Basic Energy Sciences Perspective

Committee on the Decadal Assessment of Plasma Physics

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For Basic Energy Sciences

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Outline

- **BES Overview**
- **Plasma Sciences in BES:**

  Then vs. Now & Future Outlook

Basic Energy Sciences

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

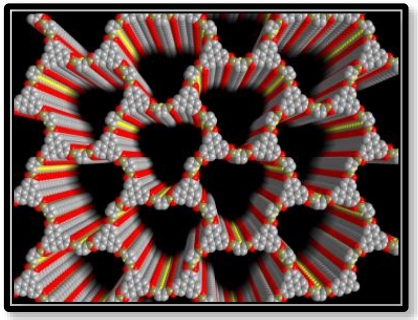
Chemical sciences, geosciences, and biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

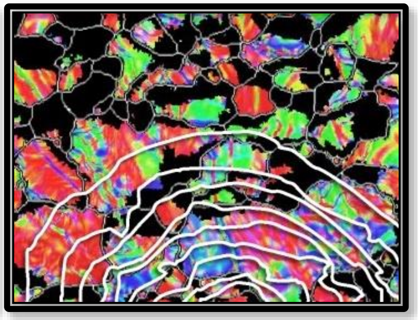
Scientific User Facilities
The largest collection of facilities for x-ray and neutron scattering and nanoscience tools in the world

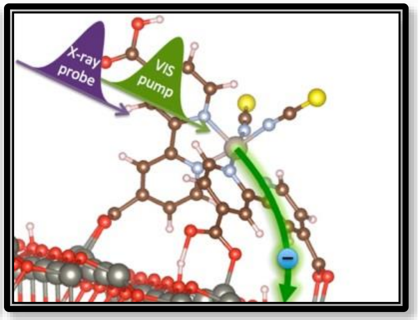
The Scientific Challenges:

- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

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







Basic Energy Sciences At a Glance (2018)

BES RESEARCH SPANS

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

15 DOE NATIONAL LABORATORIES | **45** STATES AND WASHINGTON, D.C.

25 CORE RESEARCH AREAS

46 ENERGY FRONTIER RESEARCH CENTERS

SUPPORTED RESEARCHERS

~6,200 Ph.D. SCIENTISTS | **~2,100** STUDENTS SUPPORTED

BES | BY THE NUMBERS

FY 2018

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

2 ENERGY INNOVATION HUBS

$787 MILLION RESEARCH BUDGET

~26% AVERAGE NEW GRANT SUCCESS RATE

OVER **1,100** CORE RESEARCH PROJECTS

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

$934 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET

OPERATIONS FOR SCIENTIFIC USER FACILITIES 45%

FACILITY UPGRADES, CONSTRUCTION 17%

38% RESEARCH

49% UNIVERSITIES

51% DOE LABS

$369 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET

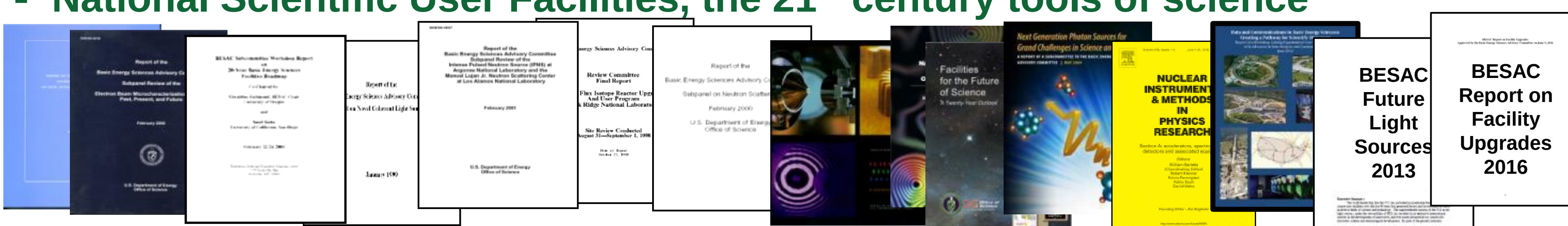
BES strategic planning activities provide the foundation for program strategy

2016 - 2018

- **Science for Discovery**

- **Science for National Needs**

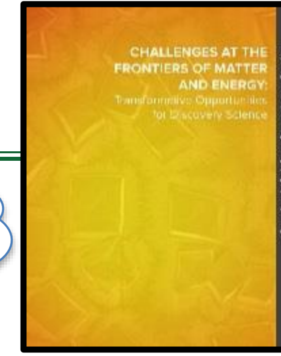
- **National Scientific User Facilities, the 21st century tools of science**



Grand Science Challenges:
Directing and Controlling Matter and Energy

- Synthesize, atom by atom, new forms of matter with tailored properties
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
- Control the quantum behavior of electrons in materials
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
- Control matter very far away from equilibrium

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

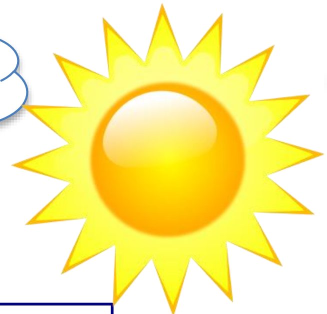


2015

Instrumentation & Tools

Human Capital

Synthesis



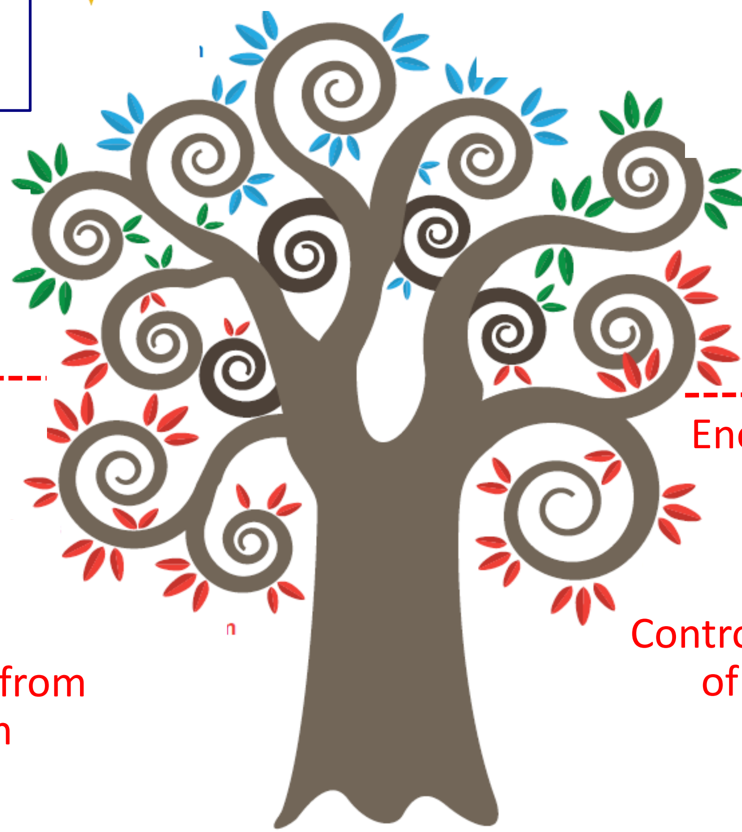
Beyond Ideal Materials and Systems

Mastering Hierarchical Architectures

Harnessing Coherence in Light and Matter

Imaging Matter across Scales

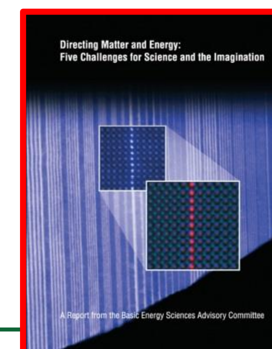
Data, Algorithms and Computing



Efficient Synthesis for Tailored Properties

Energy and Information on the Nanoscale

2007



Correlated Systems

Control at the Level of Electrons

Systems Away from Equilibrium

“Basic Research Needs ...” Workshops 2002 - 2017

>20 reports; >>2,000 participants from academia, industry, and DOE labs

2002

BRN to Assure a Secure Energy Future (BESAC)

- **BRN for Hydrogen Economy (2003)**
- **BRN for Solar Energy Utilization (2005)**
- **BRN for Superconductivity (2006)**
- **BRN for Solid State Lighting (2006)**
- **BRN for Advanced Nuclear Energy Systems (2006)**
- **BRN for Geosciences (2007)**
- **BRN for Clean and Efficient Combustion (2007)**
- **BRN for Electrical Energy Storage (2007)**
- **BRN for Catalysis for Energy Applications (2007)**
- **BRN for Materials under Extreme Environments (2007)**
- **BRN for Carbon Capture (2010)**
- **New Science for Sustainable Energy Future (2008)**
- **Computational Materials Science and Chemistry (2010)**
- **Science for Energy Technology (2010)**
- **Controlling Subsurface Fractures and Fluid Flow (2015)**
- **BRN for Environmental Management (2016)**
- **BRN for Quantum Materials (2016)**
- **BRN for Synthesis Science (2016)**
- **BRN for Transformative Experimental Tools (2016)**
- **BRN for Next Generation Electrical Energy Storage (2017)**
- **BRN for Future Nuclear Energy (2017)**
- **BRN for Energy and Water (2017)**
- **BRN for Catalysis Science (2017)**

Basic Research Needs – Use Inspired Basic Research

- **Transformative, not incremental research directions**
- **Fundamental science challenges to move the technology forward**
- **New techniques and methods**
- **10-30 years out**

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

Increasing scope and size

- **Core Research (>1,100 projects, ~$600M/yr)**
  Single investigators ($150K/year) and small groups ($500K-$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing.

- **Energy Frontier Research Centers ($110M/yr)**
  $2-4M/year research centers for 4-year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.

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

- **Energy Innovation Hubs ($39M/yr)**
  Research centers for 5-year award terms, established in 2010 ($15-25M/year), engage in research topics that have proven challenging for traditional funding modalities and in which success could be transformative to science and technology. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.

National Quantum Initiative Act
H.R. 6227 passed by Congress on 12/13/2018 and signed into law on 12/21/2018

TITLE IV—DEPARTMENT OF ENERGY QUANTUM ACTIVITIES
SEC. 401. QUANTUM INFORMATION SCIENCE RESEARCH PROGRAM.

(a) IN GENERAL.—The Secretary of Energy shall **carry out a basic research program on quantum information science**.
(b) PROGRAM COMPONENTS.—In carrying out the program under subsection (a), the Secretary of Energy shall—
(1) <u>formulate goals for quantum information science research</u> to be supported by the Department of Energy;
(2) <u>leverage the collective body of knowledge from existing quantum information science research</u>;
(3) <u>provide research experiences and training for additional undergraduate and graduate students</u> in quantum information science, including in the fields of—

- (A) **quantum information theory**;
- (B) **quantum physics**;
- (C) **quantum computational science**;
- (D) applied mathematics and algorithm development;
- (E) quantum networking;
- (F) **quantum sensing and detection; and**
- (G) **materials science and engineering**;

(4) **coordinate research efforts funded through existing programs** across the Department of Energy, including—

- (A) the Nanoscale Science Research Centers;
- (B) the Energy Frontier Research Centers;
- (C) the Energy Innovation Hubs;
- (D) the National Laboratories;
- (E) the Advanced Research Projects Agency; and
- (F) the National Quantum Information Science Research Centers; and

(5) **coordinate with other** Federal departments and agencies, research communities, and potential users of information produced under this section.

The bill directs the President to implement a 10-year National Quantum Initiative Program.

The bill defines QIS as the storage, transmission, manipulation, or measurement of information that is encoded in systems that can only be described by the laws of quantum physics.

U.S. DEPARTMENT OF ENERGY | Office of Science

https://www.congress.gov/115/bills/hr6227/BILLS-115hr6227enr.pdf

National Quantum Initiative Act

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Department of Energy

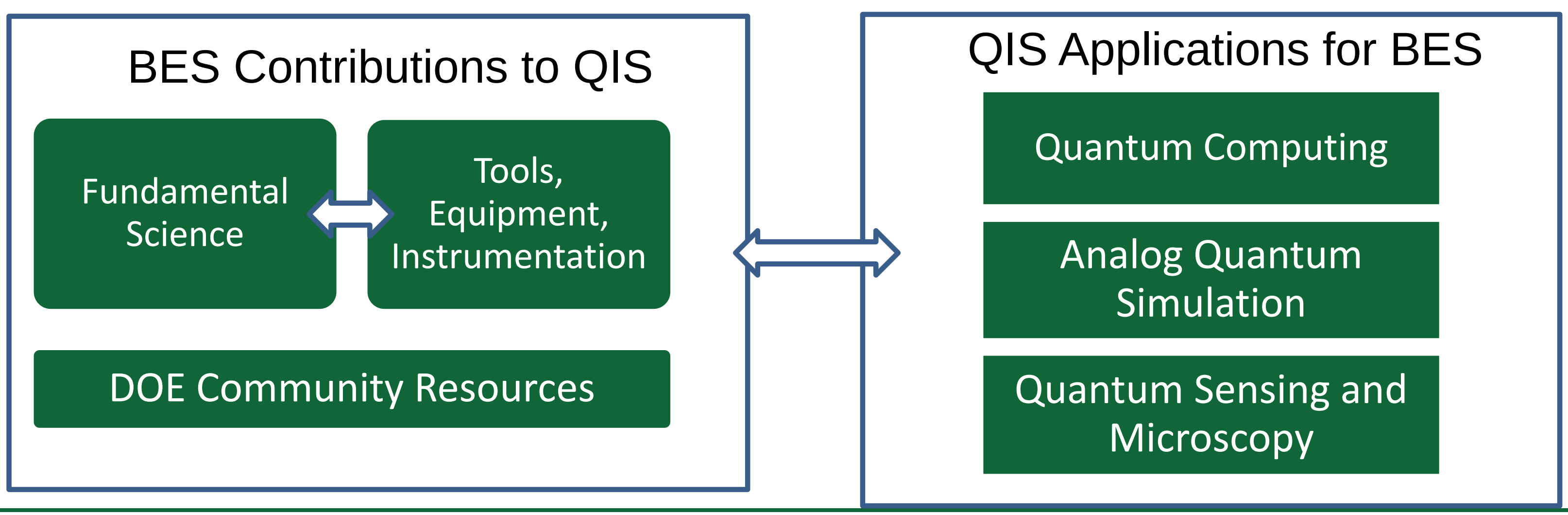
The Committee recognizes **DOE's capabilities, research infrastructure, and expertise in materials science, physics, applied mathematics, and computer science provide a foundation** for significant advances in QIS research and technological development. In particular, the **DOE National Laboratories,** which **operate world class, open-access user facilities** around the country, provide access to the supercomputers, x-ray light sources, photon sources, and neutron sources that are necessary to conduct ground-breaking quantum research. … **The Committee supports DOE's current efforts to increase investment in QIS across the Office of Science**, including for proposed programs in Biological and Environmental Research, High Energy Physics, Nuclear Physics, Basic Energy Sciences, and Advanced Scientific Computing Research (ASCR), as requested in the President's fiscal year 2019 Budget.

Sec. 402. National Quantum Information Science Research Centers

This section directs the DOE Office of Science to establish and operate **up to five National Quantum Information Science Research Centers to conduct basic research to accelerate scientific breakthroughs in quantum information science and technology.** This section also outlines criteria for establishment, collaborations, and other requirements. The Centers are directed to carry out activities for a period of five years. This section authorizes appropriations of $625,000,000 over five years for the Office of Science to carry out this section, which shall include $125,000,000 for each fiscal years 2019 through 2023.

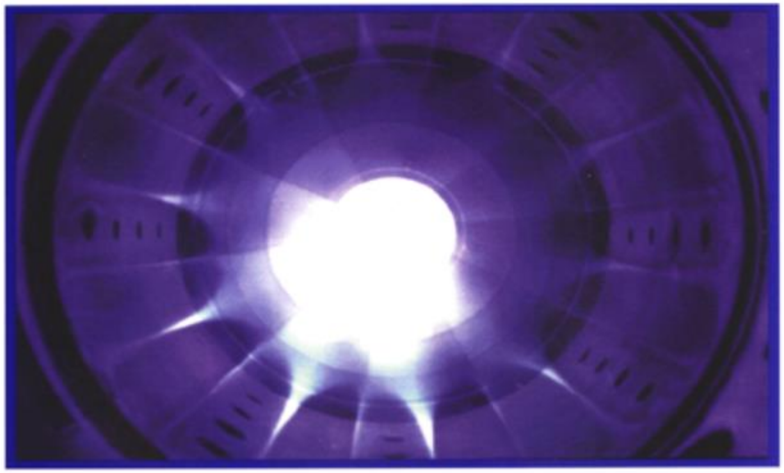
Quantum Information Science Activities in BES

- **NEXT GENERATION QUANTUM SYSTEMS**: Develop understanding leading to control of quantum phenomena in chemical and materials systems to advance quantum-based science and technology.
- **QUANTUM COMPUTING**: Develop quantum computing algorithms and utilize emerging quantum computing capabilities to address major scientific problems in chemical and materials sciences.
- **USER CAPABILITIES:** Research and infrastructure at the Nanoscale Science Research Centers, enabling next-generation qubit concepts, innovative quantum and classical architectures.



Plasma-Based Research Supported by Basic Energy Sciences 1980s and 1990s

- In the 1980s and 1990s, BES supported research developed plasma-based processes for use-inspired analytical and synthetic applications, and plasma physics (including development of tools and scientific foundations related to fusion energy science)
- Plasma-related research was throughout the portfolios for materials, chemistry, engineering, and advanced energy project programs
- Focused on specific classes of materials (ceramics, intermetallics, photovoltaics and semiconductors) or were targeted towards specific technology or engineering topics (fusion energy, combustion, corrosion, and welding/joining)
- The advent of pulsed laser deposition for high temperature superconductor synthesis in the late 1980s spurred growth in plasma-related research in BES



Plasma Processing

During the processing of computer chips, plasmas created by microwave heating can both etch away unwanted material and lay down new material. Oak Ridge National Laboratory teamed with ASTeX, PlasmaQuest, and the University of Cincinnati to develop a new plasma source for a SEMATECH advanced plasma processing program (From a 1996 BES Report “BES Science: Serving the Present, Shaping the Future”).

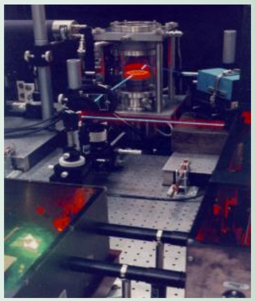
Notable Accomplishments in Plasma-Based Research 1980s and 1990s

- **Plasma source ion implantation** (PSII, LANL) to directly implant ions for surface modification and as a method for generating graded interfaces to enhance the adhesion of surface coatings
- Development of **Inductively Coupled Plasma/Mass Spectrometry** (Ames Lab) for elemental analysis of metals (commercialized and used in >17,000 analytical labs worldwide)
- Developments related to **high repetition rate plasmas for X-ray lithography** (LLNL)
- Development of tunable lasers and amplifiers used for inertial confinement fusion by LLNL was based on BES-supported basic research on **excited state absorption mechanisms** of Cr ions and isoelectronic V ions in various crystalline hosts
- Development of degenerate **four wave mixing technique** to monitor non-equilibrium concentrations of certain important species in plasmas used for materials processing (Stanford)
- SNL developed the first detailed model of the **Chemical Vapor Deposition** process ("Surface Chemkin" and reacting flow software) as well as in situ diagnostic tools to obtain a detailed understanding of semiconductor growth chemistry
- Demonstration that **inductively coupled plasma** that is essentially **containerless** can be used to grow **high purity ceramic oxide** crystals at temperatures >2000 K - use of real-time video monitoring coupled with computer controlled crystal motion allowed precise positioning of the crystal to preserve the shape during crystal growth (Ames Lab)
- Development of **arc plasma spraying for growth of ohmic contacts** for solar cells (small business research)

Solid-State Lighting

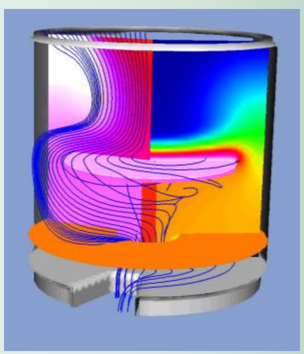
BES Basic Science

Detailed mechanistic research on semiconductor deposition



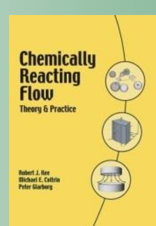
In-situ diagnostics of growth chemistry

UHV surface studies



First detailed model of coupled gas-phase / surface chemistry and transport in CVD (Chemkin software)

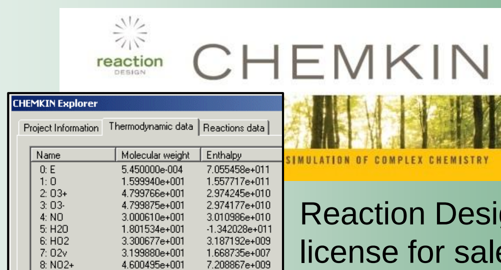
Silicon CVD chemistry research (~4,800 citations)



Sandia National Laboratories

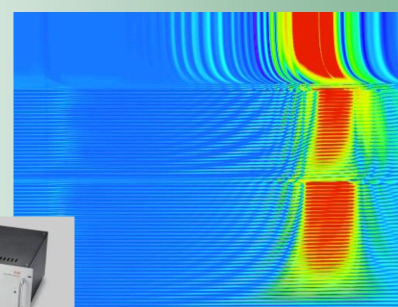
Applied R&D

Software and in-situ diagnostic tools licensed & commercialized



Name	Molecular weight	Enthalpy
0: E	5.450000e-004	7.055458e+011
1: O	1.599940e+001	1.557717e+011
2: O3+	4.799766e+001	2.974245e+010
3: O3-	4.799875e+001	2.974177e+010
4: NO	3.000610e+001	3.010986e+010
5: H2O	1.801534e+001	-1.342028e+011
6: HO2	3.300677e+001	3.187192e+009
7: O2v	3.199880e+001	1.668735e+007
8: NO2+	4.600495e+001	7.208867e+009

Reaction Design license for sales & support of Chemkin



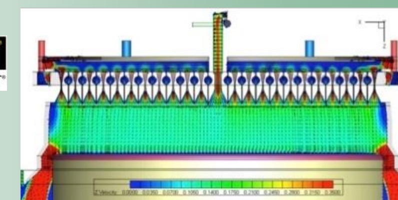
R&D 100 Award

In-situ monitor licenses: Filmetrics, LayTec, K-Space, and Emcore

Manufacturing (EERE)

New MOCVD systems and models of the growth process enable improved manufacturing and material properties

ANSYS FLUENT

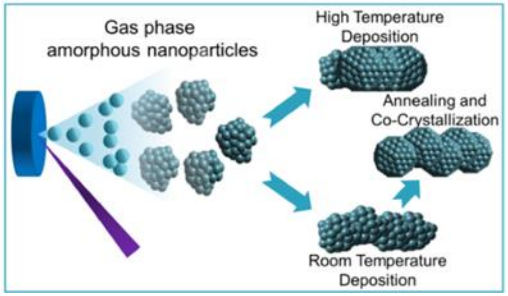


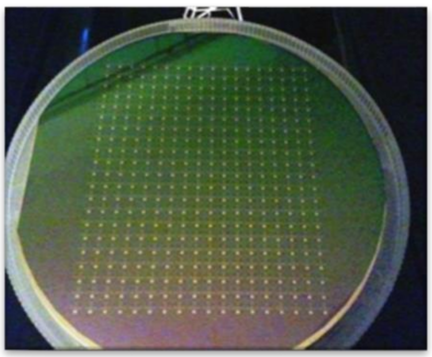
Sandia transferred modeling and *in situ* monitoring expertise to Veeco

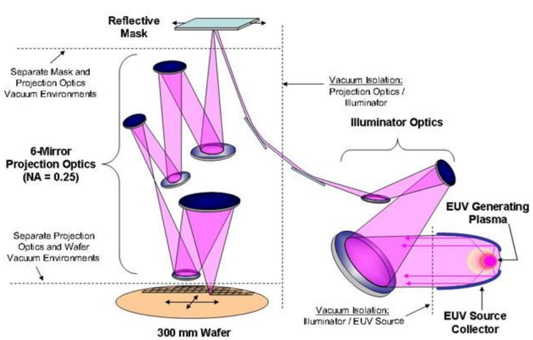
New reactor design improved throughput and reproducibility.

Veeco new 465i reactor enables~70% reduction in epi-materials growth cost.

Current BES Plasma-Related Research

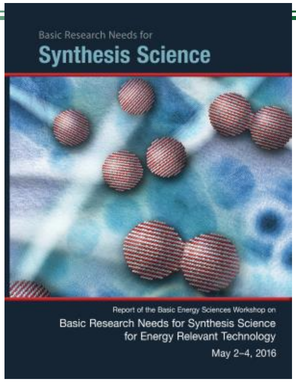


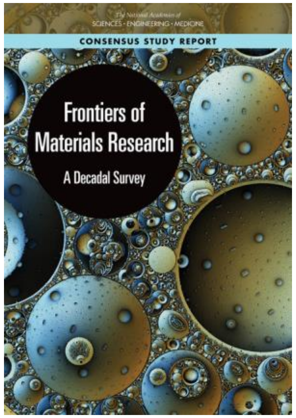


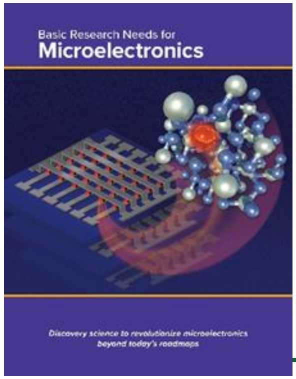


- BES-supported research related to plasma-based processes focuses on scientific foundations and use of plasma techniques as tools
  - Synthesis and processing science, laser sources, characterization tools and diagnostics, theory, combustion science, and catalysis
  - Plasma-based fabrication of materials used for investigations of other scientific phenomena
  - LCLS end station, Matter in Extreme Conditions, provides opportunities for high energy density plasma research
- Recent development and commercialization of low-temperature diamond deposition technology that began in materials science research, was further developed by the Center for Nanoscale Materials, ANL
- Industrial use of the EUV Lithography facility at the Advanced Light Source to develop new advanced nanoelectronic manufacturing capability

Looking Towards the Future of Plasma Sciences in BES







New plasma synthesis and related capabilities are discussed in recent DOE-BES Basic Research Needs and Academy reports

- 2016 BES Report on Basic Research Needs in Synthesis Science
  - Use of high-energy plasmas as new synthesis methods for kinetic trapping of atoms and/or molecules in metastable configurations
  - Synthesis under extreme or non-equilibrium conditions (e.g., plasmas) for understanding phenomena beyond thin film growth
  - New characterization and modeling methods to probe reactions in far-from-equilibrium conditions
- 2019 National Academy materials decadal report
  - Synthesis methods under extreme conditions with in situ characterization of reactions coupled to computational modeling for real-time control of synthesis
- 2019 BES Report on Basic Research Needs for Microelectronics
  - Plasma processing techniques have been widely used in semiconductor manufacturing and will likely play a role in addressing the future priority research directions identified in this report

DOE Office of Basic Energy Sciences: Scientific User Facilities

- Available to all researchers ***at no cost*** for non-proprietary research, regardless of affiliation, nationality, or source of research support
- Access based on external peer merit review of brief proposals
- Coordinated access to co-located facilities to accelerate research cycles
- Collaboration with facility scientists an optional potential benefit
- Instrument and technique workshops offered periodically
- A variety of on-line, on-site, and hands-on training available
- Proprietary research may be performed at full-cost recovery

Light Sources

- Advanced Light Source (LBNL)
- Advanced Photon Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source-II (BNL)
- Stanford Synchrotron Radiation Laboratory (SLAC)

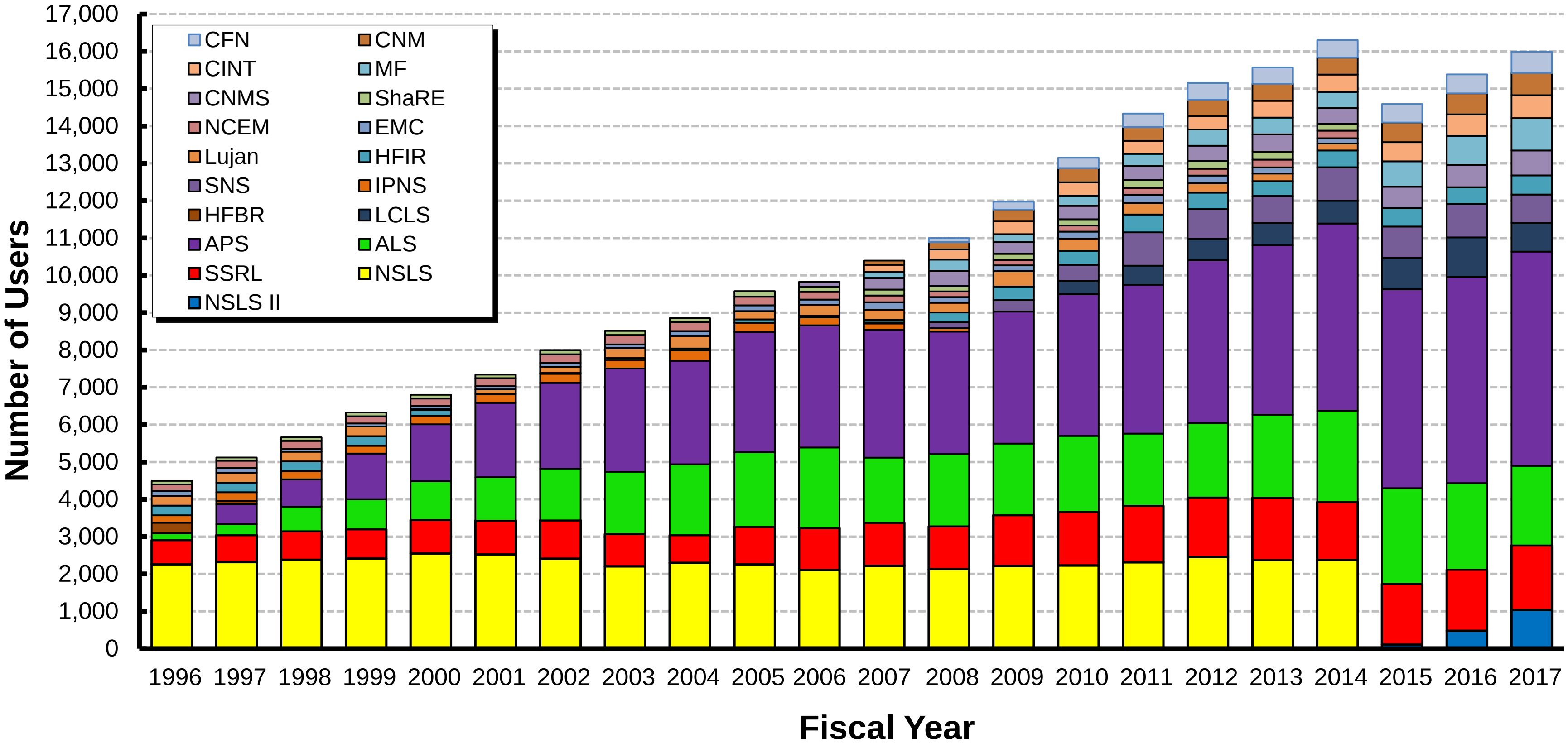
Neutron Sources

- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)

Nanoscale Science Research Centers

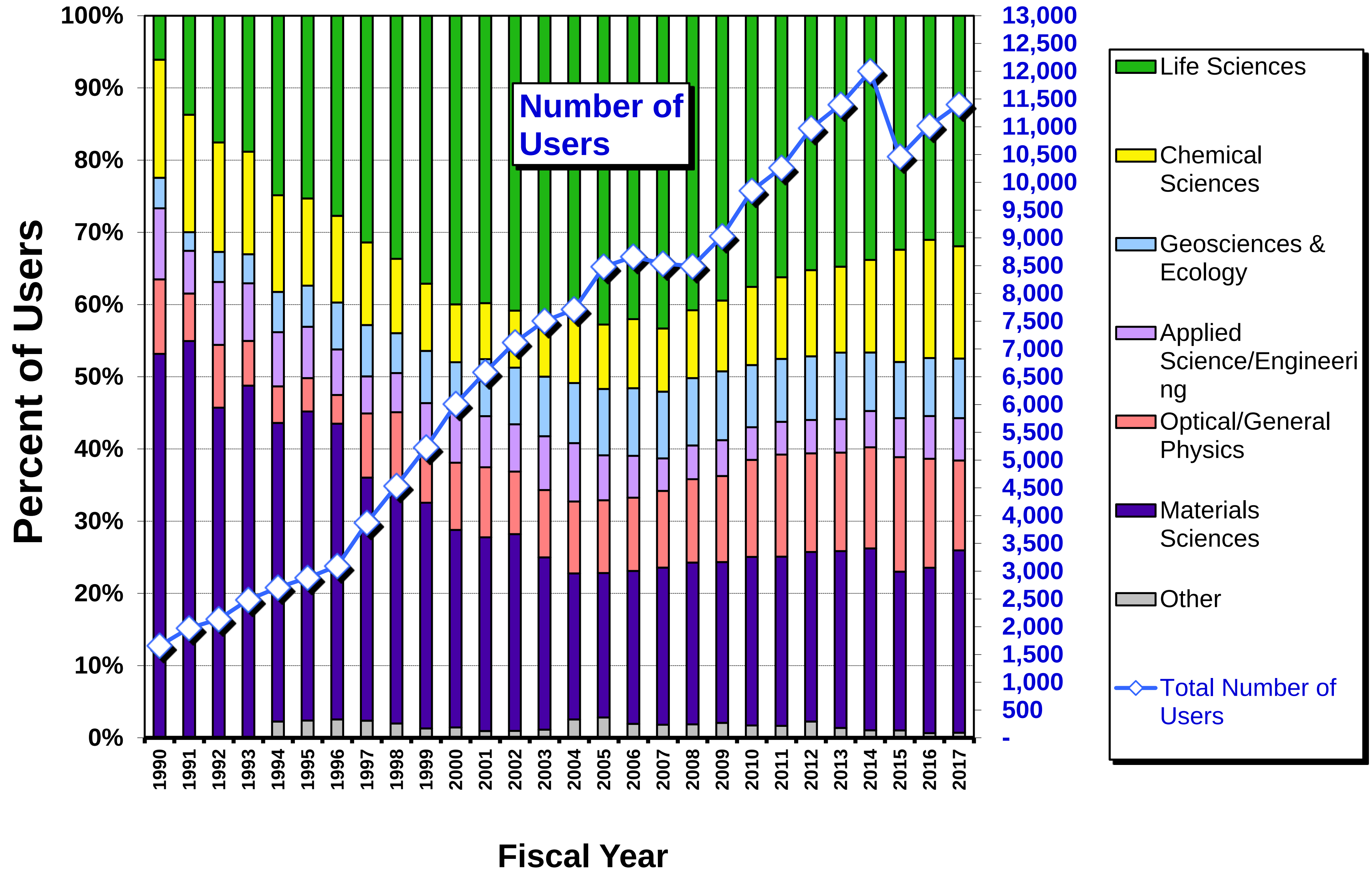
- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL & LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)

BES User Facilities Hosted Nearly 16,000 Users in FY 2017



- The newly constructed NSLS-II started early operations in FY 2015 (hosted 110 users); NSLS closed on 9/30/14.
- The three electron beam microcharacterization centers were merged administratively with their respective neighboring NSRCs in FY 2015.
- BES operations at the Lujan Neutron Scattering Center ceased in FY 2014.

Users by Discipline at the Light Sources



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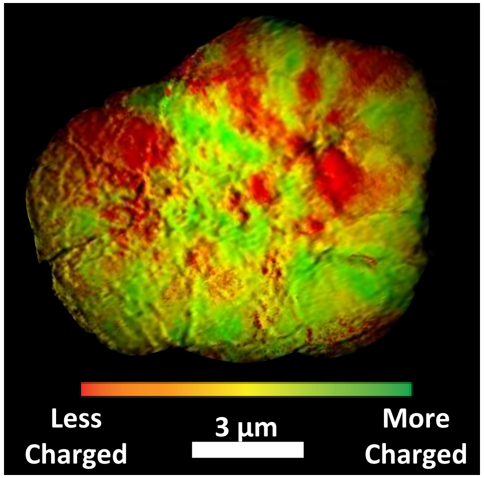
Motivation: Desire to Probe Nature at Atomic Lengths (Å) & Time Scales (fs)

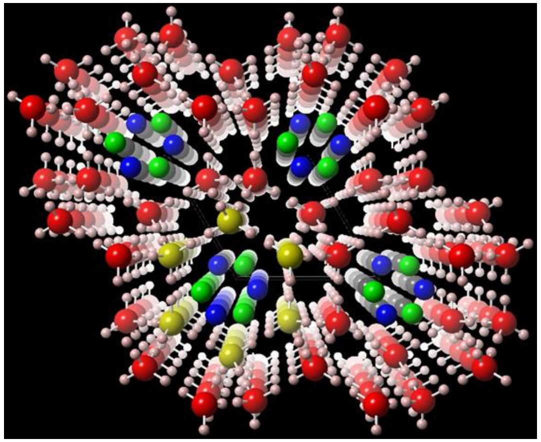
Seeing the Invisible in Real Materials



Compositional heterogeneity in $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ battery hundreds of hours after charging

Adv. Materials (2016)

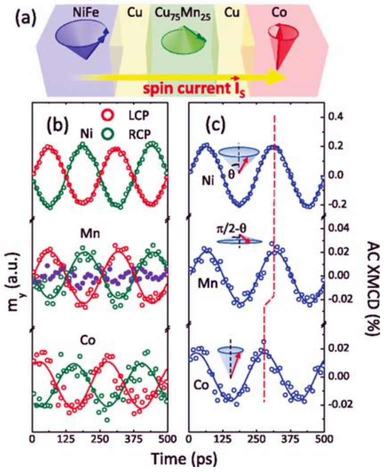
Where are the Atoms?



Newly discovered structure of a hydrogen-stuffed, quartz-like form of ice

JACS (2016)

Where are the Electrons & Spins?



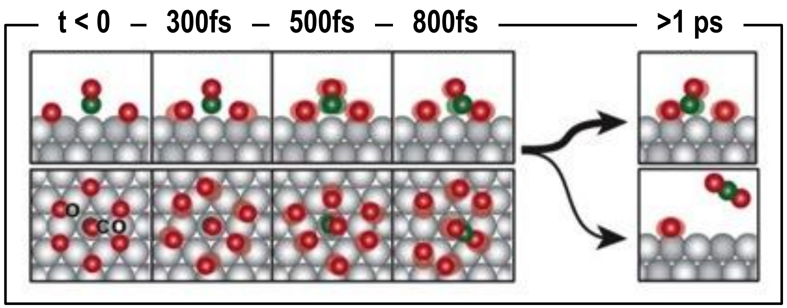
Direct measurements of "pure" ac spin currents (flow of spin angular momentum without flow of charge)

PRL (2016)

What are the Dynamics?

Capturing the transient behavior of catalytic bond formation

Science (2015)



Light Sources: Global Race to the Top

60+ Facilities Worldwide and Growing

Neutron Scattering Facilities Worldwide:
Reactors & Spallation Sources

US Neutron Scattering Facilities

European Neutron Scattering Facilities

Asian Neutron Scattering Facilities

BESAC Report on Facility Upgrades (June 2016)

Project	ANL APS-U	LBNL ALS-U	ORNL SNS PPU	ORNL SNS STS	SLAC LCLS-II	SLAC LCLS-II-HE
Proposed Project	Hard X-ray ~Diffraction Limited 6 GeV MBA Ring	Soft X-ray ~Diffraction Limited 2 GeV MBA Ring	Proton Power Upgrade to 2.5 MW (W Target) 1.3 GeV SC Linac	High Resolution Neutron Science; Second Target Station	High Rep-Rate, Soft X-ray FEL, 4 GeV SC Linac	High Rep-Rate, Medium Energy X-ray FEL, 8 GeV SC Linac
Current Status of Facility	APS is operational since 1996; ring will be replaced	ALS is operational since 1993; ring will be replaced	SNS Linac is operational since 2006 at 0.94 GeV	SNS is operational since 2006	LCLS is operational since 2010; LCLS-II is under construction	LCLS is operational since 2010; LCLS-II is under construction
Worldwide Competition	EU **ESRF** Germany **PETRA3,4** Japan **SPring-6** China **HEPS**	Sweden **MAX-IV** Brazil **SIRIUS** CH **SLS-II**	EU **ESS** Japan **JPARC** China **CSNS** UK **ISIS**	EU **ESS** Japan **JPARC** China **CSNS** UK **ISIS**	EU **XFEL** Japan **SACLA** Korea **PAL XFEL** CH **Swiss FEL**	EU **XFEL** China **SCLF**
Status Q2/19	CD-2 CD-3B	CD-1	CD-1 CD-3A	CD-0	CD-3	CD-1
FY19 Approp	✓	✓	✓	✓	✓	✓

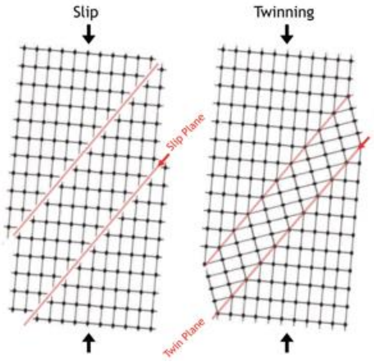
LCLS is a 2-mile long atomic & molecular camera with a femtosecond "shutter speed"

LCLS operates 24 hours/day with 95% beam availability as an open-access User Facility for the DOE Office of Science

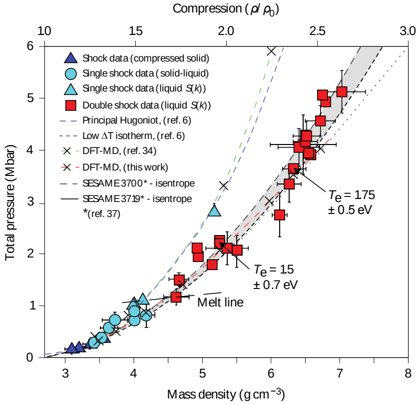
MEC has delivered a wide range of quantitative and impactful science, in the "extreme materials" and "dense plasma" areas

Shock formation of diaplectic glass

Observing twinning deformation

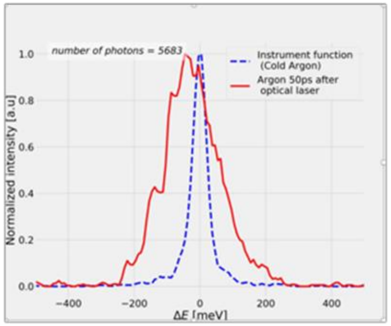


WDM EOS

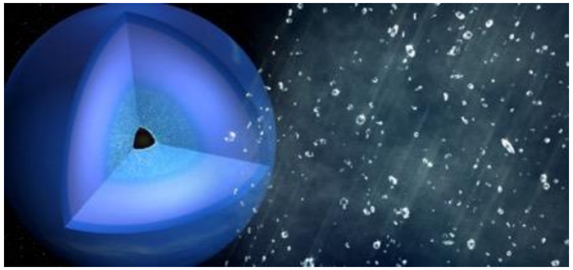


Al

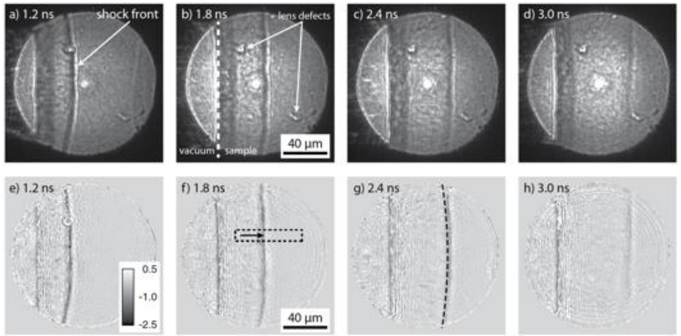
Ion feature in dense plasma



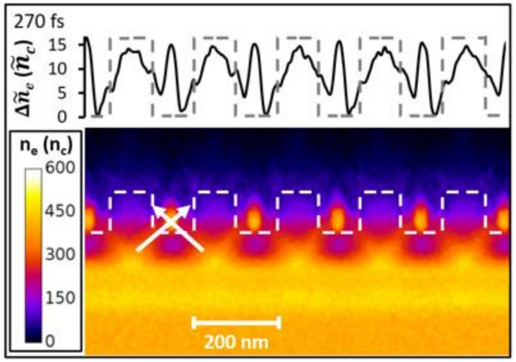
"Diamond rain" induced and observed in the lab (replicating Neptune)



Imaging shock waves in solid matter



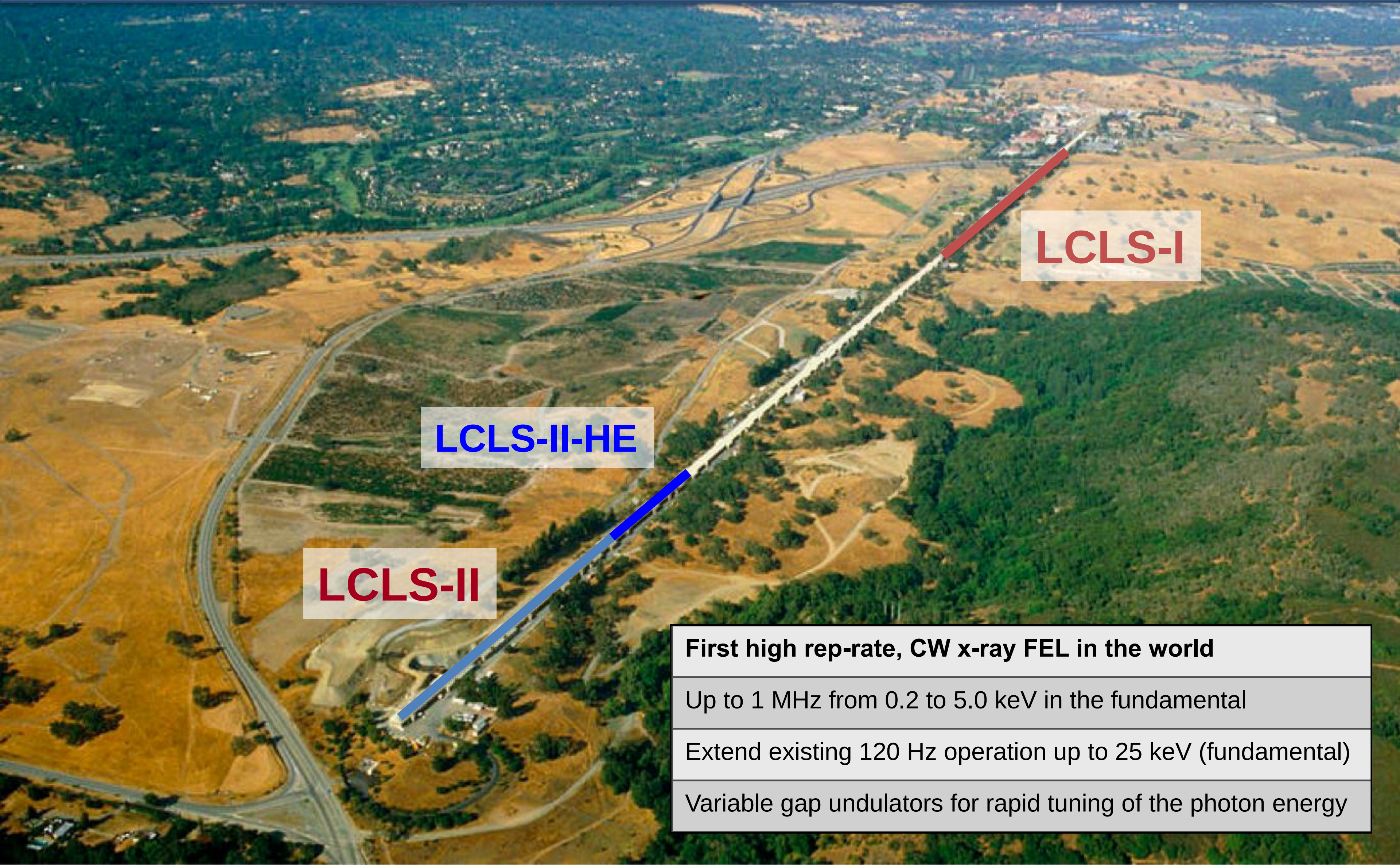
Nanostructured dense plasma feature evolution observed by SAXS



Example application areas at LCLS

- **LCLS provides a platform for studying beam-plasma interactions that are of fundamental interest, and have applications in areas such as:**
- **Physics of ICF**
- **Plasma/wall interactions for fusion reactors**
- **High strain-rate, high-pressure material science, with applications for fusion, NNSA, geo-science, and extreme industrial applications (e.g. experiments conducted at LCLS by Rolls-Royce PLC).**
- **Basic science exploration of particle beam generation, with potential for medical imaging and hadron therapy.**
- **Development of high brightness sources of secondary radiation with application in industrial and security imaging**
- **Exploration of next-generation particle accelerators for light source and/or HEP applications.**

Future Outlook: LCLS-II will increase the X-ray repetition rate from 120 Hz to 1 MHz, bringing transformative capabilities to the fields of atomic, chemical, material and plasma science

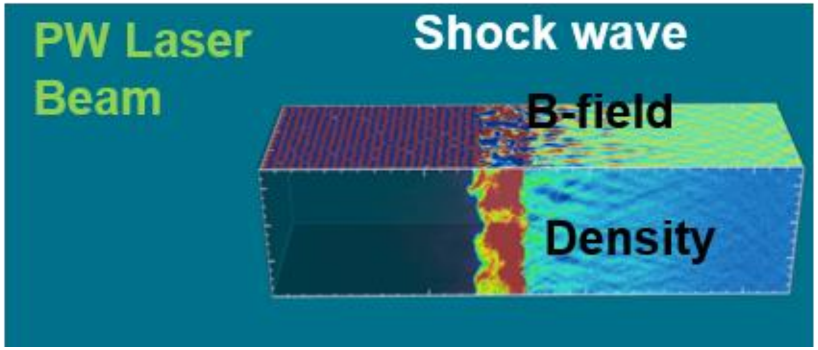


First high rep-rate, CW x-ray FEL in the world
Up to 1 MHz from 0.2 to 5.0 keV in the fundamental
Extend existing 120 Hz operation up to 25 keV (fundamental)
Variable gap undulators for rapid tuning of the photon energy

Future Outlook: the addition of a Petawatt Laser at LCLS will access important physics regimes

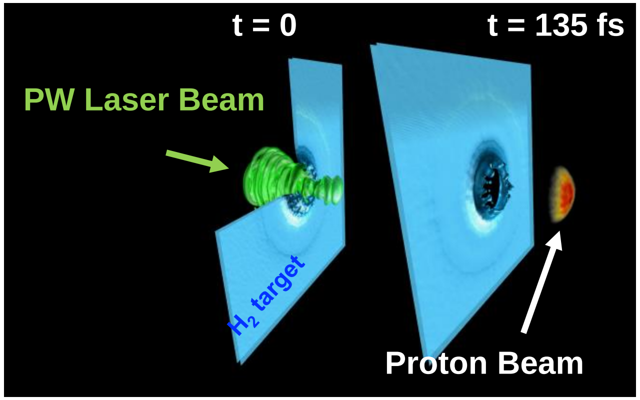
Basic Plasma Science

- Probe relativistic shocks at the nanoscale using the ultrafast, coherent X-ray beam



Extreme Conditions

- Create ion beams for stopping power measurements in well-characterized plasmas



Materials for Fusion Research

- Resolve damage cascade on the atomic scale for the first time