Office of Basic Energy Sciences -

Science Underpinning Hydrogen and Fuel Cells

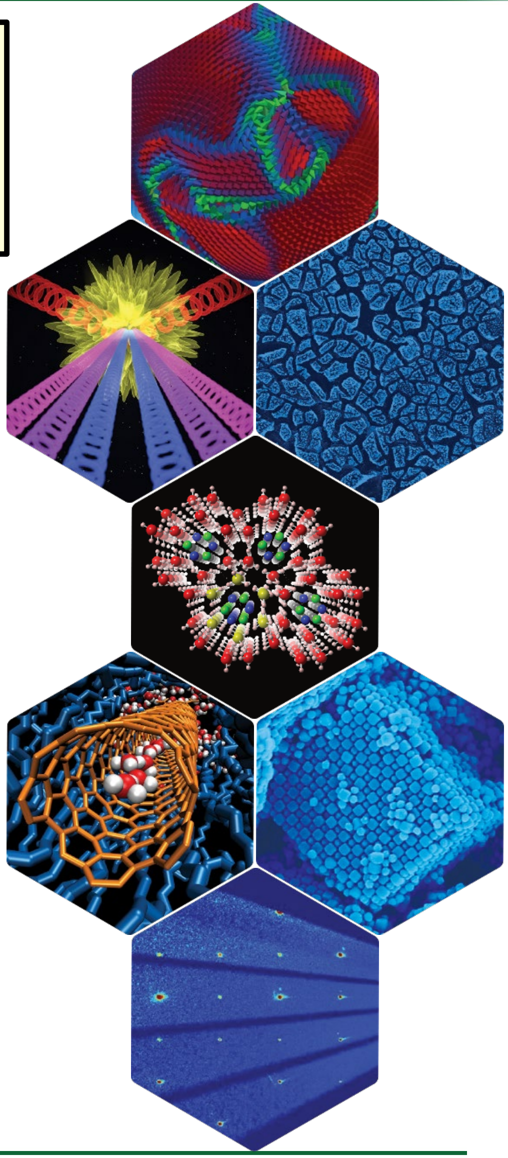
June, 2020

HFTO Annual Merit Review

John Vetrano
Program Manager
Division of Materials Sciences and Engineering

Basic Energy Sciences Mission

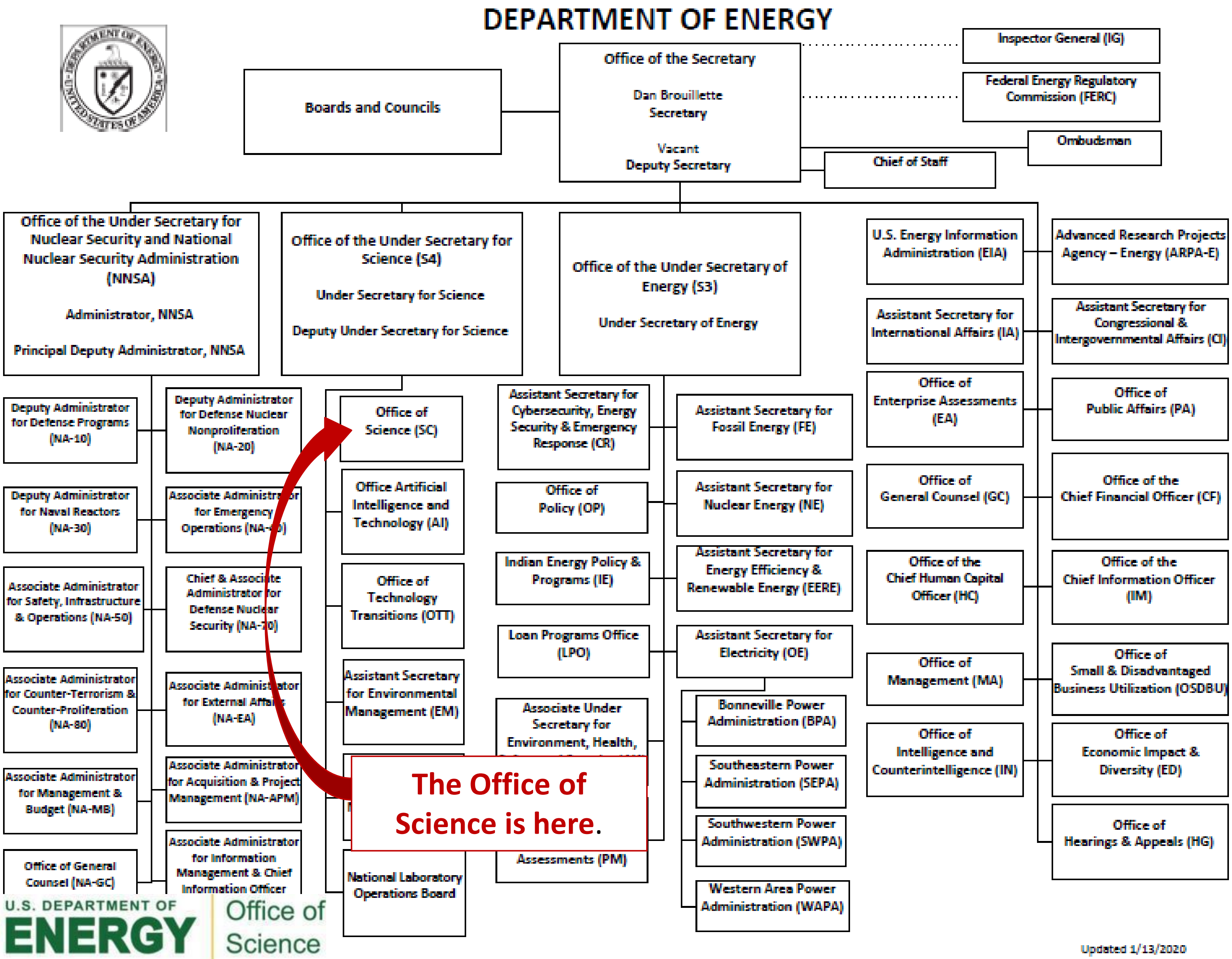
To understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels



BES fulfills its mission through:

- Supporting basic research to discover new materials and design new chemical processes that underpin a broad range of energy technologies
- Operating world-class scientific user facilities in x-ray, neutron, and electron beam scattering as well as in nanoscale research
- Managing construction and upgrade projects to maintain world-leading scientific user facilities

Department of Energy Organizational Structure



Office of Basic Energy Sciences (BES)

Office of Basic Energy Sciences
Linda Horton, Director

- **Materials Sciences and Engineering Division (MSE)**
  Vacant
  - Materials Discovery, Design and Synthesis
  - Condensed Matter and Materials Physics
  - Scattering and Instrumentation Sciences
- **Scientific User Facilities Division (SUF)**
  Vacant
  - X-ray and Neutron Scattering Facilities
  - Nanoscience and Electron Microscopy Centers
  - Facility Construction and Major Items of Equipment
- **Chemical Sciences, Geosciences and Biosciences Division (CSGB)**
  Bruce Garrett, Director
  - Fundamental Interactions
  - Photochemistry and Biochemistry
  - Chemical Transformations

Research grouped by scientific topics, not by specific energy technologies

DOE Office of Basic Energy Sciences: Scientific User Facilities

More than 16,000 users in FY 2019

- **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)

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)

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)

Basic Energy Sciences At a Glance (2019)

BES RESEARCH SPANS

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

15 DOE NATIONAL LABORATORIES

47 STATES AND WASHINGTON, D.C.

25 CORE RESEARCH AREAS

46 ENERGY FRONTIER RESEARCH CENTERS

SUPPORTED RESEARCHERS

~6,100 Ph.D. SCIENTISTS

~2,100 STUDENTS SUPPORTED

BES | BY THE NUMBERS

FY 2019

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

2 ENERGY INNOVATION HUBS

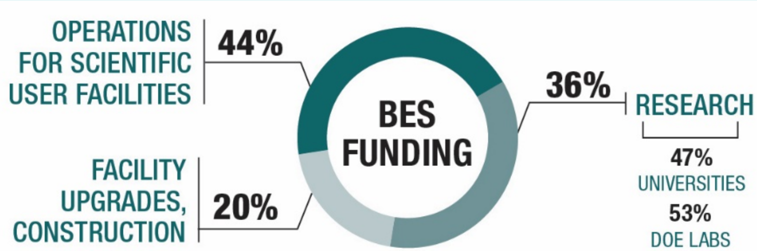
$784 MILLION RESEARCH BUDGET

~21% AVERAGE NEW GRANT SUCCESS RATE

NEARLY **1,400** CORE RESEARCH PROJECTS

MORE THAN **16,000** USERS AT **12** BES FACILITIES

$955 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET



$427 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET

BES Research and Funding Modalities:
Informed by Community-Based Strategic Planning

Increasing scope and size

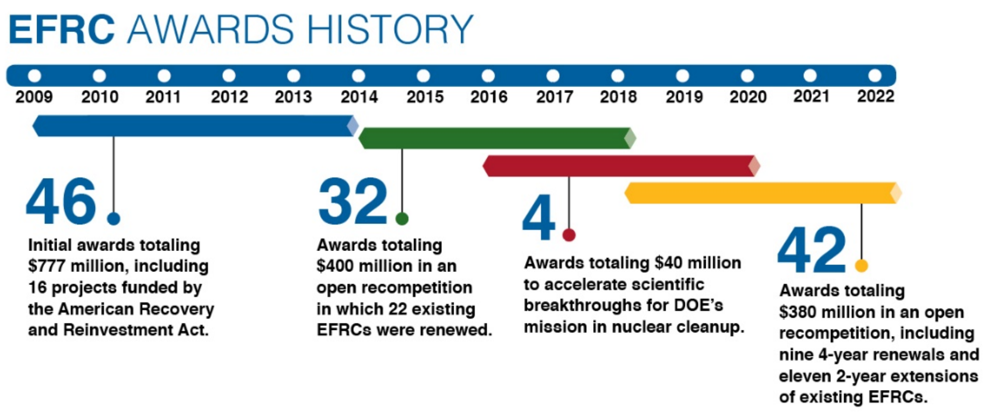
- **Core Research (>1,300 projects, ~$600M/yr)**
  Single investigators ($150K/year) and small groups ($500K-$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing.

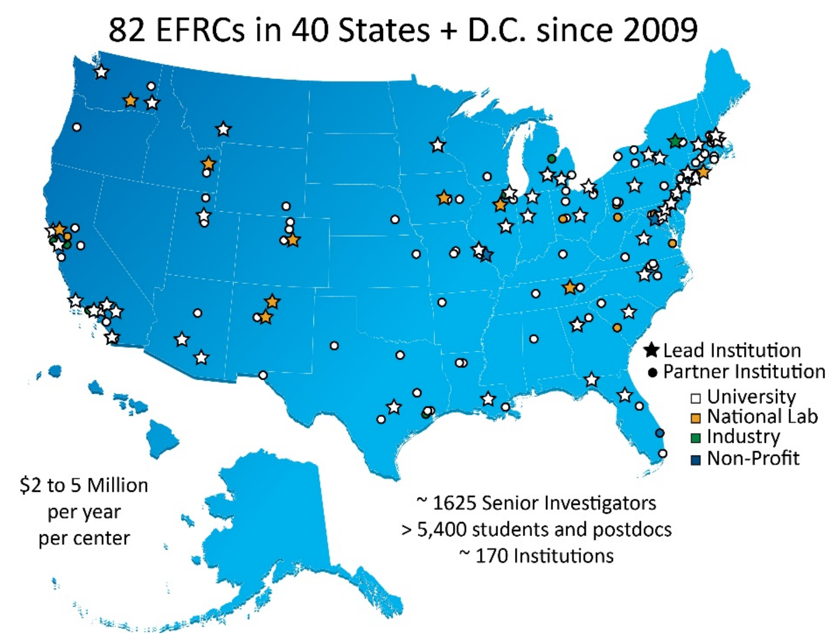
- **Computational Materials & Chemical Sciences ($26M/yr)**
  Core awards are $2-4M/year research activities for 4-year terms; focus on delivering open-source software for materials and chemistry by design in preparation for exascale computing.

- **Energy Frontier Research Centers (46, $115M/yr)**
  $2-4M/year research centers for 4-year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.

- **Energy Innovation Hubs ($39M/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.

Energy Frontier Research Centers (2009 – 2019)





Cumulative Investment (2009 – 2019): $1.4B

Cumulative Accomplishments (Aug 2009 – May 2019)

- Over 11,600 peer-reviewed scientific publications
- ~110 companies have benefited from EFRC research
- Over 770 disclosures, 610 U.S. patent applications, and 480 foreign patent applications
- Over 210 patents issued
- Over 1,600 senior investigators at ~170 institutions (university, lab, industry, non-profit)
- At least 5,400 students and postdocs trained in EFRCs

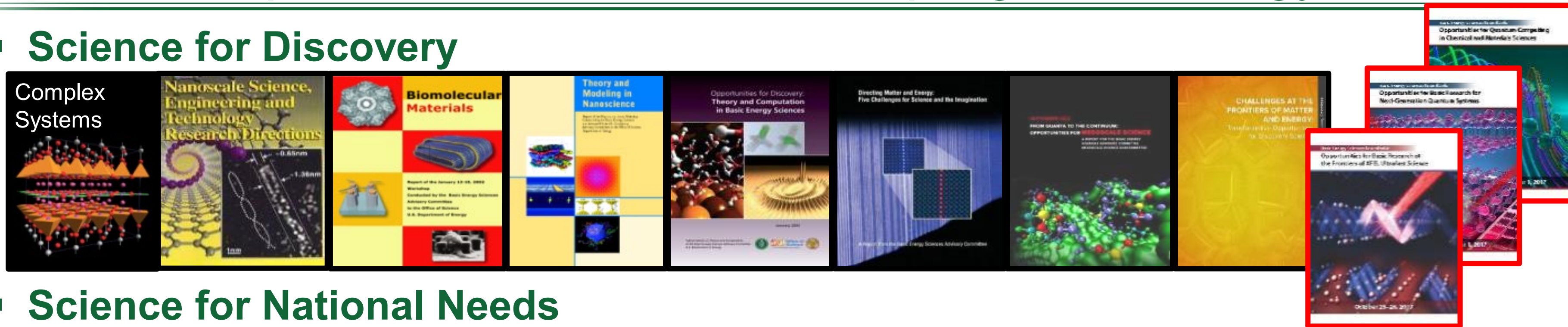
Hydrogen and Fuel Cell Underpinning Science and Coordination

- BES support for fundamental research underpinning fuel cells and hydrogen has remained steady between $20M and $25M for several years.
- Research topics include science related to hydrogen storage, catalysts, membranes/ separations, bio-inspired and solar hydrogen production
- Annual solicitations applicable for basic research in these areas are in the “open” annual SC FOA and Early Career Research Program FOA. The Energy Frontier Research Center Program also includes these topics.
- BES coordinates with other DOE Offices through the internal working group, and with other government agencies through participation in the Interagency Working Group
- The core of BES strategic planning is “Basic Research Needs” workshops and roundtables, such as the 2017 Catalysis Science workshop (report on the BES web site)

BES strategic planning activities provide the foundation for program strategy

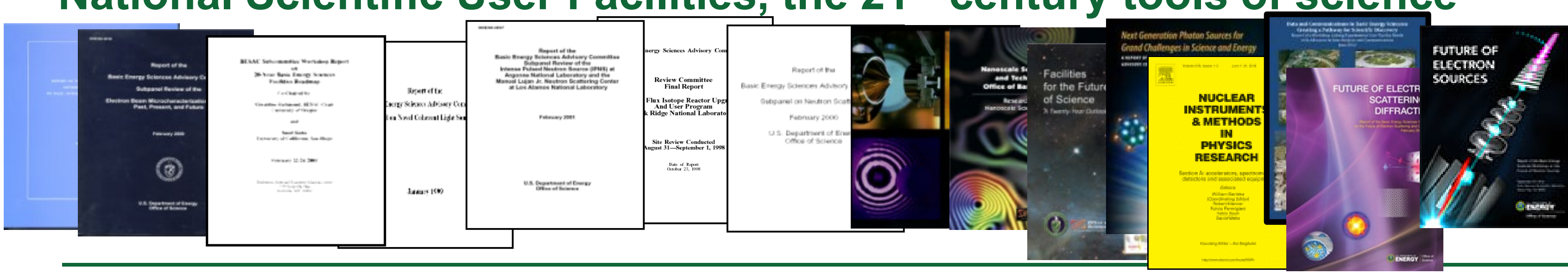
2016 - 2019

- **Science for Discovery**



- **Science for National Needs**

- **National Scientific User Facilities, the 21st century tools of science**

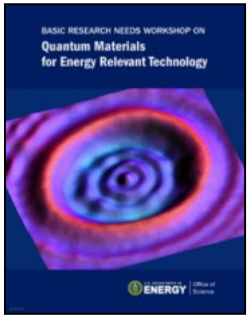


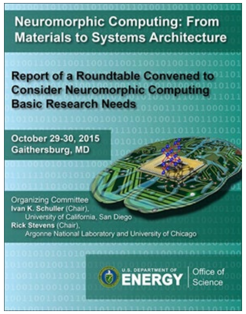
BESAC Future Light Sources 2013

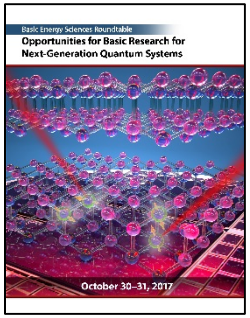
BESAC Report on Facility Upgrades 2016

Strategic Planning Workshops and Roundtables Provide Insights on Priority Research Areas

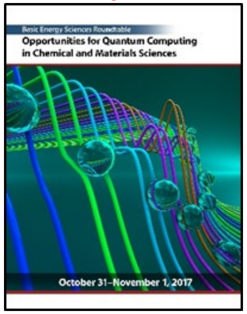
- Quantum Science

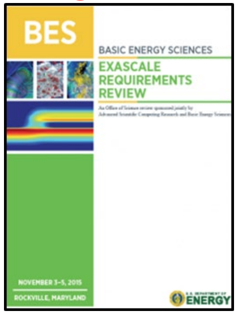




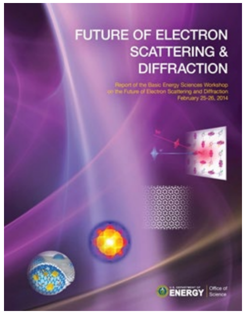


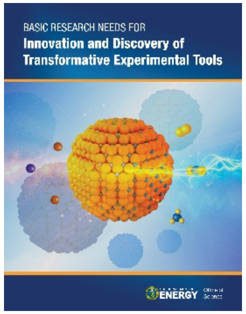
Theory, Modeling and Computation



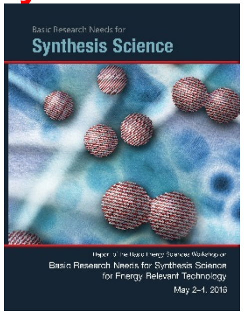


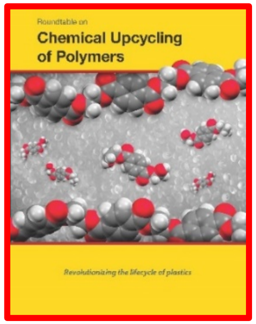
- Characterization



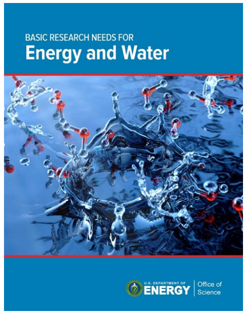


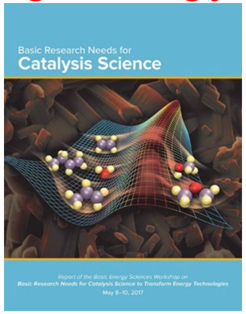
Synthesis

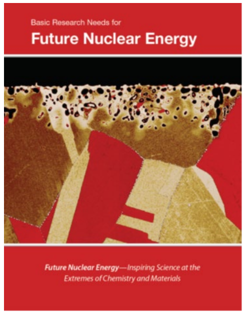


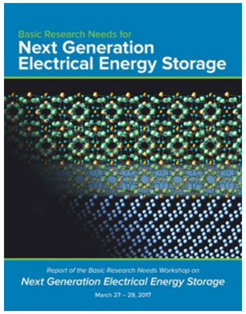


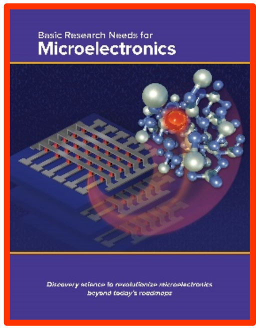
- Cross-Cutting Energy

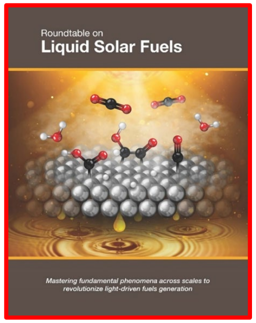






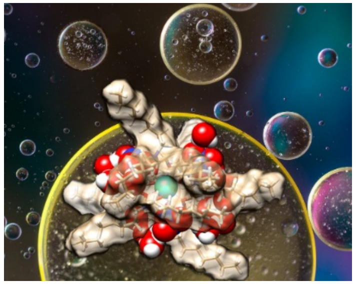




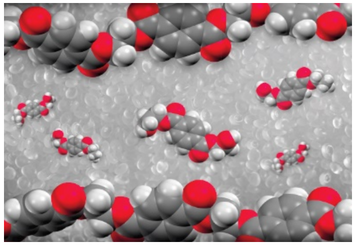


Basic Energy Sciences – FY 2021 Priorities

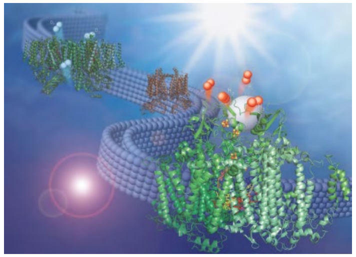
- Critical materials (+$25M) - advance our understanding of fundamental properties of these materials, identify methodologies to reduce their use and to discover substitutes, and enhance chemical processing and separation science for rare earths
- AI/ML (+$10M) - accelerate fundamental research for the discovery of new chemical mechanisms and material systems with exceptional properties and function
- Polymer upcycling (+$8.25M) - provide the foundational knowledge for designing chemical components and processes that enable efficient conversion of plastic waste to high-value chemicals, fuels, and materials; investments informed by BES Roundtable on Chemical Upcycling of Polymers
- Next-generation biology (+$3.75M) - cross-fertilize and leverage discoveries and approaches across the biological, physical, and computational sciences to develop bio-inspired, biohybrid and biomimetic systems; emphasis on neuromorphic computing, programmable biomaterials and biocatalysts, and tools for characterization of chemical, biological, biomaterial, and biohybrid systems



Critical materials: Peculiar outer-sphere water coordination of trivalent lanthanide complexes is shown to correlate with the lanthanide selectivity



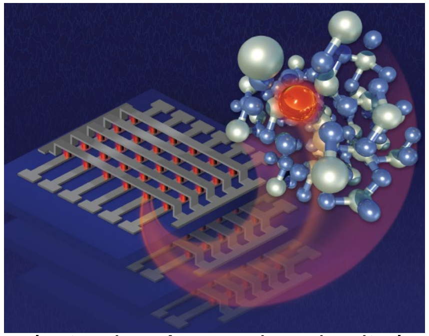
Polymer upcycling: A circular polymer lifecycle would make it easy to recycle polyethylene terephthalate (PET)



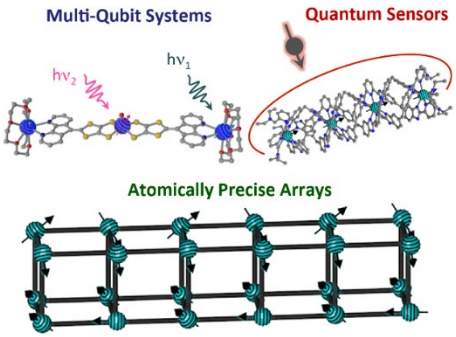
Next-gen biology: Z-scheme solar water splitting via self-assembly of photosystem I-catalyst hybrids in thylakoid membranes

Basic Energy Sciences – FY 2021 Priorities

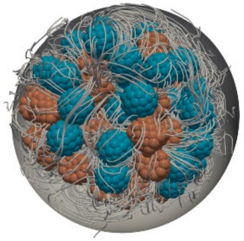
- Microelectronics (+$25M) - focus on materials, chemistry, and fundamental device science; multi-disciplinary research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem in which materials, chemistries, devices, systems, architectures, algorithms, and software are developed in a closely integrated fashion
- Quantum information science – investments in core research and the interdisciplinary SC QIS Center(s) started in FY 2020 are maintained at $72M
- Exascale computing – investments in Computational Chemical and Materials Sciences are maintained at $26M



Microelectronics: A cross-bar circuit element designed for future low power, non-volatile memory or neuromorphic computing applications.



QIS: Coordination compounds as qubits

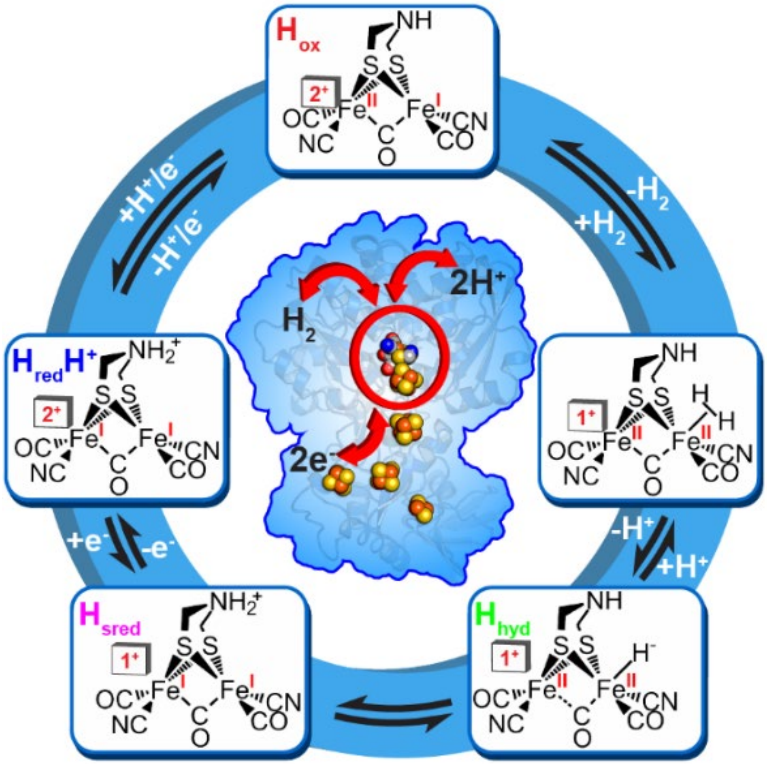


Preparing for Exascale: Computational modeling of the motion of spherical (blue) and cylindrical (orange) nanoparticles in a solvent

Research Highlights

- Highlights are a representative of research across BES that can impact hydrogen and fuel cell technologies
- These illustrate the broad underpinning research supported by BES
- It is common for BES research awards to advance science that can impact an array of technologies.

Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases



Catalytic H_2 evolution by [FeFe]-hydrogenase. Inner: Structure of [FeFe]-hydrogenase I from *Clostridium pasteurianum*, which includes an arrangement of electron transfer center and active-site hydrogen cluster (red circle) for the interconversion of H_2 from $2e^-$ and $2H^+$(red arrows). Differences in the electrostatic environment at the active site tune the relative stability of key intermediates, changing the relative propensity to oxidize (outer cycle, clockwise direction) or produce hydrogen (inner cycle, counter-clockwise direction).

Scientific Achievement

Developed a simple, yet elegant model that explains how [FeFe]-hydrogenases tune the tendency to oxidize or produce molecular hydrogen (catalytic bias).

Significance and Impact

This work provides a blueprint for engineering catalytic bias in synthetic oxidation-reduction catalysts.

Research Details

- Three [FeFe]-hydrogenases with the same cofactor active site show catalytic bias differences over six orders of magnitude.
- This work elucidated structure-activity relationships using a combination of electron paramagnetic resonance, infrared spectroscopy, X-ray powder diffraction, X-ray damage-free data from the Linac Coherent Light Source, electrochemistry, enzymatic assays, and computational methods.
- Results support a unifying model based on the relative stability of oxidation states and speciation as a function of reduction potential.

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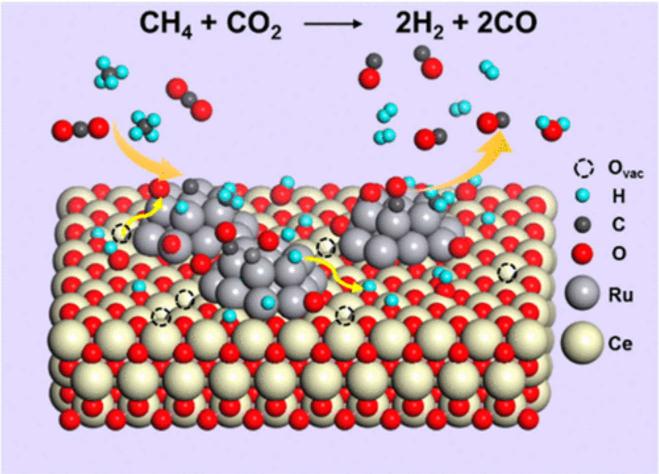
Artz JH, OA Zadvornyy, DW Mulder, et al. (2020) Tuning Catalytic Bias of Hydrogen Gas Producing Hydrogenases *J. Am. Chem. Soc.* 142, 1227−1235. DOI: 10.1021/jacs.9b08756

Research performed at WSU, NREL, PNNL, SSRL, XFEL/LCLS, ASU, and UGA

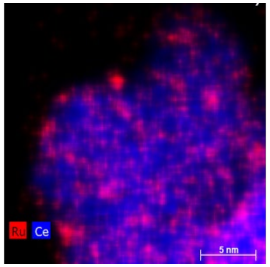
$Ru^{\delta+}$–Ce^{3+} Interactions for Enhanced Dry Reforming of Methane

Scientific Achievement

Discovered a Ru/CeO_2 catalyst with good performance and stability in the Dry Reforming of Methane (DRM) reaction to produce syngas $CO + H_2$ from $CO_2 + CH_4$ and elucidated $Ru^{\delta+}$–Ce^{3+} interaction of Ru nanoclusters (<1nm) as key.



$Ru^{\delta+}$–CeO_{2-x} interactions (top) stabilize and activate Ru clusters and improve oxygen mobility. Ru clusters on ceria imaged by EDX (right).



Significance and Impact

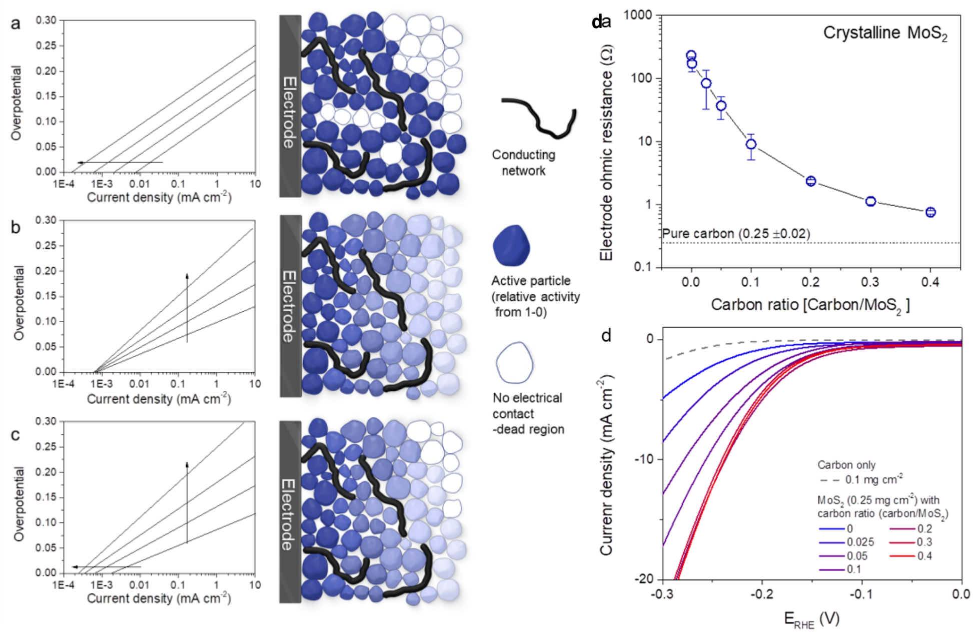
DRM is desirable to utilize mixed sources of methane and CO_2 but requires high temperature with challenges of catalyst stability. In-situ studies of Ru/CeO_2 found $Ru^{\delta+}$ – Ce^{3+} interactions at cluster interfaces selectively activate C-H bonds, stabilize small clusters in reaction conditions and correlate with oxygen transfer for oxidation of surface carbon to resist coking. Small metal particle size and tuning metal–oxide interactions are important for improved DRM catalysts.

Research Details

- A 0.5wt% Ru–CeO_2 catalyst activated methane at temperatures as low as 150 °C.
- In-situ XAFS, AP-XPS and XRD show charged Ru clusters stabilized by reduced ceria ($Ru^{\delta+}$–CeO_{2-x})
- Excellent activity/stability from stable small (<1nm) Ru clusters and improved oxygen mobility produced by metal–support interactions.

Z. Liu, F. Zhang, R. Ning, L. Lin, L.E. Betancourt, D. Su, W. Xu, J. Cen, K. Attenkofer, H. Idriss, J.A. Rodriguez, S.D. Senanayake
***ACS Catalysis*, 9(4) (2019) 3349-3359.**

Poorly Conductive Electrochemical Interfaces



Three typical models for electrochemical activity change depending on the electrode resistance: (Left) Log[current] versus overpotential (arrow indicates the deviation with increasing electrode ohmic resistance), and (right) scheme of each scenario: (a) Not all particles are active sites, (b) potential variation model due to ohmic loss of applied potential, (c) mixture of models (a) and (b). (d) Electrode ohmic resistance measured by 4-point probe method as a function of carbon additive ratio for crystalline MoS_2, and current-potential plots of the electrochemical hydrogen evolution reaction (HER) activity for the same material.

Dong Young Chung, Subin Park, Pietro P. Lopes, Vojislav R. Stamenkovic, Yung-Eun Sung, Nenad M. Markovic and Dusan Strmcnik, "Electrokinetic Analysis of Poorly Conductive Electrocatalytic Materials", *ACS Catal. 2020, 10, 4990–4996*

Scientific Achievement

A model of the impact of poor material conductivity on the evaluation of its electrochemical properties was developed. A systematic evaluation of such materials is reported, and facilitates the link between fundamental and functional properties .

Significance and Impact

Mitigation of poorly conductive materials employed at electrochemical interfaces enables development of sustainable systems for energy conversion. Key electrochemical parameters for the hydrogen evolution reaction, such as Tafel slope and intrinsic activity were revealed by high precision electrochemistry.

Research Details

– Model developed for MoS_2 HER catalyst
– MoS_2 needed to be mixed with conductive carbon to obtain correct kinetic parameters.

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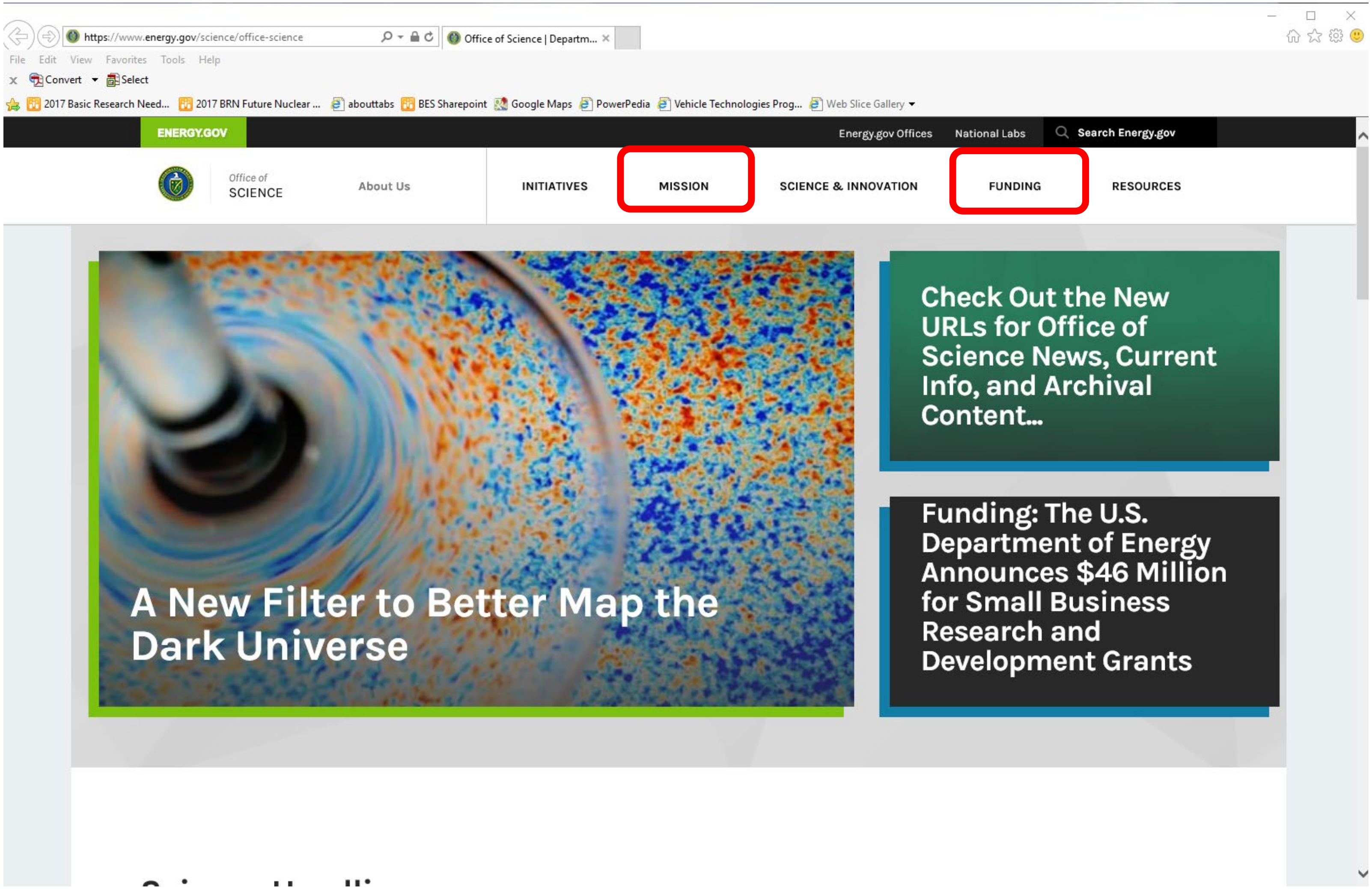
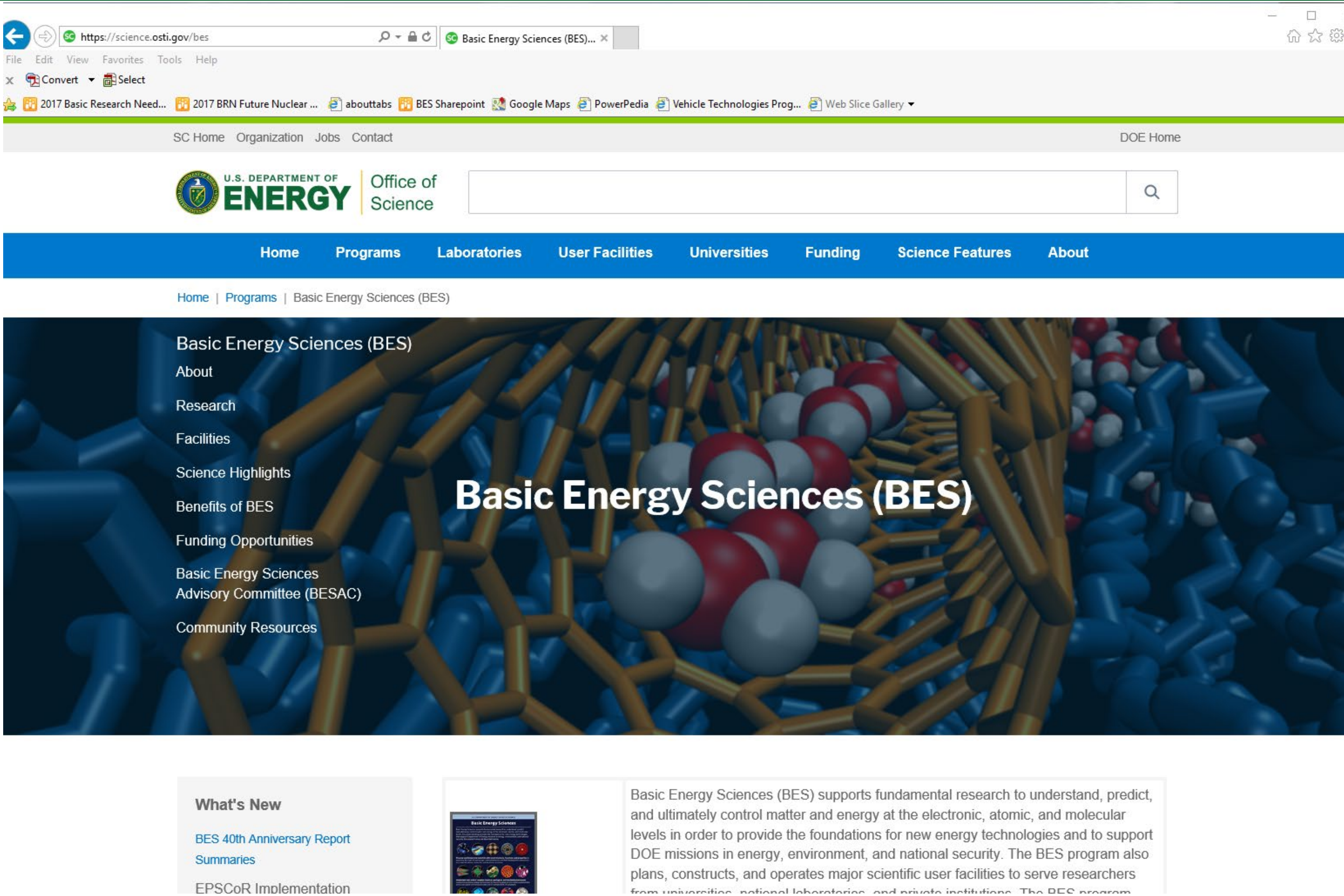
Argonne NATIONAL LABORATORY

Office of Science Home Page has Links to Budgets and Programs (https://www.energy.gov/science/office-science)



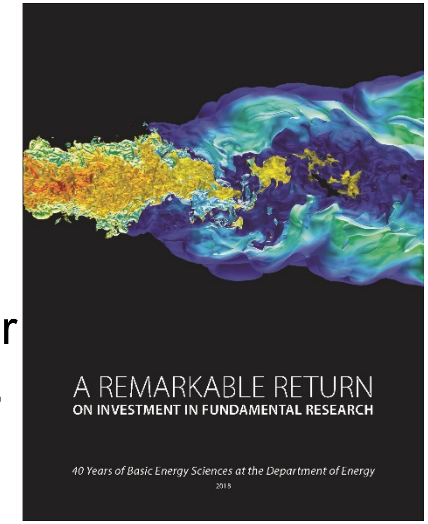
BES Home Page

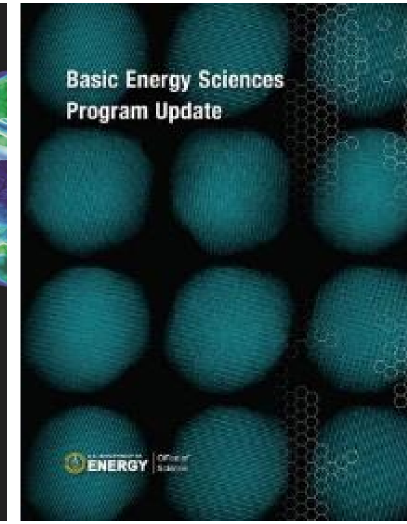
https://science.osti.gov/bes



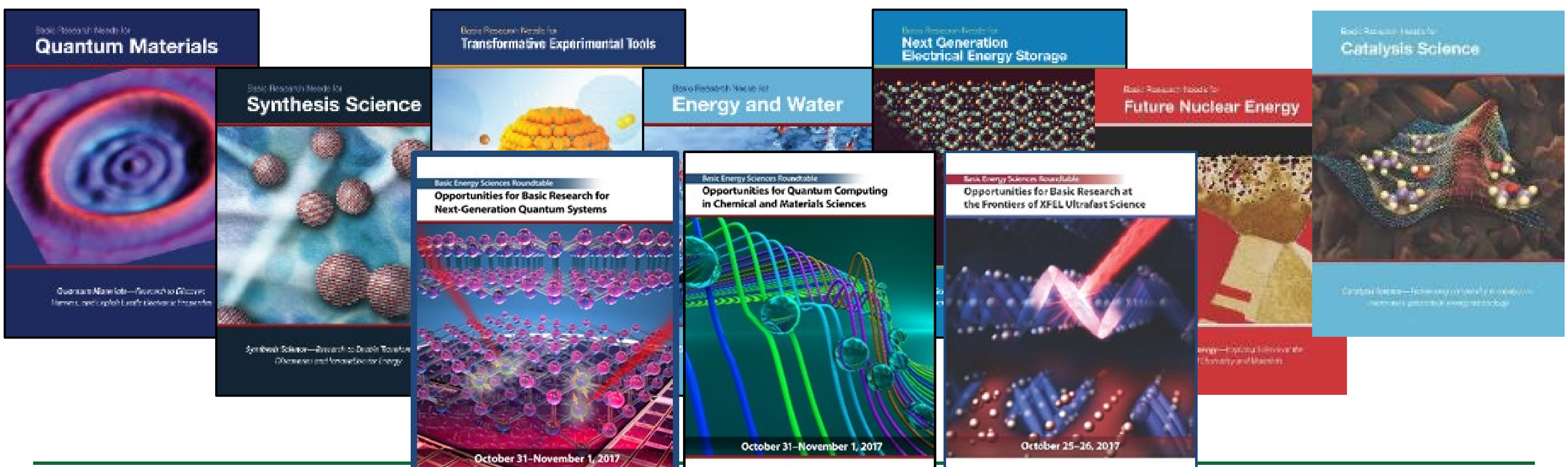
On-Line Resources

- BES at 40
  - Highlights on the impact of BES
- 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 and Roundtable Reports



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https://science.osti.gov/bes/community-resources/

Thank you

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