Basic Energy Sciences Update

BES Advisory Committee Meeting
July 12, 2018

Harriet Kung
Director, Basic Energy Sciences
Office of Science, U.S. Department of Energy
Outline

- BES Staffing Update
- FY 2018 Appropriation & FY 2019 Budget Status
- FY 2018 Solicitations Update
- Program Highlights
FY 2017 – FY 2019 BES Budget

FY 2017 Enacted: $1.871B
FY 2018 Enacted: $2.09B (Request: $1.554B)
FY 2019 President’s Request: $1.85B (HEWD: $2.129B; SEWD: $2.193B)

Priorities:

- Continue support of all Core Research Areas, EFRCs, Hubs, and CMS/CCS
- Continue support of all 12 scientific user facilities at near optimal operation level
- Expand quantum information science (an SC-wide QIS initiative) and other research priorities following strategic planning reports
- Support facility upgrades per 2016 BESAC prioritization study
<table>
<thead>
<tr>
<th>Budget Element</th>
<th>FY 2017 Enacted</th>
<th>FY 2017 % of Total</th>
<th>FY 2018 Enacted</th>
<th>FY 2018 % of Total</th>
<th>President's Request</th>
<th>FY 2019 % of Total</th>
<th>vs. FY18 $ Change</th>
<th>vs. FY18 % Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Research</td>
<td>755,669</td>
<td>40.4%</td>
<td>821,403</td>
<td>39.3%</td>
<td>746,269</td>
<td>40.3%</td>
<td>-75,134</td>
<td>-9.1%</td>
</tr>
<tr>
<td>Facility Operations</td>
<td>877,331</td>
<td>46.9%</td>
<td>898,597</td>
<td>43.0%</td>
<td>878,331</td>
<td>47.5%</td>
<td>-20,266</td>
<td>-2.3%</td>
</tr>
<tr>
<td>Projects (Const/MIE)</td>
<td>237,500</td>
<td>12.7%</td>
<td>369,000</td>
<td>17.7%</td>
<td>224,400</td>
<td>12.1%</td>
<td>-144,600</td>
<td>-39.2%</td>
</tr>
<tr>
<td>Other</td>
<td>1,000</td>
<td>0.1%</td>
<td>1,000</td>
<td>0.0%</td>
<td>1,000</td>
<td>0.1%</td>
<td>0</td>
<td>0.0%</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>1,871,500</strong></td>
<td><strong>100.0%</strong></td>
<td><strong>2,090,000</strong></td>
<td><strong>100.0%</strong></td>
<td><strong>1,850,000</strong></td>
<td><strong>100.0%</strong></td>
<td><strong>-240,000</strong></td>
<td><strong>-11.5%</strong></td>
</tr>
</tbody>
</table>

*Other includes GPP.*
Research programs

- Core Research ($551M; \( \Delta = +$62.9M \))
  - New and supplemental awards in key priority areas
  - Early Career Research Awards
  - New Solicitations in QIS, Ultrafast Science
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($110M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).

Scientific user facilities

- Operations of 12 facilities at \( \geq 95\% \) optimal level ($898.6M; \( \Delta = +$21.3M \))
- $1M Lujan equipment disposition; $8.5M Long Term Surveillance and Maintenance

Construction/MIE* \( \Delta = +$131.5M \)

- LCLS-II ($200M)
- Advanced Photon Source Upgrade($93M)
- Three new starts: LCLS-II-HE ($10M) and ALS-U ($30M); PPU ($36M)

*includes OPC
BES strives to maintain a balanced portfolio of research, facility operations, and construction.
<table>
<thead>
<tr>
<th>Project</th>
<th>ANL APS-U</th>
<th>LBNL ALS-U</th>
<th>ORNL SNS PPU</th>
<th>ORNL SNS STS</th>
<th>SLAC LCLS-II</th>
<th>SLAC LCLS-II-HE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current Status of Facility</td>
<td>APS is operational since 1996; ring will be replaced</td>
<td>ALS is operational since 1993; ring will be replaced</td>
<td>SNS Linac is operational since 2006 at 0.94 GeV</td>
<td>SNS is operational since 2006</td>
<td>LCLS is operational since 2010; LCLS-II is under construction</td>
<td>LCLS is operational since 2010; LCLS-II is under construction</td>
</tr>
<tr>
<td>Worldwide Competition</td>
<td>EU ESRF Germany PETRA3,4 Japan SPring-6 China HEPS</td>
<td>EU ESS MAX-IV Brazil SIRIUS CH SLS-II</td>
<td>EU ESS Japan JPARC China CSNS UK ISIS</td>
<td>EU ESS Japan JPARC China CSNS UK ISIS</td>
<td>EU XFEL Japan SACLA Korea PAL XFEL CH Swiss FEL</td>
<td>EU XFEL</td>
</tr>
<tr>
<td>Status Q2/18</td>
<td>CD-3b</td>
<td>CD-0</td>
<td>CD-1</td>
<td>CD-0</td>
<td>CD-3</td>
<td>CD-0</td>
</tr>
<tr>
<td>FY18 Approp</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>
FY 2018 – FY 2019 BES Research Priorities*

- **Quantum Information Science (QIS) – FY18 = $20M; FY19 = $32M**
  - 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 FY18 = $10M; FY19 = $10M**
  - 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 - FY18 = $26M; FY19 = $26M**
  - 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 BES 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.

*FY19 funding at President’s request levels, including SBIR/STTR
In the FY 2018 Enacted budget, LCLS was increased by 1.3% or $1.7M over FY 2017 Enacted in preparation for completion of the LCLS-II construction project.

The remaining light sources were decreased by 0.5% or $1.9M.

Neutron facilities were increased by 5.2% or $13.8M.
  
  - SNS increased by 2% or $4.1M; HFIR increased by 14.9% or $9.7M

NSRCs were increased by 6.3% or $7.7M, supporting optimal operations.

<table>
<thead>
<tr>
<th>% Optimal Operations</th>
<th>FY 2017 Enacted</th>
<th>FY 2018 Enacted</th>
<th>FY 2019 President’s Request</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linac Coherent Light Source</td>
<td>97%</td>
<td>97%</td>
<td></td>
</tr>
<tr>
<td>All Other Light Sources</td>
<td>97%</td>
<td>95%</td>
<td>95%</td>
</tr>
<tr>
<td>Spallation Neutron Source</td>
<td></td>
<td>99%</td>
<td></td>
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<tr>
<td>High Flux Isotope Reactor</td>
<td></td>
<td>&gt;100%</td>
<td></td>
</tr>
</tbody>
</table>

* After applicable reductions due to SBIR/STTR.
<table>
<thead>
<tr>
<th>FY 2019 House Mark</th>
<th>FY 2019 Senate Mark</th>
</tr>
</thead>
<tbody>
<tr>
<td>EFRCs, Hubs flat funded; Batteries Hub encouraged to focus on grid storage applications, particularly on chemistries with low cost reagents.</td>
<td>EFRCs, Hubs, CMS, CCS flat funded; submit a 10-year solar fuels research initiative strategic plan within 120 days of enactment.</td>
</tr>
<tr>
<td>Funding levels for NSRCs, light sources, neutron sources specified (+$12M over FY 2018)</td>
<td>Funding levels for NSRCs, light sources (NSLS-II), neutron sources specified (+$45M over FY 2018); submit a plan for beamline buildout at NSLS-II as part of the FY 2020 budget</td>
</tr>
<tr>
<td>$20M for EPSCoR; annual or biennial Implementation Grant solicitations encouraged with a report due on BES’s plan within 90 days of enactment.</td>
<td>$20M for EPSCoR; annual or biennial Implementation Grant solicitations encouraged with a report due on BES’s plan within 90 days of enactment.</td>
</tr>
<tr>
<td>Encourages support for basic research in polymers and polymer-based materials for energy applications, and implementation of neutron research efforts for polymeric materials.</td>
<td>Supports funding for emergent polymer optoelectronic technologies</td>
</tr>
<tr>
<td>$10M for research of artificial light harvesting systems that promise to significantly increase computational processing power and speed.</td>
<td></td>
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</tbody>
</table>
## Status of BES FY 2019 Appropriation – HEWD & SEWD vs. FY 2018 Enacted

<table>
<thead>
<tr>
<th></th>
<th>FY 2018</th>
<th>FY 2019</th>
<th>FY 2019 House Mark vs. FY 2018 Enacted</th>
<th>FY 2019 Senate Mark vs. FY 2018 Enacted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Enacted</td>
<td>House Mark</td>
<td>Senate Mark</td>
<td></td>
</tr>
<tr>
<td>Core Research</td>
<td>555,768</td>
<td>581,068</td>
<td>535,051</td>
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<tr>
<td>EPSCoR</td>
<td>19,270</td>
<td>19,270</td>
<td>19,270</td>
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</tr>
<tr>
<td>EFRCs/Hubs/CMS/CCS/GPP</td>
<td>176,088</td>
<td>176,088</td>
<td>176,088</td>
<td></td>
</tr>
<tr>
<td>Facility Operations</td>
<td>898,597</td>
<td>910,500</td>
<td>944,009</td>
<td></td>
</tr>
<tr>
<td>MIEs/Construction/OPC</td>
<td>369,000</td>
<td>379,400</td>
<td>456,400</td>
<td></td>
</tr>
<tr>
<td>LTSM</td>
<td>8,500</td>
<td>...</td>
<td>...</td>
<td></td>
</tr>
<tr>
<td>SBIR/STTR</td>
<td>62,777</td>
<td>62,907</td>
<td>62,582</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2,090,000</td>
<td>2,129,233</td>
<td>2,193,400</td>
<td>39,233</td>
</tr>
<tr>
<td>FY 2019 House Mark vs. FY 2018 Enacted</td>
<td>4.6%</td>
<td>-20,717</td>
<td>-3.7%</td>
<td></td>
</tr>
<tr>
<td>FY 2019 Senate Mark vs. FY 2018 Enacted</td>
<td>1.3%</td>
<td>45,412</td>
<td>5.1%</td>
<td></td>
</tr>
</tbody>
</table>

**FY 2018 ENACTED**
- Projects: 18%
- Research: 39%
- Facility Ops: 43%

**FY 2019 HEWD**
- Projects: 18%
- Research: 39%
- Facility Ops: 43%

**FY 2019 SEWD**
- Projects: 21%
- Research: 37%
- Facility Ops: 42%
History: 20+ community workshops since early-2000s with over 2,000 participants describing “basic research needs” for energy applications and “grand-challenge science”

Establishment of EFRCs in 2009
- 46 awards: 30 funded at $100M/year; 16 fully funded by ARRA at $277M; $2-5M/year each for a 5-year term

Recompetition in 2014
- 32 awards funded at $100M/year (22 renewal, 10 new); $2-4M/year each for a 4-year term, with competitions now every 2 years

Targeted FOA in 2016 – Emphasizing science related to environmental management
- 4 new awards funded at $10M/year; $2-4M/year each for a 4-year term;

Recompetition in 2018
EFRC History (2009-2018)

Cumulative

60 EFRCs in 40 States + D.C. since 2009

Current EFRCs

- Over 115 participating institutions, located in 34 states and DC
- 610 senior investigators and more than 1,600 postdocs, grad students, undergrads, and technical staff
- >240 scientific advisory board members from 12 countries and 40 companies

Initial Awards

- Initial awards totaling $777 million, including 16 projects funded by the American Recovery and Reinvestment Act.

Re-competition

- Awards totaling $400 million in an open recompetition in which 22 existing EFRCs were renewed.

EM-Related

- Additional awards totaling $40 million to accelerate scientific breakthroughs for DOE’s mission in nuclear cleanup.
The 2016 EFRC booklet describes the history and outcomes from the first seven years of the EFRC program, including representative scientific highlights, academic publications, intellectual property, and science commercialization.

- **Solar concentrators based on quantum dots**
  Core-shell quantum dots were rationally designed for efficient light collection and transmission.

- **Building precision nanobatteries by the billions**
  Batteries constructed in nanopores promise to deliver energy at much higher power and longer life.

- **Examining the enzyme complex that makes cellulose fibrils**
  Imaging and computational modeling revealed new structural insights.

- **Accurately modeling materials for energy applications**
  Optimal method identified for multiscale simulations of carbon nanostructures.

- **Viability of long-term carbon sequestration in the subsurface**
  The Bravo Dome gas field was used to estimate CO$_2$ dissolution rates over millennia.

- **Nanoscale control of uranium for solvent-free recovery**
  Water-soluble uranium-oxygen clusters are large enough to be filtered using commercial membranes.
EFRC Impact – IP and Company Interactions (May 2016)

**EFRC IMPACT BY THE NUMBERS**

- Now over 10,000
- Over 7,500 Peer-reviewed publications
- Over 490 Invention disclosures
- Over 50 Patents issued
- Over 250 Foreign patent applications
- Over 380 U.S. patent applications
- At least 100 Licenses
- About 90 Companies have benefited from EFRC research

**DISTRIBUTION OF COMPANIES THAT HAVE BENEFITTED FROM EFRC RESEARCH**

- ~33% Start-ups
- ~23% Mid-sized companies
- ~44% Large companies

General criteria for claiming company’s benefits from EFRCs:
Licensed EFRC IP; Established CRADA; Used EFRC ideas in their business; Provided follow-on funding; Substantial interactions, involving personnel or sample exchange
EFRC FY2018 Recompetition Timeline

Proposal Statistics (3 preproposals per institution as lead)
- Lead institutions: 76% university, 24% national laboratory
- >150 unique partner institutions in 45 states, DC, Puerto Rico, and 10 foreign countries

Awards
- 31 four-year awards – 22 New and 9 Renewal; 9 led by Labs, 22 by Universities
- Additional 11 two-year extensions to existing centers to support the completion of valuable research
Topical Distribution of 42 EFRCs

Synthesis/Mat-Chem by Design – Foundational science underpinning materials and chemical synthesis for broad energy applications.

Subsurface – New geophysics and geochemistry for enhanced oil/gas and geothermal applications.

Solar – Cutting-edge innovation for the capture of solar energy and conversion into electricity and fuels.

Separations – Advances to enhance gas separations and address energy-water issues.

Catalysis – Enhanced selectivity and efficiency in production of fuels and chemicals.

Energy Storage – New materials and chemistries for next-generation electrical energy storage.

Nuclear – Advanced fuels and radiation-tolerant materials for future nuclear energy.

Quantum Materials – Novel materials for innovative electronics, sensors, and communications.

4 additional EM-related EFRCs funded 2016-2020
<table>
<thead>
<tr>
<th>Director</th>
<th>Lead Institution</th>
<th>Center Name</th>
<th>Topical Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>McQueeney</td>
<td>Ames</td>
<td>Center for the Advancement of Topological Semimetals (CATS)</td>
<td>Quantum Materials</td>
</tr>
<tr>
<td>Basov</td>
<td>Columbia</td>
<td>Programmable Quantum Materials (Pro-QM)</td>
<td></td>
</tr>
<tr>
<td>Broholm</td>
<td>Johns Hopkins</td>
<td>Institute for Quantum Matter</td>
<td></td>
</tr>
<tr>
<td>Moore</td>
<td>LBNL</td>
<td>Center for Novel Pathways to Quantum Coherence in Materials</td>
<td></td>
</tr>
<tr>
<td>Cheng</td>
<td>Univ of Florida</td>
<td>Center for Molecular Magnetic Quantum Materials</td>
<td></td>
</tr>
<tr>
<td>Schuller</td>
<td>UC San Diego</td>
<td>Quantum Materials for Energy Efficient Neuromorphic Computing (Q-MEEN-C)</td>
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<tr>
<td>Abruna</td>
<td>Cornell</td>
<td>Center for Alkaline-Based Energy Solutions (CABES)</td>
<td>Energy Storage</td>
</tr>
<tr>
<td>Savinell</td>
<td>Case Western Reserve</td>
<td>Breakthrough Electrolytes for Energy Storage (BEES)</td>
<td></td>
</tr>
<tr>
<td>Dai*</td>
<td>ORNL</td>
<td>Fluid Interface Reactions, Structures and Transport (FIRST) Center</td>
<td></td>
</tr>
<tr>
<td>Takeuchi*</td>
<td>SUNY Stony Brook</td>
<td>EFRC: Center for Mesoscale Transport Properties</td>
<td></td>
</tr>
<tr>
<td>Tolbert</td>
<td>UC Los Angeles</td>
<td>EFRC Center for Synthetic Control Across Length-scales for Advancing Rechargeables (SCALAR)</td>
<td></td>
</tr>
<tr>
<td>Uberuaga</td>
<td>LANL</td>
<td>Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)</td>
<td>Nuclear</td>
</tr>
<tr>
<td>Hurley</td>
<td>INL</td>
<td>Center for Thermal Energy Transport under Irradiation (TETI)</td>
<td></td>
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<tr>
<td>Wishart</td>
<td>BNL</td>
<td>Molten Salts in Extreme Environments</td>
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* Renewal Award
<table>
<thead>
<tr>
<th>Director</th>
<th>Lead Institution</th>
<th>Center Name</th>
<th>Topical Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beard</td>
<td>NREL</td>
<td>Center for Hybrid Organic-Inorganic Semiconductors for Energy (CHOISE)</td>
<td>Solar</td>
</tr>
<tr>
<td>Scholes</td>
<td>Princeton</td>
<td>Bioinspired Light-Escalated Chemistry (BioLEC)</td>
<td></td>
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<tr>
<td>Dionne</td>
<td>Stanford</td>
<td>Photonics at Thermodynamic Limits</td>
<td></td>
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<tr>
<td>Friend*</td>
<td>Harvard</td>
<td>INTEGRATED MESOSCALE ARCHITECTURES FOR SUSTAINABLE CATALYSIS (IMASC)</td>
<td>Catalysis/Bioscience</td>
</tr>
<tr>
<td>Cosgrove*</td>
<td>Penn State</td>
<td>Center for Lignocellulose Structure and Formation (CLSF)</td>
<td>Catalysis/Bioscience</td>
</tr>
<tr>
<td>Vlachos*</td>
<td>Univ of Delaware</td>
<td>Catalysis Center for Energy Innovation (CCEI)</td>
<td>Catalysis/Bioscience</td>
</tr>
<tr>
<td>Gagliardi*</td>
<td>Univ of Minnesota</td>
<td>Inorganometallic Catalyst Design Center</td>
<td>Catalysis/Bioscience</td>
</tr>
<tr>
<td>Bullock*</td>
<td>PNNL</td>
<td>EFRC for Center for Molecular Electrocatalysis</td>
<td>Catalysis/Bioscience</td>
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<tr>
<td>Strano</td>
<td>MIT</td>
<td>The Center for Enhanced Nanofluidic Transport (CENT)</td>
<td></td>
</tr>
<tr>
<td>Darling</td>
<td>ANL</td>
<td>Advanced Materials for Energy-Water Systems</td>
<td>Separations</td>
</tr>
<tr>
<td>Walton*</td>
<td>Georgia Tech</td>
<td>Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)</td>
<td>Separations</td>
</tr>
<tr>
<td>Freeman</td>
<td>UT Austin</td>
<td>Center for Materials for Water and Energy Systems</td>
<td></td>
</tr>
<tr>
<td>Kovscek</td>
<td>Stanford</td>
<td>Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations</td>
<td>Subsurface</td>
</tr>
<tr>
<td>Butt</td>
<td>Univ of Utah</td>
<td>Multi-Scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)</td>
<td>Subsurface</td>
</tr>
<tr>
<td>Stupp*</td>
<td>Northwestern</td>
<td>Center for Bio-Inspired Energy Science (CBES)</td>
<td>Synthesis/Mat-Chem by Design</td>
</tr>
<tr>
<td>Parise</td>
<td>SUNY Stony Brook</td>
<td>GENESIS: A Next Generation Synthesis Center</td>
<td>Synthesis/Mat-Chem by Design</td>
</tr>
<tr>
<td>Baneyx</td>
<td>Univ of Washington</td>
<td>CSSAS: The Center for the Science of Synthesis Across Scales</td>
<td>Synthesis/Mat-Chem by Design</td>
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</tbody>
</table>

* Renewal Award
## 11 Two-Year Extensions

<table>
<thead>
<tr>
<th>Director</th>
<th>Lead Institution</th>
<th>Proposal Title</th>
<th>Topical Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peters</td>
<td>Washington State</td>
<td>Biological Electron Transfer and Catalysis EFRC</td>
<td>Catalysis/Bioscience</td>
</tr>
<tr>
<td>Fenter</td>
<td>ANL</td>
<td>CENTER FOR ELECTROLYTE-ELECTRODE INTERFACE SCIENCE</td>
<td>Energy Storage</td>
</tr>
<tr>
<td>Whittingham</td>
<td>SUNY Binghamton</td>
<td>NorthEast Center for Chemical Energy Storage (NECCES)</td>
<td></td>
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<tr>
<td>Rubloff</td>
<td>Univ of Maryland</td>
<td>Precision Ion-electron Control in Solid State Storage (PICS3)</td>
<td></td>
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<tr>
<td>Zhang</td>
<td>ORNL</td>
<td>Energy Dissipation to Defect Evolution</td>
<td>Nuclear</td>
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<tr>
<td>Long</td>
<td>UC Berkeley</td>
<td>Center for Gas Separations</td>
<td>Separations</td>
</tr>
<tr>
<td>Wasielewski</td>
<td>Northwestern</td>
<td>Center for Light Energy Activated Redox Processes (LEAP)</td>
<td>Solar</td>
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<tr>
<td>Meyer</td>
<td>UNC Chapel Hill</td>
<td>Alliance for Molecular PhotoElectrode Design for Solar Fuels (AMPED)</td>
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<tr>
<td>Perdew</td>
<td>Temple</td>
<td>Center for Complex Materials from First Principles (CCM)</td>
<td>Synthesis/Mat-Chem by Design</td>
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<tr>
<td>Shi</td>
<td>UC Riverside</td>
<td>Spins and Heat in Nanoscale Electronic Systems (SHINES)</td>
<td></td>
</tr>
<tr>
<td>Tumas</td>
<td>NREL</td>
<td>Center for Next Generation of Materials Design</td>
<td></td>
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</tbody>
</table>
Two Roundtable Reports (October 2017) defined a BES research agenda for emerging quantum systems and computing research opportunities:

**BES Science for Quantum Systems**
- Advance artificial quantum-coherent systems
- Enhance creation and control of coherence in quantum systems
- Novel approaches for quantum-to-quantum transduction
- New quantum methods for advanced sensing and process control

**Quantum Computing for BES Science**
- Control the quantum dynamics
- Unravel the physics and chemistry of strongly correlated electron systems
- Embed quantum hardware in classical frameworks
- Bridge the classical–quantum computing divide
BES QIS Funding Opportunity Announcement (1)

Materials and Chemical Sciences Research for Quantum Information Science

DE-FOA-0001909 and LAB 18-1909

FOA Scope:
Fundamental research in materials and chemical sciences to:
- Advance understanding of quantum phenomena in systems that could be used for QIS
- Use today’s quantum computers for chemical and materials sciences research.
- Topics related to BES roundtable reports on QIS.

Application requirements:
- A maximum of 2 applications were accepted per institution as lead
- Single investigator/small group and team proposals: $150K to $1.5M per year, up to 3 year awards
- Projected up to 30 awards and $20M in FY 2018 funding ($60M over 3 years)

U.S. DEPARTMENT OF ENERGY
Office of Science

BES Leads: Jim Horwitz and Jeff Krause
Quantum Integration Across Scales

- BES Nanoscale Science Research Centers user facilities are key to the synthesis and characterization of materials and structures from nano-components to prototype-scale quantum systems.
  - Integration and testing couple closely to theory, design, and systems efforts
  - Development and testing of physical models of behavior of quantum devices
  - Co-located with National Lab x-ray, neutron, computing, and microfabrication facilities for understanding and scale-up of quantum structures
  - Next-generation qubits and sensors
BES QIS Funding Opportunity Announcement (2)
QUANTUM INFORMATION SCIENCE AND RESEARCH INFRASTRUCTURE (LAB 18-1910)

FOA Scope:

**Research Infrastructure:** includes funding for metrology, fabrication, and prototypes (measurement science instrumentation, modeling and simulation, and shared DOE-lab based user facilities).

**Research:** Topics related to BES roundtable reports on QIS.

**Application requirements**
- A maximum of 3 pre-applications were accepted per Nanoscale Science Research Center
- Team proposals: $500K - $2M per year, up to 3 year awards
- Projected up to 8 awards and $10M in FY 2018 funding ($30M over 3 years)
Fundamental research in materials and chemical sciences enabled by new ultrafast x-ray free electron laser (XFEL) capabilities at LCLS-II and its prospective upgrades:

- Probing and controlling electron motion within a molecule
- Discovering novel quantum phases through coherent light-matter coupling
- Capturing rare events and intermediate states in the transformation of matter

Application requirements:

- A maximum of 2 applications were accepted per institution as lead
- Small groups and team proposals: $300K to $1.5M per year, up to 3 year awards
- Projected up to 15 awards and $10M in FY 2018 funding ($30M over 3 years)

**Timeline:**

- **April**
  - 4/2/2018: FOA & Lab announcement issued

- **May**
  - 4/30/2018: Letters of Intent Received
  - 5/21/2018: Full Proposals Received

- **June**
  - Late May – Early July: Merit Review and Assessment (ongoing)

- **July**
  - Mid - Late July: Proposals Recommended for Funding
  - 7/31/2018: Target Awards Announcement
  - 9/30/2018: Award Start

**BES Leads:** Helen Kerch and Jeff Krause
BES Exascale Computing Initiative Funding Opportunity Announcement
COMPUTATIONAL CHEMICAL SCIENCES RESEARCH

DE-FOA-0001912 and LAB 18-1912

FOA Scope:
Fundamental research to develop validated, public access codes and databases and to advance new approaches to use large complex data sets for deriving fundamental knowledge from calculations and advanced characterization of chemical systems.

Application requirements:
- A maximum of one application was accepted from each institution (as lead)
- Small groups and team proposals: $150K to $2M per year, up to 4 year awards
- Projected up to 15 new awards and $13M/year in total FY 2018 funding

April
4/13/2018
FOA & Lab announcement issued

May
5/16/2018
Letters of Intent Received
6/18/2018
Full Proposals Received

June
Mid June – Early July
Merit Review (ongoing)
Mid - Late July
Proposals Recommended for Funding

July
07/31/2018
Award Packages due
September 30
Awards Start

BES Lead: Mark Pederson
DE-FOA-0001897

Partnerships to advance fundamental, early-stage energy research collaborations between the EPSCoR jurisdictions and the DOE national laboratories

- Research must be within DOE’s mission-space
  - Office of Science
  - Energy Technology Offices

Application requirements:
- A maximum of 1 application was accepted per institution
- Requires (unfunded) collaboration with a DOE National Laboratory
- Small team proposals: up to $750,000 over three years
- Up to 20 fully funded awards; up to $15M in FY 2018 funding

BES Lead: Tim Fitzsimmons
National Synchrotron Light Source-II on a Path to Mature Operations

- Reliable accelerator operation
  - Operating at 375 mA and will increase to 400 mA by the end of July
  - FY2018 reliability to date is over 97%

- Steady increase in both the number of beamlines and the number of users
  - 18 beamlines in General User Program and 8 beamlines in commissioning
  - 28 beamlines will be in operation by the end of CY2018
  - Over 1,000 unique users for FY2017 and already nearly 1,000 unique users for FY2018 to date

- 5,000 planned operating hours for users for FY2019

**Mesoporous Catalysts for Hydrogen Production**

Mesoporous Co/CeO2 catalysts were characterized and found the catalysts to be active for water-gas shift reactions at 300 – 500°C.

*Figure:* Co K-edge XANES and FEFF 9 models of Co atom on top of CeO2 particle.

*J. Phys. Chem. C (2018)*

**3D Nanoscale Imaging of Defects in a Nanowire**

In a single nanowire, the 3D distribution of both strain and stacking defects was measured using coherent x-rays, revealing structural heterogeneity from nano- to micrometer scales.

*Figure:* (Left) a SEM image of a nanowire with diffraction geometry and (right) cutouts from 3D images sensitive to stacking defects.

*Nano Letters (2018)*

**Unexpected Architecture of a Membrane Protein Revealed**

The crystal structure of a channel-forming O-antigen polysaccharide transporter called Wzm-Wzt was revealed and showed an unexpected, non-traditional architecture.

*Figure:* Wzm forms six transmembrane helices and the cytoplasmic loop (CH) forms the coupling helix. The periplasmic loop, between helices 5 and 6, generates two periplasmic gate helices (PG1 and PG2). Gray box indicates likely membrane boundaries.

*Nature (2018)*
Transmission X-ray Microscope

- TXM achieved a complete 3D nanotomography measurement in 1 min., at ~50 nm resolution
- with 20 ms exposures and 3°/s rotation speed
- World-leading capabilities, based on cutting-edge in-house design that leverages NSLS-II nanopositioning capability

Tracking 3D nano-dendritic growth in real time

In-situ reaction: \( \text{Cu} + \text{AgNO}_3 \rightarrow \text{Ag} + \text{Cu(NO}_3\text{)}_2 \)

0 min

1 min

2 min

3 min

20 um
Helical Superconducting Undulator: 
Sending Electrons on a Rollercoaster Ride

Technical Achievement

- A first-of-its-kind x-ray source based on superconducting undulator technology has been designed and built at the Advanced Photon Source (APS). The new source -- the Helical Superconducting Undulator (HSCU) -- forces the 7-GeV electron beam into a helical trajectory.

Significance and Impact

- Light produced by electrons moving on a helical trajectory is unlike that from planar undulators. It is circularly polarized and monochromatic (with no harmonics on axis), and still high-brightness. This x-ray beam can be used directly, i.e. without any optics, for experiments.
- The flux from the HSCU surpasses the flux from planar APS undulators with monochromators by several orders of magnitude.

Research details

- The integration of the HSCU into the APS storage ring went flawlessly
- The measured spectrum confirmed the predicted ratio of flux for 1st and 2nd harmonics. (A very weak 2nd harmonic arises from the finite beam emittance; it is not strong enough to affect user experiments.)
Single-pulse X-ray White-Beam Imaging Using HSCU at the APS 7-ID

- Fuel-spray research requires single-pulse (100 ps) white-beam to image high-speed, transient liquid jets.
- Undulator A at 6 keV: power density > 100 W/mm², > 90% is unwanted higher-energy (HE) photons.
  - Requires a mirror to reject HE photons and to reduce power, but it introduces artifacts and additional noise.
- HSCU white beam at 6 keV: low power density < 15 W/mm², much lower HE contents, so NO need of a mirror.
  - 5x beam intensity and 8x S/N compared to UA

HSCU beam enables quantitative imaging analysis and simulation.
Magnetic quasicrystals are both ordered and disordered nanomaterials

Researchers observed that quasicrystals made of nanomagnets form magnetic states having both an ordered, rigid 'skeleton' spanning the entire network, and smaller domains with configurations that are switchable without energy cost.


Tailored Nanotubes for Sensors and Lasers

Low temperature single defect photoluminescence spectroscopy and quantum chemistry modeling revealed existence of six distinct chemical binding configurations for sp³ defects as the source of diverse spectral behavior. This provides a rational strategy toward controllable creation and manipulation of individual covalent quantum defects with desired optical functionalities.

Any functional groups (gray dots) can bind to nanotubes (gray lattice) in six distinct configurations (white circles) leading to defect states emitting photons at different energies (red, orange and yellow stars). Wavefunction spread of the lowest energy exciton states are plotted in red and blue.

Dynamic Lens-on-MEMS Brings New Vision to Optics

Integration process of a metasurface-based flat lens onto a MEMS scanner. Integration process: an FIB probe was used to cut, grab and weld the lens onto the MEMS scanner.

Flat lens mounted on 2-axis MEMS scanner.

Metasurfaces were dynamically controlled by integrating them onto Micro-Electro-Mechanical Systems (MEMS).


Sugar-coated Peptoid Nanosheets Selectively Detect Multivalent Proteins

A model of a glycosylated peptoid nanosheet binding a multivalent protein.

A team led by Foundry researchers has developed a method to engineer the surface of peptoid nanosheets, mimicking some of the properties of cell membranes, to interact with multivalent proteins.

This work was performed in part at the Molecular Foundry.