U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Update

Basic Energy Sciences Advisory Committee Meeting

August 24, 2021

Linda Horton, Bruce Garrett, and Andy Schwartz

Office of Basic Energy Sciences

Exciting Times Continue

- Organization Changes and Progress…
- FY 2020 statistics summary
- FY 2021 funding, FY 2021 Facilities Highlights and Projects Update
- FY 2021 FOA Updates plus cross SC coordination (Andy Schwartz)
- FY 2021 FOA Updates plus cross DOE coordination and related strategic planning workshops/RTs (Bruce Garrett)
- FY 2022 Funding Request (Linda Horton)

DEPARTMENT OF ENERGY

Boards and Councils

Secretary

Deputy Secretary

Jennifer Granholm

David Turk

nergy Regulatory
ission (FERC)

or General (IG)

nbudsman

Under Secretary for Nuclear Security and Administer, NNSA

- Deputy Administrator for Defense Programs (NA-10)
- Deputy Administrator for Defense Nuclear Nonproliferation (NA-20)
- Deputy Administrator for Naval Reactors (NA-30)
- Associate Administrator for Emergency Operations (NA-40)
- Associate Administrator for Safety, Infrastructure & Operations (NA-50)
- Chief & Associate Administrator for Defense Nuclear Security (NA-70)
- Associate Administrator for Counter-Terrorism & Counter-Proliferation (NA-80)
- Associate Administrator for External Affairs (NA-EA)
- Associate Administrator for Management & Budget (NA-MB)
- Associate Administrator for Acquisition & Project Management (NA-APM)
- Office of General Counsel (NA-GC)
- Associate Administrator for Information Management & Chief Information Officer (NA-IM)

Under Secretary for Science and Energy (S-4) Nominee: Geri Richmond

- Assistant Secretary for Cybersecurity, Energy Security & Emergency Response (CR)
- Office Artificial Intelligence and Technology (AI)
- Arctic Energy Office (AE)
- **Nominee SC-1: Asmeret Berhe**
- National Laboratory Operations Board
- Transitions (OTT)
- Assistant Secretary for Nuclear Energy (NE)
- Assistant Secretary for Energy Efficiency & Renewable Energy (EERE)
- Assistant Secretary for Fossil Energy (FE)
- Loan Programs Office (LPO)
- Indian Energy Policy & Programs (IE)
- Assistant Secretary for Electricity (OE)
  - Bonneville Power Administration (BPA)
  - Southwestern Power Administration (SWPA)
  - Southeastern Power Administration (SEPA)
  - Western Area Power Administration (WAPA)

Under Secretary (S-3)

- Associate Under Secretary for Environment, Health, Safety and Security (AU)
- Office of Project Management Oversight and Assessments (PM)

for
ion

anced Research Projects
ency – Energy (ARPA-E)

- Assistant Secretary for International Affairs (IA)
- Assistant Secretary for Congressional & Intergovernmental Affairs (CI)
- Office of Enterprise Assessments (EA)
- Office of Public Affairs (PA)
- Office of General Counsel (GC)
- Office of the Chief Financial Officer (CF)
- Office of the Chief Human Capital Officer (HC)
- Office of the Chief Information Officer (IM)
- Office of Management (MA)
- Office of Small & Disadvantaged Business Utilization (OSDBU)
- Office of Intelligence and Counterintelligence (IN)
- Office of Economic Impact & Diversity (ED)
- Office of Legacy Management (LM)
- Office of Hearings & Appeals (HG)
- Assistant Secretary for Environmental Management (EM)
- Office of Strategic Planning and Policy (OSPP)

Updated 1/20/2021

Office of Basic Energy Sciences

Associate Director
Linda Horton

BES Budget and Planning
- Kara Beles, Financial Management
- Donetta Herbert, Financial Management
- (Vacant, Senior Technical Advisor)
- Thomas Russell, Senior Technical Advisor

BES Operations
- Teresa Crockett, Program Analyst
- Robin Hayes, Program Manager
- Kerry Hochberger, Program Analyst / BESAC*
- (Vacant, Program Support Specialist)
- 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

Materials Discovery, Design, and Synthesis
Mike Markowitz
- Materials Chemistry: Craig Henderson, Michael Sennett
- Biomolecular Materials: Mike Markowitz, (Vacant)
- Synthesis and Processing Science: Tim Fitzsimmons, (Vacant)
- Batteries and Energy Storage Hub; Technology Coordination: Craig Henderson, John Vetrano

Condensed Matter and Materials Physics
Michael Pechan, Acting
- Experimental Condensed Matter Physics: Michael Pechan, (Vacant)
- 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

Rocio Meneses, Program Support Specialist

Operations
- X-ray and Neutron Scattering Facilities: Eliane Lessner, (Vacant), 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/ Advanced Light Source Upgrade: Ed Stevens, (Vacant)
- Advanced Photon Source/ SNS Proton Power Upgrade: ★ Hannibal Joma, (Vacant)
- Facilities Upgrades and MIE*** Projects: Ed Stevens, ★ Hannibal Joma, (Vacant)

*** Major Items of Equipment

Chemical Sciences, Geosciences, and Biosciences Division
Bruce Garrett, Director

Brandon Rohnke, AAAS Fellow

Fundamental Interactions
Gregory Fiechtner, Acting
- Atomic, Molecular, and Optical Sciences: Tom Settersten, ■ Paul Parazzoli
- 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: Gail McLean, (Vacant)
- Fuels from Sunlight Energy Innovation Hub: Christopher Fecko

Chemical Transformations
Raul Miranda
- Catalysis Science: Chris Bradley, Viviane Schwartz, ● Igor Slowing
- Separation Science: Daniel Matuszak, ■ Vanda Glezakou
- Heavy Element Chemistry: Philip Wilk
- Geosciences: James Rustad

LEGEND
- ■ (red) Detailee (50%) from PNNL
- ■ (blue) IPA from SNL
- ▲ Detailee (70%) from SLAC
- ● Detailee (80%) from Ames
- ★ Detailee (50%) from Berkeley Site Office

August 2021

Posted August 9, 2021

BES Staffing Transitions – Welcome to Kerry Hochberger and Kara Beles

- **Kerry Hochberger** – Management and Program Analyst responsible for BESAC and other BES crosscutting activities effective June 6, 2021. She most recently was a program support specialist in the BES Associate Director's office, including responsibilities for support of the Energy Frontier Research Centers and Early Career Research Program. Bachelor of Arts, James Madison University.

- **Kara Beles** – A Financial Management Specialist, joined BES on August 2, 2021 to co-anchor the BES budget office focusing on execution. She is an experienced budget analyst with over 10 years of service in the area of federal budgeting, with specific experience in budget formulation, justification, execution, and analysis of annual and multi-year budgets. She was most recently with the Office of Science Budget Office. Master of Business Administration and Bachelor of Arts in Management and International Economics from Hood College.

New IPA– Atomic Molecular and Optical Science Program

Paul Parazzoli

IPA, Atomic Molecular and Optical Science

Chemical Sciences, Biosciences, and Geosciences Division

Expertise

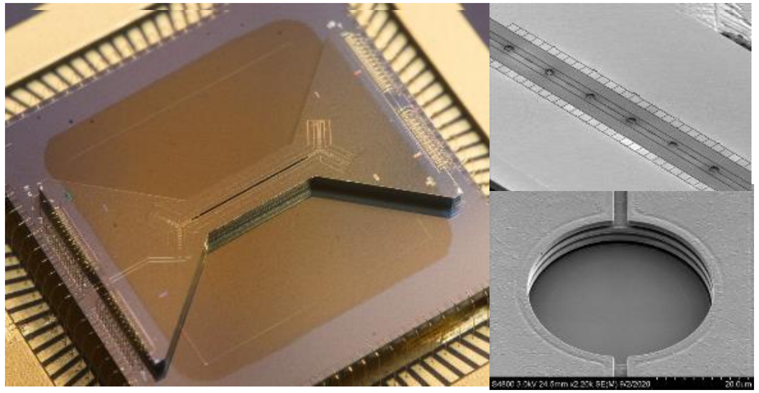
- Atomic physics and quantum information sciences
- Experimental quantum computing, atomic inertial sensing, and atomic clocks

Experience

- Principal Member of Technical Staff, Sandia National Laboratories
- Postdoctoral Fellow, Sandia National Laboratories
- Ph.D. in Physics, U Colorado

Paul joined BES in February 2021

Science highlight



Surface ion traps offer a scalable quantum computing platform with unparalleled fidelities. Recent advances include the integration of photonics for individual addressing and readout.

Sandia National Laboratory

New AAAS Fellow

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

Expertise
- Materials research including mechanics of polymer thin films, charge-containing polymers, membranes for filtration/fuel cells
- Polymer physics
- Development and use of novel characterization tools

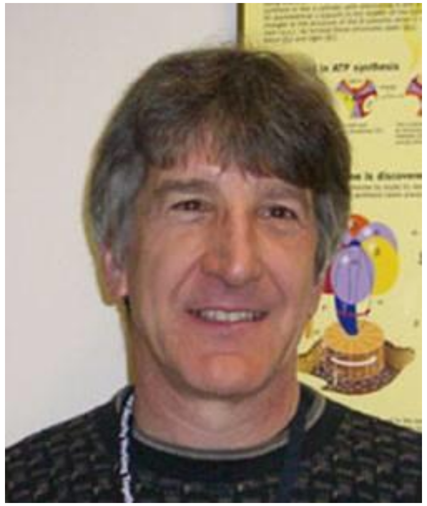
Joining BES in September 2021

Experience
- Northwestern University, Ph.D. in Materials Science and Engineering
- University of California San Diego, BS in NanoEngineering

U.S. DEPARTMENT OF ENERGY
Office of Science

AAAS
AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE

BES Staffing Transitions – Congratulations to Retirees!



- **Bob Stack**– Physical Biosciences program manager, retired from federal service (2009-2021). Before becoming a Federal Program Manager, Bob served as a detailee for the BES Biosciences programs. Prior to joining DOE, Bob worked at several San Francisco Bay Area biotechnology firms and, prior to his biotech career, at the USDA Agricultural Research Service in Illinois.

- **Jeff Krause** – Fundamental Interactions team lead, retired from federal service (2008-2021). Before becoming team lead, Jeff was the Atomic, Molecular, and Optical Sciences program manager. Prior to joining DOE, he was a detailee at NSF from his home institution, the University of Florida, where he was a member for the Chemistry Department faculty and contributor to the Quantum Theory Project.

Gail McLean (Photochemistry & Biochemistry team lead) and **Gregory Fiechtner** (Condensed Phase and Interfacial Molecular Science program manager) are filling these roles on an interim basis

BES Staffing Transitions – Congratulations to Retirees and Staff Launching New Life Adventures!

- **Jim Horwitz**– Team Lead for Condensed Matter and Materials Physics retired from federal service (1986-2021). Jim joined DOE in 2003 as the program manager for Experimental Condensed Matter Physics. Prior to coming to DOE, Jim was a staff member at the Naval Research Laboratory in the Surface and Modification Branch of the Materials Science Division.

- **Bonnie Gersten** – Synthesis and Processing Science program manager left federal service in August (2006-2021). Before joining DOE, Bonnie was an Assistant Professor at City University of New York - Queens College in the Chemistry and Biochemistry Department. Prior to Queens College, she served as a Materials Engineer at the US Army Research Laboratory.

Mick Pechan (Experimental Condensed Matter Physics program manager) and **Tim Fitzsimmons** (EPSCoR program manager) are filling these roles on an interim basis

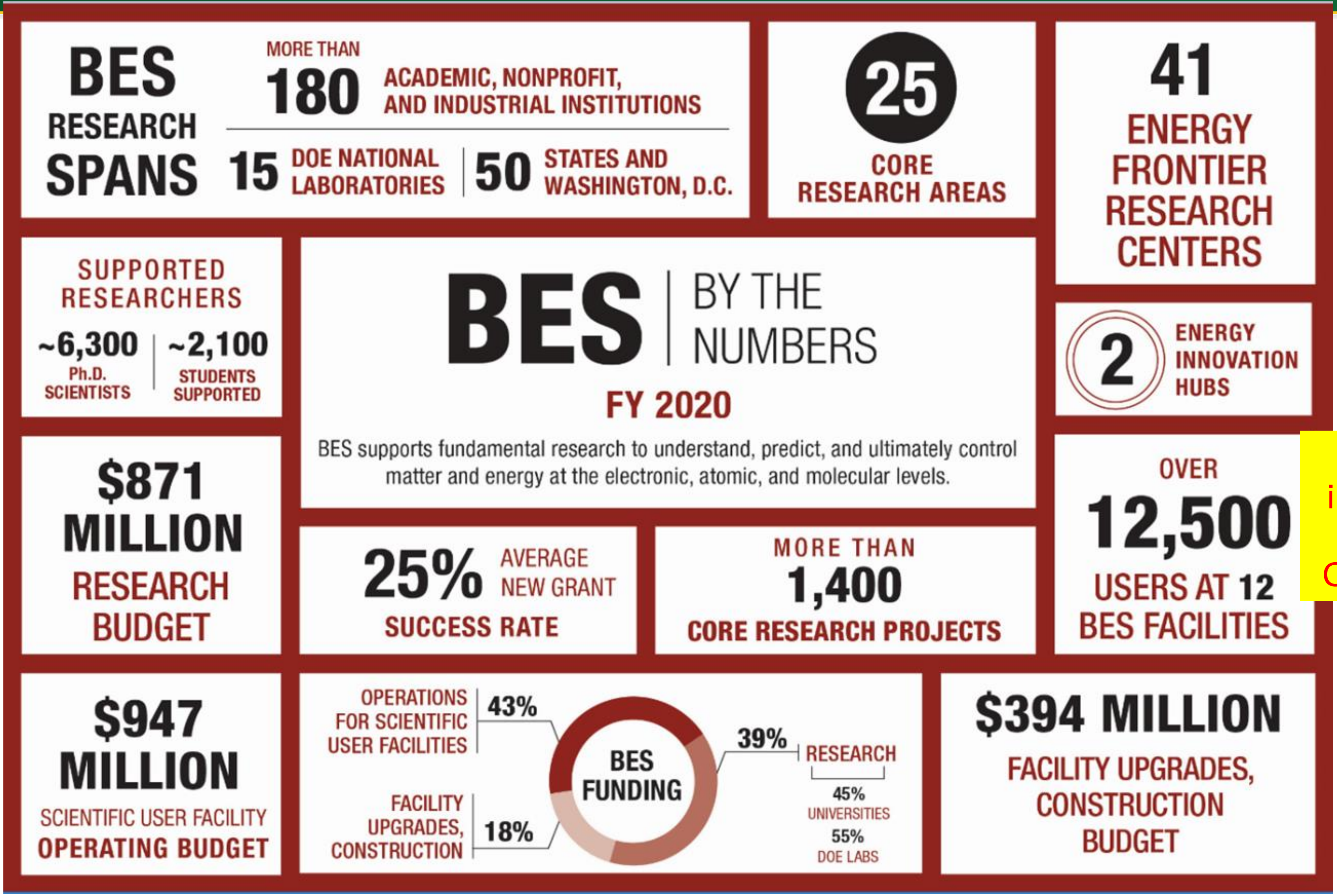
BES Staffing Transitions – Congratulations to Retirees!

- **Peter Lee** – X-ray program manager, retired from federal service (2010-2021). Before joining DOE, Peter worked at APS as beamline scientist and served as lead scientist for the Structural Science Program in the Argonne National Laboratory X-ray Science Division. Prior to ANL, he managed beamlines and was an instrument scientist at NSLS.

- **Phil Kraushaar** – Construction program manager, retired from federal service (2010-2021). Before joining DOE, Phil worked at four of DOE's national laboratories, which include Fermi National Accelerator Laboratory (thesis research), the Superconducting Super Collider Laboratory (Collider Machine Group and Accelerator String Test Facility), Oak Ridge National Laboratory (Spallation Neutron Source Project) and Argonne National Laboratory (Office of Project Management).

Thiyaga Thiyagarajan (Neutron scattering program manager) and **Hannibal Joma** (50% detail from DOE Bay Area Site Office) are filling these roles on an interim basis

Updates: Basic Energy Sciences At a Glance (2020)

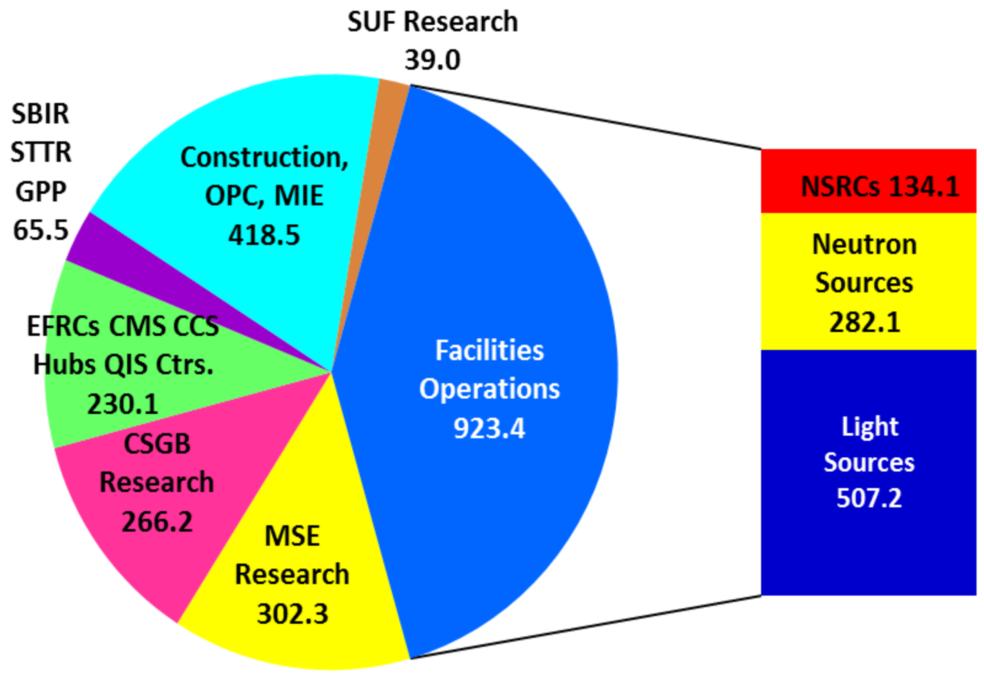


COVID impacts on User Community

FY 2021 Enacted Appropriation: $2,245M (+$32M or +1.4% above FY 2020)

Research programs Δ = +$30.8M

- Core Research ($607.5M) includes new investments ($73M) in critical materials, data/AI/ML, polymer upcycling, micro-electronics, next-generation biology, accelerator R&D, CO_2 Direct Air Capture
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($115M)
- Energy Innovation Hubs continue (~$44M)
- National QIS Research Centers (~$45M, +$18M)



Scientific user facilities Δ = -$23.8M

- Operations of 12 facilities continue at ~95% of optimal (~$923M)
- Facilities research continues for AI/ML; increases for accelerator R&D (~$39M)

Construction/MIE* Δ = +$25M

- APS-U ($160M); LCLS-II-HE ($54M); ALS-U ($62M); PPU ($55M); STS ($42M); CRMF ($2M)
- MIEs: NSRC Recap ($5M); NEXT-II ($5.5M)
- LCLS-II Rebaseline: $33M

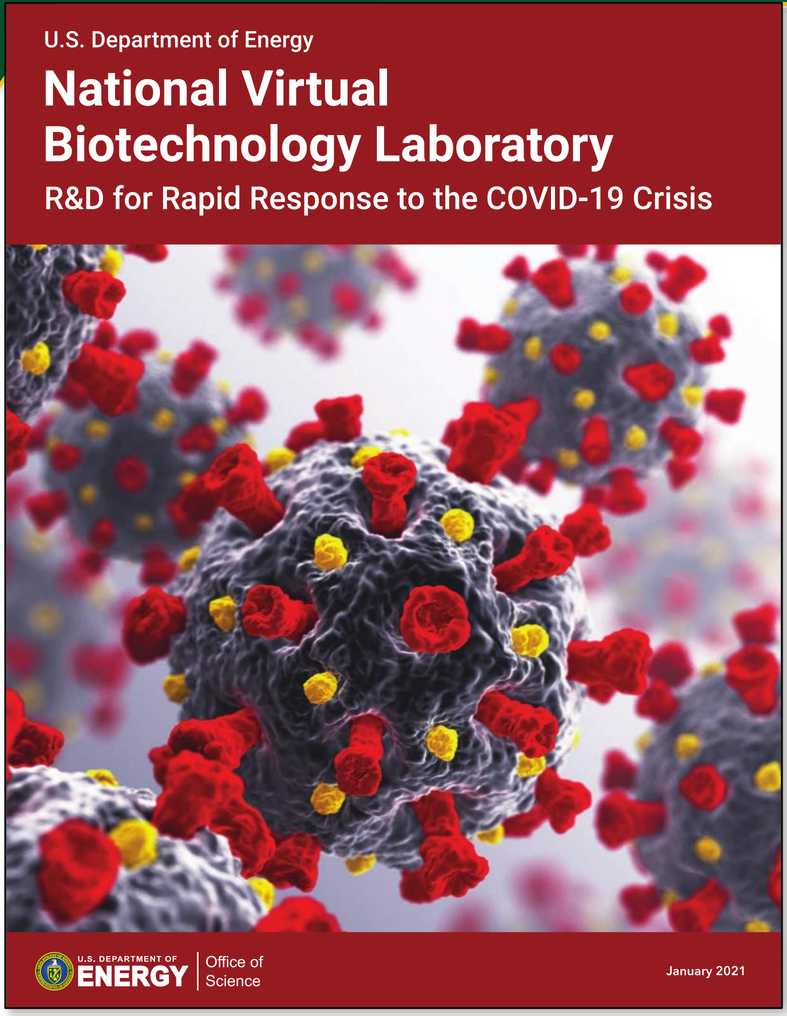
*includes OPC

FY 2021: Continued Remote Operations Accommodated User/Staff Science with COVID-19 Restrictions

- Funding supported BES user operations at ~95% optimal. All have continued curtailed user operations due to COVID-19 restrictions, mostly through remote access with limited on-site users.
  - APS, NSLS-II and SSRL have delivered better than 97% of their planned operating user hours.
  - ALS had a 3-month major shutdown in January-April for preparation activities for the ALS upgrade.
  - LCLS has operated with ~95% reliability since resuming user operation in August 2020. Delivered soft x-rays for RIXS instruments.
  - SNS has continued operating stably with ~86% reliability, and HFIR resumed operations for Cycle 490 on March 2, 2021 with 100% reliability.
  - NSRCs adopt virtual reality, telepresence and remote instrument access to maintain access for lab-based users.

- In recognition that remote operation is likely a "new normal" now and into the future – an Office of Science User Facilities Roundtable focused on Lessons from the COVID Era and Visions for the Future.

The DOE National Virtual Biotechnology Laboratory (NVBL) Provided Broad Capabilities for Addressing the COVID-19 Crisis

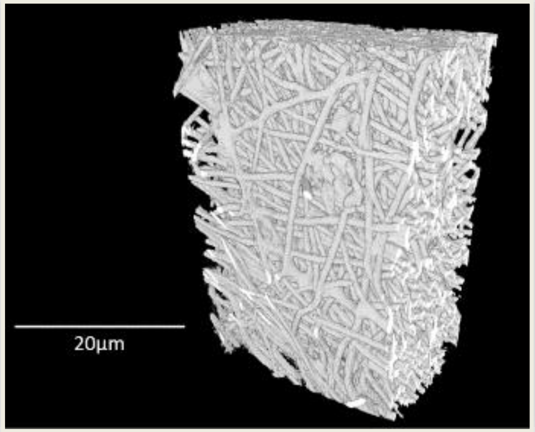


https://science.osti.gov/nvbl

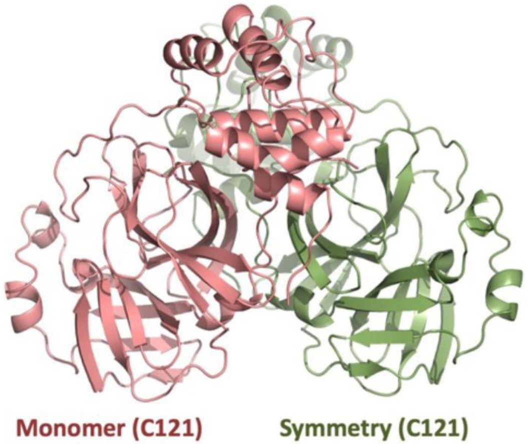
- Took advantage of user facilities, materials science, chemistry, and biological and environmental research expertise.
- Leveraged partnerships and R&D in manufacturing and transportation.
- Funded by CARES Act, activities included:
  - Addressing supply chain bottlenecks by harnessing advanced manufacturing
  - Medical therapeutics: computational drug discovery and structural biology
  - Innovations in testing capabilities
  - Understanding fate and transport of virus in the environment
  - Epidemiological modeling and logistical support

BES Light and Neutron Sources Have Been Instrumental in the Fight Against COVID-19

- User facilities rapidly shifted to remote access and mail-in in March 2020 to support critical research
  - Macromolecular crystallography to study atomic-scale interactions of viral proteins with drug candidates and human proteins
  - Solution state analysis of large and transient macromolecular assemblies
  - Observation of cellular infection
  - Characterization of respirator filter materials to aid manufacturing – complementary research at Nanoscale Science Research Centers
- Research at light sources underpinned development of several compounds granted Emergency Use Authorization; more are in clinical trials
  - Pfizer scientists used NSLS-II to research certain structural properties of their vaccine
  - Research at ALS and SSRL supported GlaxoSmithKline and Vir Biotechnology development of the antibody therapeutic sotrovimab
  - A decade of studies at APS and SSRL on spike proteins were key to the rapid development and effectiveness of all three vaccines in use in the United States
- NSLS-II and APS operated ~10% more hours in FY 2020 using CARES Act funding to support COVID-19 research
- More than 700 unique users from >125 groups (including most major Pharma companies) using ~55 different beamlines, determined >450 structures of SARS CoV-2 proteins with/without potential antivirals or antibodies (+ other research), leading to >80 peer-reviewed publications to-date
- Support for certain of these bioscience capabilities is a great example of BES' collaboration with BER and NIH



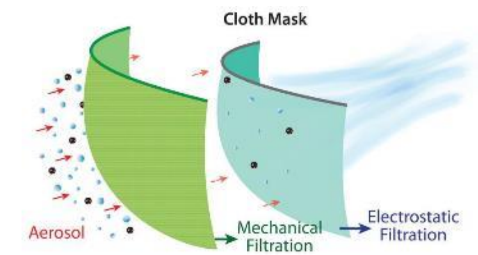
Nanotomography image of N95 electrospun filter media acquired at APS



SARS-CoV-2 main protease structure at near-physiological temperature to guide drug discovery, determined at LCLS using serial femtosecond crystallography (Durdagi, bioRxiv, https://doi.org/10.1101/2020.09.09.287987)

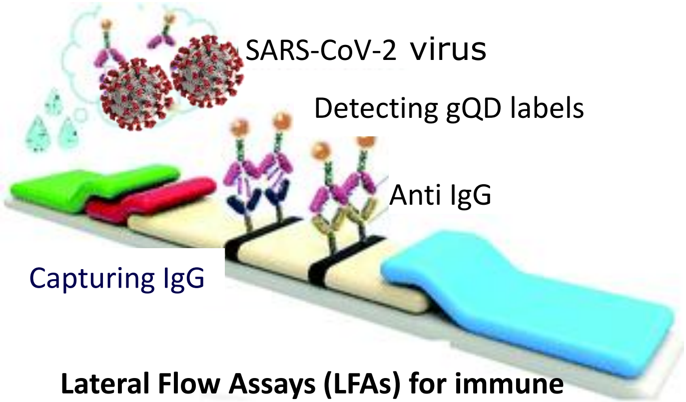
Nanoscale Science Research Centers Support COVID-19 Research

- The Nanoscale Science Research Centers supported research to understand the virus and develop novel detection methods (fast, nanotechnology-based portable diagnostics sensors), synthesize custom nanoparticles for vaccine encapsulation and delivery, improve effectiveness of personal protective equipment (masks, nanoparticle-based antiviral coatings) and develop epidemiological models to predict virus spread. A decade development of peptoid libraries at NSRCs used for new COVID therapeutics.

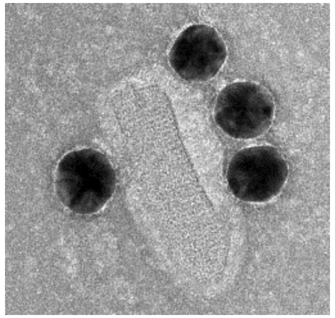


Mask fabrics combining mechanical and electrostatic filtration, such as a layer of high thread count cotton followed by a layer of silk, performed best. (CNM, Image courtesy of American Chemical Society)

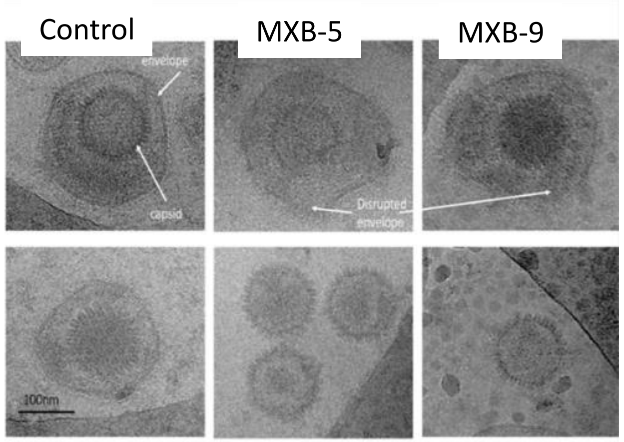
Characterization of exhaled breath. Hydrogel bed housed in a 3D printed "whistle" allows capture of cells, bacteria, fungi, and live virus from breath. Modeling and testing determined impact of surface topography, composition, and airflow on pathogen capture. (CNMS)



Lateral Flow Assays (LFAs) for immune response. Demonstration of a LFA platform for inexpensive yet high-sensitivity/high-reliability rapid diagnostics for COVID virus and antibodies. (CINT)



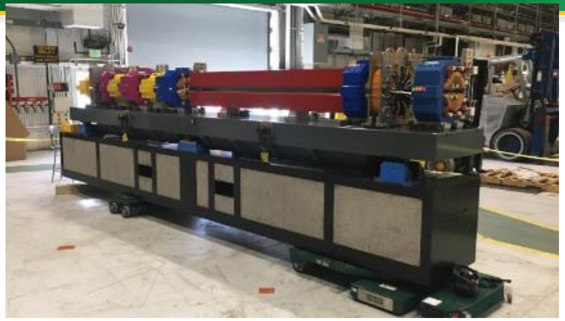
Virus tagging for optical detection. rVSV virus expressing SARS-CoV-2 spike is tagged with anti-spike antibody functionalized 50 nm Au nanoparticles for optical detection. (CFN)

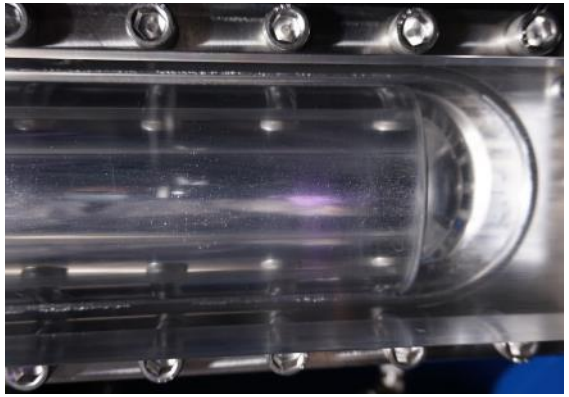


Cryo-EM imaging identified antimicrobial peptoids that can disrupt the viral envelope. Samples treated with peptoid libraries synthesized at the Molecular Foundry disrupted envelopes (top panels) compared to naked capsids (bottom).

BES - FY 2021 Highlights – Construction Projects

- ***Linac Coherent Light Source-II:*** Re-baseline (10/13/2020). New TPC $1,136M; Upgrade for high-repetition-rate(1 MHz), ultra-bright, transform-limited femtosecond x-ray pulses (0.25-5 keV). Installation of accelerator and x-ray systems and commissioning activities. Both soft and hard x-ray undulators operational. Completion (CD-4) projected for 2Q FY 2024.
- ***Advanced Photon Source Upgrade****:* CD-3 (7/25/2019). Continued procurement, testing of storage ring and experimental equipment, and long beamline building construction; COVID-related delays moved dark time for installation to ~3Q FY 2023. Completion (CD-4) projected for 2Q FY 2026.
- ***Proton Power Upgrade****:* CD-2/3 (10/6/2020). Construction to double the Spallation Neutron Source accelerator beam power to 2.8 MW. Completion (CD-4) projected for 4Q FY 2028.
- ***Advanced Light Source Upgrade****:* **CD-2 (4/2/2021).** Upgrade to multi-bend achromat lattice to reduce emittance and generate 1,000 times brighter soft x-rays with higher coherence. Long-lead procurements, design, and prototyping activities underway. CD-3 projected for 3Q FY 2022; CD-4 for 4Q FY 2029.





BES - FY 2021 Highlights – Construction Projects

- ***Linac Coherent Light Source-II – High Energy**:* CD-1 (9/21/2018), Long Lead Procurements 3A (5/12/2020). Increase the linac energy to 8 GeV at 1 MHz and deliver ~1,000-fold higher average brightness for hard x-rays (5-12 keV). New scope added to provide additional instruments and a low emittance superconducting electron gun (current TPC estimate is $660M). Baseline/Start of Construction (CD-2/3) projected for 4Q FY 2022; CD-4 projected 2Q FY 2030.
- ***Second Target Station**:* CD-1 (11/23/2020). Continued design, R&D, and engineering activities for a complementary pulsed source with an order of magnitude higher brightness cold neutrons at the Spallation Neutron Source. TPC range is $1,800M to $3,000M; Preliminary point estimate of $2,242M. Start of Construction (CD-2/3) projected for 2Q FY 2025. CD-4 projected 2Q FY 2037.
- ***Cryomodule Repair and Maintenance Facility**:* CD-0 (12/6/2019). Conceptual design and alternatives analysis for a facility to enable repair and maintenance of cryomodules and other accelerator components requiring clean environments and cryogenic capabilities. TPC range is $70M to $98M. Alternative section and cost range approval (CD-1) projected 1Q FY 2023.
- ***HFIR-Pressure Vessel Replacement***: Mission Need (CD-0) (Oct 2020). ORNL has begun internal assessments of replacement of the pressure vessel pending funding. Cost range estimate is $300M - 550M. (Direct outcome of BESAC assessment and report)
- *Major Items of Equipment:* **NEXT-II**: CD-1 (9/30/2020). Builds out 3 priority beamlines at the NSLS II. TPC range is $65M to $95M. **Start of construction (CD-2/3) projected for 1Q 2022**. **NSRC Recap**: – **CD-1/3A, Long Lead Procurements (4/15/2021)**. Provides 17 instruments to upgrade capabilities at the Nanoscale Science Research Centers. TPC range is $70M to $95M. CD-2/3 projected 2Q FY 2022.

FY 2021 Annual, Early Career, and EPSCoR FOAs

- **Continuation of Solicitation for the Office of Science Financial Assistance Program (annual "Open Call")** – The annual, broad, open solicitation that covers all research areas in the Office of Science and is open throughout the Fiscal Year; for BES, the solicitation includes brief descriptions of 22 core research areas, with current priorities and areas of interest and contact information for cognizant program managers – **OPEN for proposals!**

- **Early Career Research Program** – Support the research of outstanding scientists early in their careers, for five years at U.S. academic institutions and DOE national laboratories; an applicant must be an untenured, tenure-track assistant or associate professor at a U.S. academic institution or a full-time employee at a DOE national laboratory, who has received a Ph.D. within the past ten years (5-year awards) – **83 Awards Announced (34 in BES); FY 2022 FOA in preparation**
  https://science.osti.gov/-/media/early-career/pdf/ECRP2021-PI-list-v2.pdf

- **Established Program to Stimulate Competitive Research (DOE EPSCoR) FY 2021 Implementation Grants** – Implementation grants to help institutions in EPSCoR-eligible states to conduct research through support of groups working on a common science or technology theme, while building capabilities to enable these regions to compete more successfully for other federal funding; collaboration with DOE National Labs and leveraging of DOE Office of Science user facilities are encouraged. (Fully funded, 2-year awards) – **9 Awards Announced; FY 2022 FOA will focus on partnering with National Labs**
  https://science.osti.gov/-/media/bes/pdf/Funding/2021/EPSCoR_2021_awardees.pdf

SC Early Career Research Program

FOA Scope:

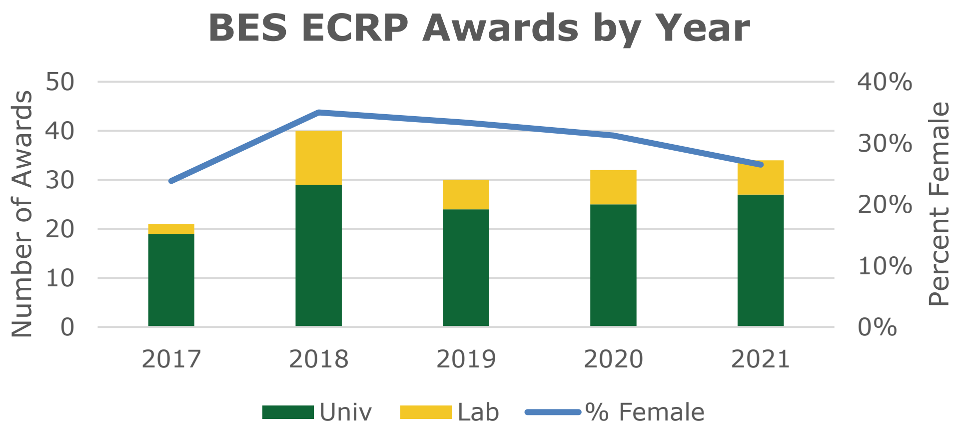
- Support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by SC.
- All BES core research areas participate, including SUF
- Topics alternate to maintain reasonable applicant pool, ease reviewer burden, 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; extension for major life events of at least 3 months
- **Typical funding**: University: $150K/yr for 5 years; DOE Lab: $500K/yr for 5 years
- **Timeline**: FY 2022 FOA in preparation for release in Fall 2021

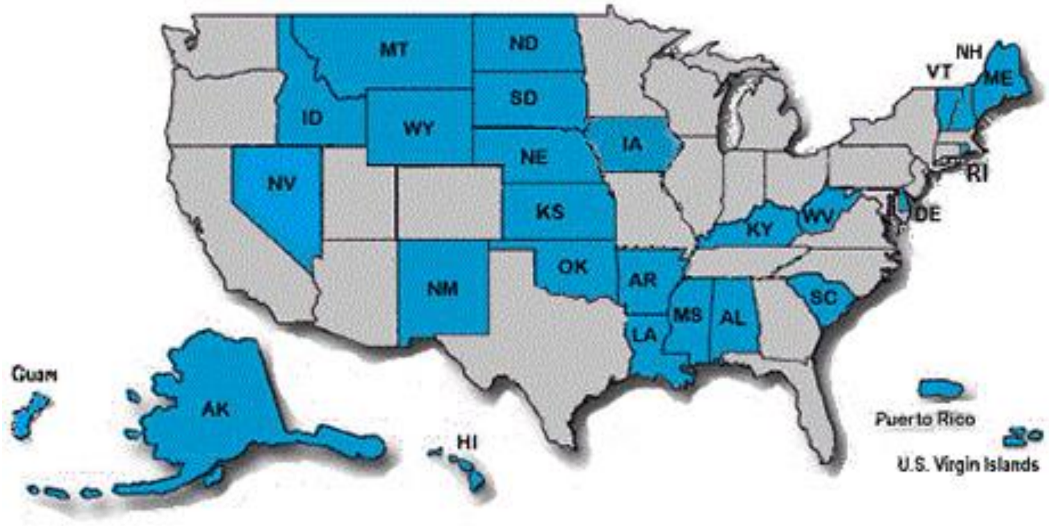
Active BES Awards (2017 – 2021)

- 37 states and 77 unique institutions
- 4 new institutions in 2021 (since program inception)
- 30 awards to EPSCoR institutions; 7 new in 2021
- 1 HBCU & 15 HSI awards; 1 HBCU & 4 HSI new in 2021



https://science.osti.gov/early-career

FY 2021 EPSCoR Implementation Awards



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 FOAs biennially; coordination across DOE
- FY 2022 FOA will focus on partnerships between EPSCoR institutions and DOE National Labs

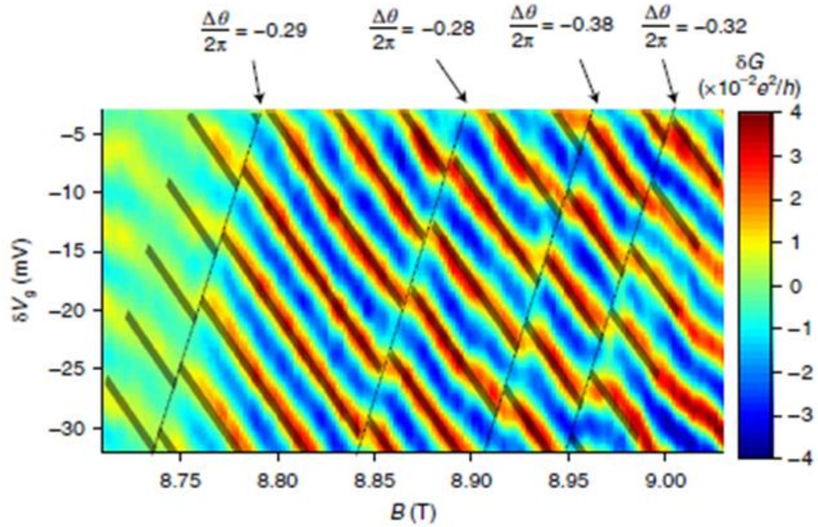
FOA Details:

- **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
- **9 Awards Announced**

FY 2021 SciDAC, QIS, and Microelectronics FOAs

- **Scientific Discovery through Advanced Computing (SciDAC) –** Collaborations among BES researchers and ASCR experts in computer science/applied math to understand quantum phenomena of many-particle systems and reaction pathways for chemical reactions and materials synthesis ($28M for 4 yrs) – **5 Awards Announced** https://science.osti.gov/-/media/bes/pdf/Funding/2021/2441_SciDAC_Awards_List.pdf
- **QIS Research –** Chemical and materials science research on quantum phenomena to aid in discovery/design of new quantum information systems; use of quantum computers or emulators to solve complex problems in chemistry and materials sciences ($73M for 3 yrs) – **29 Awards Announced** https://science.osti.gov/-/media/bes/pdf/Funding/2021/2449_BES_QIS_Awards_List.pdf
- **QIS Infrastructure –** QIS-related research instrumentation at NSRCs for synthesis, fabrication, metrology, and modeling/simulation to develop a flexible and enabling infrastructure for accelerated discoveries and innovations toward QIS technologies (NSRCs only; $30M for 3 yrs) – **8 Awards Announced** https://science.osti.gov/-/media/bes/pdf/Funding/2021/QIS-NSRC_Award_List.pdf
- **Microelectronics –** Multi-disciplinary, cross-SC 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 (National Labs only, multiple SC offices; ~$54M for 3 yrs) – Closed; award announcement expected soon.

Anyons Found – Best Evidence Yet for Long-Sought Particles



Map of the conductance (color scale) versus magnetic field (B) and gate voltage in a 2D electronic device. Each dashed line denotes a jump in the phase of the quantum-mechanical wave of the system, corresponding to a rotation of a fraction (1/3) of 2π. This fractional rotation is the smoking gun for the presence of exotic particle-like objects called anyons.

J. Nakamura, S. Liang, G. C. Gardner, and M. J. Manfra, *Nature Physics* **16**, 931 (2020).

Work was performed at Purdue University

Scientific Achievement

New experimental evidence of collective behavior of electrons to form "anyons,“ particle-like quantum objects first predicted theoretically in the 1970s

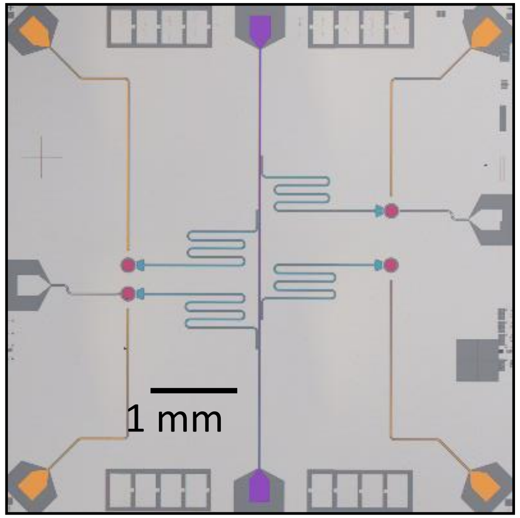
Significance and Impact

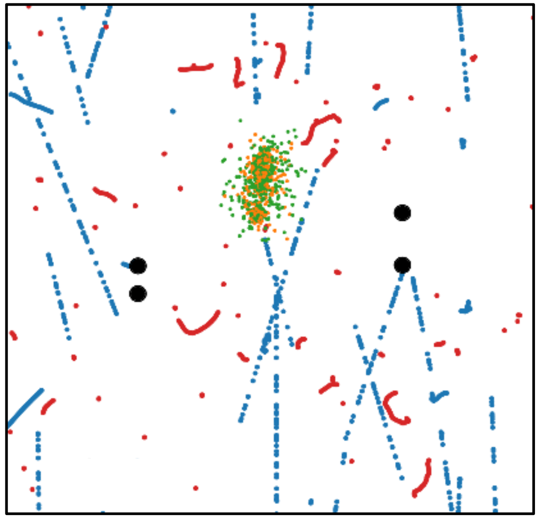
Many-anyon systems can build collective memories, which serve as the basis for topological quantum computing.

Research Details

- Interferometer made in a 2D electron gas.
- Sample at 10 mK, subject to a gate voltage and a strong magnetic field. Resulting quasiparticles flow only on the edge of the sample.
- The looping quasiparticles acquired a phase depending on the number of standing quasiparticles encircled.
- The interferometer currents interfere to yield phase sensitivity consistent with anyons.

Correlated Errors in Superconducting Qubits





LEFT: Superconducting multiqubit (red circles) chip used to probe correlated errors.
RIGHT: Simulated tracks from γ-ray (red) and cosmic-ray muon (blue) impacts in the qubit chip, with generated electrons (green) and holes (orange) shown for one muon track.

C.D. Wilen *et al., Nature* **594**, 369 (2021)

Work was performed in the Department of Physics at UW-Madison, with theory support from Fermilab, Lawrence Livermore National Lab, INFN Rome, and Google.

Scientific Achievement

Identified and characterized correlated phase and bit-flip errors due to radiation impacts in superconducting multiqubit chips.

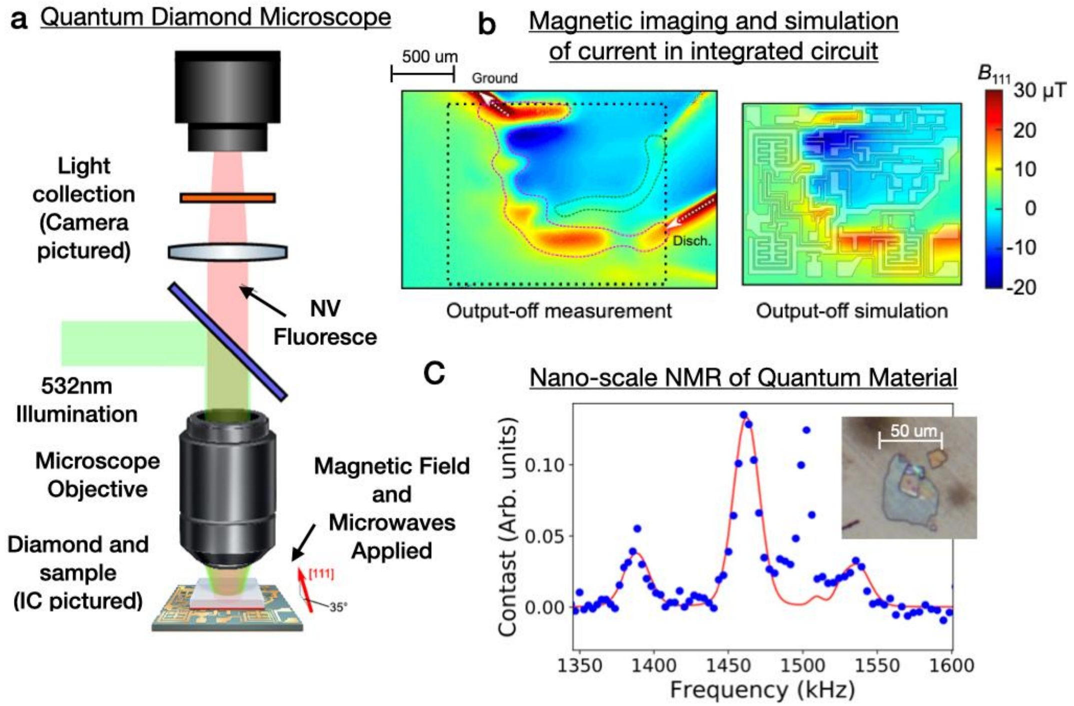
Significance and Impact

Correlated errors in multiqubit arrays are fatal for quantum error correction; a detailed understanding of the physics of these events points the direction to robust mitigation strategies for scalable quantum computing.

Research Details

- Cosmic ray muons and gamma rays impact multiqubit chips with combined rate of order 1/minute/cm^2.
- Impact events deposit roughly 100 keV of energy, liberating the order of 10^5 charge carriers that induce correlated dephasing errors across multiple qubits.
- Ultimately, energy is transferred to phonons in the substrate which propagate throughout the chip, inducing correlated relaxation errors.

Quantum Sensed Nuclear Magnetic Resonance (QSNMR)



(a) Cartoon of Quantum Diamond Microscope experimental implementation at CINT. (b) Widefield quantum-sensed magnetic fields from integrated circuit and complete modeling of device.[2] (c) NMR spectrum for ^{11}B in hBN as detected by nitrogen vacancy ensembles. (inset) 100nm thick hBN flake on nitrogen vacancy rich diamond. [3]

[1] P. Kehayias, A. M. Mounce, *et al.*, J. Applied. Phys. 127, 203904 (2020).
[2] P. Kehayias, A.M. Mounce et al Simulation and Measurement of the Magnetic Fields from a 555 Timer Integrated Circuit using a Quantum Diamond Microscope and Finite Element Analysis. In preparation (2021).
[3] J. Henshaw, A.M. Mounce et al. High Sensitivity Nanoscale Nuclear Quadrupolar Resonance of 11B in h-BN Through Optimized Nitrogen Vacancy Ensembles. In preparation (2021)

Scientific Achievement

The first example of solid-state nuclear magnetic resonance (NMR) using nitrogen vacancy (NV) ensembles was demonstrated. Quantum sensing (QS) using NV-rich diamonds was launched as the QSNMR Discovery Platform (a) for several quantum sensing applications.

Significance and Impact

The high sensitivity, high resolution imaging on large samples enables new measurements of magnetic states, current flow and strain in quantum electronic devices and materials. This work sets the stage for further quantum materials discovery at the nanoscale. Applications include device failure localization and counterfeit detection.

Research Details

- This NMR measurement is the first example of solid-state NMR using NV ensembles, which demonstrated significantly improved nanoscale NMR sensitivity for quantum materials discovery (a).
- The integrated circuit (IC) is the first complete widefield (micron-scale) example (b) of a quantum-based diagnostic used for device failure localization.
- QSNMR spectroscopy (c) of ^{11}B in h-BN exfoliated 2D flakes on diamond was demonstrated with very high sensitivity and resolution of the NQR frequency.
- CINT's new QSNMR capability has created high demand for access by users.

National QIS Research Centers

Q-NEXT • Next Generation Quantum Science and Engineering
(David Awschalom, ANL)

C^{2}QA • Co-design Center for Quantum Advantage
(Andrew Houck, BNL)

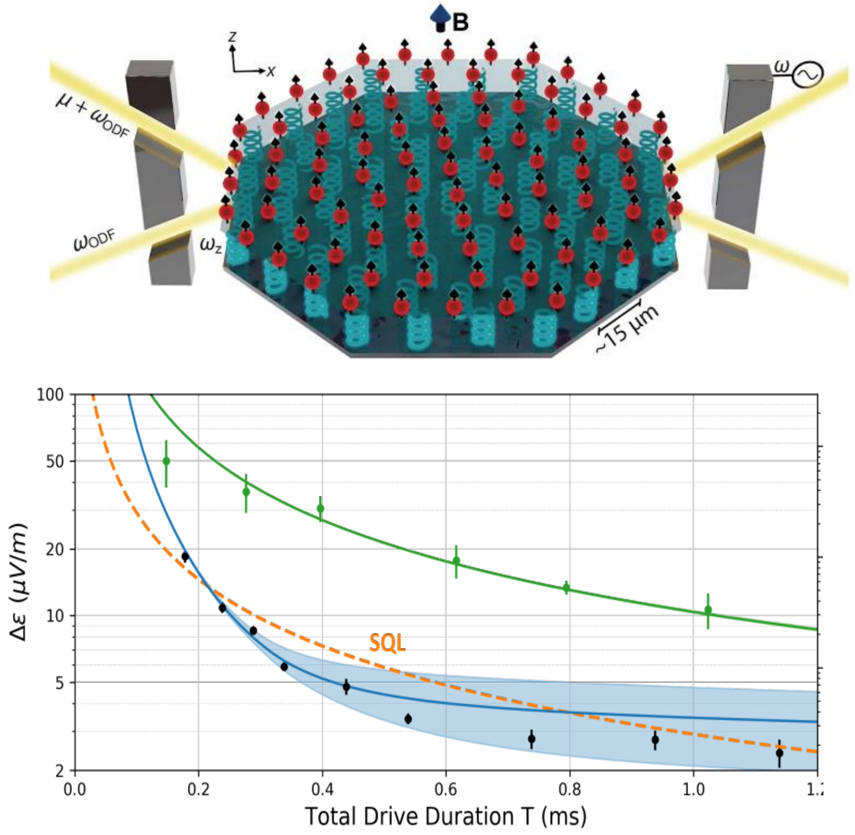
SQMS • Superconducting Quantum Materials and Systems Center
(Anna Grassellino, FNAL)

QSA • Quantum System Accelerator
(Irfan Siddiqi, LBNL)

QSC • The Quantum Science Center
(David Dean, ORNL)

https://science.osti.gov/Initiatives/QIS/QIS-Centers

Quantum-enhanced sensing of displacements and electric fields with two-dimensional trapped-ion crystals



A) Beryllium ions (red dots) confined within a Penning trap. The valence electron spin (black arrows) of the ions realizes a collective spin that serves as the measurement device.
B) Electric field sensitivity Δϵ as a function of the drive duration T. Experimental data from both classical (green) and quantum (black) protocols. Theoretical models of both protocols (green and blue solid lines). As reference, we show the SQL (orange). The quantum protocol attains an electric field sensitivity of 240±10 nV $m^{-1}/\sqrt{Hz}$.

Accomplishment

Realization of a sensor that uses quantum entanglement to achieve sensitivities that exceed the standard quantum limit (SQL).

Significance and Impact

This demonstration of quantum advantage for displacement and electric field sensing enables the measurement of previously undetectable signals.

Details

- The team achieved sensitivity of 8.8 ± 0.4 decibels below the SQL for displacements and 240 ± 10 nanovolts per meter in a second for electric fields using a crystal of ~150 trapped ions.
- This sensitivity was achieved by entangling the center-of-mass vibrational mode with the crystal collective spin, mapping the displacement into a spin rotation while avoiding quantum back-action and thermal noise.
- Potential applications include dark matter searches.

K.A. Gilmore, et. al. *Science* 06 Aug 2021: Vol. 373, Issue 6555, p. 673.
Work performed at University of Colorado / JILA and partner institutions.

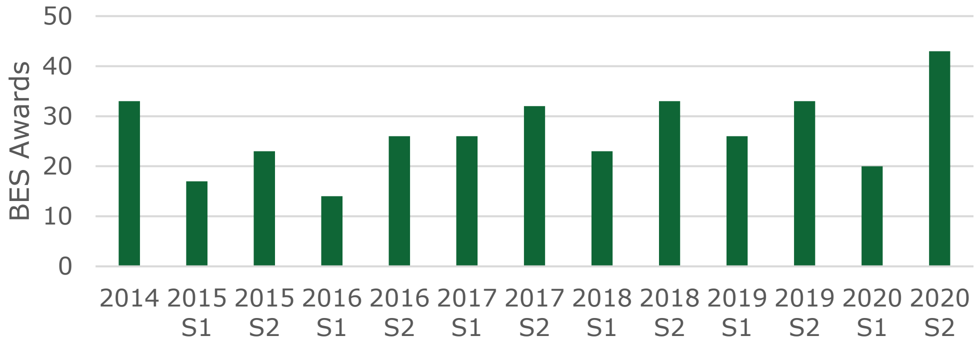
University of Colorado Boulder

QUANTUM SYSTEMS ACCELERATOR
Catalyzing the Quantum Ecosystem

DOE Office of Science Graduate Student Research (SCGSR) Program

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

- **Research** must be aligned with a SCGSR priority research area.
- **Current topics in BES**: Advanced Manufacturing; Clean Energy and Decarbonization; Data Science; Electrochemistry; Gas Phase Chemical Physics; Geosciences; Microelectronics; QIS; Radiation Effects and Radioactive f-elements; Accelerator and Detector R&D; Electron and Scanning Probe Microscopy Instruments R&D; Neutron and X-ray Facilities Instruments R&D; Convergence (Accelerators; Data Science; Microelectronics)
- **Award Benefits:** (1) A monthly stipend of up to $3,000/month for general living expenses; (2) Reimbursement of inbound/outbound traveling expenses to/from the host DOE laboratory/facility of up to $2,000.
- **Two solicitations per year. 2021 Solicitation 2 – Application Due November 10, 2021, 5:00 PM ET**



- 349 BES awards since 2014
- 116 unique graduate institutions
- 15 unique host DOE laboratories
- 272 unique DOE laboratory mentors

Cross SC Coordination Activities

- **Quantum Information Science**
  - SC Coordination Committee and Working Groups
  - Joint funding of National QIS Research Centers
  - Active engagement with interagency groups
- **Microelectronics**
  - SC Basic Research Needs Workshop (ASCR, BES, HEP)
  - FY 2021 National Lab Funding Announcement (ASCR, BES, FES, HEP, NP)
  - Coordination across DOE and with interagency groups
- **Early Career Research Program**
  - Annual FOA coordinated across all SC programs
- **SC Graduate Student Research Program**
  - Convergence topics designed to encourage research across SC programs
- **Scientific Discovery through Advanced Computing (SciDAC)**
  - Partnership with ASCR to support collaborations between BES domain scientists and ASCR experts in computer science/applied math

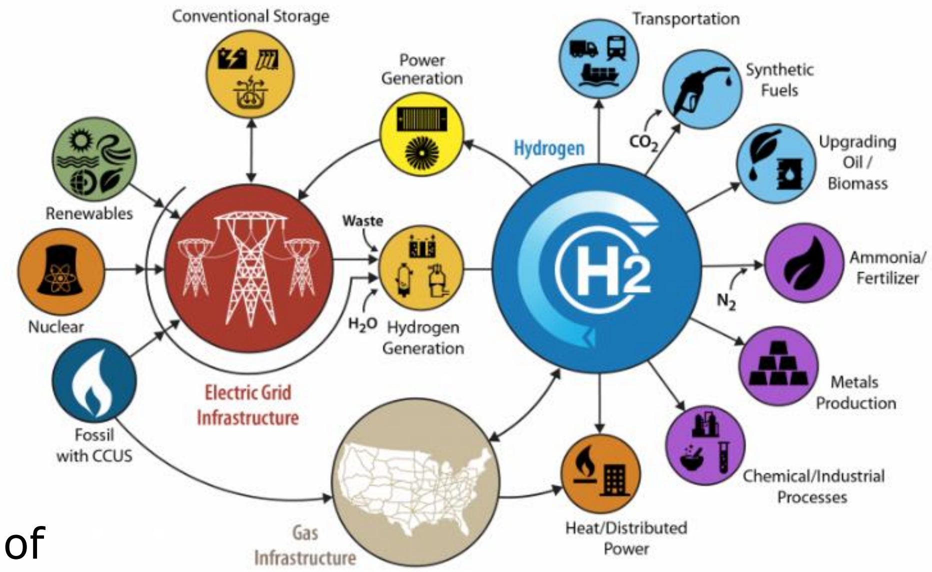
Small Business Innovation Research (SBIR) and Technology Transfer (STTR)

- By Congressional statute, SBIR/STTR is supported by 3.65% of the BES research budget line – SBIR 3.20%, STTR 0.45%
- **Phase I awards:** Maximum $200K for 1 year; **Phase II awards:** Maximum $1.1M for 2 years
- **FY 2021 awards:** Phase I – 72 SBIR, 12 STTR; Phase II – 35 SBIR, 6 STTR; **Total funding – $64M**
- **FY 2022 Phase I Release 1 FOA:** **Required Letters of Intent due August 30, 2021;** **Applications due October 12, 2021**
  - **Topics:** https://science.osti.gov/-/media/sbir/pdf/TechnicalTopics/FY22-Phase-I-Release-1-TopicsV407232021.pdf, **Solicitation:** https://science.osti.gov/-/media/grants/pdf/foas/2022/DE-FOA-0002554.pdf
  - **Accelerator and Detector Research topics:** (1) Manufacturing of ultra-high quality x-ray mirrors, (2) Strain-free processing and mounting of ultra-thin diamond crystals for applications at next generation X-ray sources, (3) Novel manufacturing capabilities for high resolution X-ray gratings, (4) Hollow-core fiber based ultrafast high-power laser beam delivery system, (5) Superconducting undulator with high heat-load limit, (6) Visible wavelength-tunable photocathode drive laser
  - **Nanoscale Science Research Centers topics:** (1) Ultra-high resolution electron monochromator for applications in TEM, STEM, and LEEM; (2) Theoretical tools to accelerate discovery and improve control of multi-modal autonomous correlative nanoscale measurements; (3) FAIR data management software tools for user facilities; (4) Low cost, solution processible perovskite materials for high performance X-ray imaging
  - **Instrumentation and tools for materials research using neutron scattering**
  - **Membranes for electrochemical energy storage applications**
  - **Design of color centers for spin qubit devices**
  - **Capabilities for sharing, mining and extracting knowledge from chemical and geochemical data (managed by ASCR)**
  - **Technology Offices topics funded by BES:** High performance materials for nuclear application (NE), Advanced subsurface energy technologies (EERE/FECM), Advanced fossil energy technology research (FECM), Rare earth elements (FECM)
  - **Technology transfer opportunity funded by BES:** Split laser sensor for harsh environment sensing applications (NETL)
- **FY 2022 Phase II Release 1 FOA:** **Will be issued October 18, 2021**

Coordination across DOE – Science & Energy Tech Teams (SETT)

Hydrogen SETT

- Cross-DOE activity
  - Led by Energy Efficiency and Renewal Energy's Hydrogen and Fuel Cells Technology Office (EERE-HFTO)
  - Co-leads: SC-BES and Fossil Energy and Carbon Management (FECM)
  - Participants: Nuclear Energy (NE), Advanced Research Project Agency – Energy (ARPA-E)
- Advances DOE's Hydrogen@Scale Initiative and clean energy priorities
  https://www.energy.gov/eere/fuelcells/h2scale
- Launched Hydrogen Energy Earthshot June 7
  Goal: $1 per 1 kg in 1 decade (1-1-1)
  https://www.energy.gov/eere/fuelcells/hydrogen-shot
- Roundtable on Foundational Science for Carbon-Neutral Hydrogen Technologies (August 2-5)
- Hydrogen Shot Summit (August 31–September 1)
  https://www.energy.gov/eere/fuelcells/hydrogen-shot-summit
  - BES participating in organizing Advanced Pathways Panel:
    - Topics include advanced approaches for electrolysis, conversion of fossil, biomass, and waste-streams, photoelectrochemical processes, and solar/thermochemical processes



BES Roundtable – Foundational Science for Carbon-Neutral Hydrogen Technologies

Co-chairs: Morris Bullock (PNNL)
Karren More (ORNL)
Date: August 2-5, 2021
Format: Virtual


Led by BES in partnership with DOE Offices of Energy Efficiency and Renewal Energy, Fossil Energy and Carbon Management, and Nuclear Energy

Priority Research Opportunities for Basic Energy Sciences

Discover and Control Materials and Chemical Processes to Revolutionize Electrolysis Systems

- How do we co-design multiple components that work together to enable stable, efficient electrolysis for the carbon-free production of hydrogen from water?

Manipulate Hydrogen Interactions to Harness the Full Potential of Hydrogen as an Energy Carrier

- How do we acquire fundamental insights across the entire range of energies to allow selective tuning of hydrogen interactions with molecules and materials?

Elucidate the Structure, Evolution, and Chemistry of Complex Interfaces for Energy and Atom Efficiency

- How can co-existing and evolving interfaces be tailored at multiple length scales to achieve energy-efficient, selective processes and enable carbon-neutral hydrogen technologies?

Understand and Limit Degradation Processes to Enhance the Durability of Hydrogen Systems

- How do we identify and understand the complex mechanisms of degradation to obtain foundational knowledge that enables the predictive design of robust hydrogen systems?

Fuels from Sunlight Hub Program (2010 – today)

Energy Innovation Hubs

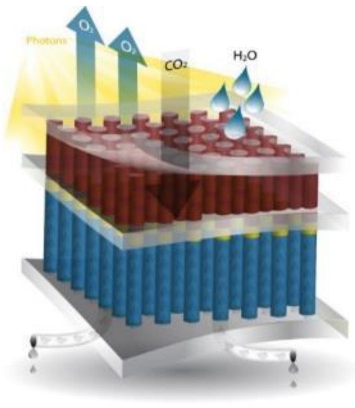
- Multi-investigator, multi-disciplinary integrated centers that focus on overcoming the scientific barriers to development of a complete energy system that has potential for implementation into a transformative energy technology.
- The objective of the Fuels from Sunlight Hub program is to develop an effective solar energy to chemical fuel conversion system. The system should operate at an overall efficiency and produce fuel of sufficient energy content to enable transition from bench-top discovery to proof-of-concept prototyping.

FY 2010-2020 award: Joint Center for Artificial Photosynthesis (JCAP)

- Goal: Discovery of robust, earth-abundant light absorbers, catalysts, membranes, and scale-up science required to for an integrated system to produce fuels from sunlight
- Launched in September 2010 (~$25 M/year for 5 years)
- Renewal in September 2015 ($15 M/year for up to 5 years; No Cost Extension to September 2021)
- Led by Caltech with LBNL as primary partner; additional partners were SLAC, UC San Diego and UC Irvine

FY 2020 Recompetition: 2 Awards Led by Caltech and U. North Carolina

- Goal**:** Build the scientific foundation for a scalable technology that converts carbon dioxide into renewable transportation fuels with only solar added energy
- Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) – led by U North Carolina
- Liquid Sunlight Alliance (LiSA) – led by Caltech



Photoelectrochemical Solar-Fuel Generator

Tuning Catalytic Bias of Hydrogenases for Hydrogen Production or Oxidation

Scientific Achievement

Developed a mechanistic understanding of catalytic bias – nature's ability to tune enzymes that can perform redox reactions in either direction. Discovered that different protein secondary interactions around the same active site in [FeFe]-hydrogenases tunes the relative stabilization/destabilization of the active site's oxidation states, which accounts for rates for either hydrogen oxidation or production that span a remarkable 6 orders of magnitude.

Significance and Impact

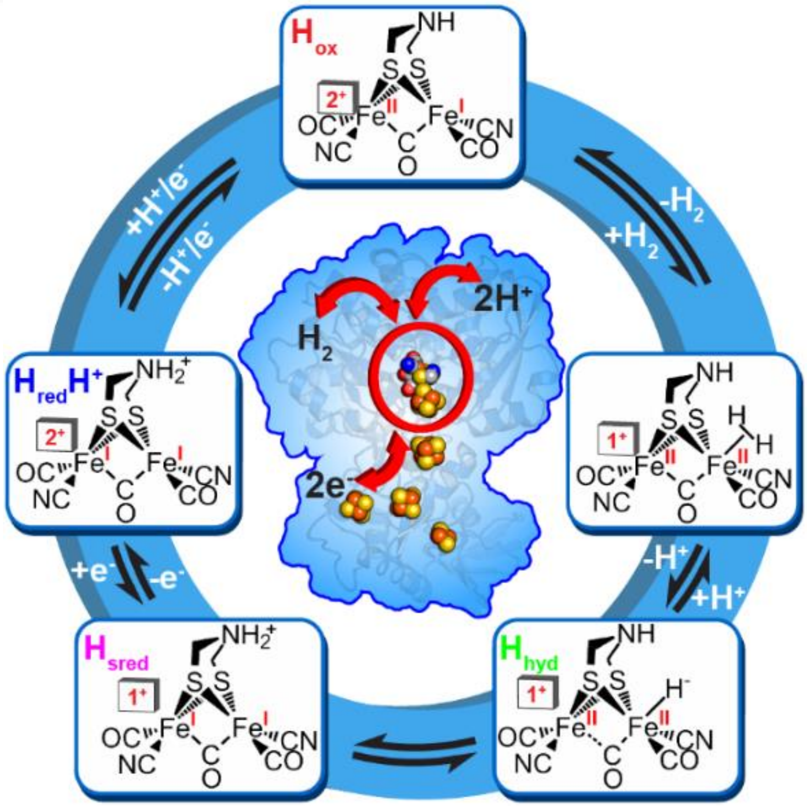
This work provides a blueprint for engineering catalytic bias in synthetic oxidation-reduction catalysts, such as those used in hydrogen fuel cells.

Research Details

- This work elucidated structure-activity relationships using a combination of high-resolution structural work, biochemical analyses, and computational modeling.
- Results support a unifying model based on the relative stability of oxidation states and speciation as a function of reduction potential.

Artz, Zadvornyy, Mulder, Keable, Cohen, Ratzloff, Williams, Ginovska, Kumar, Song, McPhillips, Davidson, Lyubimov, Pence, Schut, Jones, Soltis, Adams, Raugei, King, Peters (2020) *J. Am. Chem. Soc*. 142, 1227. DOI: 10.1021/jacs.9b08756

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

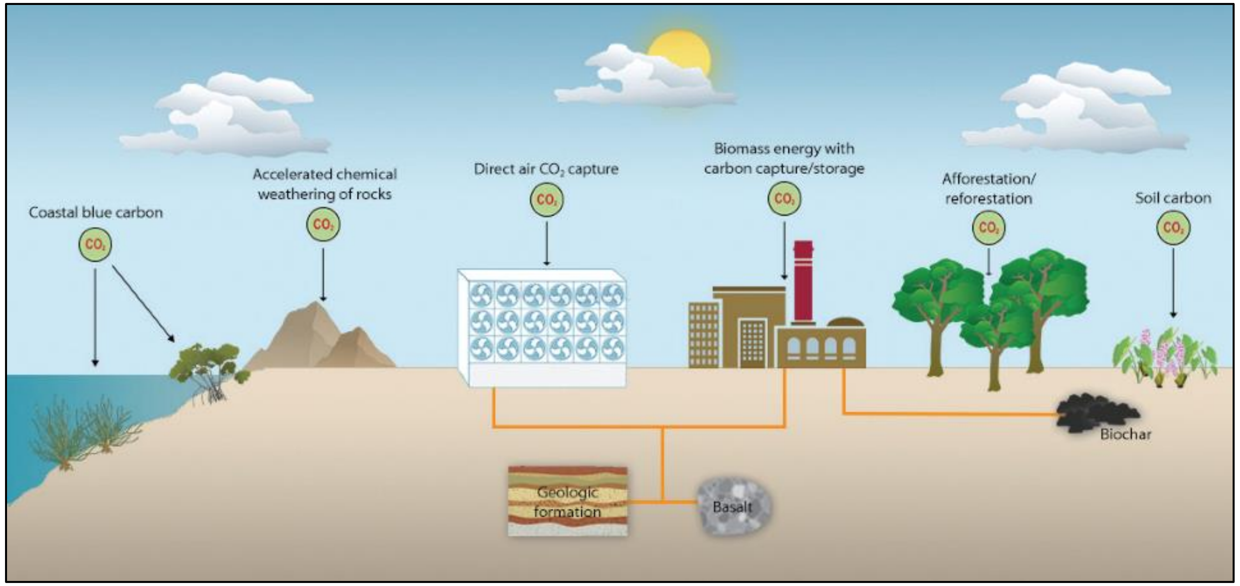


Catalytic H_2 evolution by [FeFe]-hydrogenase. Inner: Structure of [FeFe]-hydrogenase I from *Clostridium pasteurianum*, which includes an arrangement of electron transfer centers and active-site cluster (red circle) for the interconversion of H_2 with 2e- and 2H+(red arrows). Differences in the electrostatic 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).

Coordination across DOE – Science & Energy Tech Teams

Carbon Management SETT

- Crosses multiple DOE offices
  - Led by FECM
  - Co-leads: SC-BES and EERE's Bioenergy Technology Office (BETO)
- Advances clean energy and climate priorities and addresses National Academies report on Negative Emissions Technologies (NET)*
- Responds to congressional direction for DOE to develop an implementation plan coordinated across EERE, FECM, and SC that advance NET and carbon dioxide removal (CDR)

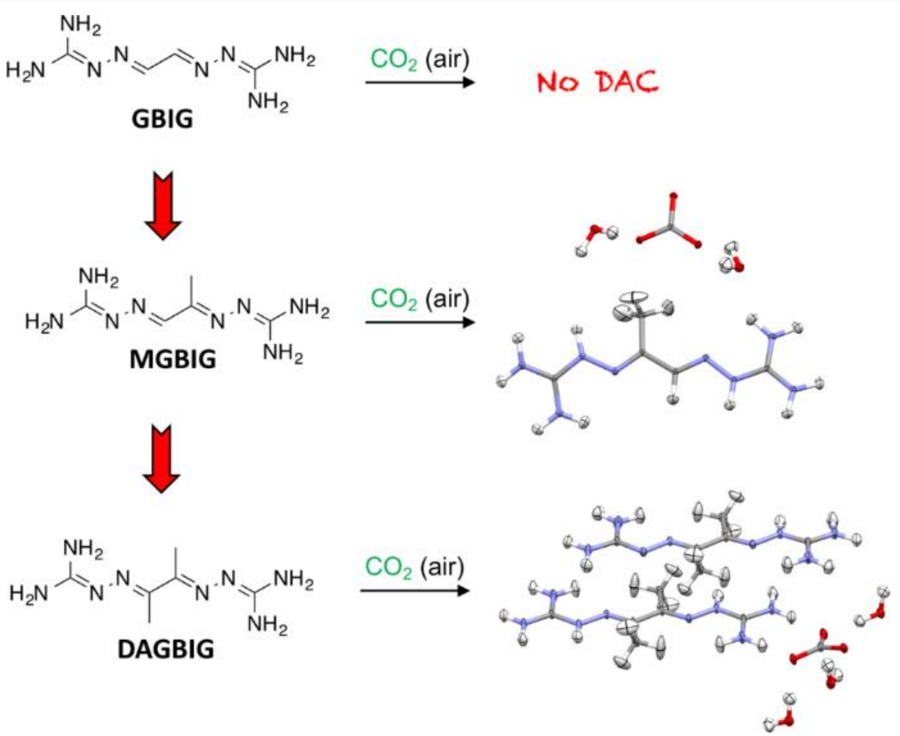


CDR Technologies

- Coastal blue carbon: manage land use to enhance carbon stored in living plants or sediments in coastal ecosystems.
- Advanced chemical weathering of rocks: accelerate chemical reactions of CO_2 with reactive minerals. (**BES Geosciences**)
- **Direct air capture: capture and concentrate CO_2 from ambient air – BES Focus.**
- Biomass energy with carbon capture/storage: combine energy production from biomass with CO_2 capture and storage.
- Afforestation/reforestation & Soil carbon: manage land use to enhance soil carbon storage.

* https://www.nap.edu/catalog/25259/negative-emissions-technologies-and-reliable-sequestration-a-research-agenda

Crystal Engineering Turns On Direct Air Capture (DAC) of Carbon Dioxide



DAC of CO_2 via crystallization of BIG carbonate salts is switched on by small structural modifications of BIG's molecular structures. While no DAC was observed with glyoxal-bis-iminoguanidine (GBIG), methyl substitution for H atoms led to major changes in the crystal structures of the corresponding methylglyoxal-bis-iminoguanidine (MGBIG) and diacetyl-bis-iminoguanidine (DABIG) complexes, as determined by X-ray and neutron diffraction (crystal structures shown on the right). This led to greatly enhanced aqueous solubilities of MGBIG and DABIG, thereby switching on DAC.

Custelcean, Williams, Wang, Garrabrant, Martin, Kidder, Ivanov, *ChemSusChem*,13, 6381 (2020) DOI: 10.1002/cssc.202001114

Scientific Achievement

The direct air capture of CO_2 can be dialed in by subtle structural modifications of bis-iminoguanidine (BIG) crystals, resulting in major improvements in their aqueous solubilities and DAC performance.

Significance and Impact

DAC of CO_2 via BIG crystal engineering provides key design principles for future DAC approaches to negative emissions technologies.

Research Details

—Structure-property relationships in DAC by crystallization of BIG carbonate salts have been elucidated. X-ray and neutron diffraction provided key structural parameters including molecular conformations, hydrogen bonding, and π-stacking.

—Thermodynamic measurements, such as aqueous solubilities, regeneration energies and temperatures, were complemented by first-principles calculations of lattice and hydration energies, and ΔG of CO_2 capture and release.

Direct Coupled Electrochemical System for Capture and Conversion of Carbon Dioxide from Ocean Water

Scientific Achievement

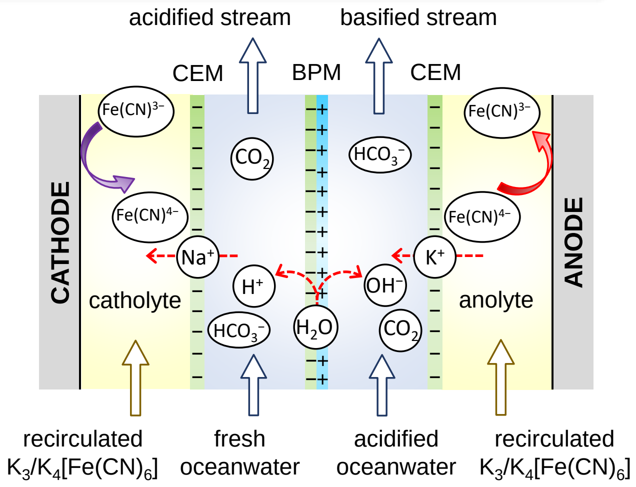
A direct coupled system captures CO_2 from ocean water using electrochemical energy of 0.98 kWh/kg CO_2 and converts CO_2 to CO at a Faradaic efficiency of up to 95% in vapor-fed cells.

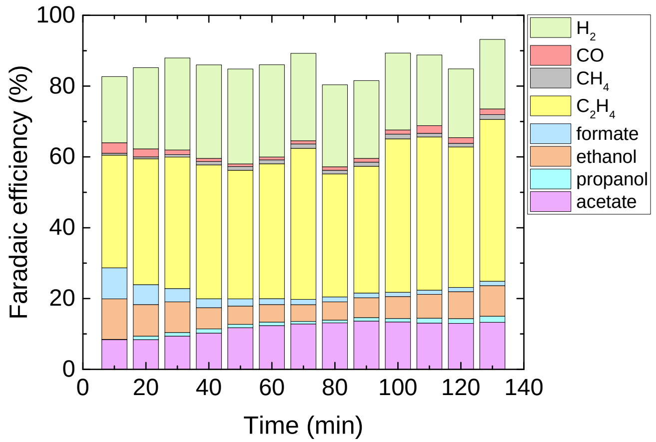
Significance and Impact

The bipolar membrane (BPM) electrodialysis cell replaces the commonly used water splitting reaction with a one-electron redox couple at the electrodes, significantly lowering the electrochemical energy consumption. Tandem vapor-fed cells were used to eliminate O_2 and convert CO_2 at high Faradaic yields.

Research Details

- Parasitic losses due to water splitting reaction is eliminated by using a one-electron redox couple at the electrodes of the electrodialysis cell.
- Electrochemical energy for CO_2 capture from ocean water as low as 0.98 kWh/kg CO_2 with ~70% efficiency; gas output composition >90% CO_2
- Ag-based vapor-fed cell converts CO_2 to CO with up to 95% Faradaic efficiency; Cu-based vapor-fed cell converts CO_2 to conversion to fuels and chemicals with up to 73% Faradaic efficiency.





Schematic illustration of the BPM electrodialysis cell, and gas/liquid product distribution of converted CO_2 from ocean water..

Digdaya, Sullivan, Lin, Han, Cheng, Atwater, Xiang, *Nat. Commun.* **2020**, *11*, 4412

Coordination across DOE – Energy Storage Grand Challenge

Energy Storage

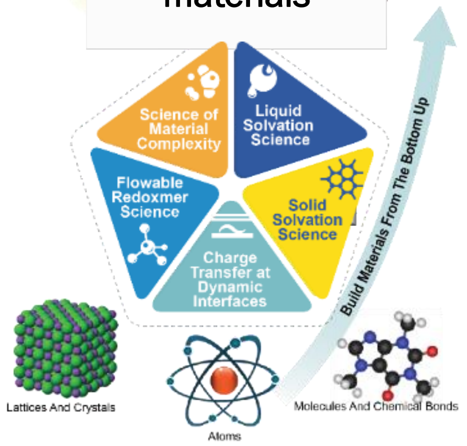
- Crosses multiple DOE offices
  - Led by Offices of Electricity (OE) and Energy Efficiency and Renewable Energy (EERE)
  - Participation by multiple offices including SC, FECM, ARPA-E, NE
- Advances DOE’s Energy Storage Grand Challenge
  https://www.energy.gov/energy-storage-grand-challenge/energy-storage-grand-challenge
- Recognizes Grid storage is now the critical technology constraint to electricity decarbonization
  - A highly decarbonized grid could require 1200-2300 GWh of storage (from <300 GWh today)
  - Long duration (10+ hours) storage will be increasingly important (<4-hour systems typical today)
- Launched Long Duration Storage Energy Earthshot in July 2021

Reduce storage costs by	...in storage systems that deliver	...in
90%	10+	1
from 2020 Li-ion baseline...	hours of duration	decade

https://www.energy.gov/eere/long-duration-storage-shot

Batteries and Energy Storage Hub (2012 – today)
Scientific Foundations for Next-Generation Electrical Energy Storage

Transformative energy storage materials

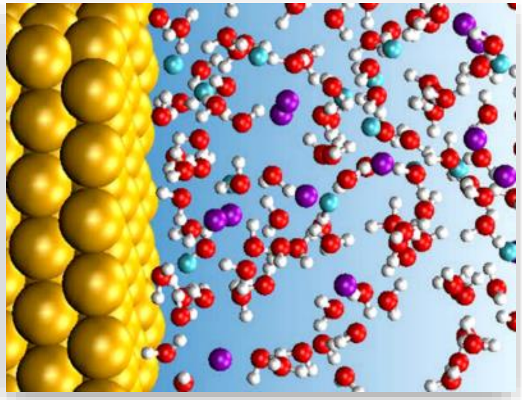


Energy Innovation Hubs

- Multi-investigator, multi-disciplinary integrated centers that focus on overcoming the scientific barriers to development of a complete energy system that has potential for implementation into a transformative energy technology.
- The Batteries and Energy Storage Hub will provide the scientific foundation for disruptive high-performance battery materials constructed from the bottom up to enable a diversity of batteries that simultaneously meet challenging, and often conflicting, performance requirements for grid or transportation applications.

Joint Center for Energy Storage Research (JCESR)

- Launched in December 2012 (~$24 M/year for 5 years)
  - Over 430 publications and >10,000 citations, >100 invention disclosures and patent applications
  - 3 spin-off companies to commercialize key technologies: solid electrolytes, microporous polymer (PIM) membranes, and air-breathing sulfur battery
- Renewal in July 2018 (~$25 M/year for up to 5 years)
  - Multidisciplinary team research developing and using innovative tools to understand, design, and build materials where each atom or molecule has a prescribed role in energy storage systems with targeted behavior
  - Led by ANL in partnership with four other national labs, eleven universities, one industry and the Army Research Laboratory

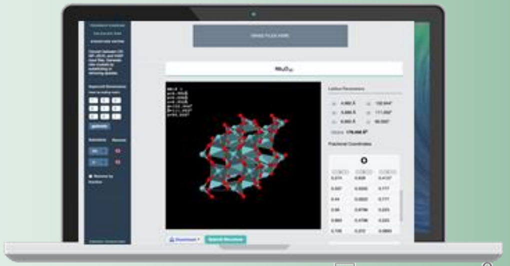


Electrified Interfacial Structure

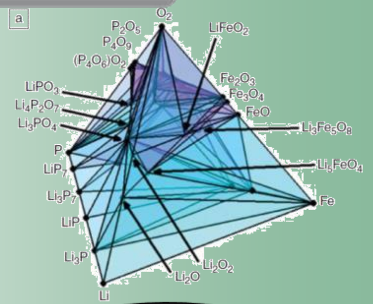
The Materials Project: Powerful Computing and Analysis To Discover Novel Materials (https://materialsproject.org/)

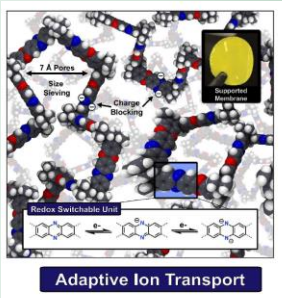
Basic Science

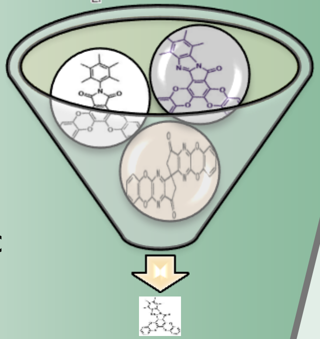
Focused on first principles theory research to develop computer codes and data screening tools to advance discovery of materials with specific functionality



Calculated ground state phase diagrams





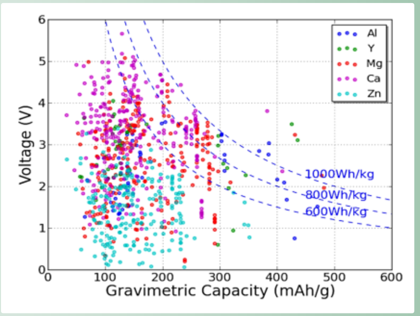


The Electrolyte Genome for calculation of organic electrolyte components

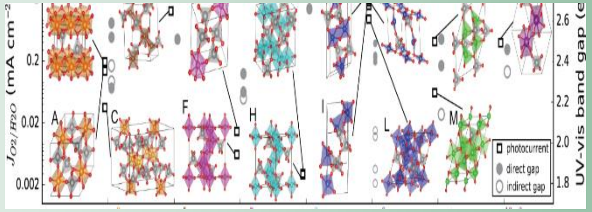
Supported by BES and NSF

Applied R&D

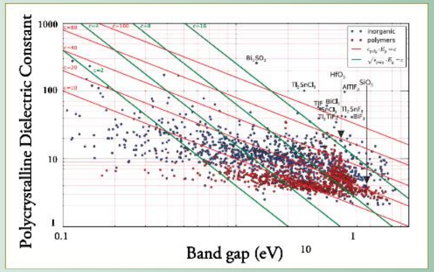
Developed the computational data and screening approaches for specific technologies



Multivalent cathodes for energy storage



A landscape of photoactive structures identified by computational screening



Discovery of novel dielectric materials

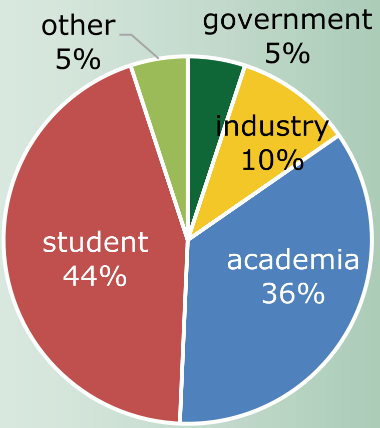
Supported by DOE-EERE, DoD, and Industry

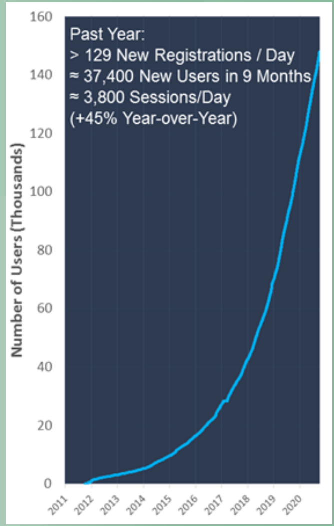
Web-Based Resource

Available to users through the National Energy Research Scientific Computing Center

144,595	76,240	63,876	530,243
INORGANIC COMPOUNDS	BANDSTRUCTURES	MOLECULES	NANOPOROUS MATERIALS
14,072	3,402	4,730	16,128
ELASTIC TENSORS	PIEZOELECTRIC TENSORS	INTERCALATION ELECTRODES	CONVERSION ELECTRODES

Growing use by both academia and industry



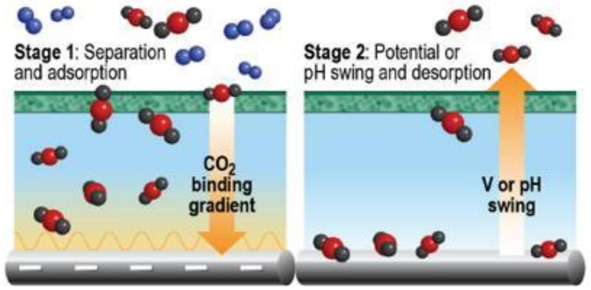


"Now you instantly have it [data] in your browser…It's a huge increase in efficiency"
- product development engineer, 3M

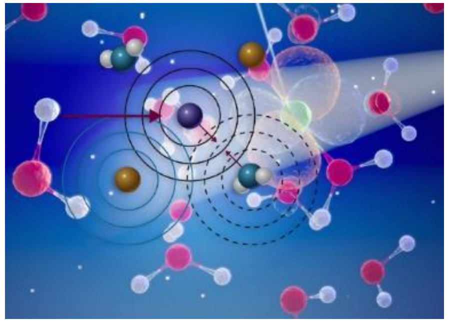
NERSC supported by ASCR

FY 2021 FOAs: Advancing Science and Capabilities for Clean Energy Stewardship

Materials and Chemical Sciences Research for Direct Air Capture of Carbon Dioxide – Experimental and computational research to provide foundational understanding for design of high-selectivity, high-capacity, and high-throughput chemical separations; data-science-driven synthesis and assembly of materials for direct air capture; and understanding of temporal changes that occur during separations.

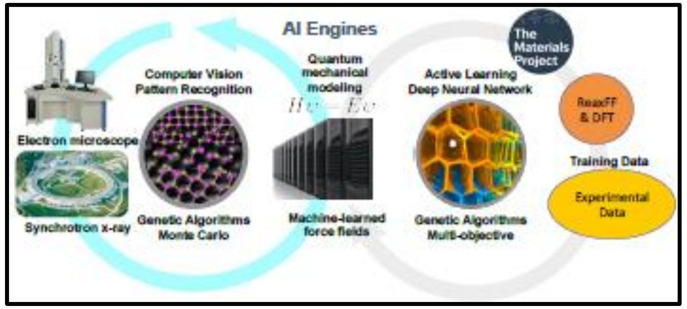


9 Awards Announced (2 Lab, 7 University); $24M over 3 years
https://science.osti.gov/-/media/bes/pdf/Funding/2021/FY2021_DAC_Awards_20210722.pdf



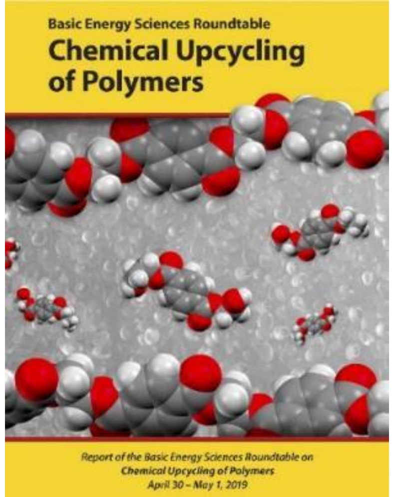
Computational Chemical Sciences – Research to develop open-source computational chemistry codes that enable full use of exascale computers to accurately describe chemistry in complex environments and provide the science foundations to advance clean, efficient energy technologies.
9 Awards Announced (3 Lab, 6 University); $29M over 4 years
https://science.osti.gov/-/media/bes/pdf/Funding/2021/2426_BES_Computational_Chemical_Sciences_Award_List.pdf

Data Science to Advance Chemical and Materials Sciences – Collaborations of BES domain scientists with experts in data science (e.g., AI/ML) and/or applied math to increase the use of data science across the BES research portfolio focusing on cross-cutting phenomena important in clean-energy systems.
Awards will be announced soon; up to $21M over 3 years



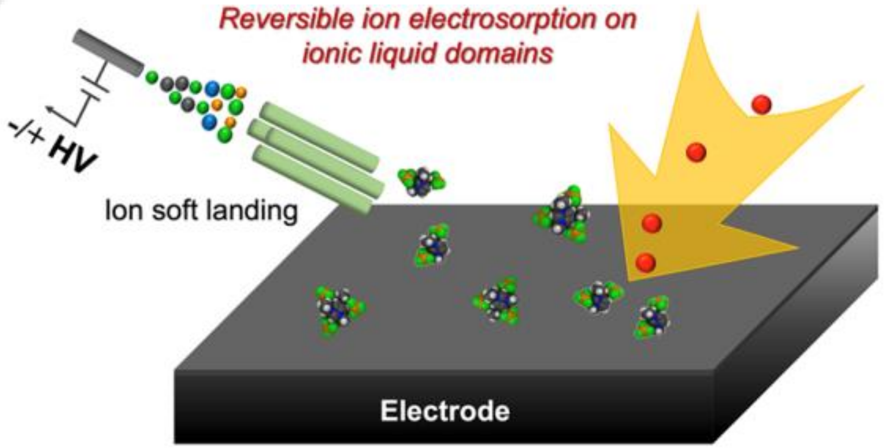
Coordination across DOE – Advanced Manufacturing

- **Advanced manufacturing and industrial processes (coordination with EERE Advanced Manufacturing Office)**
  - Workshop on Basic Research Needs for Transformative Manufacturing (March 2020) with goal of developing a basic science strategy that underpins applied technology research and lays the scientific foundation to go beyond incremental improvements to create new, transformative technologies for manufacturing that are energy efficient and sustainable.
- **Polymer upcycling working group (EERE, SC, FECM, ARPA-E)**
  - Connects BES directions identified in Roundtable on Chemical Upcycling of Polymers with DOE-wide Plastics Innovation Challenge (PIC).
  - PIC R&D strategy being finalized.
- **Critical minerals/materials working group (EERE, SC, FECM, ARPA-E, IA)**
  - BES research provides foundational knowledge that will allow discovery/development of substitutes, diversification of supply, and efficient use to reduce or eliminate criticality.



https://science.osti.gov/bes/Community-Resources/Reports
for brochures and reports

Structure and Stability of Ionic Liquid Clusters: Implications for Electrochemical Separations



Dissolved ILCs are ionized by electrospray ionization and then deposited onto the electrode surfaces. Once adsorbed, the ILCs reduce the amount of energy needed for other ions from solution to adsorb and separate on the electrode.

Zhang, Baxter, Nguyen, Prabhakaran, Rousseau, Johnson, and Glezakou, *Journal of Physical Chemistry Letters* (2020) **11** (16), 6844-6851

Work performed at Pacific Northwest National Laboratory

Scientific Achievement

Understanding of the structure, abundance, and growth motifs of ionic liquid clusters (ILCs) led to an optimized choice of deposited cluster size for maximizing charge transfer during ion electrosorption and separation on a working electrode.

Significance and Impact

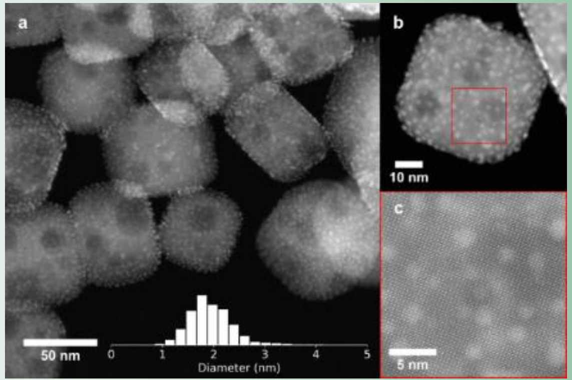
Predictions from simulations, supported by experimental evidence, provide the fundamental understanding necessary to lower overpotentials for electrosorption and discover novel processes for industrial separations.

Research Details

- High mass resolution mass spectrometry determined relative cluster abundance and stability using collision-induced dissociation experiments.
- Computational studies predicted structures and growth patterns of ILCs with one to nine cations.
- ILC functionalized electrodes were prepared via a specialized ion soft landing technique developed at the Pacific Northwest National Laboratory.
- Electrochemical measurements showed lower charge transfer resistances for ILC functionalized electrodes.

BES-EERE Coordination to Transform Plastic Waste into New Products

Basic Science



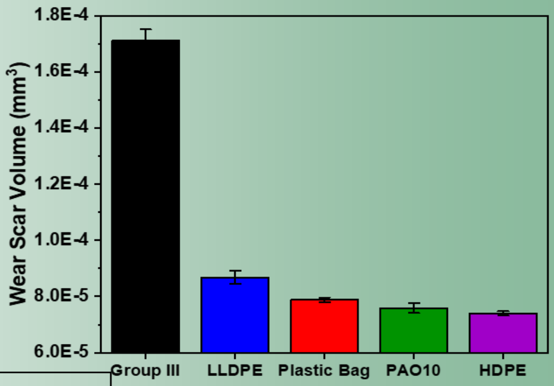
Electron micrographs of Pt NPs with an average size of 2.0 ± 0.5 nm, deposited by ALD on $SrTiO_3$ nanocuboids

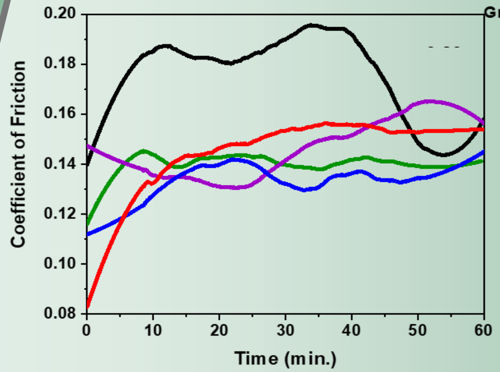
Platinum nanoparticles on a perovskite support catalyze *selective* hydrogenolysis of carbon-carbon bonds in polyethylene under mild conditions. Selective catalytic hydrogenolysis yields macro-molecules of uniform chain length that are ideal as lubricants and with negligible formation of undesired byproducts.

Celik et al., ACS central science 5 (11), 1795-1803 (2019)

Applied R&D

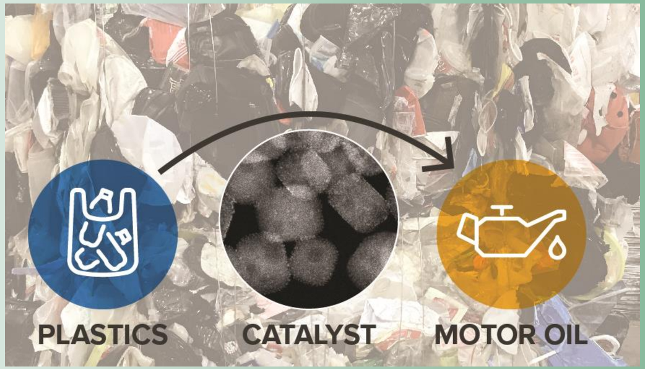
EERE-funding enabled the design and evaluation of the economic viability of a manufacturing process for converting polyolefin waste to premium synthetic lubricants. It is estimated this process will have a much lower product cost compared to that of the refinery-based counterpart.





Measured wear rate volume and coefficient of friction for ball-on-disk tests using various base oils and upcycled products from waste polyolefins.

Manufacturing/Commercialization



In 2021, EERE-supported work with Chevron-Phillips Chemical Company to improve carbon and energy efficiency to enable a circular plastic economy, by creating innovative deconstruction pathways for existing polymers that generate high value products, such as high-performance lubricants.

Argonne NATIONAL LABORATORY

Chevron Phillips Chemical Company LP

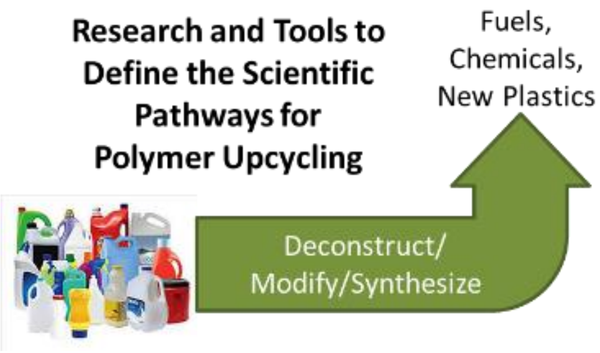
AMES LABORATORY Creating Materials & Energy Solutions U.S. DEPARTMENT OF ENERGY

Northwestern University

FY 2021 FOAs: Science to Transform Manufacturing

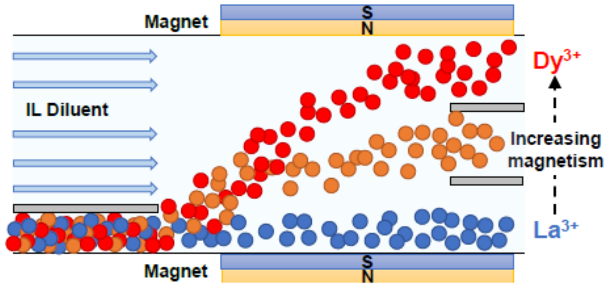
Polymer upcycling – Provide the foundational knowledge for designing chemical components and processes that enable efficient conversion of plastic waste to high-value chemicals, fuels, and materials; investments informed by BES Roundtable on Chemical Upcycling of Polymers.

Awards will be announced soon; up to $25M over 3 years

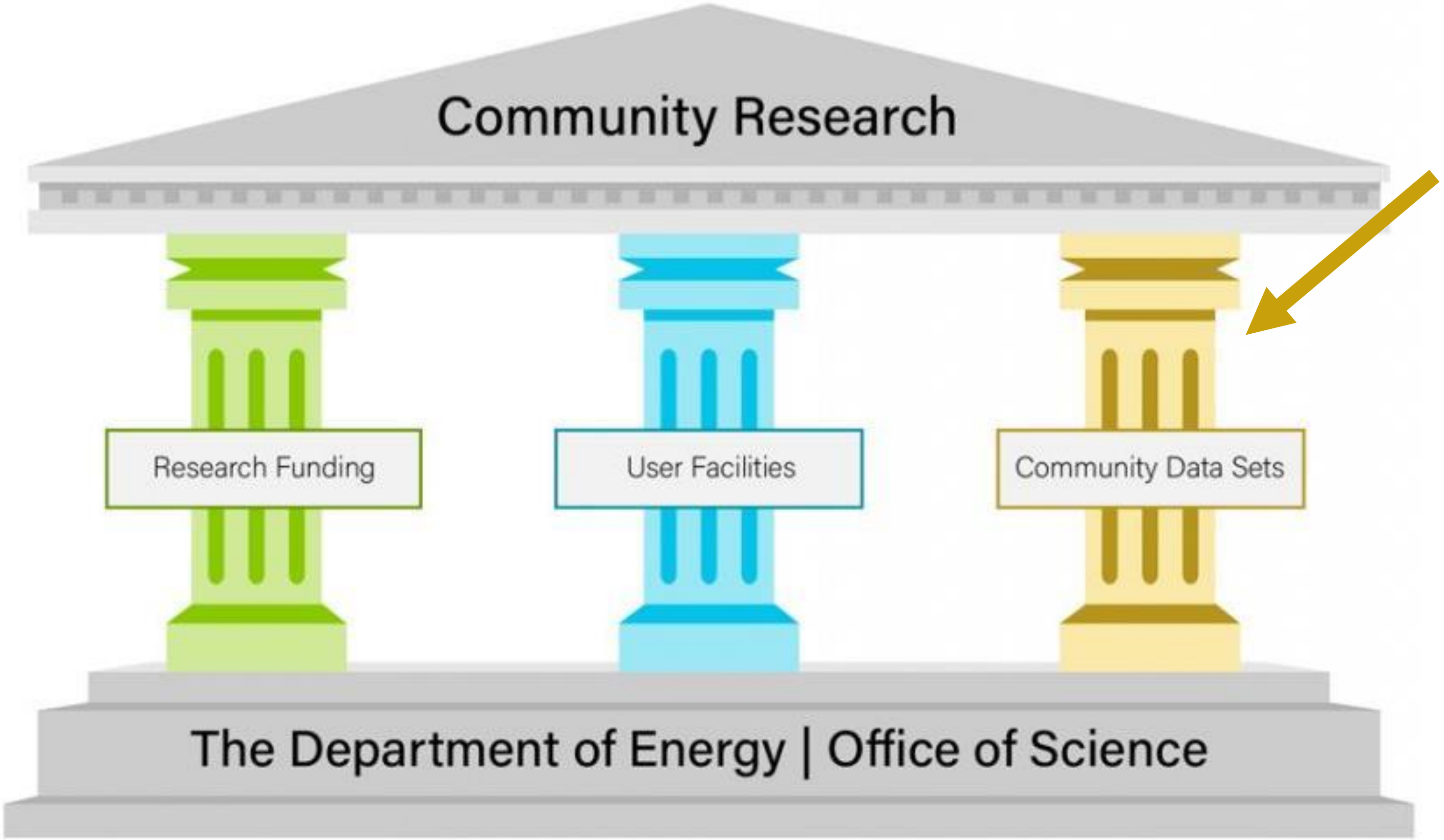


Critical materials: Rare earth/platinum – Advance the understanding of fundamental properties of these materials, identify methodologies to reduce their use and to discover substitutes, and enhance chemical processing and separation science for rare earths.

Awards will be announced soon; up to $30M over 3 years



Data is the Third Pillar of the DOE SC Enterprise



https://www.energy.gov/science/office-science-pure-data-resources

Public Reusable Research (PuRe) Data Resources are:

- data repositories,
- knowledge bases,
- analysis platforms,
- and other activities

that aim to make data **publicly available** in order to advance scientific or technical knowledge.

PuRe Data Resource designations **highlight** and **improve stewardship** of SC-supported community data efforts with strategic impact on the SC mission.

PuRe Data Resources at a Glance

PuRe Data Resources

https://science.osti.gov/Initiatives/PuRe-Data/Resources-at-a-Glance

- Initially designated resources:
  - Atmospheric Radiation Measurement Data Center
  - Joint Genome Institute
  - **Materials Project**
  - National Nuclear Data Center
  - Particle Data Group
  - Systems Biology Knowledgebase (KBase)

JGI JOINT GENOME INSTITUTE

NNDC

PDG particle data group

The Materials Project

ARM

KBase PREDICTIVE BIOLOGY DOE Systems Biology Knowledgebase

The Materials Project

The Materials Project is a recognized leader of **data generation, storage, and distribution in the domain of materials science.**

- Computational materials science database and analysis platform
- Provides scientists information of known and predicted materials and chemistries and inspires the design of novel structures and processes
- Allows researchers to data-mine scientific trends in properties

Sponsored by the office of Basic Energy Sciences (BES)

https://materialsproject.org/

Accelerates innovation in materials and chemistry research

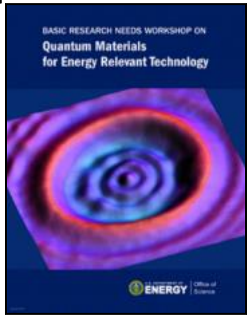
Predicts materials and chemical properties before they are synthesized in a laboratory

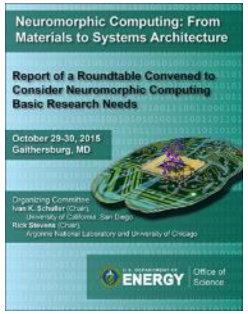
>200,000 registered users, ~ 10,400 distinct daily users, and data for ~145,000 inorganic compounds

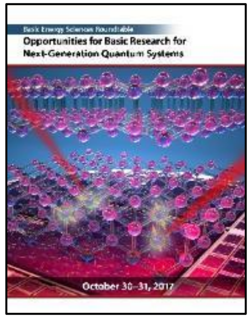
Primary single publication associated with the Materials Project has been cited >4,000 times

Defining Research Priorities: Basic Research Needs Strategic Planning Workshops and Roundtables

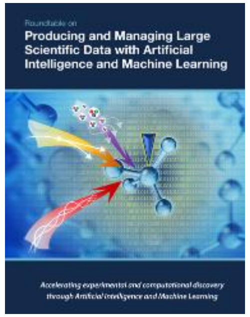
- Quantum Science



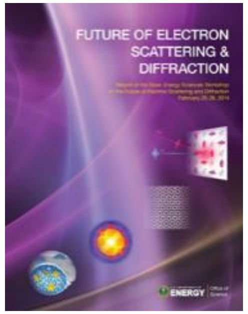


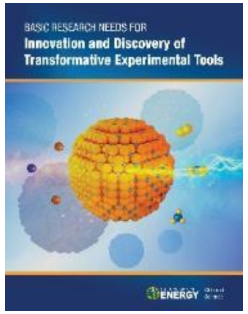


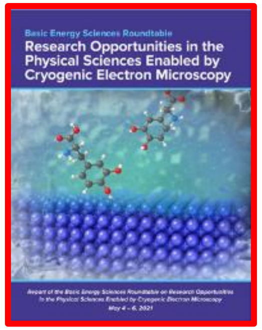
Theory, Modeling and Computation



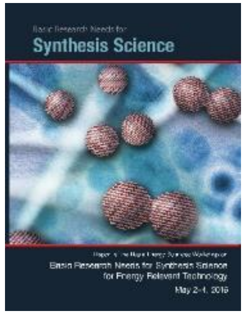
- Characterization

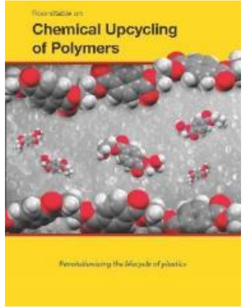




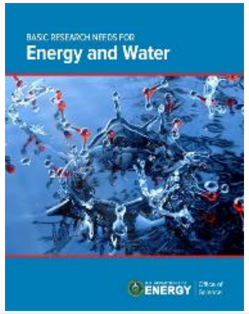


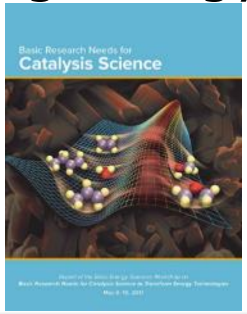
Synthesis

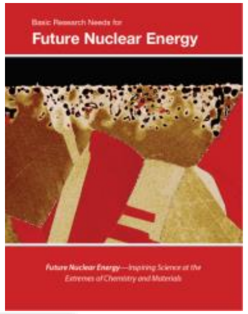


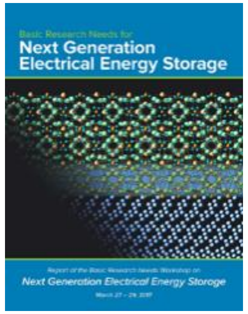


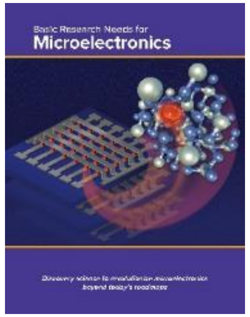
- Cross-Cutting Energy

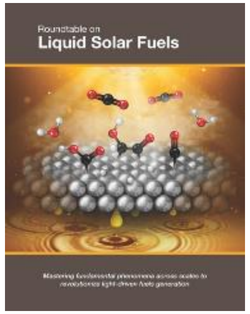












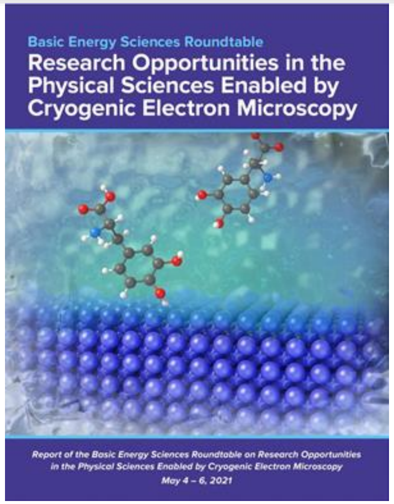
Science for Carbon-Neutral Hydrogen

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

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

Date: May 4-6, 2021

Format: Virtual



Charge:

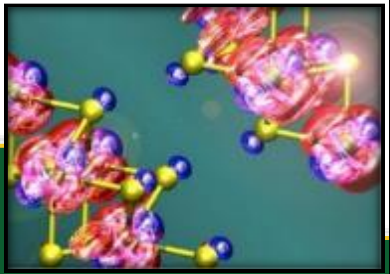
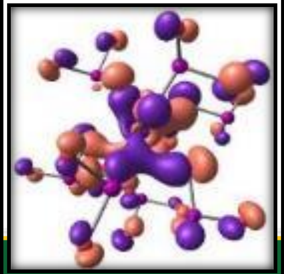
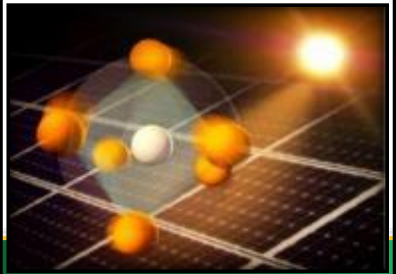
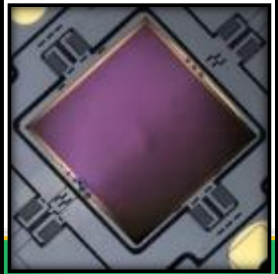
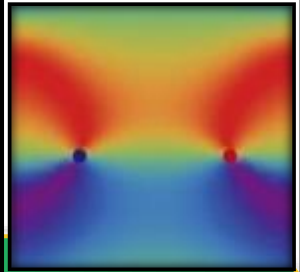
- Articulate research opportunities, key science drivers, and research strategies for the BES physical sciences research portfolio in the area of cryo-EM
- Assess the current status of BES electron microscopy science at cryogenic temperatures and define a path for optimal utilization of these capabilities 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

FY 2022 Budget Request: Department of Energy

- The President's 2022 discretionary request includes **$46.1 billion** for DOE, a **$4.3 billion** or **10.2 percent** increase from the 2021 enacted level.
- **Expands Foundational Research, Emphasizing Climate and Clean Energy Science.** The discretionary request invests **$7.4 billion**, an increase of more than **$400 million** over the 2021 level, in the Office of Science to: better understand the changing **climate**; identify and develop **novel materials and concepts for clean energy** technologies of the future; advance **artificial intelligence and computing** to enhance prediction and decision-making across numerous environmental and scientific challenges; and support the National Laboratory network with **cutting-edge scientific facilities**.
- **Invests in Minority-Serving Institutions.** The discretionary request creates and enhances **research funding opportunities** and invests in infrastructure such as laboratory facilities and information technology upgrades for Historically Black Colleges and Universities (HBCUs) and Minority-Serving Institutions (MSIs).The discretionary request also increases resources for **workforce development programs** to augment pathways to good-paying science, technology, engineering, and math careers for students attending these schools. New grant awards, including a research center focused on climate, would expand research capacity and create new opportunities at HBCUs and other MSIs.

FY 2022 Request: Basic Energy Sciences

- The BES FY 2022 Request of $2,300M focuses resources on the highest priorities in early-stage fundamental research, operation and maintenance of scientific user facilities, and facility upgrades.
- Research priorities include:
  - Clean Energy Stewardship: critical materials/minerals, direct air capture, hydrogen, solar, energy storage
    - Advanced Manufacturing: science to transform manufacturing including polymer upcycling, microelectronics
    - Reaching a New Energy Sciences Workforce (RENEW)
  - Computing and Data: Exascale computing, artificial intelligence and machine learning (AI/ML)
  - Quantum Information Science: National QIS Research Centers, Materials and Chemistry R&D, Infrastructure
  - Facilities-related Research and Capabilities: integrated computational and data infrastructure, accelerator science and technology, biopreparedness research virtual environment

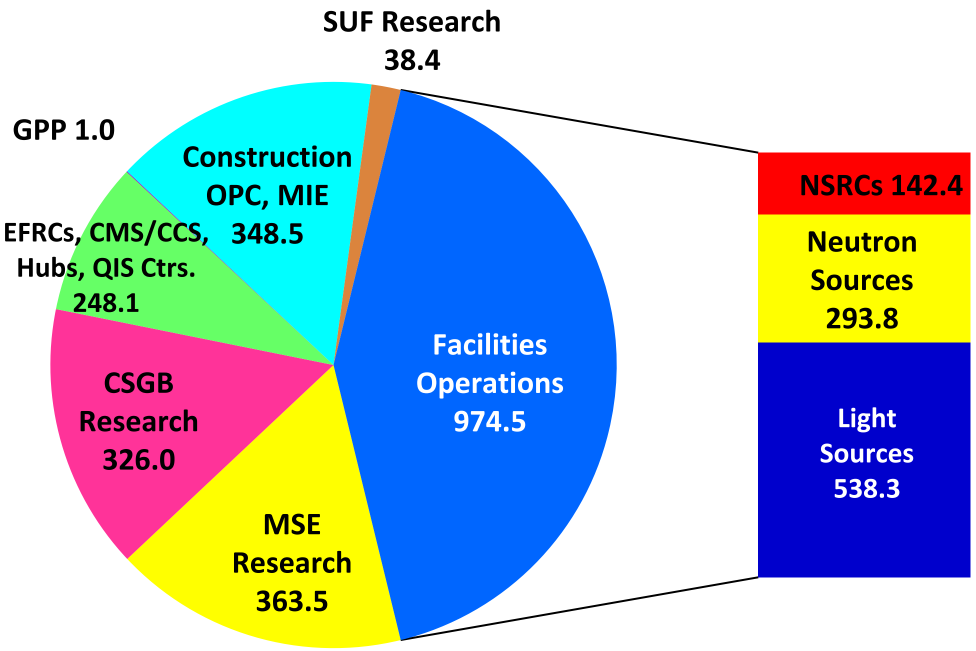
FY 2022 President's Request: Marks Similar to Request
$2,300M (+$55M or +2.4% above FY 2021 Enacted)

Research programs Δ = +$109.3M

- Core Research ($735.5M,+$79M) includes new and expanded investments in research for clean energy, manufacturing, microelectronics, and RENEW (Reaching a New Energy Sciences Workforce)
- Computational Materials and Chemical Sciences, Energy Innovation Hubs, and National QIS Research Centers continue (~$118M)
- Energy Frontier Research Centers continue (~$130M, +$15M)
- EPSCoR continues ($25M)

Scientific user facilities Δ = +$15.7M

- Operations of 12 facilities continue at ~97% of optimal ($974.5M)
- Facilities research continues for AI/ML; increases for accelerator R&D ($38.4M)



Construction/MIE* Δ = -$70.0M

- APS-U ($106M); LCLS-II ($32.4M); LCLS-II-HE ($53M); ALS-U ($75.1M); PPU ($17M); STS ($32M); CRMF ($3M)
- MIEs: NSRC Recap ($15M); NEXT-II ($15M)

*includes OPC

U.S. DEPARTMENT OF ENERGY | Office of Science

FY 2022 Funding Opportunity Announcements

- New Collaborator Template
  - Excel file submitted by the lead applicant listing collaborators for all individuals listed as senior/key personnel on the proposal.
  - Information used to manage reviewer selection.
  - Requested for all FY 2022 funding opportunities and lab calls.
- Biosketches and Current and Pending Support
  - Office of Science is working with SciENcv to develop a DOE SC template for biosketches and current and pending support.
  - Expected to be available on or before January 2022.
  - SciENcv can be linked to ORCID accounts to leverage existing data.

Call for Nominations: 2021 E.O. Lawrence Awards

- **Recognizes:** Mid-career U.S. scientists and engineers for exceptional contributions and achievements in research, technical, and engineering supporting the broad missions of DOE and its programs to advance the national, economic, and energy security of the U.S.
- **Awards considered in nine categories:**
  - Atomic, Molecular, and Chemical Sciences
  - Biological and Environmental Sciences
  - Computer, Information, and Knowledge Sciences
  - Condensed Matter and Materials Sciences
  - Energy Science and Innovation
  - Fusion and Plasma Sciences
  - High Energy Physics
  - National Security and Nonproliferation
  - Nuclear Physics
- **Eligibility:**
  - Mid-career, defined as within 20 years of earning highest degree
  - United States citizen
  - Recognized for achievement in research principally funded by DOE
  - Recognized primarily on the scientific impact and technical significance of their work relative to its discipline and/or related mission
- **Deadline for nominations: Tuesday, September 21st, 2021, 5:00 PM (ET)**
  - Nominations made online: https://apps.orau.gov/Award/Lawrence
  - Additional information (eligibility, category descriptions, review process): https://science.osti.gov/lawrence

Questions: SCLawrence.Award@science.doe.gov

Questions?