Overview of the US Department of Energy's Office of Basic Energy Sciences

John Vetrano

Program Manager

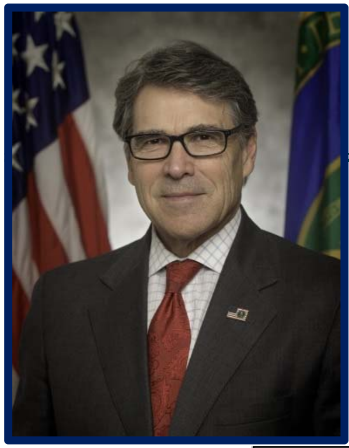
Office of Science - Basic Energy Sciences

U.S. Department of Energy

Presentation Outline

- Overview of DOE and BES Organization and Budget
- Description of BES Science and Organization
- Strategic Planning and Research Priorities
- Funding Opportunities and Process

Department of Energy Organizational Structure



Office of the Secretary

Rick Perry
Secretary

Dan Brouillette
Deputy Secretary

- Federal Energy Regulatory Commission
- Inspector General
- Ombudsman
- Chief of Staff

Office of the Under Secretary for Nuclear Security and National Nuclear Security Administration

Under Secretary for Nuclear Security (S5) / Administrator, NNSA

- Deputy Administrator for Defense Nuclear Nonproliferation
- Deputy Administrator for Defense Programs
- Deputy Administrator for Naval Reactors
- Deputy Under Secretary for Counter-terrorism & Counter-proliferation
- Associate Administrator for Defense Nuclear Security
- Associate Administrator for Emergency Operations
- Associate Administrator for External Affairs
- Associate Administrator for Safety, Infrastructure & Operations
- Associate Administrator for Management & Budget
- Associate Administrator for Acquisition & Project Management
- Office of General Counsel
- Associate Administrator for Information Management & Chief Information Officer

Office of the Under Secretary for Science (S4)

Under Secretary for Science

- Office of Science
- Office of Technology Transitions
- Office of the Assistant Secretary for Environmental Management
- Office of Legacy Management
- National Laboratory Operations Board

Office of the Under Secretary of Energy (S3)

Under Secretary

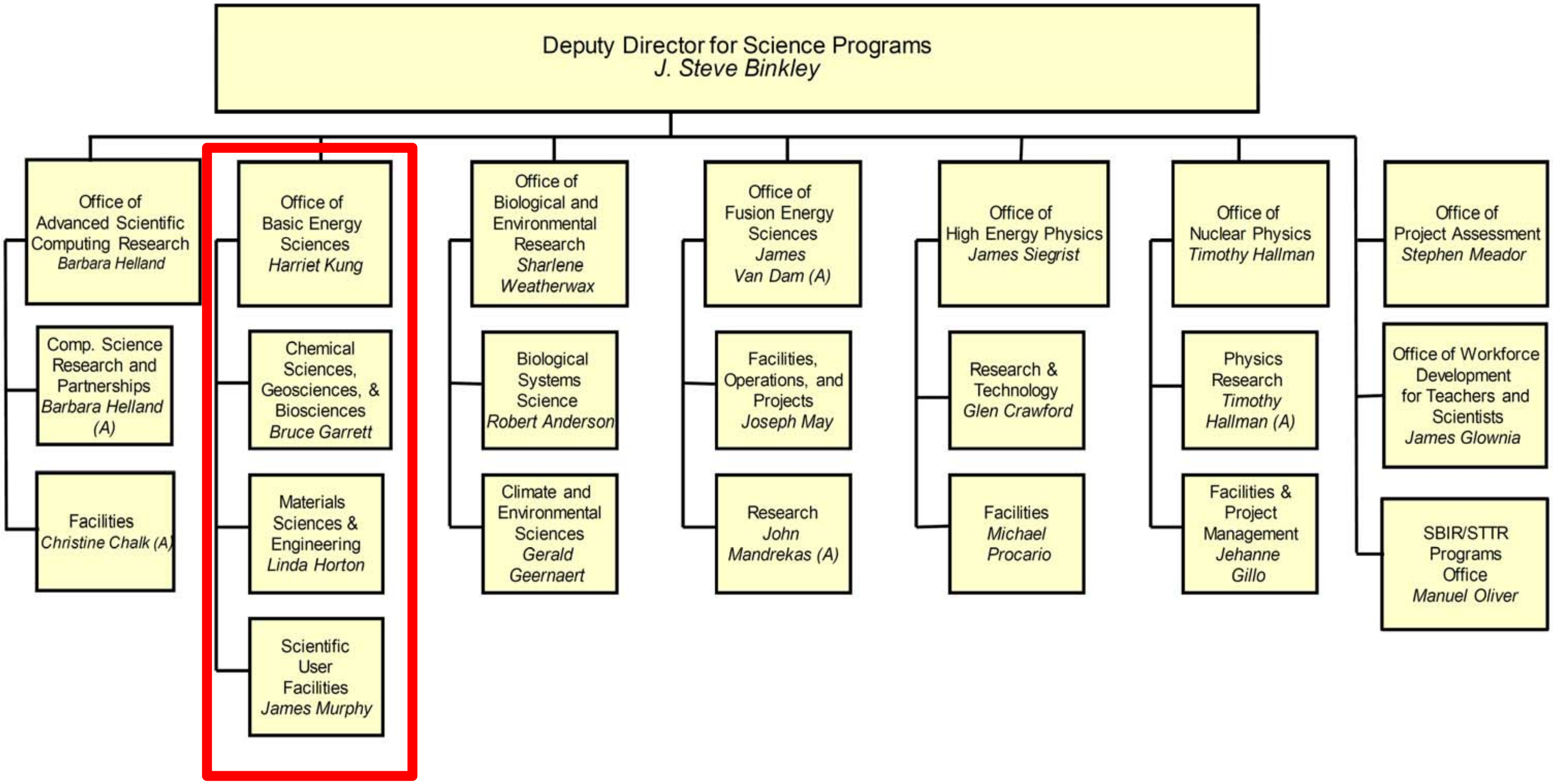
- Office of Policy
- Office of the Assistant Secretary for Energy Efficiency & Renewable Energy
- Office of the Assistant Secretary for Electricity Delivery & Energy Reliability
- Office of the Assistant Secretary for Fossil Energy
- Office of the Assistant Secretary for Nuclear Energy
- Office of Indian Energy Policy and Programs
- Loan Programs Office
- Office of Project Management Oversight & Assessments
- Office of the Associate Under Secretary for Environment, Health, Safety & Security

Offices reporting to the Secretary

- U.S. Energy Information Administration
- Advanced Research Projects Agency - Energy
- Bonneville Power Administration
- Southeastern Power Administration
- Southwestern Power Administration
- Western Area Power Administration
- Office of the Assistant Secretary for International Affairs
- Office of the Assistant Secretary for Congressional & Intergovernmental Affairs
- Office of Enterprise Assessments
- Office of Public Affairs
- Office of the General Counsel
- Office of the Chief Financial Officer
- Office of the Chief Human Capital Officer
- Office of the Chief Information Officer
- Office of Management
- Office of Small and Disadvantaged Business Utilization
- Office of Intelligence & Counterintelligence
- Office of Economic Impact & Diversity
- Office of Hearings & Appeals

The Office of Science is here.

Office of Science – Science Programs

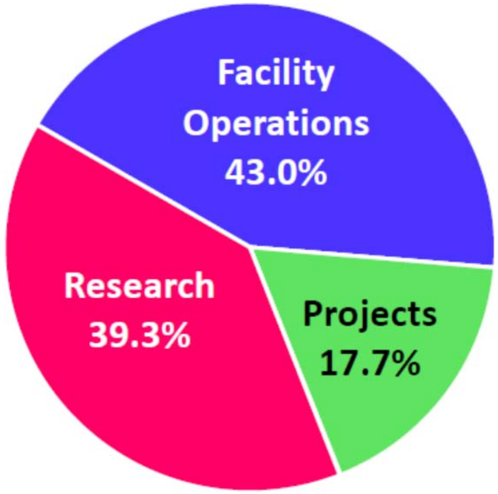


BES Program Overview

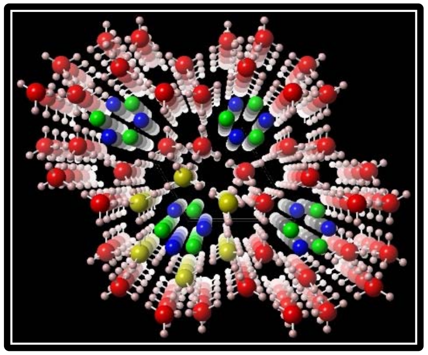
Understanding, predicting, and controlling matter and energy at the electronic, atomic, and molecular levels

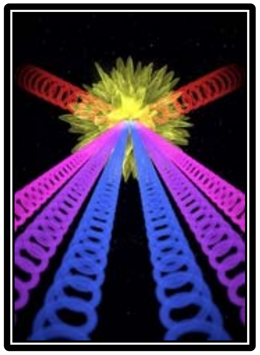
Research: condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences—to discover new materials and design new chemical processes that touch virtually every important aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation.

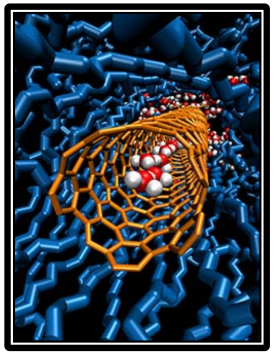
Facilities: x-ray light sources, neutron sources, nanoscale science research centers for the atomic-level visualization and characterization of materials of all kinds, including biological molecules. Construction of the next-generation facilities to maintain international competitiveness.

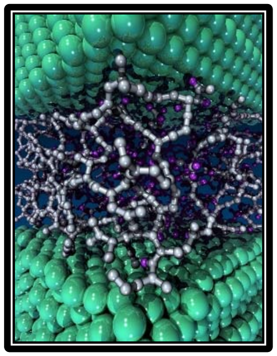


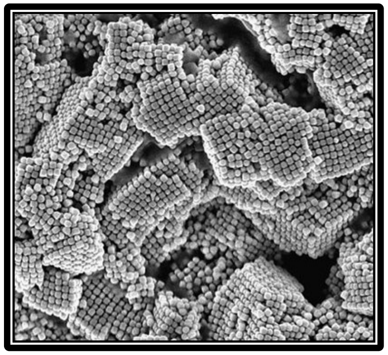
FY 2018 BES $2.09 B











BES By the Numbers

BES RESEARCH SPANS

MORE THAN **150** ACADEMIC, NONPROFIT, AND INDUSTRIAL INSTITUTIONS

17 DOE NATIONAL LABORATORIES | **47** STATES AND WASHINGTON, D.C.

25 CORE RESEARCH AREAS

36 ENERGY FRONTIER RESEARCH CENTERS

SUPPORTED RESEARCHERS

~5,600 Ph.D. SCIENTISTS | **~1,800** STUDENTS

BES | BY THE NUMBERS

FY 2017

BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels.

2 ENERGY INNOVATION HUBS

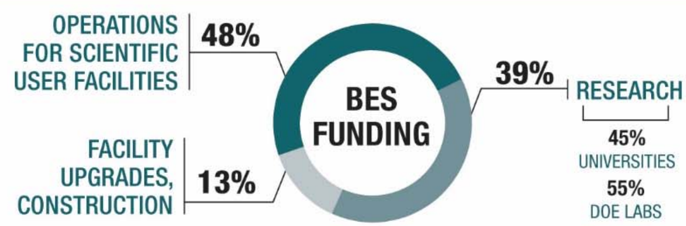
$724 MILLION RESEARCH BUDGET

~15% AVERAGE NEW GRANT SUCCESS RATE

OVER **1,000** CORE RESEARCH PROJECTS

NEARLY **16,000** USERS AT **12** BES FACILITIES

$915 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET



$233 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET

6

BES-Supported Research Activities

Increasing scope and size

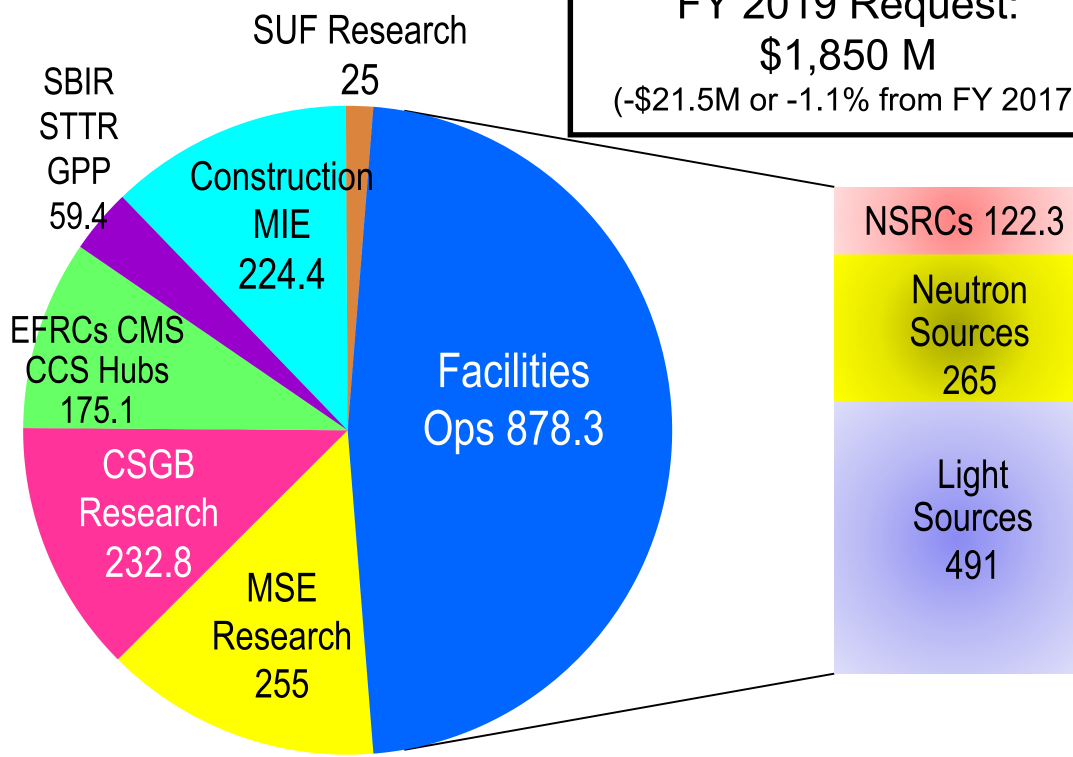
- **Core Research (>1,000 projects, ~$500M/yr)**
  Single investigators (~$150K/year) and small groups ($500K-$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing. Annual FOA open year-round. Includes awardees under the SC Early Career Research Program (separate FOA with annual proposal due dates).
- **Energy Frontier Research Centers ($110M/yr)**
  $2-4 million/year research centers for 4-year award terms; focus on fundamental research described in Basic Research Needs Workshop reports. Recompetition underway in FY 2018
- **Computational Materials & Chemical Sciences ($26M/yr)**
  $2-4 million/year research centers for 4-year award terms; focus on delivering open-source software for materials and chemistry by design in preparation for exascale computing. Recompetition anticipated in FY 2019 for CMS.
- **Fuels from Sunlight & Batteries and Energy Storage Hubs ($38M/yr)**
  Research centers for 5-year award terms, established in 2010 ($15-25M/year), engage in research topics that have proven challenging for traditional funding modalities and in which success could be transformative to science and technology. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.

FY 2019 BES Budget Request

Research programs

- Core Research will emphasize quantum materials and chemistry, ultrafast science, and BRN topics.
- Computational Materials and Chemical Sciences continue ($26M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).
- Energy Frontier Research Centers continue ($110M)

FY 2019 Request:
$1,850 M
(-$21.5M or -1.1% from FY 2017)



Scientific user facilities

- Operations of 12 facilities at 95% optimal level
- No funding is requested for Lujan equipment disposition or Long Term Surveillance and Maintenance

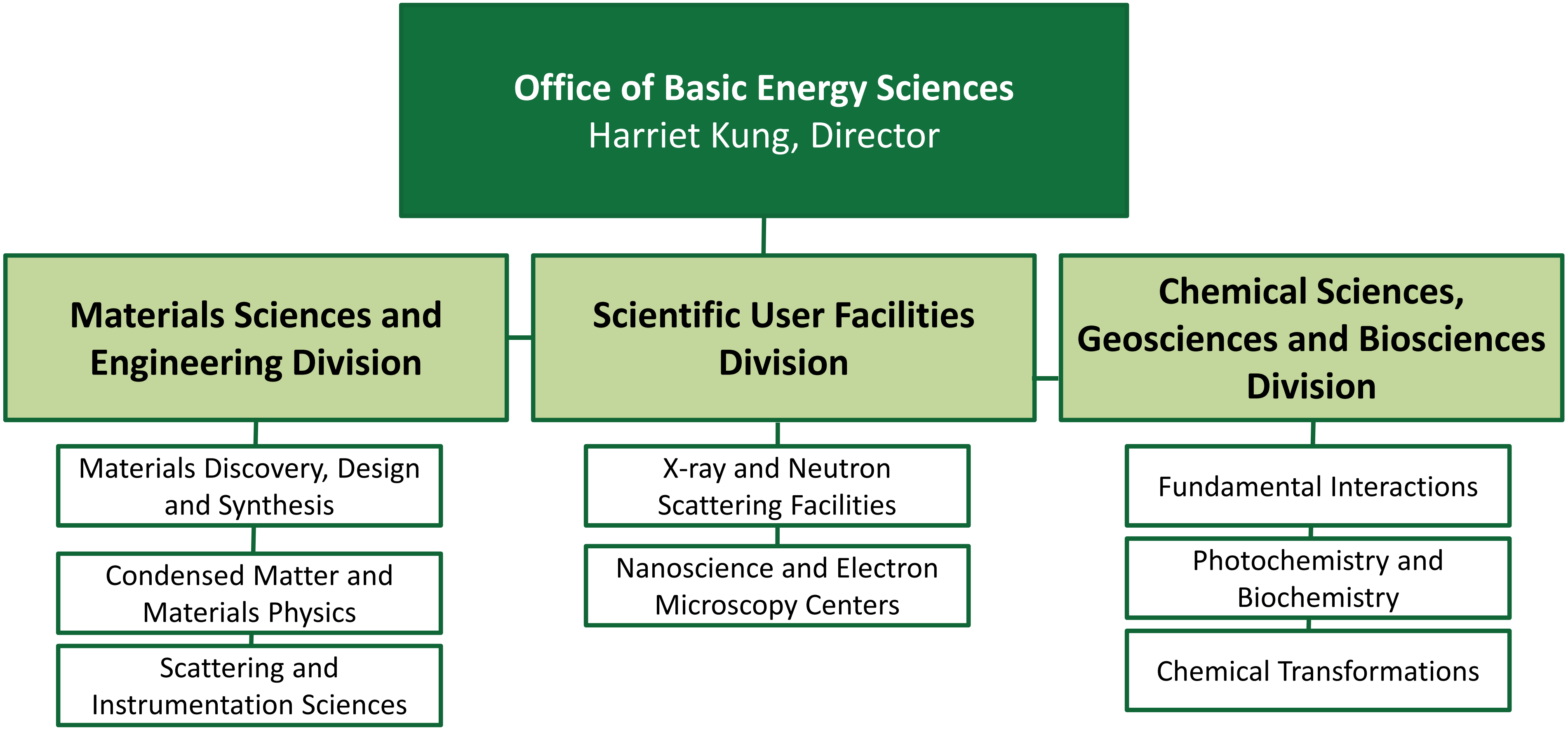
Construction

- Last year of funding for LCLS-II (Δ = -$45M)
- Advanced Photon Source Upgrade(Δ = +17.5M)
- Two new starts: LCLS-II-HE ($7M) and ALS-U ($12M)

Presentation Outline

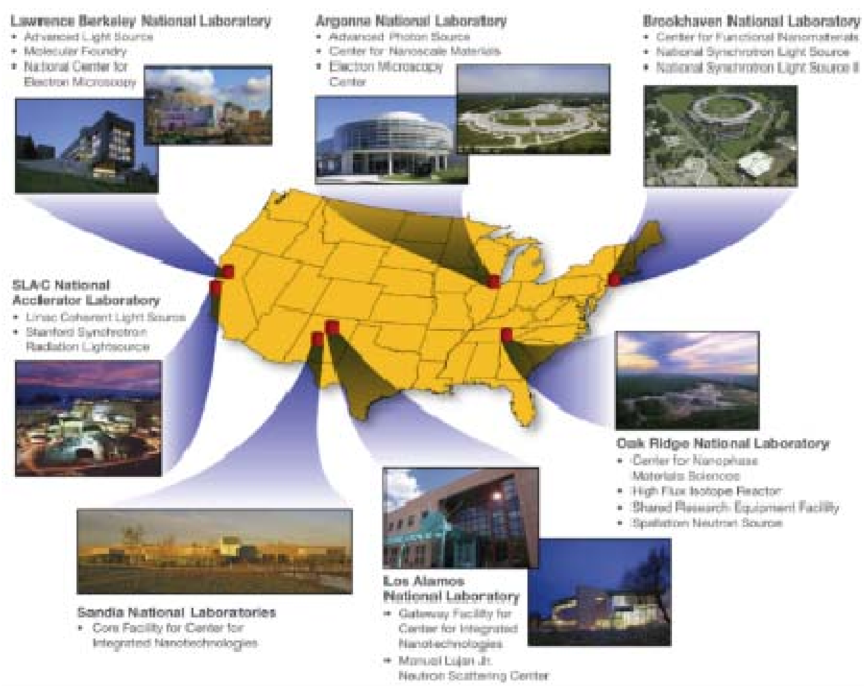
- Overview of DOE and BES Organization and Budget
- Description of BES Science and Organization
- Strategic Planning and Research Priorities
- Funding Opportunities and Process

Office of Basic Energy Sciences



DOE Office of Basic Energy Sciences: Scientific User Facilities

Nearly 16,000 users in FY 2017



- 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

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)

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)

Administrative Staff
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

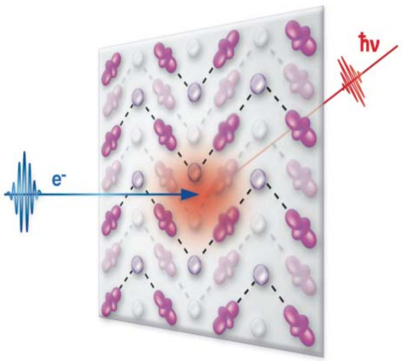
Jane Zhu

DOE EPSCoR Program

Tim Fitzsimmons

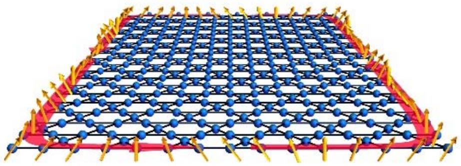
Scattering and Instrumentation Sciences

Science Driven Tools and Techniques for Foundational Materials Studies



- Electron and Scanning Probe Microscopy
  - Using electron beams and scanning probes to study local atomic and electronic structures and the spatial and chemical inhomogeneities in materials

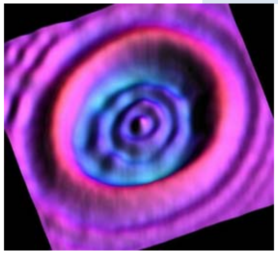
- X-ray Scattering including Ultrafast Science
  - Fundamental interactions of photons with matter with an emphasis on x-ray scattering, spectroscopy and imaging and ultrafast science

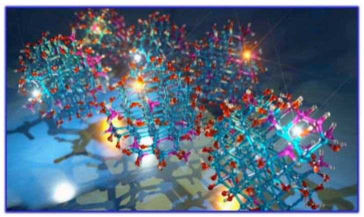


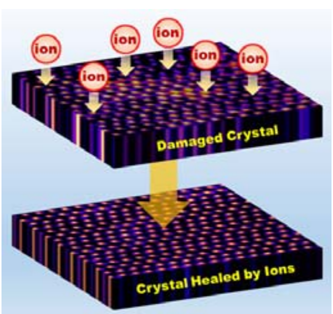
- Neutron Scattering
  - Harnessing the unique properties of neutrons to investigate hard and soft condensed matter

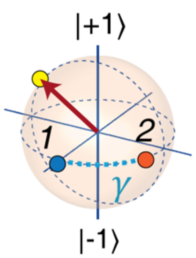
Condensed Matter and Materials Physics

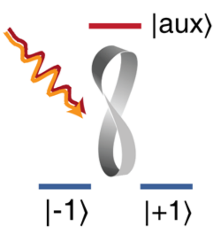
Experimental and theoretical research to advance our understanding of phenomena in condensed matter







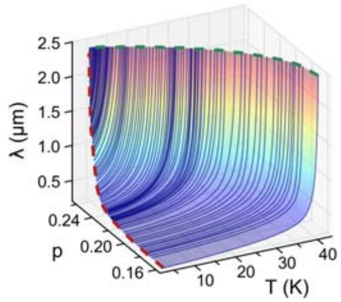




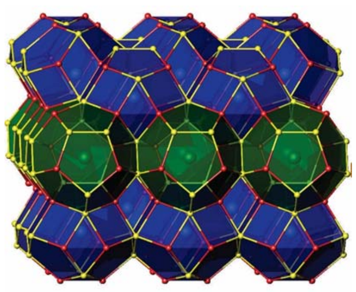
- Experimental Condensed Matter Physics
  - Understanding relationships among electronic structure; properties such as topology, superconductivity, and magnetism; reduced dimensionality; and interfacial behavior
- Theoretical Condensed Matter Physics
  - Electronic correlations, emphasizing quantum phenomena, non-equilibrium and ultrafast phenomena, materials discovery, and computational materials sciences
- Mechanical Behavior and Radiation Effects
  - Understanding defect formation, growth, and migration and their effects on strength, structure, deformation, and failure over a wide range of spatial and temporal scales
- Physical Behavior of Materials
  - Understanding response to external environments, emphasizing the relationships among electrical, magnetic, optical, electrochemical, and thermal performance

Materials Discovery, Design, and Synthesis

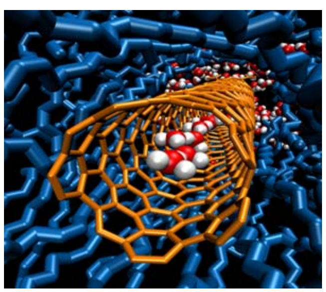
Synthesis and assembly science, controlling properties, and discovering new, unprecedented phenomena and functionalities



- Synthesis and Processing Science
  - Atomic-level control to advance understanding of the physical mechanisms of synthesis and processing, with development of real-time monitoring tools playing a critical role



- Materials Chemistry
  - Chemical aspects of composition-structure-property relationships across length scales to design and tailor materials, morphologies, and properties from first principles



- Biomolecular Materials
  - Translate biological concepts into new approaches for design and synthesis of materials with remarkable properties found only in nature (e.g., self-regulation, adaptability to changing environments)

Program Assistants
Teresa Crockett
Gwen Johnson

Chemical Sciences, Geosciences & Biosciences Division

Bruce Garrett, Division Director

Fundamental Interactions Team

Team Lead – Jeff Krause

Atomic, Molecular, and Optical Sciences

Tom Settersten

Gas Phase Chemical Physics

Wade Sisk

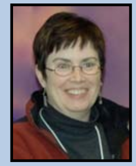
Condensed Phase and Interfacial Molecular

Gregory Fiechtner

Computational and Theoretical Chemistry

Mark Pederson

Photochemistry and Biochemistry Team

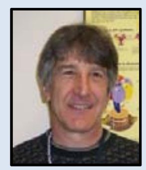


Team Lead – Gail McLean

Photosynthetic Systems

Stephen Herbert

Physical Biosciences



Robert Stack

Solar Photochemistry

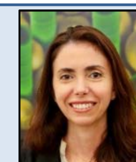
Chris Fecko

Fuels from Sunlight Energy Innovation Hub

Chemical Transformations Team

Team Lead – Raul Miranda

Catalysis Science



Viviane Schwartz

Chris Bradley

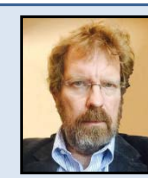
Separations and Analysis

Philip Wilk (Acting)

Heavy Element Chemistry

Philip Wilk

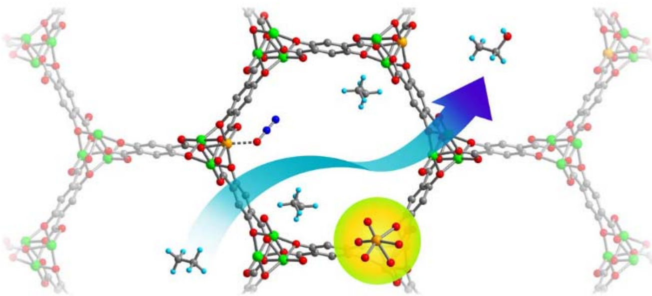
Geosciences

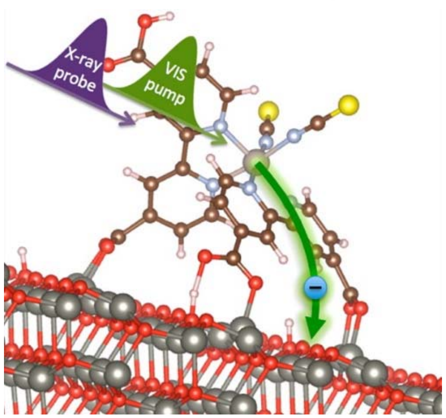


James Rustad

Fundamental Interactions Team Programs

Understanding reactive chemistry at full quantum detail



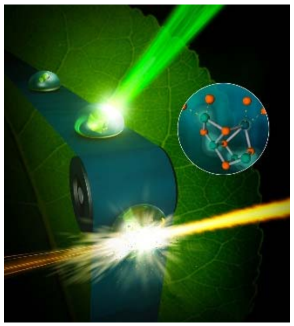


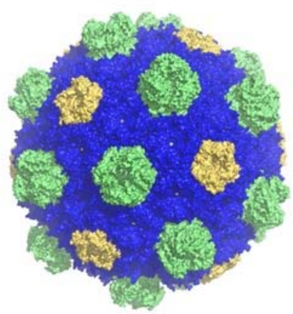
Upper figure: Oxidation of ethane to ethanol by N_2O in a metal–organic framework. Lower figure: X-ray photoelectron spectroscopy at the LCLS provides an atomic perspective of ultrafast interfacial charge transfer.

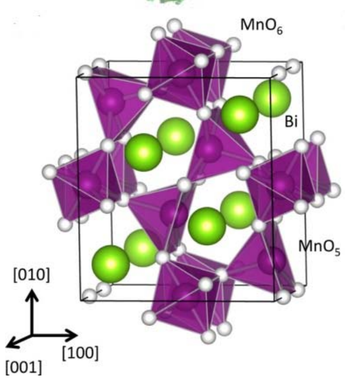
- **Atomic, Molecular, and Optical Sciences**
  - Fundamental interactions of atoms, molecules, and nanostructures with photons and electrons to characterize, understand and control their behavior
- **Gas Phase Chemical Physics**
  - Dynamics and rates of chemical reactions at conditions characteristic of combustion, and the chemical and physical properties of key intermediates, to enable computational models of combustion systems
- **Condensed Phase and Interfacial Molecular Science**
  - Understand and ultimately control chemical processes and dynamics in liquids and at interfaces at a molecular level, and confront the transition from molecular-scale chemistry to collective phenomena in complex systems.
- **Computational and Theoretical Chemistry**
  - Development and integration of theoretical and computational approaches for the accurate and efficient description of chemical processes

Photochemistry and Biochemistry Team Programs

Light energy capture and conversion into chemical and electrical energy through biological and chemical pathways



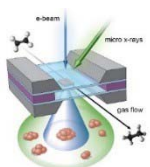


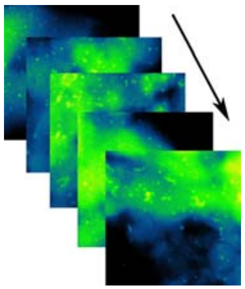


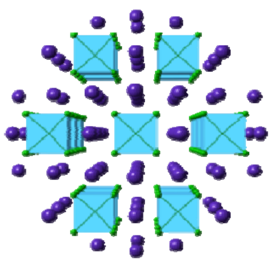
- **Photosynthetic Systems:** Brings together biochemistry, chemistry, biology, and biophysics to uncover the fundamental science of biological capture of sunlight and its conversion to and storage as chemical energy in plants, algae, and microbes.
- **Physical Biosciences:** Combines experimental and computational tools from physical sciences with biochemistry, chemistry and molecular biology to increase basic understanding of processes to capture, convert and store energy in living systems; placing an increasing emphasis on redox biochemistry
- **Solar Photochemistry:** Investigates solar photochemical energy conversions focused on the elementary steps of light absorption, electrical charge generation, charge transport and energy harvesting within a number of chemical systems
- **Fuels from Sunlight Hub: Joint Center for Artificial Photosynthesis (JCAP):** Advances basic scientific research and development on systems for the conversion of sunlight, water and carbon dioxide into a range of commercially useful fuels.

Chemical Transformations Team Programs

Understand and control the synthesis, conversion, stabilization and transport processes in chemical systems, from atomic to geologic scales







Na_3PaF_8

- **Catalysis Science**
  - Mechanisms for the efficient and clean catalytic conversion of feedstocks into fuels, chemicals, materials and energy. Principles of structure-reactivity of inorganic, organic, and hybrid complexes; interfacial, multiscale, and bio-inspired processes.
- **Heavy Element Chemistry**
  - Fundamental chemistry of the actinides and transactinide elements. Spectroscopy, bonding, and reactivity.
- **Separations and Analysis**
  - Chemical separations of complex energy carriers, actinides, carbon compounds. Coordination chemistry; molecular recognition. Cages, interfaces. Chemical imaging.
- **Geosciences**
  - Geochemistry and geophysics of surface and subsurface energy resources. Mineral-fluid interactions and reactions; rock fracture; flow/transport phenomena.

Presentation Outline

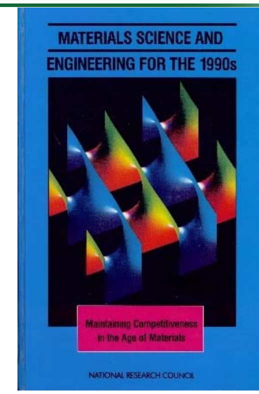
- Overview of DOE and BES Organization and Budget
- Description of BES Science and Organization
- Strategic Planning and Research Priorities
- Funding Opportunities and Process

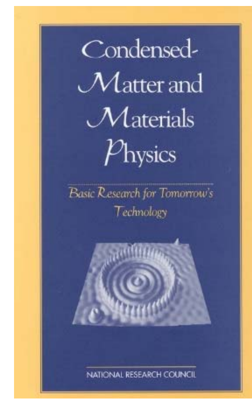
Extensive Strategic Planning provides Research Direction and is Critical to Programmatic Impact

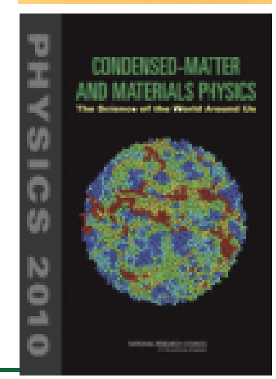
- National Academy
  - Decadal Study supported by BES-MSE and NSF-DMR
- DOE strategic planning and priorities
- BES strategic planning – an ongoing process...
  - Basic Research Needs Workshops and Reports
    - Quantum materials, Synthesis Science, Instrumentation, Environmental Management, Energy-Water Nexus
    - Next Generation Energy Storage, Catalysis, Future Nuclear Energy
  - Roundtables and Reports
    - Neuromorphic computing, Common problems in condensed matter and high energy physics, Ammonia Synthesis, Ultrafast, Quantum Information Science

Frontiers of Materials Research 2020: A Decadal Survey

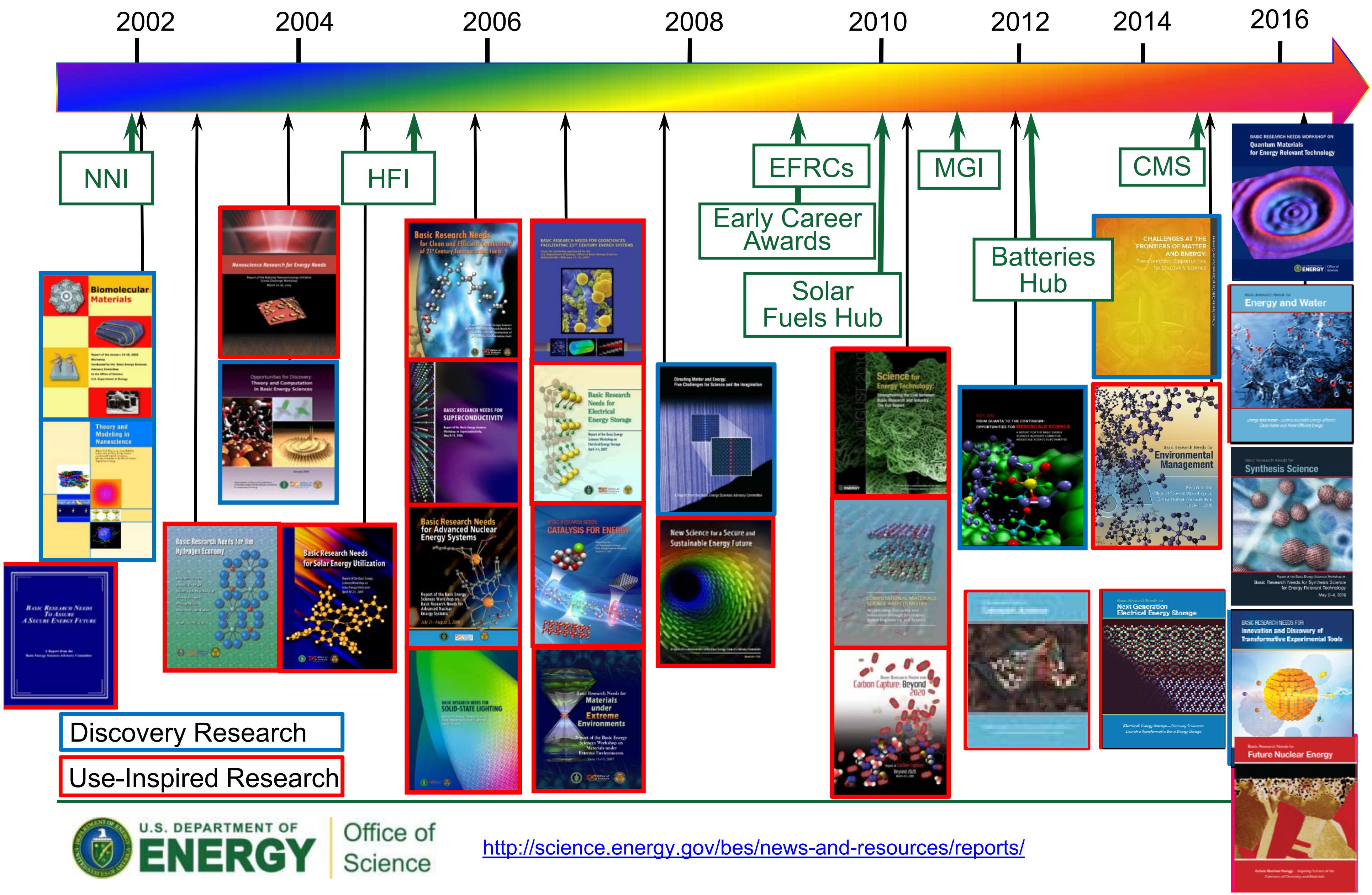
- Assess the progress in materials research over the past decade and promising new directions for 2020-2030
- Discuss the impacts that materials research has had and is expected to have on emerging technologies, national needs, and science, broadly
- Use case studies of selected fields that have had or are anticipated to have near-term growth to evaluate recent investment trends in materials research in the United States relative to similar research abroad
- Town Halls or similar forums held at APS, MRS, Materials Week, ... to gather community input
- Supported by DOE and NSF
- Led by the NA Condensed Matter and Materials Research Committee (NSF and DOE-BES-MSE supported) and the National Materials and Manufacturing Board
- Report anticipated late in 2018







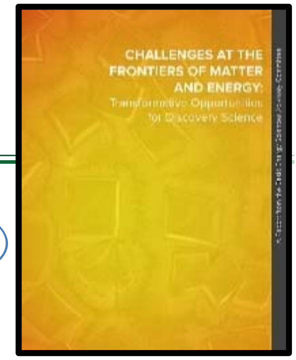
BES Budget Requests and FOAs are Informed by Strategic Planning and Program Development



U.S. DEPARTMENT OF ENERGY | Office of Science

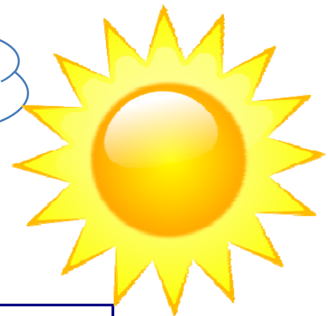
http://science.energy.gov/bes/news-and-resources/reports/

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



2015

Instrumentation & Tools



Human Capital

Synthesis

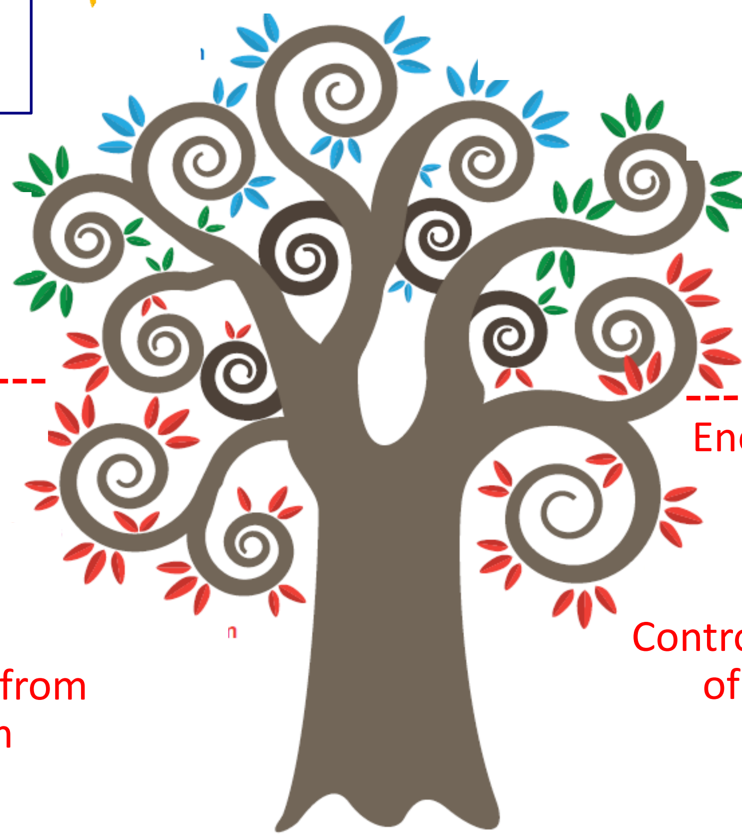
Beyond Ideal Materials and Systems

Mastering Hierarchical Architectures

Harnessing Coherence in Light and Matter

Imaging Matter across Scales

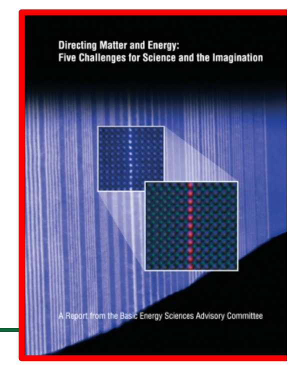
Data, Algorithms and Computing



Efficient Synthesis for Tailored Properties

Energy and Information on the Nanoscale

2007

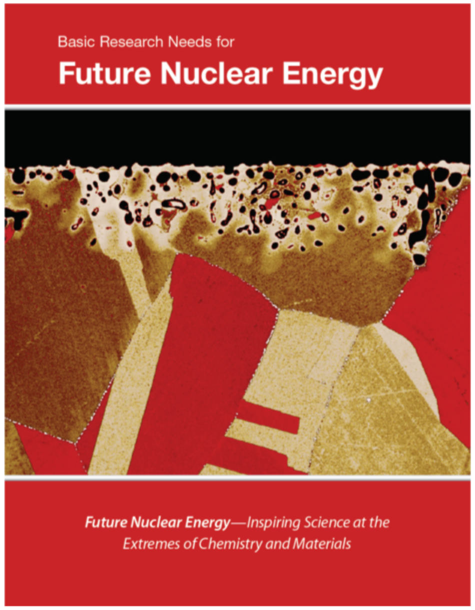


Correlated Systems

Control at the Level of Electrons

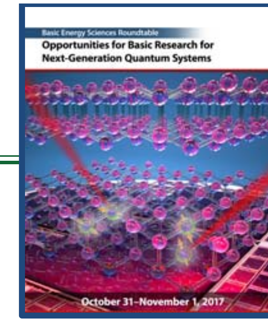
Systems Away from Equilibrium

BRN for Future Nuclear Energy – Priority Research Directions



- Enable design of revolutionary molten salt coolants & liquid fuels
  How can we characterize and predict the structure, dynamics, and energetics of molten salts including evolving chemical composition across length and time scales?
- Master the hierarchy of materials design and synthesis for complex, reactor environments
  How do we design, synthesize, and process superior materials able to function and perform over decades in the extreme environments of advanced nuclear reactors?
- Tailor interfaces to control the impact of nuclear environments
  How can the multitude of inextricably linked chemical and physical processes that occur at interfaces be controlled?
- Reveal multiscale evolution of spatial and temporal processes for coupled extreme environments
  How can computational and experimental techniques be integrated to bridge spatial, temporal, and energy scales that underpin materials' behavior and chemical transformations in coupled extreme environments?
- Identify and control unexpected behaviors from rare events and cascading processes
  How do we identify, anticipate and control rare events that initiate cascading processes and cause aberrant properties and materials responses?

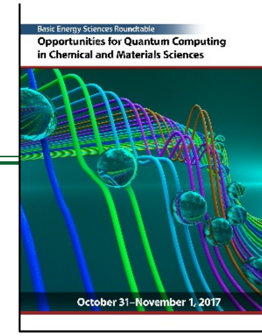
Quantum Information Science: Opportunities for Basic Research for Next Generation Quantum Systems



Roundtable in October 2017 defined a BES research agenda for quantum systems for QIS and provided input on priority research opportunities:

- Advance artificial quantum-coherent systems with unprecedented functionality
  - Develop new capabilities for synthesis that couple theoretical predictions and real-time measurements of targeted quantum characteristics, including coherence
  - Explore robotic synthesis of layered materials, design of quantum properties for hybrid (organic and inorganic) systems, creation of topological states of matter, and precise control to position atomic defects
- Enhance creation and control of coherence in quantum systems
  - Understand scaling of coherence lengths and times with system size and complexity, and identify new signatures of quantum states in artificial quantum-coherent systems
  - Investigate mechanisms to prevent decoherence, leading to discovery and exploitation of novel entangled excitations
- Discover novel approaches for quantum-to-quantum transduction
  - Advance new capabilites for coherent transfer of complete wavefunctions between disparate physical systems, the core of quantum measurement and information processing
  - Develop new techniques for generation and stabilization of nonclassical states of light and matter; high fidelity transfer of quantum wavefunctions; and quantum state replication and entanglement
- Implement new quantum methods for advanced sensing and process control
  - Design new quantum-based sensors, detectors, and imaging systems for precise measurements of time, space, and fields to probe material properties and chemical processes
  - Create novel methods to use squeezed states for metrology and understand the connections of entanglement, thermodynamics, and many-body localization/diffusion

Quantum Information Science: Quantum Computing Opportunities in Chemical and Materials Sciences

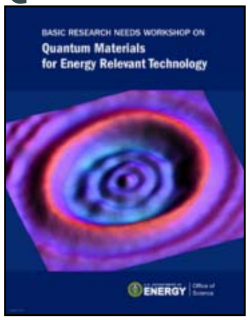


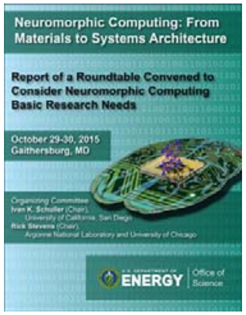
Roundtable in October 2017 defined a BES research agenda for emerging quantum computing and provided input on priority research opportunities:

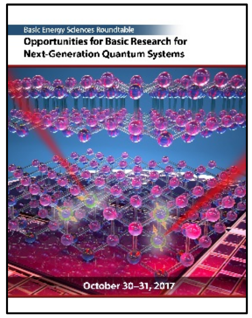
- Controlling the quantum dynamics of nonequilibrium chemical and materials systems
  - Elucidate the fundamental principles underlying chemical reactions and catalytic pathways; discover dynamical phases of matter; and understand how to prepare entangled states across many quantum degrees of freedom
- Unraveling the physics and chemistry of strongly correlated electron systems
  - Enable a correct description of the quantum behavior of strongly entangled electrons to allow discovery of the principles controlling superconductivity, magnetic states and the dynamics of electronic states
- Embedding quantum hardware in classical frameworks
  - Develop efficient hybrid algorithms that embed quantum computing for strongly correlated quantum components in classical computing for more weakly correlated parts, thus enabling simulations of molecular and materials problems containing thousands of atoms
- Bridging the classical–quantum computing divide
  - Improve the efficiency of quantum computing using approximate results from classical computing as input, and improve the accuracy of classical computing using high-accuracy results from quantum computing to parameterize and optimize complex models

Recent Strategic Planning Workshops and Roundtables Cross the Breadth of the MSE Division

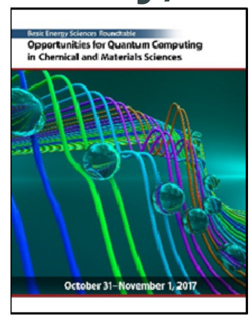
- **Quantum Science**

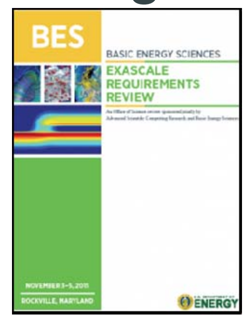






Theory, Modeling and Computation

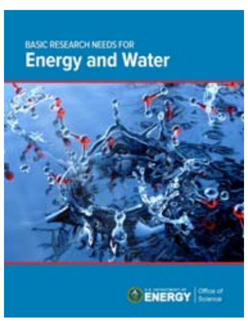


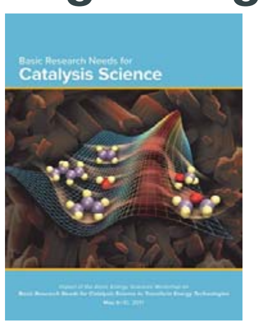


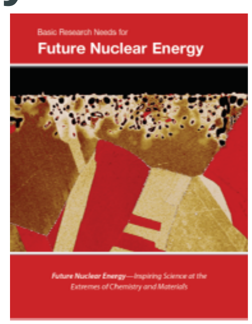
- **Characterization**

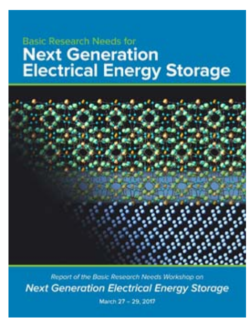
Synthesis

- **Cross-Cutting Energy**



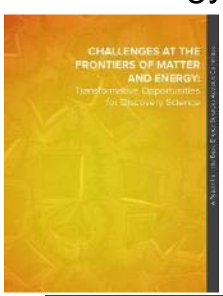


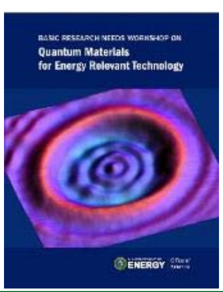


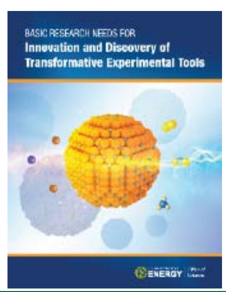


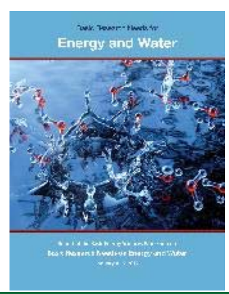
FY 2018 – FY 2019 BES Research Priorities

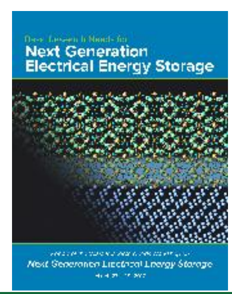
- **Quantum Information Science (QIS)**
  - By exploiting the intricate quantum mechanical phenomena, QIS will create fundamentally new ways of obtaining and processing information and open new vistas of science discovery and technology innovation. Research priorities were identified in two QIS roundtables held in October 2017.
- **Ultrafast Science**
  - Ultrafast science remains a priority in both research divisions to position the U.S. leadership in this critical field of science and in anticipation of the completion of the LCLS-II construction project. Research priorities were identified in a roundtable held October 2017.
- **Computational Materials and Chemical Sciences**
  - Computational Materials Sciences (CMS) and Computational Chemical Sciences (CCS) are maintained in support of the Exascale Computing Initiative. CCS was funded in FY 2017 and is moved to a new budget line in the FY 2019 Request.
- **Materials and Chemical Sciences for Future Nuclear Energy**
  - Research will be supported to achieve a multi-scale spatial and temporal understanding of fundamental physical and chemical processes that govern the properties and performance of novel material systems and fuels required for advanced reactors.
- **Priorities identified by Advisory Committee and Basic Research Needs Reports**
  - Both the core research and EFRCs will emphasize emerging high priorities identified by the Basic Energy Sciences Advisory Committee and recent Basic Research Needs workshop reports.

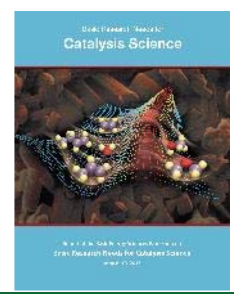


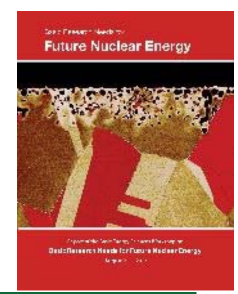












Strategic Directions are Reflected in Funding Opportunity Announcements and Program Descriptions

- Reports are available via the BES home page: https://science.energy.gov/bes
- Annual funding opportunity announcement (FOA) is updated to reflect programmatic emphasis and topical areas that will not be supported or that are being de-emphasized. Examples:
  - Synthesis and Processing Science: The program has an increasing focus on understanding of kinetics and mechanisms of materials growth ....
  - Experimental Condensed Matter Physics: Growth in research support is expected in the areas of spin physics, magnonics, and topological states of matter.
  - Materials Chemistry: Research primarily aimed at the optimization of synthetic methods or properties of materials for applications, and research with a primary goal of device fabrication and testing will be discouraged.
  - Mechanical Behavior: Proposals emphasizing mechanics of materials, rather than materials science, will not be considered responsive.
- Priorities are also communicated through the annual budget submission, on the BES web page for each program, and at conferences during BES overview presentations

Presentation Outline

- Overview of DOE and BES Organization and Budget
- Description of BES Science and Organization
- Strategic Planning and Research Priorities
- Funding Opportunities and Process

Process: Majority of Grants and Lab Awards are 3-years with Potential Renewal (CMS and SciDAC are 4-year Awards)

Grant Program

- Mostly university single PI projects; a few multi-PI research awards with focused scientific themes
- National lab collaborators funded separately (direct to labs)
- Limited labor costs typical one month faculty summer salary, with support for post-doc and students
- Research emphasis on innovation-driven science in academic environment; Funding award may be transferred with PI move
- Includes extensive support for graduate students and postdocs

Lab Program

- Interdisciplinary, large research team approach with multiple PIs and supporting technical staff
- May include university subcontracts for team members
- Supports large fraction of investigators' salary, equipment costs, and other burden/expenses
- Building and maintaining mission-driven research capabilities, often co-sited with user facilities and other major lab research capabilities
- Resources align with Lab identified vision, priority, and strengths

Proposal Review Criteria

1. Scientific and/or technical merit of the project; for example, the influence that the results might have on the direction, progress, and thinking in relevant scientific fields of research; the likelihood of achieving valuable results; and the scientific innovation and originality indicated in the proposed research.
2. Appropriateness of the proposed method or approach; for example, the logic and feasibility of the research approaches and the soundness of the research plan.
3. Competency of the personnel and adequacy of the proposed resources; for example, the background, past performance, potential of the investigator(s), and the research facilities.
4. Reasonableness and appropriateness of the proposed budget.

Additional criteria for national laboratory and large grants (~1 M/yr)

5. Synergism among the PIs in a program and the programmatic focus of a multi-PI effort.
6. Utilization of unique facilities or capabilities.

Additional review criteria may be used for specific FOAs

Funding Opportunities: FAQs

- White papers are encouraged
  - Respond to “Open Call For Proposals” (Special Calls may have different requirements – read these carefully)
  - Hypothesis driven, fundamental science project - energy relevance
  - White papers/ are encouraged but not required for academic research
  - All proposals are peer reviewed
- Funding levels
  - Peer review will assess requests versus research needs (10 CFR 605)
  - Typical academic awards are for 1 summer month plus students/postdoc
  - Multiple PI awards are allowed
  - National Lab awards are always multiple PI, except for early career
- Open call is a continuous process (no fixed deadline for submission)
  - Reviews take 4 – 6 months to complete, awards are made based on strength of the merit review and available resources
  - Proposals can be held up to one year for consideration
- Delineation from other grants...
  - You must have separate research proposals that can “stand alone” with respect to research output

Continuing Hot Topic – Research Delineation

- **Research Delineation –**
  - Investigations, prosecution
  - "It is not a problem to apply for funds for the same research at different funding agencies, but it is illegal to accept and use the funding"
  - For all BES grants, the Program Manager must sign that:
    - *I do not find any evidence of unwarranted duplication of effort or overlap in support between the research that is the subject of this Selection Statement Memorandum and any other unclassified government supported activity with this Principal Investigator.*
  - How to tell?? <u>When in doubt, ask the Program Manager</u>. I look at it like so: are there a lot of similar terms in the abstracts? Is one project essentially within the scope of the other? Is the science essentially the same? Will most papers acknowledge both funding sources?
  - Basically, don't try to justify gray areas; it should be a BRIGHT LINE

Some Common Questions

- **Single PI or Collaborative??**
  - Depends on the project and scope. It really needs to make sense to have more than one PI because of cost (in other words, don't just add someone for the heck of it). We have no preference, but if you have a collaborative proposal it should be synergistic
- **How long should the proposal period be?**
  - We typically fund in three-year increments, and they are renewable
- **How long should the proposal be?**
  - We don't have an official page limit but the main body shouldn't be longer than 20 pages (or you will annoy reviewers → BAD!)
- **What are we looking for in a single word?**
  - IMPACT!

Office of Science Early Career Research Program

Office of Science Early Career Research Program – Started in FY 2010

- 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 2017 Program

- 700 Office of Science proposals received, 21 Basic Energy Sciences (19 universities, 2 Labs) awards out of a total of 59 awards for the Office of Science (10 in BES-Materials Sciences and Engineering)

FY 2018 Program

- **Awards announced July, 2018**

Annual FOA will be released in FY 2019 for the next opportunity. FOAs cover different topics than the annual FOA for BES – important to read the details!

DOE Office of Science Graduate Student Research (SCGSR) Program

The SCGSR Program provides supplemental awards to outstanding graduate students to spend 3 to 12 months conducting part of their doctoral thesis/dissertation research at a host DOE national laboratory/facility in collaboration with a DOE laboratory scientist.

- Graduate students must apply online through the online application system.
- The application requires a research proposal and letters of support from both the graduate student's thesis advisor and the collaborating DOE laboratory scientist.
- Student's research and proposed SCGSR project must be aligned with one of the identified SCGSR priority research areas defined by the SC Program Offices and specified in the solicitation.
- Applications proposing to use an SC user facility must apply for user facility time separately.

Award Benefits:

- A monthly stipend of up to $3,000/month for general living expenses
- Reimbursement of inbound/outbound traveling expenses to/from the host DOE laboratory/facility of up to $2,000

(Award payments are provided directly to the student)

Eligibility:

- U.S. Citizen or Lawful Permanent Resident
- Qualified graduate program & Ph.D. Candidacy
- Graduate research aligned with an SCGSR priority research area
- Establishment of a collaborating DOE laboratory scientist at the time of application

2018 Solicitation 2 – Applications Due: November 15, 2018 5:00PM ET

Full details, requirements, FAQs, and link to application at: https://science.energy.gov/wdts/scgsr/

Program Contact : sc.scgsr@science.doe.gov

SCGSR Program 2018 Solicitation 2 – Priority Research Areas

Advanced Scientific Computing Research (ASCR)

(a) Applied Mathematics

(b) Computer Science

Basic Energy Sciences (BES)

(a) Accelerator and Detector R&D

(b) Nuclear Chemistry and Radiochemical Separations

(c) Neutron Scattering Research and Instrumentation

(d) Predictive Materials Science and Chemistry

(e) Fundamental Electrochemistry related to Energy Transduction, Storage, Chemical Conversion, and Corrosion

(f) Crystal Growth

(g) Ultrafast Materials and Chemical Sciences

(h) Electron and Scanning Probe Microscopy Research and Instrumentation

(i) Basic Geosciences

(j) Gas Phase Chemical Physics

(k) Radiation Effects in Materials

(l) Catalysis Science with NMR Spectroscopy and Neutron Scattering

(m) Highly Ionizing Radiation in Chemistry

(n) Energy Transfers in Large Proteins and Protein Complexes

(o) Quantum Information Science for Experimental Condensed Matter Physics

(p) Quantum Information Science for Theoretical Condensed Matter Physics

Biological and Environmental Research (BER)

(a) Computational Biology and Bioinformatics

(b) Novel in situ Imaging and Measurement Technologies for Biological Systems Science

Biological and Environmental Research (Cont'd)

(c) Plant Science for Sustainable Bioenergy

(d) Soil Microbiology

(e) Environmental Systems Science

(f) Atmospheric System Research

(g) Earth System Modeling

Fusion Energy Sciences (FES)

(a) Burning Plasma Science & Enabling Technologies

(b) Discovery Plasma Science

High Energy Physics (HEP)

(a) Theoretical and Computational Research in High Energy Physics

(b) Advanced Technology Research and Development in High Energy Physics

(c) Experimental Research in High Energy Physics

Nuclear Physics (NP)

(a) Medium Energy Nuclear Physics

(b) Heavy Ion Nuclear Physics

(c) Low Energy Nuclear Physics

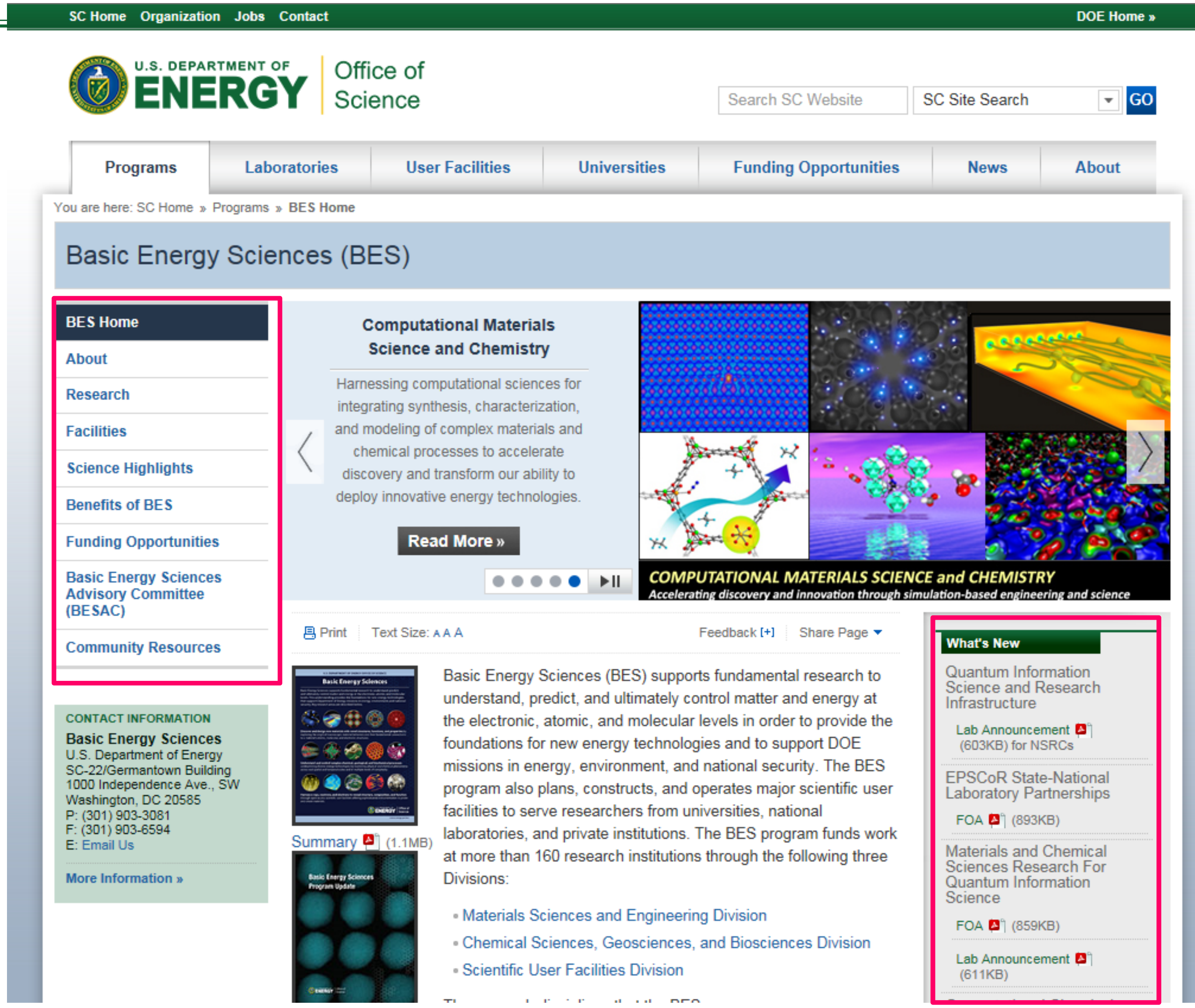
(d) Nuclear Theory

(e) Nuclear Data and Nuclear Theory Computing

(f) Isotope Development and Production for Research and Applications

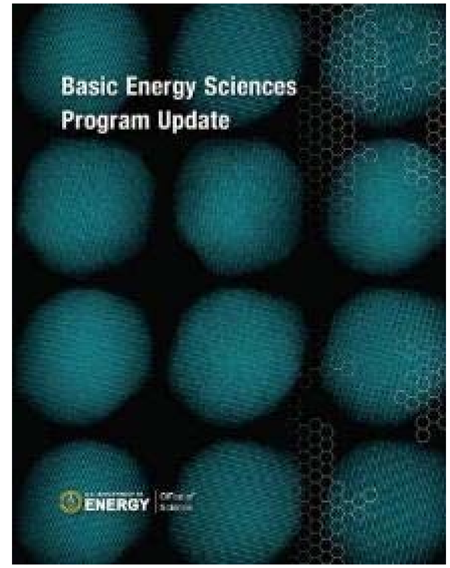
(g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

More Information Available on the BES Web Page

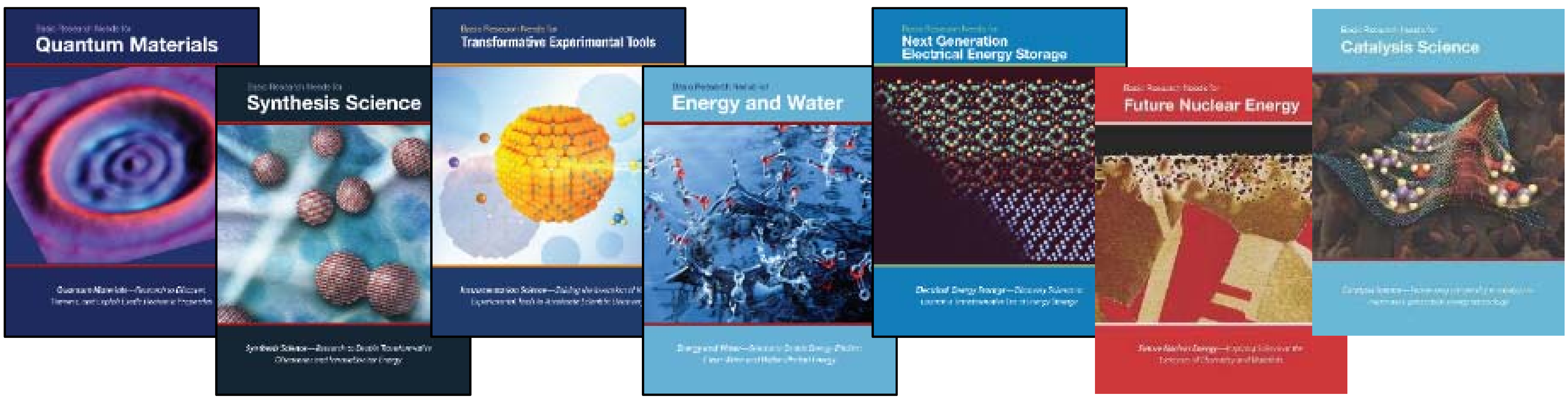


On Line Resources

- BES Program Update
  - Annual publication that describes updates to the BES program in FY 2017, including major new awards and strategic planning activities. It also describes select research highlights.

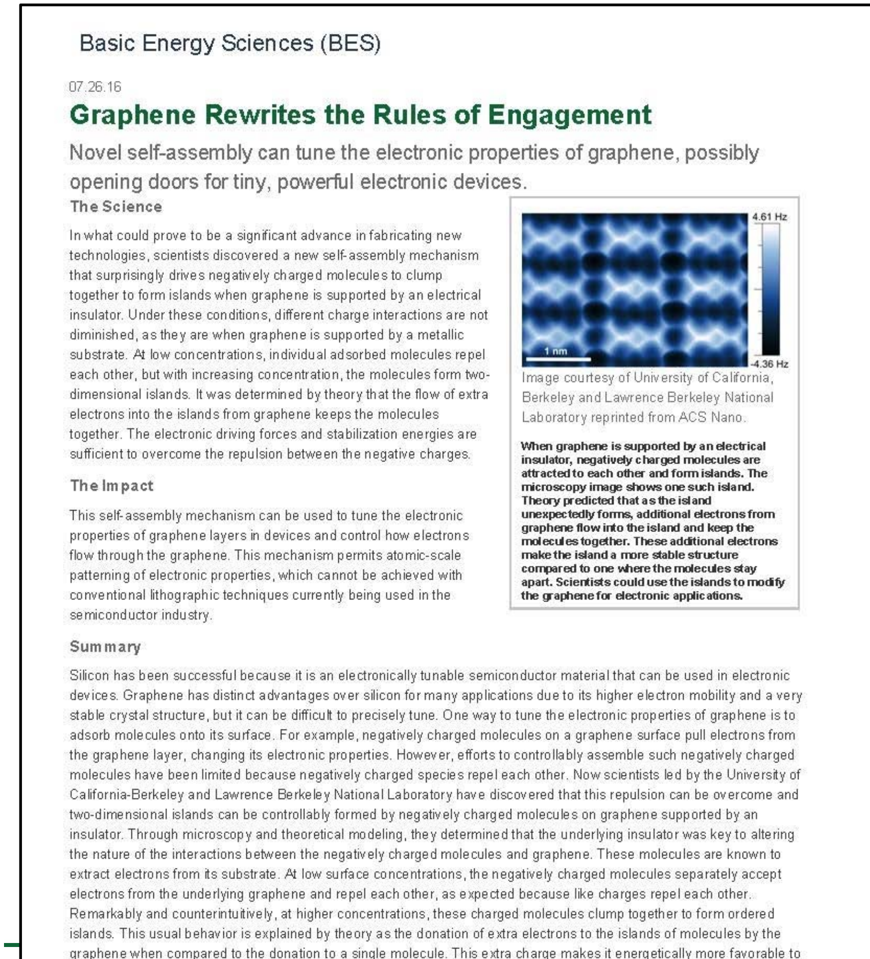


- BRN Workshop Report Brochures



Impact and Communication

- BES Communicates impact through
  - Web highlights
  - 3-panel and topical viewgraphs



Basic Energy Sciences (BES)

07.26.16

Graphene Rewrites the Rules of Engagement

Novel self-assembly can tune the electronic properties of graphene, possibly opening doors for tiny, powerful electronic devices.

The Science

In what could prove to be a significant advance in fabricating new technologies, scientists discovered a new self-assembly mechanism that surprisingly drives negatively charged molecules to clump together to form islands when graphene is supported by an electrical insulator. Under these conditions, different charge interactions are not diminished, as they are when graphene is supported by a metallic substrate. At low concentrations, individual adsorbed molecules repel each other, but with increasing concentration, the molecules form two-dimensional islands. It was determined by theory that the flow of extra electrons into the islands from graphene keeps the molecules together. The electronic driving forces and stabilization energies are sufficient to overcome the repulsion between the negative charges.

4.61 Hz

1 nm

-4.36 Hz

Image courtesy of University of California, Berkeley and Lawrence Berkeley National Laboratory reprinted from ACS Nano.

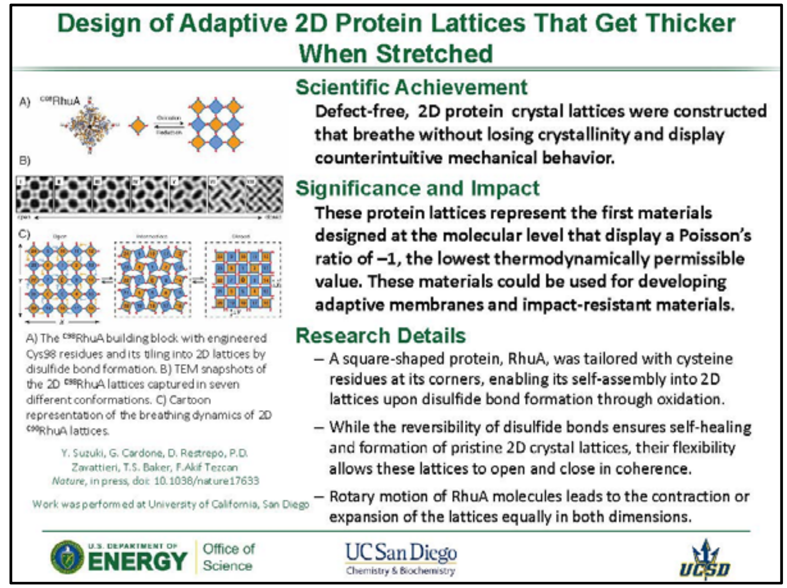
When graphene is supported by an electrical insulator, negatively charged molecules are attracted to each other and form islands. The microscopy image shows one such island. Theory predicted that as the island unexpectedly forms, additional electrons from graphene flow into the island and keep the molecules together. These additional electrons make the island a more stable structure compared to one where the molecules stay apart. Scientists could use the islands to modify the graphene for electronic applications.

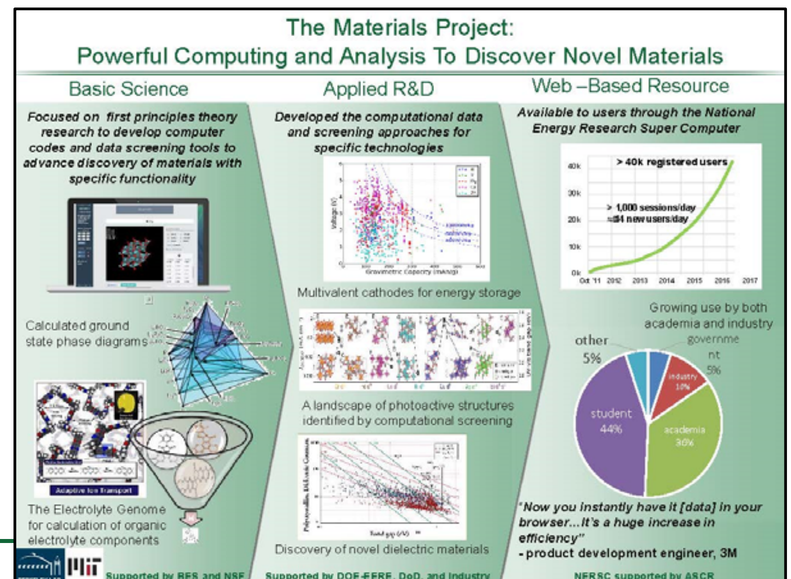
The Impact

This self-assembly mechanism can be used to tune the electronic properties of graphene layers in devices and control how electrons flow through the graphene. This mechanism permits atomic-scale patterning of electronic properties, which cannot be achieved with conventional lithographic techniques currently being used in the semiconductor industry.

Summary

Silicon has been successful because it is an electronically tunable semiconductor material that can be used in electronic devices. Graphene has distinct advantages over silicon for many applications due to its higher electron mobility and a very stable crystal structure, but it can be difficult to precisely tune. One way to tune the electronic properties of graphene is to adsorb molecules onto its surface. For example, negatively charged molecules on a graphene surface pull electrons from the graphene layer, changing its electronic properties. However, efforts to controllably assemble such negatively charged molecules have been limited because negatively charged species repel each other. Now scientists led by the University of California-Berkeley and Lawrence Berkeley National Laboratory have discovered that this repulsion can be overcome and two-dimensional islands can be controllably formed by negatively charged molecules on graphene supported by an insulator. Through microscopy and theoretical modeling, they determined that the underlying insulator was key to altering the nature of the interactions between the negatively charged molecules and graphene. These molecules are known to extract electrons from its substrate. At low surface concentrations, the negatively charged molecules separately accept electrons from the underlying graphene and repel each other, as expected because like charges repel each other. Remarkably and counterintuitively, at higher concentrations, these charged molecules clump together to form ordered islands. This usual behavior is explained by theory as the donation of extra electrons to the islands of molecules by the graphene when compared to the donation to a single molecule. This extra charge makes it energetically more favorable to





U.S. DEPARTMENT OF ENERGY | Office of Science

Questions?

John Vetrano
John.Vetrano@science.doe.gov