U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Update

Linda Horton

Associate Director

Office of Basic Energy Sciences

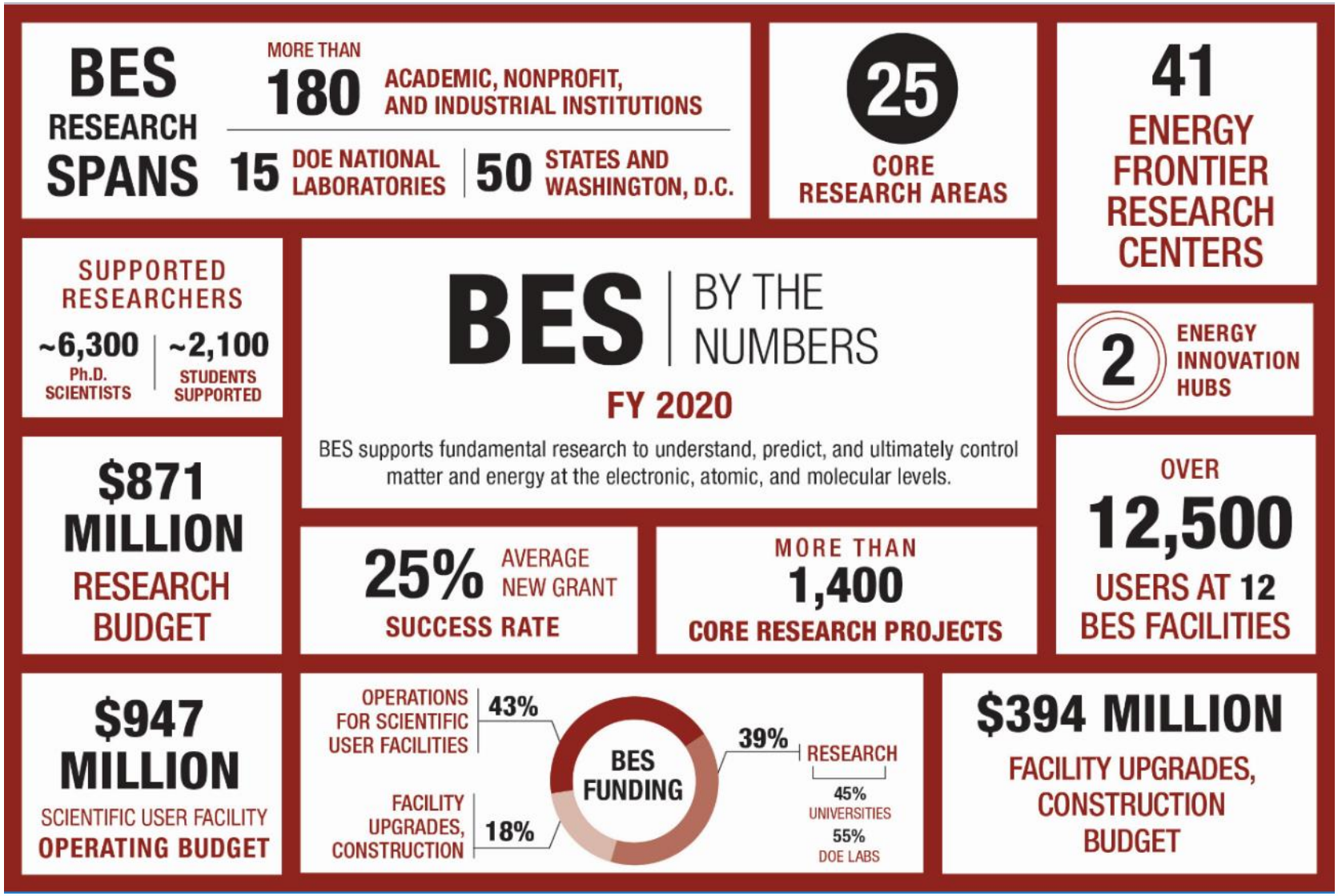
BESAC Meeting

December 9, 2020

Exciting Times for BES Continue

- Welcome to BESAC, Benchmarking Subcommittee, COVs
- BES Statistics
- People: BES Personnel, SC Distinguished Scientists
- FY 2020 Awards and Science Highlights
- FY 2020 Facilities Highlights and Projects Update
- FY 2021 Budget Status
- FY 2021 Funding Opportunity Announcements
- Strategic Planning Activities
- Impact of BESAC

Basic Energy Sciences At a Glance (2020)



Office of Basic Energy Sciences

Associate Director
Linda Horton

BES Budget and Planning
Donetta Herbert, Financial Management
(Vacant, Program Manager)
Thomas Russell, Senior Technical Advisor

BES Operations
Teresa Crockett, Program Analyst
Robin Hayes, Program Manager
Kerry Hochberger, Program Support Specialist
(Vacant, Program Analyst / BESAC*)
Andy Schwartz, Senior Technical Advisor for EFRCs**

* Basic Energy Sciences Advisory Committee
** Energy Frontier Research Centers

Materials Sciences and Engineering Division

Andy Schwartz, Acting Director
(Vacant)
Claudia Cantoni, Program Manager

Materials Discovery, Design, and Synthesis
Mike Markowitz

- **Materials Chemistry**
  Craig Henderson
  Michael Sennett
- **Biomolecular Materials**
  Mike Markowitz
  (Vacant)
- **Synthesis and Processing Science**
  Bonnie Gersten
- **Batteries and Energy Storage Hub; Technology Coordination**
  Craig Henderson
  John Vetrano

Condensed Matter and Materials Physics
Jim Horwitz

- **Experimental Condensed Matter Physics**
  Michael Pechan
- **Theoretical Condensed Matter Physics**
  Matthias Graf
  (Vacant)
- **Physical Behavior of Materials**
  Refik Kortan
  Athena Sefat
- **Mechanical Behavior and Radiation Effects**
  John Vetrano

Scattering and Instrumentation Sciences
Helen Kerch

- **X-ray Scattering**
  Lane Wilson
- **Neutron Scattering**
  Thiyaga P. Thiyagarajan
- **Electron and Scanning Probe Microscopies**
  Jane Zhu
- **Experimental Program to Stimulate Competitive Research (DOE EPSCoR)**
  Tim Fitzsimmons

Scientific User Facilities Division

Linda Horton, Acting Director
(Vacant)
Rocio Meneses, Program Support Specialist

Operations

- **X-ray and Neutron Scattering Facilities**
  Peter Lee
  Thiyaga P. Thiyagarajan
  (Vacant)
  Yiping Feng
- **NSRCs ****
  George Maracas
- **Accelerator and Detector Research**
  Eliane Lessner
- **Facilities Coordination; Metrics; Assessment**
  Van Nguyen

** Nanoscale Science Research Centers

Construction

- **Linac Coherent Light Source-II**
  Phil Kraushaar
- **Advanced Photon Source Upgrade**
  Ed Stevens
- **Facilities Upgrades and MIE*** Projects**
  Phil Kraushaar
  Ed Stevens

*** Major Items of Equipment

Chemical Sciences, Geosciences, and Biosciences Division

Bruce Garrett, Director

Brandon Rohnke, AAAS Fellow
Emily Smith, AAAS Fellow

Fundamental Interactions
Jeff Krause

- **Atomic, Molecular, and Optical Sciences**
  Tom Settersten
- **Gas Phase Chemical Physics**
  Wade Sisk
- **Condensed Phase and Interfacial Molecular Science**
  Gregory Fiechtner
- **Computational and Theoretical Chemistry**
  Aaron Holder

Photochemistry and Biochemistry
Gail McLean

- **Solar Photochemistry**
  Christopher Fecko
  (Vacant)
- **Photosynthetic Systems**
  Stephen Herbert
- **Physical Biosciences**
  Robert Stack
- **Fuels from Sunlight Energy Innovation Hub**
  Christopher Fecko

Chemical Transformations
Raul Miranda

- **Catalysis Science**
  Chris Bradley
  Viviane Schwartz
- **Separation Science**
  Daniel Matuszak
  Vanda Glezakou
- **Heavy Element Chemistry**
  Philip Wilk
- **Geosciences**
  James Rustad

LEGEND

- Detailee (50%) from PNNL
- Detailee from SBIR/STTR
- Detailee (70%) from SLAC

December 2020
Posted December 1, 2020

New Hire – Physical Behavior of Materials Program

Dr. Athena Sefat

Program Manager, Physical Behavior of Materials
Materials Sciences and Engineering Division

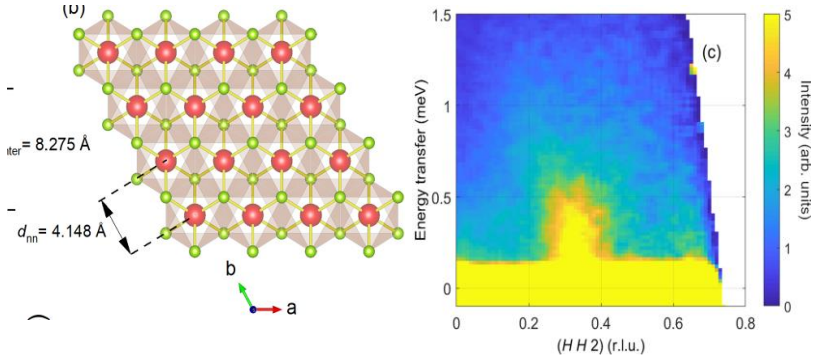
Expertise

- Experimental Condensed Matter Physics
- Chemical, electronic, and spin competitions
- Low-dimensional magnets, unconventional superconductors, quantum spin liquids

Experience

- Oak Ridge National Lab, Wigner Fellow and Senior Research Scientist
- BES 2010 Early Career Research Program awardee
- Ames Lab, Postdoc
- McMaster University, PhD

The finding of QSL behavior in $CsYbSe_2$ could inform applications in quantum communication and computation



a) Crystal structure of $CsYbSe_2$ de

b) Low-energy neutron spin excitation spectrum at 2 K confirming the absence of a long- range magnetic order.

Phys. Rev. B: Rapid Commun., **100**, 220407(R) (2019)

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https://science.osti.gov/bes/mse/About/Staff/Dr-Athena-Sefat

Dr. Brandon Rohnke

AAAS Science and Technology Policy Fellow,
Office of Basic Energy Sciences

Expertise

- Regulation of carbon concentrating mechanisms in *Fremyella diplosiphon*
- Energy cycles during natural photosynthesis
- Plant biochemistry, genetics, microbiology

Joined BES in September 2020

Experience

- Michigan State University, Ph.D.
  - Research conducted at the Plant Research Laboratory (PRL) which is funded by the US Department of Energy, Basic Energy Sciences
- St. Olaf College, BA in Chemistry and BA in Religion

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AAAS
AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE

Congratulations to DOE-SC Distinguished Scientists Fellows ! Three BES-sponsored awardees in 2019-2020

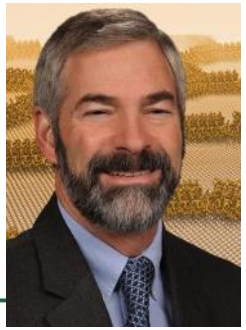
- Awards recognize DOE National Laboratory staff showing achievement, leadership, service, and impact related to the Office of Science
- 5 awards across SC in 2019; 3 awards in 2020; $1M over 3 years to each Fellow

Dr. José Rodriguez, Brookhaven National Laboratory, 2019:

- For discoveries of the atomic basis of surface catalysis for the synthesis of sustainable fuels, and for significantly advancing in-situ methods of investigation using synchrotron light sources

Dr. Jacqueline Chen, Sandia National Laboratory - California, 2020 (jointly sponsored with ASCR):

- For advancing frontiers in the fields of combustion and high-performance computing through petascale direct numerical simulations and for mentoring and inspiring generations of researchers



Dr. James De Yoreo, Pacific Northwest National Laboratory, 2020:

- For transformational discoveries that have reshaped our understanding of materials synthesis from complex nucleation pathways to hierarchical assembly, for leadership in National Laboratory-University partnerships, and for dedication to mentoring the next generation of scientists

FY 2020 Special FOAs – Awards announced since July (1/2)

- **QIS Centers:** Five 5-year SC-wide awards announced August 26, 2020
  - DOE response to National Quantum Initiative (NQI) Act, enacted December 2018
  - Lead institutions: ANL*, BNL*, FNAL, LBNL, ORNL (* BES leads DOE oversight team)
  - Each Center funded at $115M over 5 years, subject to appropriations
- **AI/ML for User Facilities:** Lab announcement with High Energy and Nuclear Physics. Eight 3-year BES awards announced August 17, 2020, total $30M over 3 years.

Scope

- Focus on research and development in artificial intelligence and machine learning methods (AI/ML) to maximize the production, mining, analysis, and control of data generated at the existing and future scientific user facilities and to optimize their scientific output

Awards

- Accelerator and Detector Research lead institutions: SLAC (2), ORNL
  - Subawards: ANL, PNNL
- Light and Neutron Source lead institutions: LBNL, BNL, ORNL
  - Subawards: ANL, BNL, LBNL, ORNL, SLAC, Purdue Univ.
- Nanoscale Science Research Center lead institutions: LBNL, ANL
  - Subawards: ANL, BNL, LBNL, ORNL, SNL

FY 2020 Special FOAs – Awards announced since July (2/2)

- **Materials and Chemical Sciences Research on Critical Materials:**
  Lab announcement. Five 3-year awards announced August 25, 2020, total $20M over 3 years.

  Scope – Fundamental materials and chemical sciences research on:

  – Physics and Chemistry of Rare Earth Elements
  – Novel Materials / Molecular Design and Synthetic Approaches
  – Advances in Separation Science

  Awards – lead institutions ANL, LBNL, LANL, ORNL, NREL

- **Materials and Chemical Sciences Research for Direct Air Capture of CO_2:**
  Lab announcement. Three 3-year awards announced August 18, 2020, total $13.5M over 3 years.

  Scope – Fundamental materials and chemical sciences research on:

  – Designing High Selectivity, Capacity, and Throughput Separations
  – Data Science Driven Synthesis and Assembly of Materials for Direct Air Capture
  – Understanding Temporal Changes That Occur During Separations

  Awards – lead institutions ANL, PNNL, LLNL

CO_2 Reduction to CO with 19% Efficiency in a Solar-Driven Gas Diffusion Electrode Flow Cell

Scientific Achievement

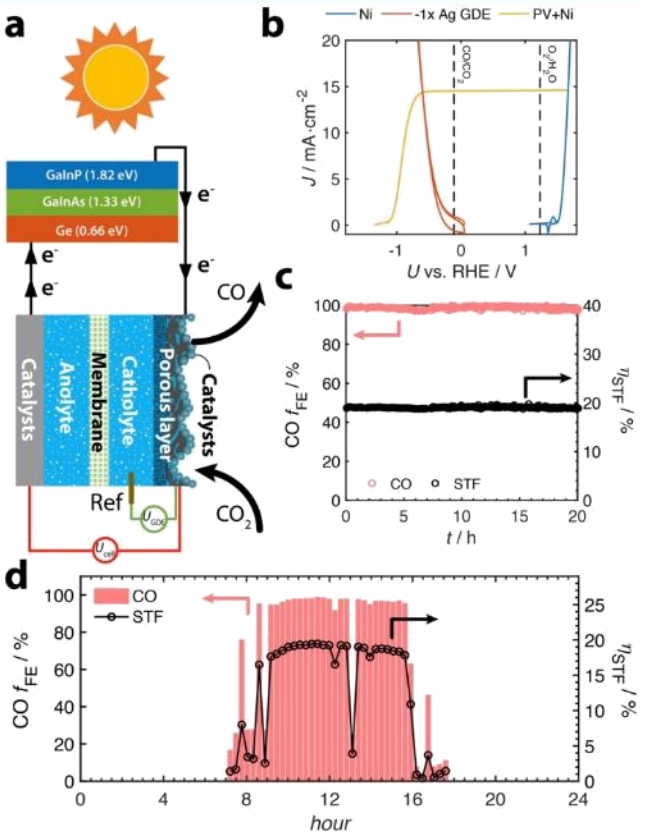
Efficient solar-driven CO_2 reduction to CO was realized by integrating high-efficiency photovoltaics with performance-matched, *reverse-assembled* gas diffusion electrodes. In reverse assembled form, the catalyst faces the gas phase CO_2 limiting flooding while overcoming the low CO_2 electrolyte solubility, enabling stable, high Faradaic efficiency operation.

Significance and Impact

The record 19% efficiency achieved in this directly-driven PV-GDE exceeds the theoretical maximum efficiency of a separately wired PV and electrolyzer using a DC-DC converter, demonstrating the benefit of component integration.

Research Details

- Similar catalytic performance in traditional and reverse-assembled GDEs.
- 150 h with no catalyst flooding in reverse-assembled GDE.
- 20 h stable 19% solar to fuel efficiency under 1 Sun illumination
- PV-GDE operates near its maximum power point by matching photoelectrode design to Ag nanoparticle catalyst loading.



(a) Wire connection between the triple junction PV and GDE cell. **(b)** *J-U* characteristic of Ni anode, photovoltaic with Ni anode, and Ag-NP gas diffusion cathode under 1 Sun. **(c)** The CO Faradaic efficiency and solar to fuel efficiency over the 20 h duration in lab under 1 Sun. **(d)** The CO Faradaic efficiency and solar to fuel efficiency for a 24h day under outdoor illumination in Pasadena, CA.

W.-H. Cheng, M. Richter, I. Sullivan, D. Larson, C. Xiang, B.S. Brunschwig, H.A. Atwater. *ACS Energy Letters*, **2020**, *5*, 470-476.

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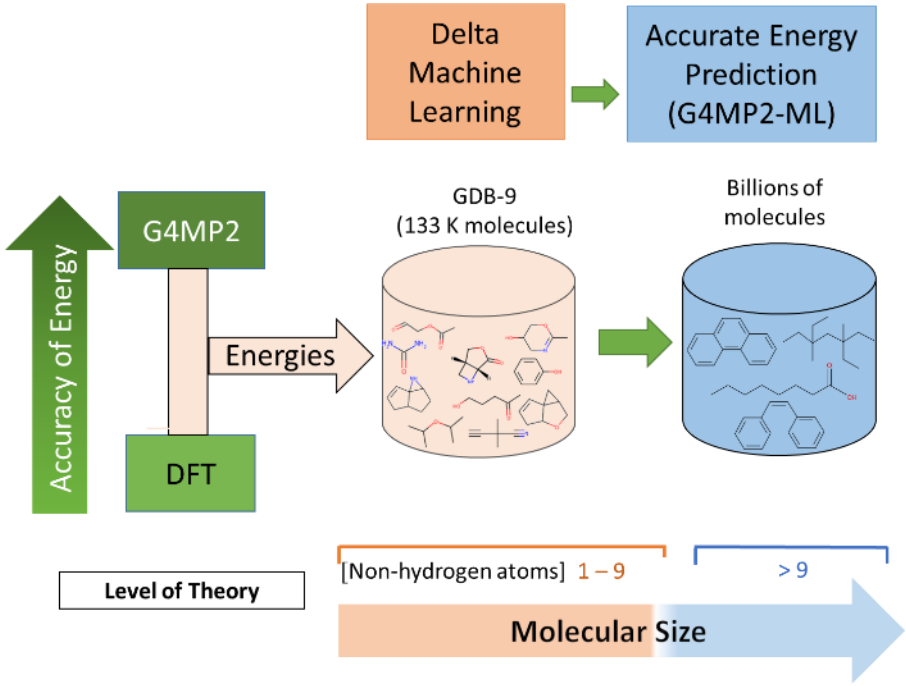
JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS
Caltech
BERKELEY LAB
SLAC

Quantum-Chemically Informed Machine Learning for Fast and Accurate Prediction of Energies of Large Molecules



Schematic of the use of delta machine learning, based on calculated G4MP4 and DFT energies for the GDB-9 set of 133,000 organic molecules with 1-9 non-hydrogen atoms, to predict energies of larger organic molecules with more than 9 non-hydrogen atoms.

Work performed at Argonne National Laboratory (JCESR managing partner)

Naveen Dandu, Logan Ward, Rajeev S. Assary, Paul C. Redfern, Badri Narayanan Ian T. Foster, Larry A. Curtiss, J. Phys. Chem A (2020)

DOI: 10.1021/acs.jpca.0c01777

Scientific Achievement

This work has demonstrated that quantum chemically informed machine learning can be used to successfully predict energies of large organic molecules with sizes beyond those in the training set at a much lower cost in computer time.

Significance and Impact

The results of this study demonstrating that machine learning methods can be accurately extended beyond the size of molecules in the training set means they can be used to explore a vast exploration space of molecules for discovery of energy storage electrolytes. The ability to quickly make these predictions greatly expands the capability of the JCESR Electrolyte Genome.

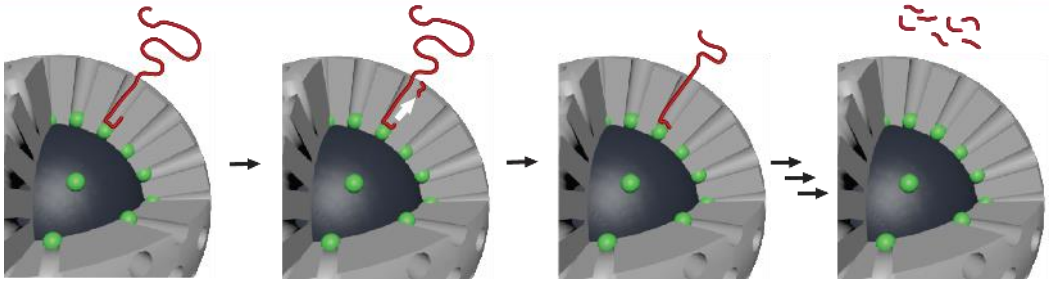
Research Details

- This work is based on a set of 191 molecules with 10-14 non-hydrogen atoms (i.e., larger than those in the training set) having accurate experimental enthalpies of formation.
- The best-performing ML method investigated in this paper, FCHL-Δ, gave atomization energies for the 191 organic molecules within about 0.4 kcal/mol of very accurate quantum chemical energies calculated by the G4MP2 method.
- This machine learning approach combined with ones being developed for anions, cations, and solvation energies will enable fast and accurate screening of properties needed to discover molecules for advanced energy storage systems.

Design of a Processive Catalyst for Polyethylene Upcycling

Scientific Achievement

A mesoporous shell/Pt/core architecture catalyzes polyethylene (PE) hydrogenolysis into a narrow distribution of hydrocarbons centered at ~C_{16} through a processive process that mimics features of enzymatic deconstruction of polymers.



Steps in the processive polymer deconstruction mechanism: (a) PE adsorption into a pore, (b) cleavage of a C-C bond via hydrogenolysis, desorption of the short hydrocarbon fragment, and repositioning of the adsorbed chain, (c) repeated cleavage, product release, and chain reorientation to convert the entire strand into a uniform distribution of shorter chains.

Significance and Impact

Processive catalysis can improve rates and selectivity in upcycling processes through the design of the mesoporous architectures to favor the synthesis of a targeted distribution of desired products.

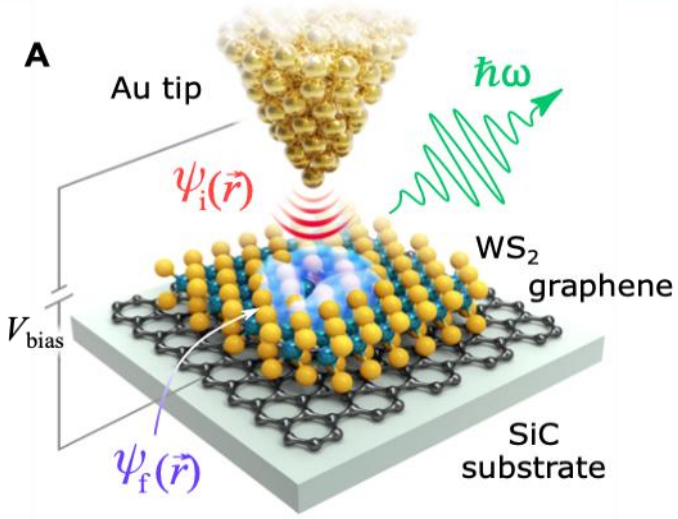
The present work is the first demonstration of processive abiotic catalysis for plastic upcycling.

Research Details

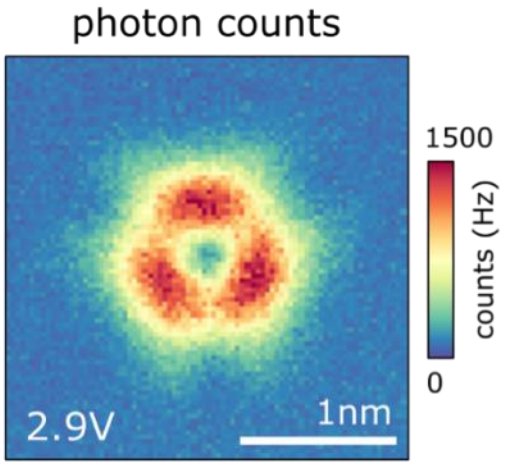
- Solid-state ^{13}C NMR spectroscopy revealed the adsorption, conformational orientation, and dynamic behavior of PE in mesoporous silica, and guided the catalyst design.
- The catalytic deconstruction of PE shows the features of a processive mechanism: long polymer chains are converted into a short, uniform conversion-independent distribution of products, and intermediate length chains are not formed.

A. Tennakoon, X. Wu, A. L. Paterson, S. Patnaik, Y. Pei, A. M. LaPointe, S. C. Ammal, R. A. Hackler, A. Heyden, I. I. Slowing, G. W. Coates, M. Delferro, B. Peters, W. Huang, A. D. Sadow, F. A. Perras *Nature Catalysis*, **2020**, *3*, 893-901.
DOI: 10.1038/s41929-020-00519-4

Visualizing single photoemission from atomic defects in 2-D WS2 with atomic resolution



Scanning Tunneling Luminescence



photoemission with atomic resolution

Scientific Achievement

Direct observation of electrically stimulated single photoemission from individual defects in 2-D WS2

Significance and Impact

The search for next generation quantum emitters is focused on 2-D systems due to the principle of higher control over the atomic environment. Here we create an ideal framework to control quantum emission from the single atomic level.

Research Details

- We directly correlated unambiguously the atomically precise morphology of defects in 2-D WS2, the electronic structure including maps of individual defect orbitals, and mapping and characterizing photons emitted from the defect orbitals
- S vacancies in 2-D WS2 act as single photo emitters when eclectically stimulated

Electrically driven photon emission from individual atomic defects in monolayer WS2 Bruno Schuler, Katherine A. Cochrane, Christoph Kastl, Edward S. Barnard, Edward Wong, Nicholas J. Borys, Adam M. Schwartzberg, D. Frank Ogletree, F. Javier Garcıa de Abajo, and Alexander Weber-Bargioni; Sci. Adv. 2020; 6 : eabb5988 16 September 2020

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Work was performed at Lawrence Berkeley National Laboratory, supported by the NPQC EFRC

npqc

BERKELEY LAB

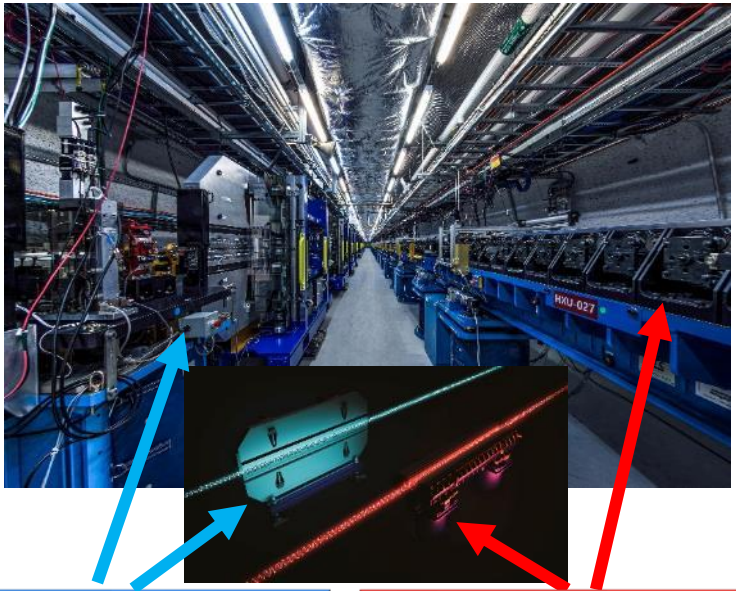
Basic Energy Sciences

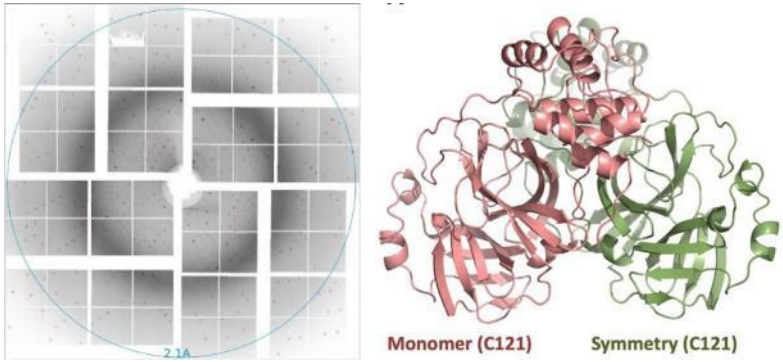
FY 2020 Facility Operation Highlights

- All 12 facilities were funded at 100% optimal level. Additional funds from the CARES Act enabled facilities to incur expenses above routine operational costs for COVID-related research. All facilities had curtailed user operations due to COVID-19 restrictions, available through remote access in supporting COVID-19 related research.
- APS and NSLS-II coordinated their operating schedules to optimize access for COVID-19 research. Both facilities delivered over 400 more operating user hours than the originally planned 5,000 hours, with better than 97% reliability.
- ALS and SSRL faced California wildfires and electricity shutdowns in addition to COVID-19 challenges; however, both facilities still delivered thousands of hours for user research, ~4,500 hours with 88% reliability for SSRL and ~3,200 hours with 84% reliability for ALS.
- On July 17, LCLS successfully produced the first light through the newly installed hard x-ray undulator after a long shutdown for LCLS-II installation activities (subsequently, on September 12, they successfully brought the new soft x-ray undulator on-line); the user operations resumed on August 16; and early experiments for COVID-19-related research were successful.
- SNS has adjusted its operation schedule to deliver over 200 hours more than the originally planned 4,600 hours, with ~95% reliability. SNS also supported COVID-19 research.
- HFIR delivered over 3,600 hours for users with 88% reliability for FY 2020. Late in the FY, scheduled user operations were delayed due to abnormal fuel plate deflections. Evaluation of the manufacturing and inspection continues.

LCLS Resumes User Operations with Two New Undulators

- LCLS-II project built and installed two new variable gap undulators
- LCLS has successfully produced the first light on July 17 through the newly installed hard x-ray undulator after long shutdown for LCLS-II installation activities
- On September 12, LCLS scientists ushered an electron beam through a second new undulator to produce “soft” X-rays
- First soft x-ray beam delivered to newly constructed Time-resolved atomic, Molecular and Optical Science (TMO) instrument on October 10, 2020

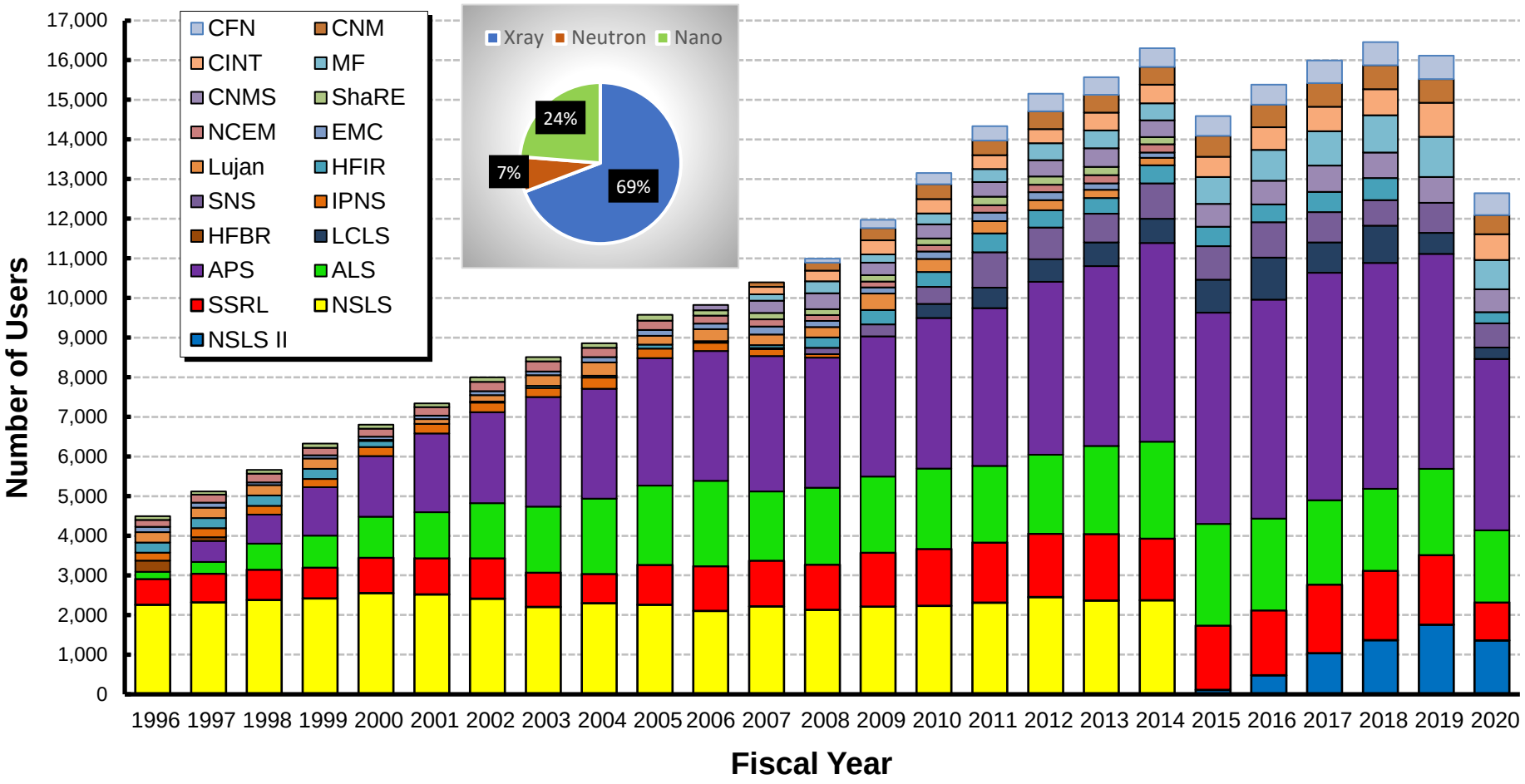




Diffraction pattern and crystal structure of SARS-CoV-2 Main Protease sample from LCLS Serial Femtosecond X-ray Crystallography experiment

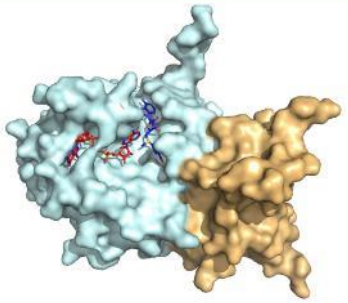
The user operations have resumed since August 16th. A number of early experiments that were COVID-19 related research have been successful.

BES User Facilities Hosted Over 12,500 Users in FY 2020 Impacted by COVID-19

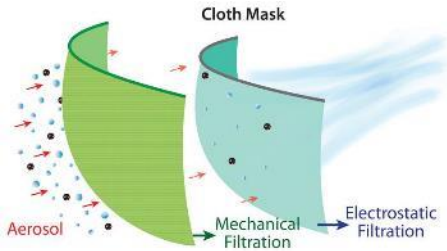


COVID-19 Related Research at BES Scientific User Facilities

- Light sources provide critical support to the development of potential therapeutic drugs and vaccines through structural studies of the proteins of the SARS CoV-2 virus, which causes COVID-19.
  - To date, a total of 146 structures of those proteins and their complexes have been determined based on data measured at BES light sources. These crucial structural information contributed to the recent success of therapeutic drug and vaccine developments.
  - At APS, there were 79 unique user groups using 21 beamlines for an accumulated total of over 10,000 hours of beamtime since late January at the start of the pandemic. Many important results have been published.
- Neutron facilities research continues high resolution structure analysis of the SARS-CoV-2 main protease enzyme, neutron reflectivity of viral protein interactions with cell membranes, and combined experiment-computational studies of potential therapeutic candidates.
- The NSRCs continue studies to improve the effectiveness of personal protective equipment (masks, nanoparticle-based antiviral coatings), develop novel methods for virus detection (quantum dot-based, 3D printed platforms for high-throughput screening) and microfluidic devices nanoparticle synthesis for vaccine encapsulation and delivery.

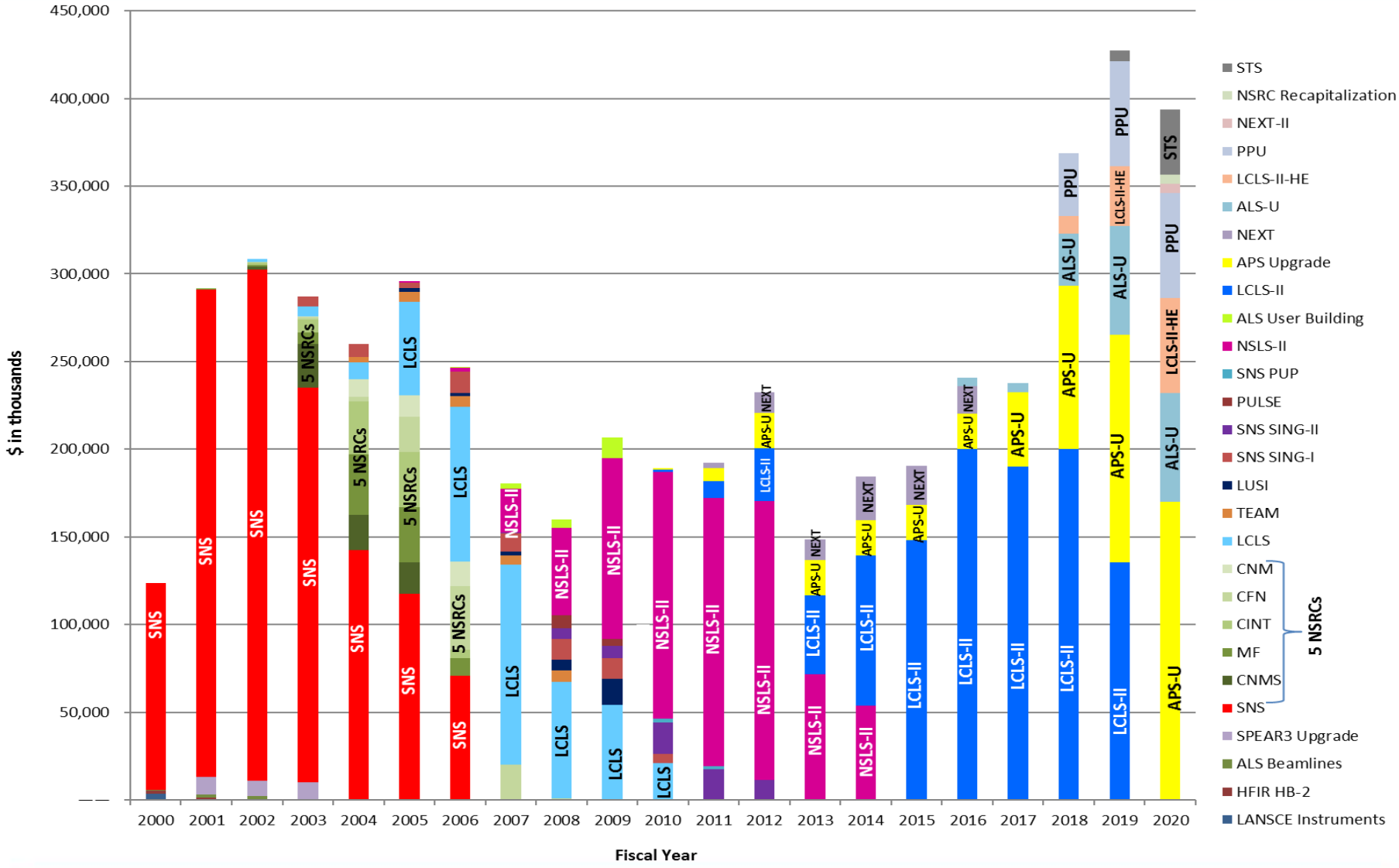


Structure of the ternary complex of SARS-CoV-2 RNA nsp16 (cyan)/nsp10 (beige) in complex with RNA cap (red) and S-adenosyl methionine or SAM (blue). **It reveals key details about how SARS-CoV-2 modifies its messenger RNA (mRNA) and evades immune responses in its host.** (Illustration courtesy of Y. Gupta)



Schematic showing filtration of aerosol particles using a combination of mechanical and electrostatic filtration from a combination of fabrics. **The study found that fabrics with a tight weave and low porosity, such as those found in cotton sheets with high thread count, performed well.** (Image courtesy of American Chemical Society)

BES Construction/MIE Funding Profiles: 2000 – 2020



Line Item Construction and Major Items of Equipment Projects (1)

Linac Coherent Light Source-II (LCLS-II) – CD-3: LCLS operation with new undulators, August 2020

- Slowly resuming construction and commissioning activities after losing ~5 months of schedule due to COVID-19.
- Performance Baseline Deviation due in part to impact of COVID-19. The Baseline Change Proposal was approved on October 13, 2020 and established a new TPC of $1,136M with a CD-4 date of Jan 2024.

Advanced Photon Source Upgrade (APS-U) – CD-3

- FY 2020 = $170M; FY 2021 request = $150M; House mark = $160M; FY 2021 Senate mark = $160M for procurement, integration, and testing of storage ring and experimental equipment and new beamline building construction. OPA status review on September 1-3, 2020.
- Some cost and schedule impacts of COVID-19.

Advanced Light Source Upgrade (ALS-U) – CD-1, 3a

- FY 2020 = $62M; FY 2021 request = $13M; FY 2021 House mark = $75M; FY 2021 Senate mark = $62M for engineering, design, R&D prototyping, and long lead procurements of construction items. OPA CD-2 review on November 17-20, 2020.
- COVID-19 impacts are being studied and mitigations put in place.

Linac Coherent Light Source-II High Energy (LCLS-II-HE) – CD-1, 3a

- FY 2020 = $54M; FY 2021 request = $16M; FY 2021 House mark = $72M; FY 2021 Senate mark = $54M for engineering, design, R&D prototyping. LCLS-II-HE received CD-3A approval in May 2020 for the long lead procurement of 18 cryomodules.
- New scope to provide for additional instruments and a new low emittance superconducting electron gun added. OPA Status review in December 2020

Line Item Construction and Major Items of Equipment Projects (2)

SNS Proton Power Upgrade (PPU) – CD-3

- FY 2020 = $60M; FY 2021 request = $8M; FY 2021 House mark = $8M; FY 2021 Senate mark = $55M for design, engineering, prototyping, fabrication, testing, and procurements. CD-2 and CD-3 approved in October 2020.
- ORNL work for PPU and STS continues onsite and remotely, helping to minimize COVID impacts.

SNS Second Target Station (STS) – CD-1

- FY 2020 = $37M; FY 2021 request = $2M; House mark = $2M; FY 2021 Senate mark = $42M for the project continues planning, R&D, and engineering activities .
- CD-1 approved in November 2020.

NSLS-II Experimental Tools-II (NEXT-II)* – CD-1

- FY 2021 Request = $1M; FY 2021 House mark = $15M; FY 2021 Senate mark = $5.5M for the project continues with R&D, prototyping, other supporting activities, and possible long lead procurements.
- The project conducted an SC Independent Project Review in August 2020 for CD-1. CD-1 was approved September 30, 2020 with a cost range of $65M - $95M and a point estimate of $89M.

Nanoscale Science Research Center (NSRC) Recapitalization* – CD-0

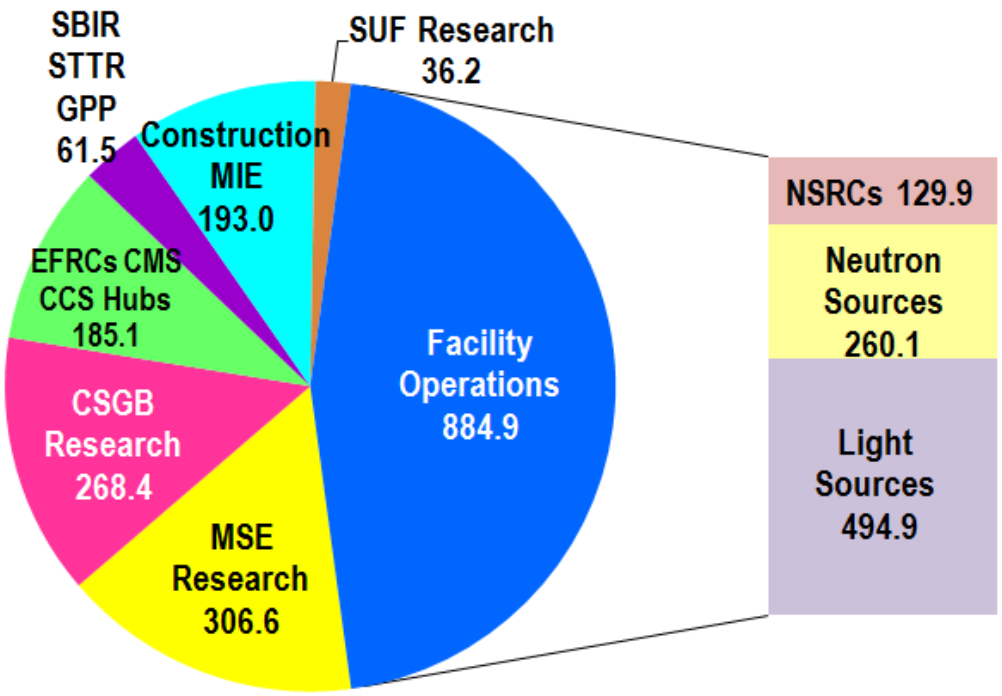
- FY 2021 Request = $1M; FY 2021 House mark = $15M; FY 2021 Senate mark = $5M for the project continues with R&D, design, engineering, prototyping, other supporting activities, and possible procurements.
- OPA CD-1 review scheduled in December 2020.

*** Major Items of Equipment (MIE) Projects**

FY 2021 President's Request: $1,935.7M (-$277.3M or -12.5% from FY 2020)

Research programs Δ = -$5.9M

- Core Research ($575M) includes new investments ($73M) in critical materials, data/AI/ML, polymer upcycling, next-generation biology, microelectronics, and accelerator R&D (Direct Air Capture of CO_2 – Marks)
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($115M)
- Energy Innovation Hubs continue ($44.1M)



Scientific user facilities Δ = -$66M

- Operations of 12 facilities continue at ~91% of optimal. LCLS at 97% of optimal ($884.9M).
- Facilities research continues for AI/ML; increases for accelerator R&D ($36.2M).

Construction/MIE* Δ = -$200.5M

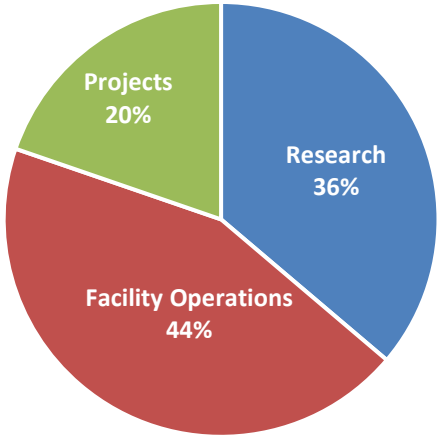
- APS-U ($150M); LCLS-II-HE ($16M); ALS-U ($13M); PPU ($8M); STS ($2M)
- MIEs: NSRC Recap ($1M); NEXT-II ($1M)
- New start: Cryomodule Repair & Maintenance Facility (CRMF) ($2M)

*includes OPC

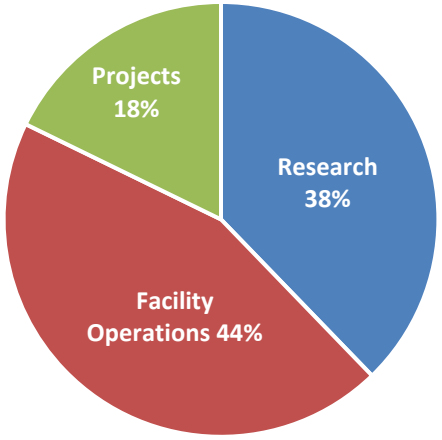
BES Budget by Budget Element: 2019 - 2021

	FY 2019 Enacted	FY 2020 Enacted	FY 2021 President's Request	FY 2021 House Mark	FY 2021 Senate Mark
Research	815,600	871,321	856,817	942,912	872,500
Facility Operations	922,000	947,179	884,856	944,088	956,000
Projects	427,400	393,500	193,000	354,000	385,500
Other	1,000	1,000	1,000	1,000	1,000
Total	2,166,000	2,213,000	1,935,673	2,242,000	2,215,000

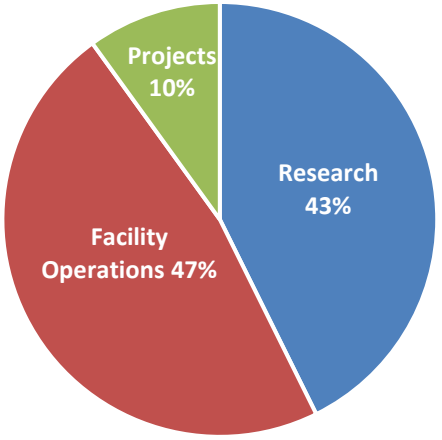
FY 2019



FY 2020



FY 2021 Request



FY 2021 Early Career Research Program FOA

FOA Scope:

- Support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by SC.
- All BES core research areas participate, including SUF (NSRCs, Accelerator/Detector Research, X-ray and Neutron Instrumentation and Technique Development)
- Technical scope developed annually, with topics alternating to maintain reasonable applicant pool, ease reviewer burden, and improve success statistics.

FOA Details:

- **Eligible Applicants**: Untenured university professors on tenure track and DOE Lab Scientists, both within 10 years of PhD; each applicant may apply a maximum of three times
- **Typical funding**: University: $150K/yr for 5 years; DOE Lab: $500K/yr for 5 years
- **Key Dates**: FOA Issued 10/20/20; Pre-applications received 11/20/20; Applications due 2/16/21

All active BES early career projects (FY 2016 – 2020)

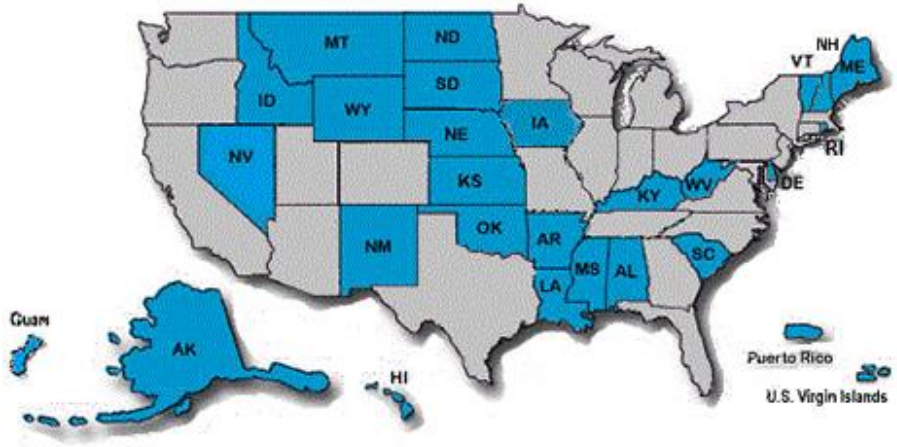
- 145 awards (113 University; 32 Lab)
- 48 female PIs (33%); 97 male PIs
- 34 States (12 EPSCoR)

https://science.osti.gov/-/media/grants/pdf/foas/2021/SC_FOA_0002421.pdf

FY 2021 EPSCoR Implementation Awards FOA

FOA Scope:

- Innovative mission relevant science and engineering enhancing capabilities of designated jurisdictions to conduct sustainable and nationally competitive energy-related research through increased human and technical resources, including training of scientists and engineers.
- BES published implementation grant FOA biennially; coordination across DOE



FOA Details:

- **Eligible Institutions**: Following NSF determinations (FY 2021 eligibility Table) within 28 jurisdictions (see map)
- **Estimated award size/duration**: Fully funded awards and renewals of existing awards. New awards $1.0-1.5M per year, renewal awards up to $2.5M per year; award duration of 2 years with a 6-year maximum period of support to promote competitive practice on part of applicants/awardees and their transition to DOE core program support.
- **Preproposals required:** Large team proposals, limited to 1/institution; option for 3-PM review
- **Key Dates**: FOA Issued 10/27/20; Pre-applications due 12/15/20; Applications due 3/2/21

https://science.osti.gov/-/media/grants/pdf/foas/2021/SC_FOA_0002431.pdf

FY 2021 Computational Chemical Science (CCS) FOA

FOA Scope:

- Small groups (2-3 PIs) and integrated multidisciplinary teams (including chemistry, applied mathematics and computer science) to develop validated, open-source codes for modeling and simulation of complex chemical processes and phenomena that allow full use of emerging exascale and future planned DOE leadership-class computers
- Topical areas cover a broad range of computational capabilities relevant to BES science, such as quantum mechanically-informed methods for describing molecular systems; methods for predicting field-driven control of molecular processes; approaches to include dissipative and (de)coherence mechanisms in molecular systems; and multi-scale methods for large molecular systems (e.g., photosynthesis)

FOA Details:

- **Eligible Institutions**: Universities/colleges, non-profit and for-profit organizations, DOE laboratories
- **Estimated total award size/duration**: $500-2,000K/yr for up to four years (new and renewal awards)
- **Estimated total funding**: $8M/yr (up to $32M for 4 years)
- **Pre-applications required:** limited to 2 per institution with a 3-PM review to identify encouraged applications
- **Key Dates**: FOA Issued 11/2/20; Pre-applications received 12/2/20; Applications due 2/8/21

FY 2021 Scientific Discovery through Advanced Computing FOA (SciDAC)

FOA Scope:

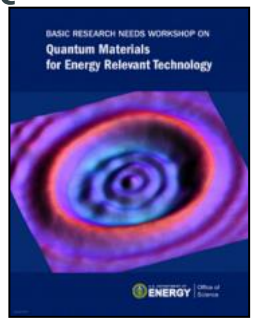
- Collaborations among domain scientists (funded by BES) and computer scientists and applied mathematicians (funded by ASCR) to accelerate scientific discovery in materials science, condensed matter physics, chemical sciences, geosciences, and energy-related biosciences through advanced HPC on ASCR facilities
- **Topical areas: (A)** 'Quantum Phenomena' of many-particle systems driven far-from-equilibrium, includes coherence, entanglement and novel states of matter; and **(B)** 'Predictive Control of Reaction Pathways' for chemical mechanisms in complex non-equilibrium and field-driven environments important in synthesis of materials and chemicals, and deconstruction of macromolecular structures such as plastics for polymer upcycling

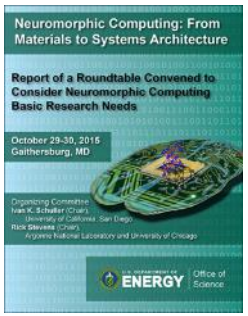
FOA Details:

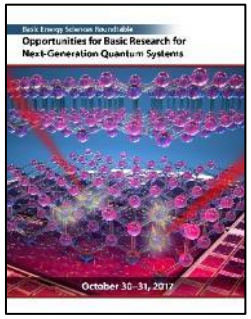
- **Eligible Institutions**: Universities/colleges, non-profit and for-profit organizations, DOE laboratories
- **Estimated total award size/duration**: $1-2M/yr for up to four years (re-competition, no renewals)
- **Estimated total funding**: $2M/yr from ASCR and $6M/yr from BES (up to $32M for 4 years)
- **Pre-applications required:** limited to 2 per institution with a 3-PM review to identify encouraged applications; Pre-applications must include partnerships/collaborations with the SciDAC Institutes
- **Key Dates**: FOA Issued 12/9/20; Pre-applications due 1/19/21; Applications due 4/6/21

Strategic Planning Workshops and Roundtables Provide Insights on Priority Research Areas

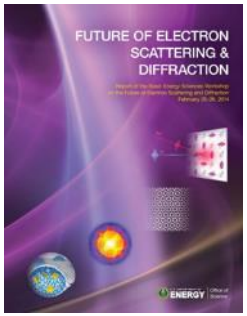
- Quantum Science

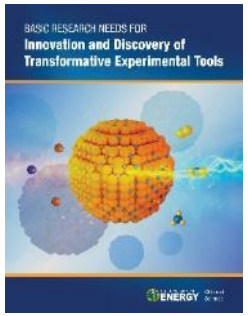




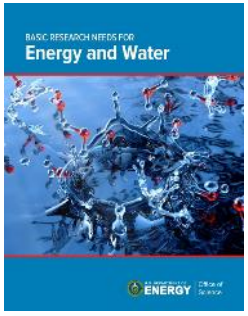


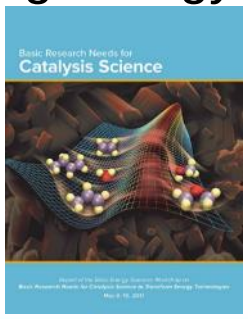
- Characterization

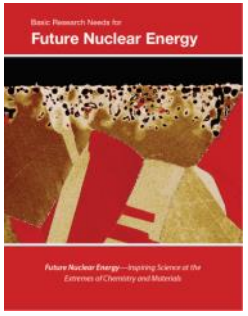


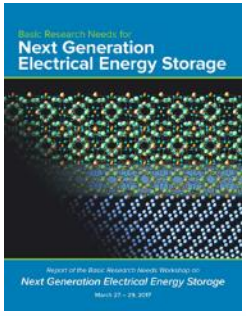


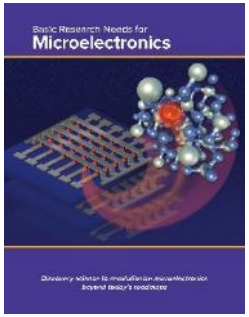
- Cross-Cutting Energy

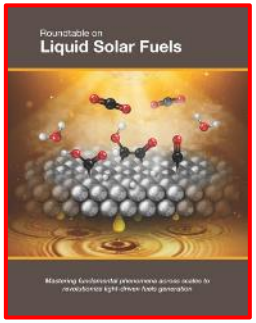




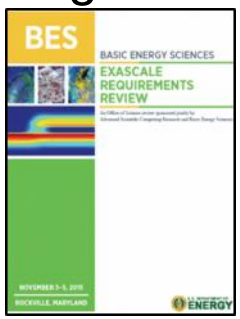


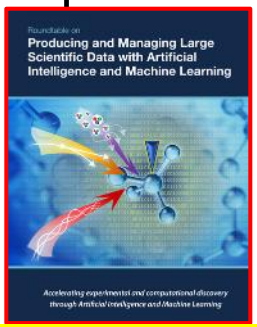






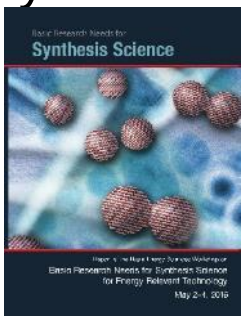
Theory, Modeling and Computation

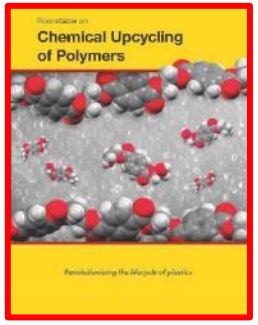


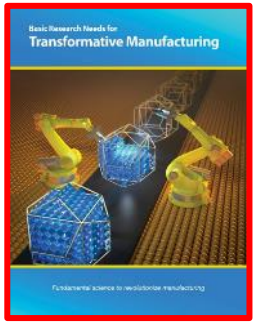


Posted in August 2020

Synthesis







Full report in review

BES Roundtable – Research Opportunities for Cryogenic Electron Microscopy in the Physical Sciences

Co-chairs: Amanda Petford-Long (ANL)
Benjamin Gilbert (LBNL)

Date: Spring 2021

Format: Virtual

Draft Charge:

- Articulate research opportunities, key science drivers, and research strategies for the BES physical sciences research portfolio in the area of cryo-EM
- Assess the current status of BES electron microscopy science at cryogenic temperatures and define a path for optimal utilization of these capabilities for physical sciences research in the 2-10 year timeframe and beyond
- Identify gaps between the current BES research portfolio and potential science that could be performed with current capabilities and instruments, as well as emerging opportunities for impactful science with these tools

Recent and future workshops sponsored by the Council on Chemical Sciences, Geosciences, and Biosciences

At the tipping point: a future of fused chemical and data science (September 2020)

- Workshop chairs – Aurora Clark (Washington State), David Kramer (Michigan State), Junko Yano (LBNL)
- Purpose – identify the current state of the art and opportunities for the seamless integration of Data Science, Chemistry and Biochemistry to fundamentally change the research lifecycle; included panels on hypothesis driven data science; integrated experimental design strategies; and understanding the topology of chemical data to shape fundamental chemical science

Synergy between chemical separations and reactions (January 2021)

- Workshop chairs – Joan Brennecke (UT Austin), Vanda Glezakou (PNNL), and Susannah Scott (UC Santa Barbara)
- Purpose – provide a critical analysis of the state of the art, insights into scientific challenges hindering progress, and an assessment of future scientific directions for integrating separations and reactions in ways that will be transformative in advancing energy science and technology

Impact of BESAC

Subcommittee charges / reports

- Neutron subcommittee study final report "The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility" posted in September
- CD-0 (mission need) for the HFIR-PVR project is a direct consequence
- International benchmarking study to be discussed at length today

HFIR-PVR CD-0 Mission Need Statement:

- Replacement vessel fabricated using improved materials that are less susceptible to radiation embrittlement, such as stainless steel, and allow HFIR to return to 100 MW operations.
- New pressure vessel with design enhancements to enable future upgrades for neutron-based research, isotopes program, and operational flexibilities.

The HFIR pressure vessel built by the former Allis-Chalmers Manufacturing Company was installed in April 1964 and has continued to operate reliably for more than 55 years.

Impact of BESAC

COV reports

- Major recommendation from the 2018 MSE Division report: "Consider implementing the flexibility to hold COVs less frequently than every 3 years"
- The recent CSGB and EFRC/Hub COVs represent BESAC Chair-approved lengthened intervals between COVs

○ CSGB COVs – 3.5 years:	September 2020	March 2017
○ EFRC/Hub COVs – 4 years:	October 2020	November 2016
○ SUF COVs – 3 years:	April 2019	April 2016
○ MSE COVs – 3 years:	April 2018	March 2015

- CSGB Division and EFRCs/Hubs reports will be presented/discussed today, providing an opportunity to consider implementing the 2018 recommendation for less frequent COVs (increase from 3 to 4 years?) going forward

Questions