

### Batteries and Energy Storage Hub & Integrated Energy Research



John Vetrano Craig Henderson

## Condensed Matter and Materials Physics Team



Team Lead - Jim Horwitz

### Experimental Condensed Matter Physics



Michael Pechan

### Theoretical Condensed Matter Physics



Matthias Graf Jim Davenport

### Physical Behavior of Materials



Refik Kortan

### Mechanical Behavior & Radiation Effects



John Vetrano

## Scattering and Instrumentation Sciences Team



Team Lead - Helen Kerch

### X-ray Scattering



Lane Wilson

### Neutron Scattering



Thiyaga P. Thiyagarajan

### Electron and Scanning Probe Microscopies



Jane Zhu

### Experimental Program to Stimulate Competitive Research (EPSCoR)



Tim Fitzsimmons

# BES Research Activities

## Energy Innovation Hubs (2)

~\$40M/year

- Research centers (\$15-25 million/year), engaged in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an FOA. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.
  - ▶ *Joint Center for Artificial Photosynthesis (JCAP), 2010 – present*
  - ▶ *Joint Center for Energy Storage Research (JCESR), 2012 – present*

## Energy Frontier Research Centers (36), 2009 – present Computational Materials Sciences Projects (5), 2015 – present

~\$122M/year

- EFRC: \$2-4 million/year for 4 year award terms; multi-disciplinary teams focused on “grand challenge” science and fundamental research described in the Basic Research Needs Workshop reports.
- CMS: \$2-4 million/year for four year award terms; multi-disciplinary teams focused on delivering open source, experimentally validated software and the associated data for predictive materials sciences in preparation for exascale computing .

## Core Foundational Research (>1,300 projects)

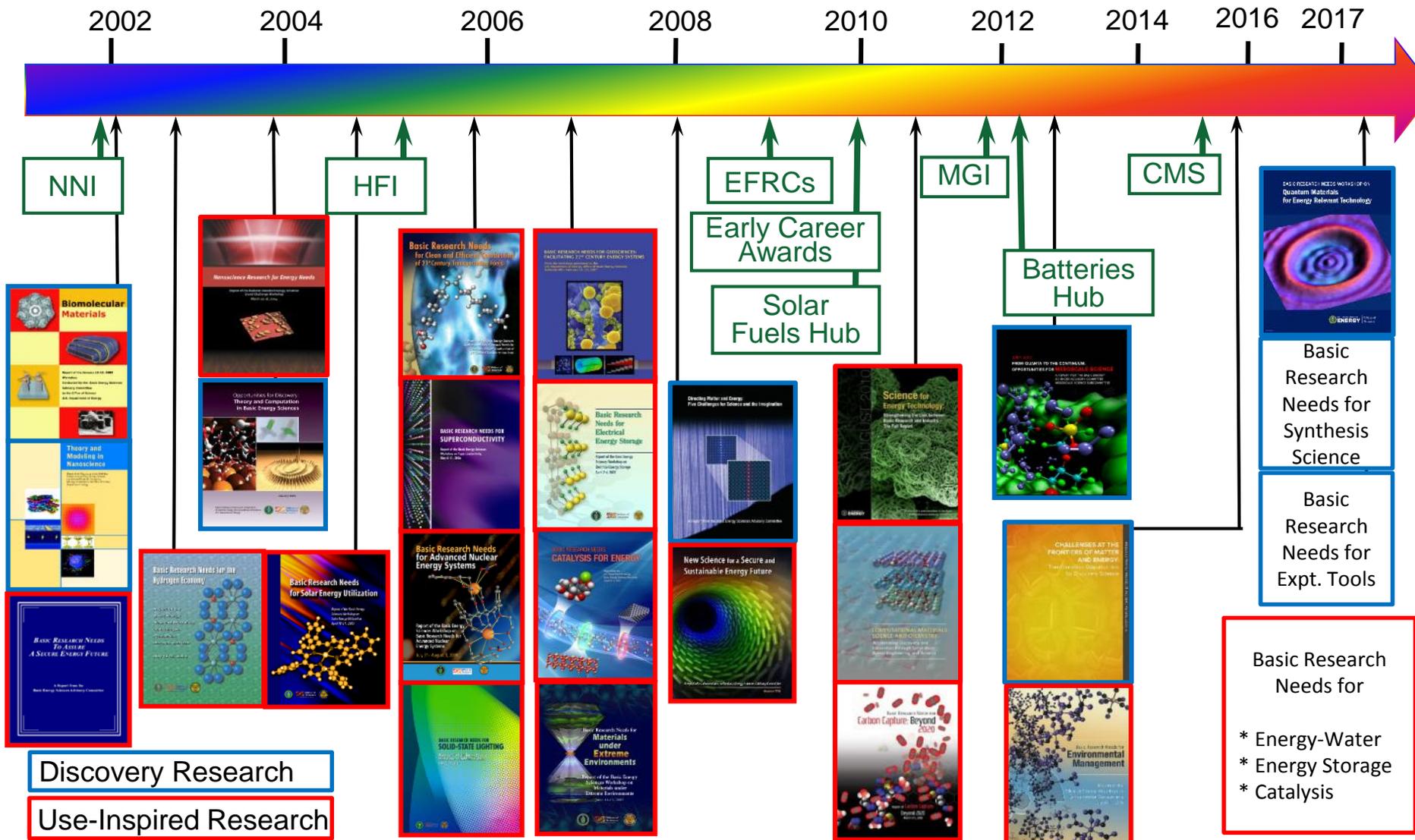
~\$520M/year

- Single investigators (~\$150K/year) and small groups (~\$500K-\$2M/year) engaged in fundamental research related to all of the BES core research areas. Investigators propose topics of their choosing in response to annual FOA.

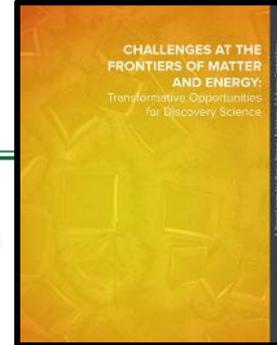
Increasing size & scope



# BES Strategic Planning and Program Development



# Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science



2015

*Instrumentation & Tools*



*Human Capital*

*Synthesis*

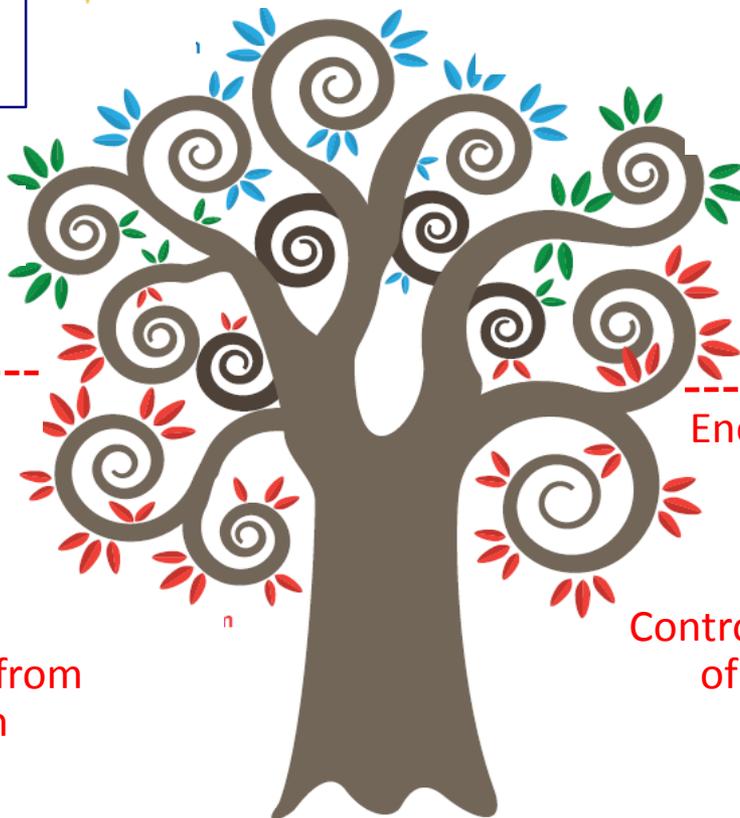
**Beyond Ideal Materials and Systems**

**Mastering Hierarchical Architectures**

**Harnessing Coherence in Light and Matter**

*Imaging Matter across Scales*

*Data, Algorithms and Computing*



Efficient Synthesis for Tailored Properties

Energy and Information on the Nanoscale

2007

Correlated Systems

Control at the Level of Electrons

Systems Away from Equilibrium

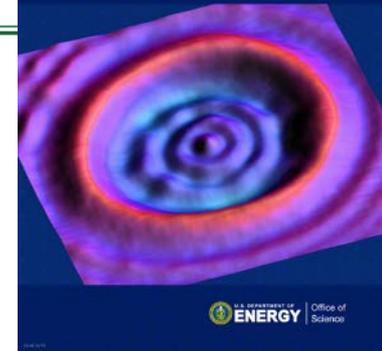


U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# Basic Research Needs for Quantum Materials for Energy Relevant Technology

BASIC RESEARCH NEEDS WORKSHOP ON  
Quantum Materials  
for Energy Relevant Technology



**CHARGE:** Identify basic research needs and priority research directions for quantum materials with a focus on new, emerging areas with potential for transformative scientific advances and for impact on energy technologies. The phenomena of quantum materials are examined in the broad categories of: (1) superconductivity and charge-related order, (2) magnetism and spin, (3) transport and non-equilibrium dynamics, (4) electronic topology, (5) nanostructure or heterogeneity.

## Priority Research Directions:

- Control and exploit fluctuations in quantum matter for the design of bulk materials with novel functionality
- Harness topological states for groundbreaking surface properties
- Drive and manipulate quantum effects (coherence, entanglement) in nanostructures for transformative technologies
- Design revolutionary tools to accelerate discovery and technological deployment of quantum materials

**Workshop Chair:** Collin Broholm (JHU); **Co-Chairs:** Ian Fisher (SLAC/Stanford); Joel Moore (UC-Berkeley/LBNL); Margaret Murnane (UC-Boulder)

**Breakout Sessions and Chairs:** *Superconductivity and charge order: Adriana Moreo (U Tennessee) and John Tranquada (BNL); Magnetism and spin: Meigan Aronson (Texas A&M) and Allan MacDonald (U Texas Austin); Transport and non-equilibrium dynamics: Dimitri Basov (UCSD) and Jim Freericks (Georgetown); Topological quantum materials: Eduardo Fradkin (U of Illinois) and Amir Yacoby (Harvard); Heterogeneous and nano-structured quantum materials: Nitin Samarth (PSU) and Susanne Stemmer (UCSB)*

# Emerging Priority Research Directions

---

## **Synthesis Science Workshop Report (to be released soon)**

- Achieve mechanistic control of synthesis to access new states of matter
- Accelerate materials discovery by exploiting extreme conditions, complex chemistries and molecules, and interfacial systems
- Harness the complex functionality of hierarchical materials
- Integrate emerging theoretical, computational and in situ characterization tools to achieve directed synthesis with real time, adaptive control

## **Experimental Tools Workshop Report (to be released soon)**

- Establish new frontiers in time, space, and energy resolution for characterization and control
- Create innovative experimental methods for investigating real-world systems
- Simultaneously interrogate form and function, bridging time, length, and energy scales
- Drive a new paradigm for instrumentation design through integration of experiment, theory, and computation

## **Recent and Upcoming Workshops**

- Energy-Water Nexus (January 2017)
- Next-Generation Electrical Energy Storage (March 2017)
- Catalysis Science to Transform Energy Technologies (May 2017)
- Future Nuclear Energy (TBD)

# Core Program Funding Opportunities: FAQs

---

- How do I get DOE/BES support?
  - Respond to “FY2017 Continuation of Solicitation for the Office of Science Financial Assistance Program” **Read all FOAs carefully!!**
  - Hypothesis driven, fundamental science with energy relevance; discovery science and use-inspired basic research
  - All eligible/responsive proposals are peer reviewed
- Can I contact/visit a program manager?
  - Initial contact by email and phone is encouraged – contact information is on the website for every program manager
  - White papers/pre-proposals are encouraged – Can be sent to program manager or submitted through the PAMS system; see FOA for details
  - BES offices located in Germantown, MD – secure facility, requires planning and additional information from foreign nationals.
- How much support can I get?
  - Peer review will assess requested budget versus research needs
  - Typical is 1 month of summer support plus graduate student/postdoc
  - Multi-PI grants are also supported – talk with the program manager

# Office of Science Early Career Research Program

(2010 – present)

- Purpose: To support individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science
- Eligibility: Within 10 years of receiving a Ph.D., either untenured academic assistant or associate professors on the tenure track or full-time DOE national lab employees
- 5-Yr Awards: University grants \$150,000/yr, National lab awards \$500,000/yr min

## FY 2016 Program

- 720 Office of Science proposals received, 22 Basic Energy Sciences (16 universities, 6 Labs) awards out of a total of 52 awards for the Office of Science (11 in BES-Materials Sciences and Engineering)

## FY 2017 Program

- Proposals currently under review

## FY 2018 Program

- Expect Funding Opportunity Announcement around July 2017
- **FOA will cover different topics than the annual FOA for BES – important to read the details!**

# DOE Office of Basic Energy Sciences: Scientific User Facilities

More than 14,000 users in FY 2015



- ★ Available to all researchers *at no cost* for non-proprietary research, regardless of affiliation, nationality, or source of research support
- ★ Access based on external peer merit review of brief proposals
- ★ Coordinated access to co-located facilities to accelerate research cycles
- ★ Collaboration with facility scientists an optional potential benefit
- ★ Instrument and technique workshops offered periodically
- ★ A variety of on-line, on-site, and hands-on training available
- ★ Proprietary research may be performed at full-cost recovery

## Neutron Sources

- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)

## Nanoscale Science Research Centers

- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL & LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)

## Light Sources

- Advanced Light Source (LBNL)
- Advanced Photon Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source-II (BNL)
- Stanford Synchrotron Radiation Laboratory (SLAC)



# Thank you

<http://science.energy.gov/bes/mse/>

The screenshot shows the website for the Materials Sciences and Engineering (MSE) Division. At the top, there is a navigation bar with links for Programs, Laboratories, User Facilities, Universities, Funding Opportunities, News, and About. Below this is a search bar and a "GO" button. The main content area features a blue header for the MSE Division and a sidebar with links to MSE Home, About, Research Areas, Reports and Activities, Science Highlights, and Principal Investigators' Meetings. The main text describes the division's mission and lists three research focus areas: Materials Discovery, Design, and Synthesis; Condensed Matter and Materials Physics; and Scattering and Instrumentation Sciences. A red box on the left highlights the text "Program Descriptions and Program Manager Contact Info" with an arrow pointing to the research focus areas.

**U.S. DEPARTMENT OF ENERGY** | Office of Science

Search SC Website    SC Site Search    **GO**

Programs    Laboratories    User Facilities    Universities    Funding Opportunities    News    About

You are here: SC Home » Programs » BES Home » MSE Home

## Materials Sciences and Engineering (MSE) Division

**MSE Home**

About

Research Areas

Reports and Activities

Science Highlights

Principal Investigators' Meetings

Print    Text Size: A A A    Feedback (+)    Share Page ▾

The Materials Sciences and Engineering (MSE) Division supports fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for the development of new materials for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. (details)

The MSE research portfolio consists of the research focus areas in the table below, which are managed within three organizational teams. Division [staff members](#) are responsible for managing these areas, conducting the reviews of research proposals, and assessing the productivity of the funded research.

- *Dr. Linda Horton*, Director of Materials Sciences and Engineering

| Materials Discovery, Design, and Synthesis  | Condensed Matter and Materials Physics  | Scattering and Instrumentation Sciences  |
|---|---|--|
| <ul style="list-style-type: none"><li>• Materials Chemistry</li><li>• Biomolecular Materials</li><li>• Synthesis and Processing Science</li></ul> | <ul style="list-style-type: none"><li>• Experimental Condensed Matter Physics</li><li>• Theoretical Condensed Matter Physics</li><li>• Physical Behavior of Materials</li><li>• Mechanical Behavior and Radiation Effects</li></ul> | <ul style="list-style-type: none"><li>• X-Ray Scattering</li><li>• Neutron Scattering</li><li>• Electron and Scanning Probe Microscopies</li></ul> |

Workshop Reports

Program Descriptions and Program Manager Contact Info