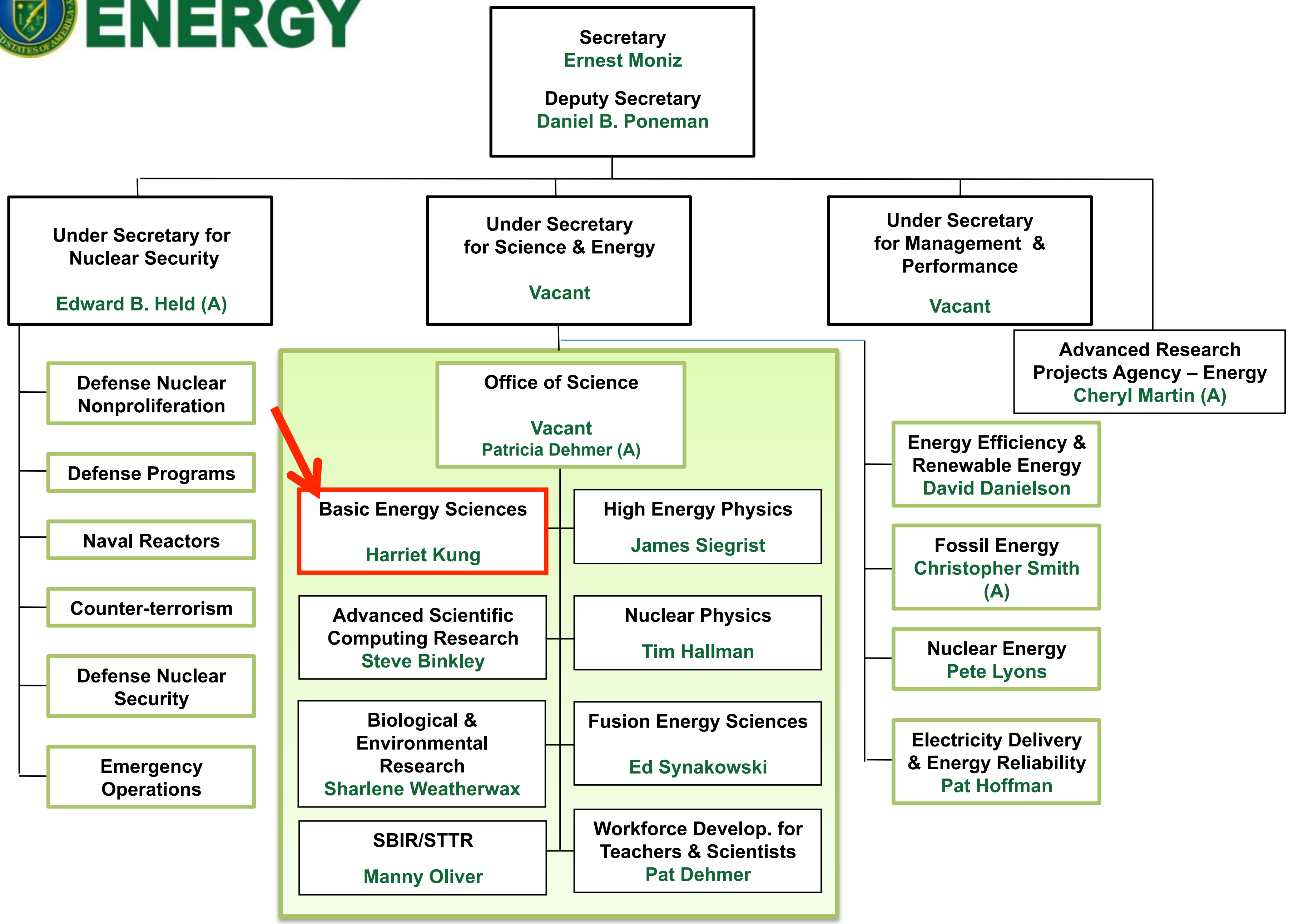
U.S. DEPARTMENT OF ENERGY | Office of Science

Computing in Basic Energy Sciences

Large Scale Production Research and Storage Requirements for Basic energy Sciences

October 8, 2013

Jim Davenport
Program Manager - Theoretical Condensed Matter Physics
Office of Basic Energy Sciences



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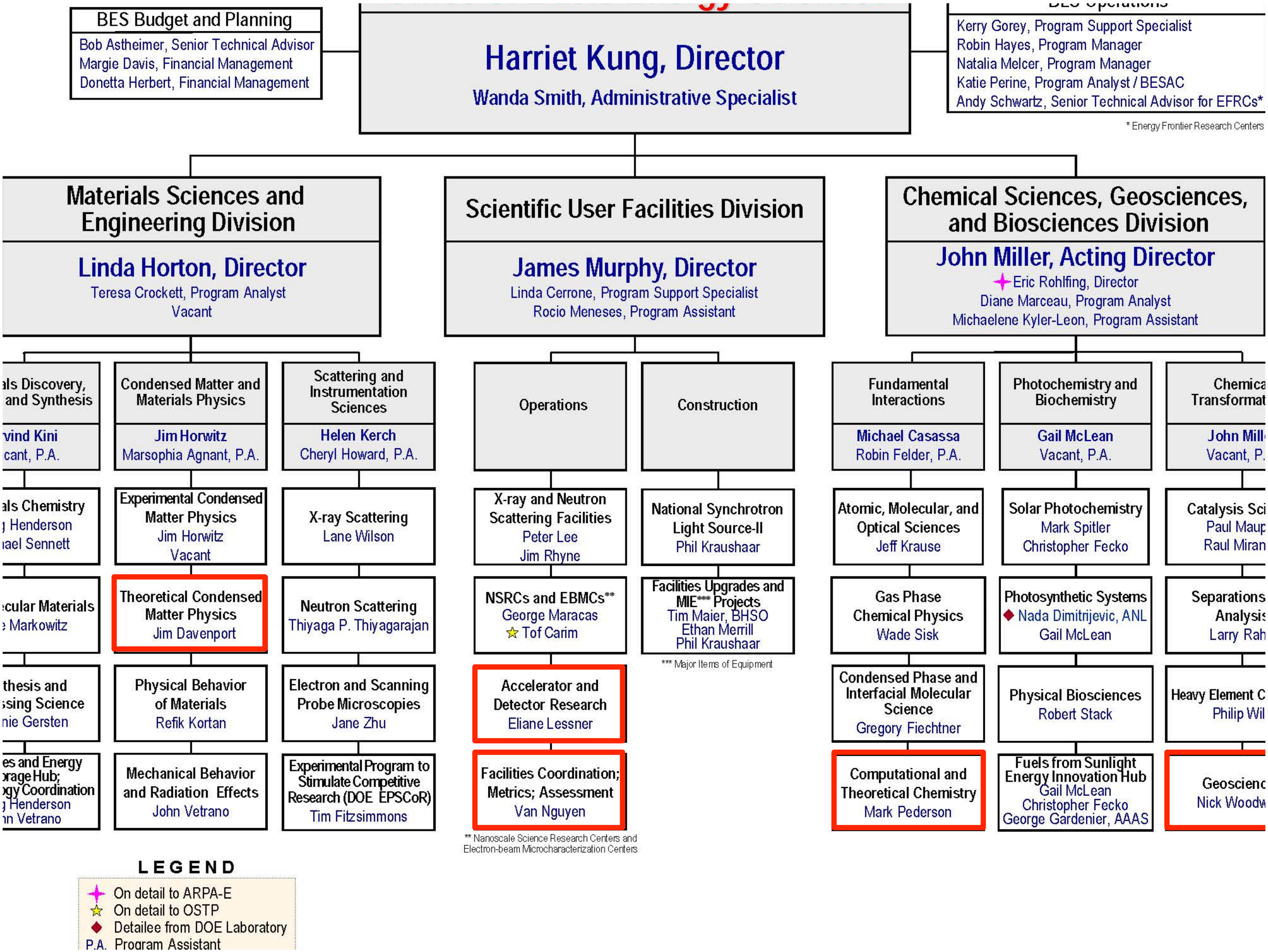

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Refik Kortan
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Jane Zhu
Accelerator and Detector Research
Eliane Lessner
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Physical Biosciences
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Mechanical Behavior and Radiation Effects
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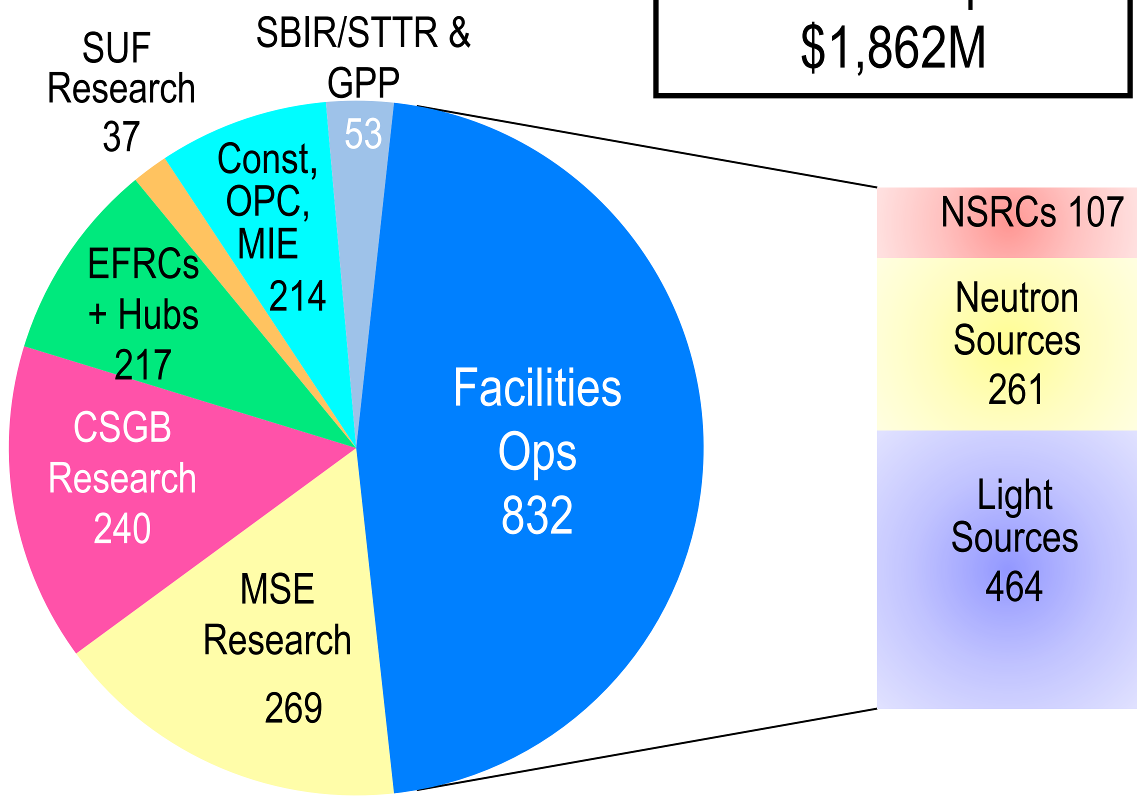
Experimental Program to Stimulate Competitive Research (DOE EPSCoR)
Tim Fitzsimmons
Facilities Coordination; Metrics; Assessment
Van Nguyen
** Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers
Computational and Theoretical Chemistry
Mark Pederson
Fuels from Sunlight Energy Innovation Hub
Gail McLean
Christopher Fecko
George Gardenier, AAAS
LEGEND
On detail to ARPA-E
On detail to OSTP
Detailee from DOE Laboratory
P.A. Program Assistant

FY 2014 BES Budget Request

- Research programs
  - Energy Innovation Hubs
  - Energy Frontier Research Centers
    - One-time $68.7M
  - Core Research
- Scientific user facilities
  - Optimum operations of facilities
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers
  - NSLS-II Early Operations ($69M)

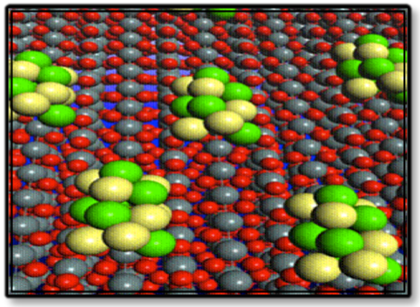
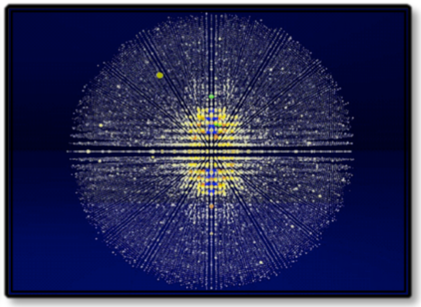
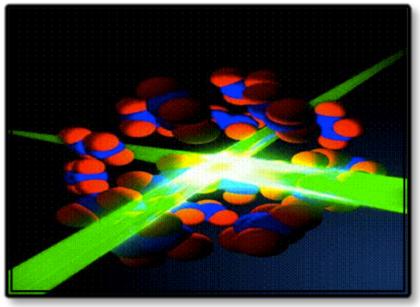
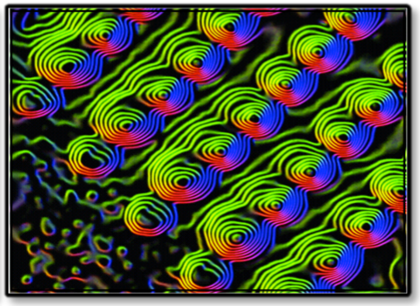
FY 2014 Request: $1,862M



- Construction and instrumentation
  - National Synchrotron Light Source-II
  - NSLS-II instrumentation (NEXT)
  - Advanced Photon Source upgrade
  - Linac Coherent Light Source-II

Basic Energy Sciences Mission
Focus on Transformational Science

- **Fundamental research** to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels
- Provide the **foundations for new energy technologies** to support DOE's missions in energy, environment, and national security
- Plan, construct, and operate world-leading scientific user **facilities** for the Nation

Basic Energy Sciences

The Program:

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

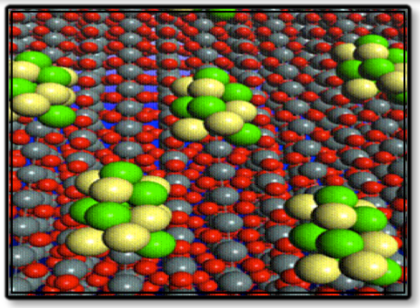
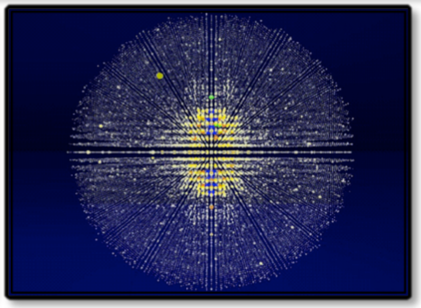
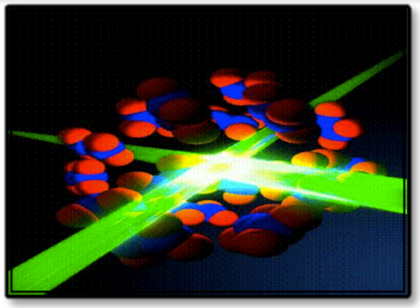
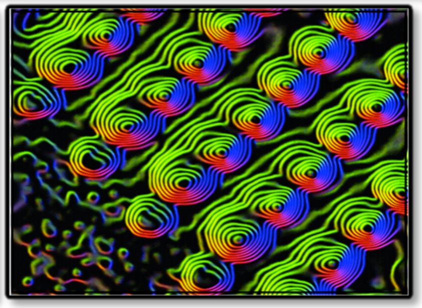
Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

Supporting:
- 46 Energy Frontier Research Centers
- Solar Fuels and Batteries and Energy Storage Hubs
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

The Scientific Challenges:

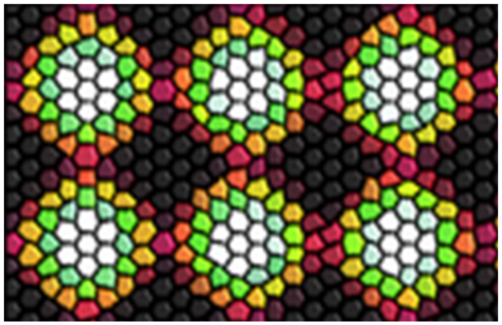
- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials and chemical 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

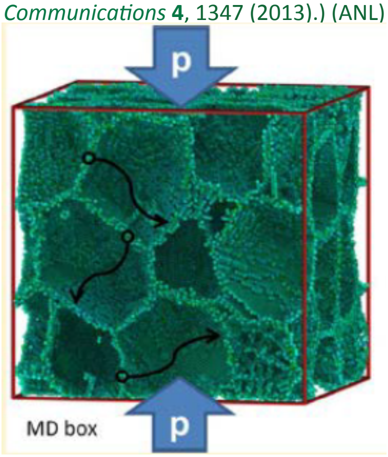





Condensed Matter and Materials Physics

Control and understanding of materials behavior and discovery of new emergent phenomena



Calculations of the distribution of superconductivity around nano-dimensioned holes (white) in a thin sheet of superconducting film in a magnetic field. Green indicates strong superconductivity. (R. Córdoba et al., *Nature Communications* **4**, 1347 (2013).) (ANL)

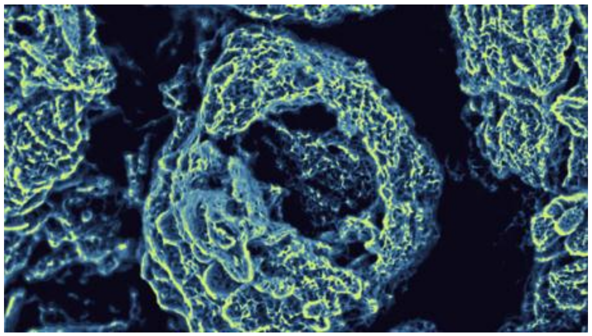


Deformation of nanocrystalline materials during irradiation (Ashkenazy and Averback, *NanoLetters* 12, 4084 (2012)) (UI-UC)

- **Experimental Condensed Matter Physics**
  - Fundamental understanding of the relationships between intrinsic electronic structure and the properties of complex materials
- **Theoretical Condensed Matter Physics**
  - Theory, modeling, and simulation of electronic correlations, emphasizing nanoscale science and materials by design
- **Mechanical Behavior and Radiation Effects**
  - Experimental and modeling studies of defects in materials and their effects on the properties of strength, structure, deformation, and failure.
- **Physical Behavior of Materials**
  - Behavior of materials in response to temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces.

Materials Discovery, Design, and Synthesis

Rational design and synthesis of materials via physical, chemical, and bio-molecular routes



Microsized pores and tunnels in the electrode facilitate free flow of oxygen molecules; nanosized pores provide sites for lithium-oxygen reactions. (Image courtesy of PNNL)

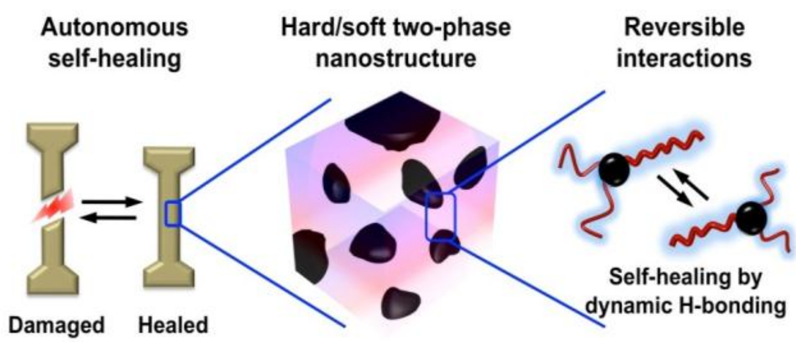
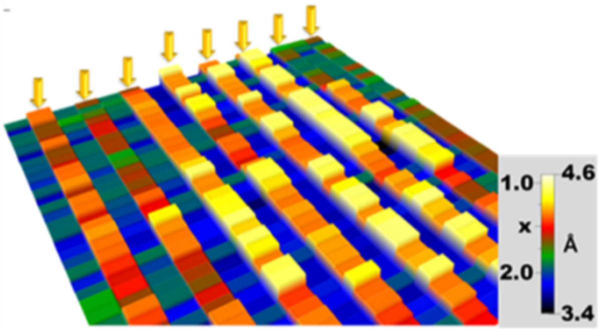


Illustration of self-healing in a fractured polymer via dynamic hydrogen bond interchange without external help from light, heat, or added healing agents
(Image courtesy of Zhibin Guan, UC Irvine)

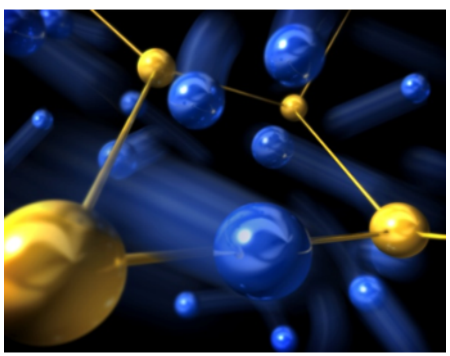
- **Synthesis and Processing Science**
  - Learn to control synthesis and processing by developing scientific foundations, *in situ* studies, and for a wide range of materials
- **Materials Chemistry**
  - Nanoscale chemical synthesis and assembly; solid state chemistry; novel polymeric materials and complex fluids; surface and interfacial chemistry
- **Biomolecular Materials**
  - Discovery, design and synthesis of biomimetic and bioinspired functional materials and energy conversion processes based on principles and concepts of biology

Scattering and Instrumentation Sciences

Study of photon, neutron, and electron interactions with matter for characterization of materials structures and excitation



Oxygen vacancy maps show overall composition and degree of oxygen order. Oxygen inhomogeneity (sidebar color scale) is high in oxygen-deficient perovskite. (Kim et al., *Nature Materials* **11**, 888–894 (2012)) (ORNL)



Depiction of superionic phase of copper (blue) diffusing through the sulfur (yellow) sublattice. (Miller et al., *Nature Communications* **4**, 1369 (2013)) (SLAC)

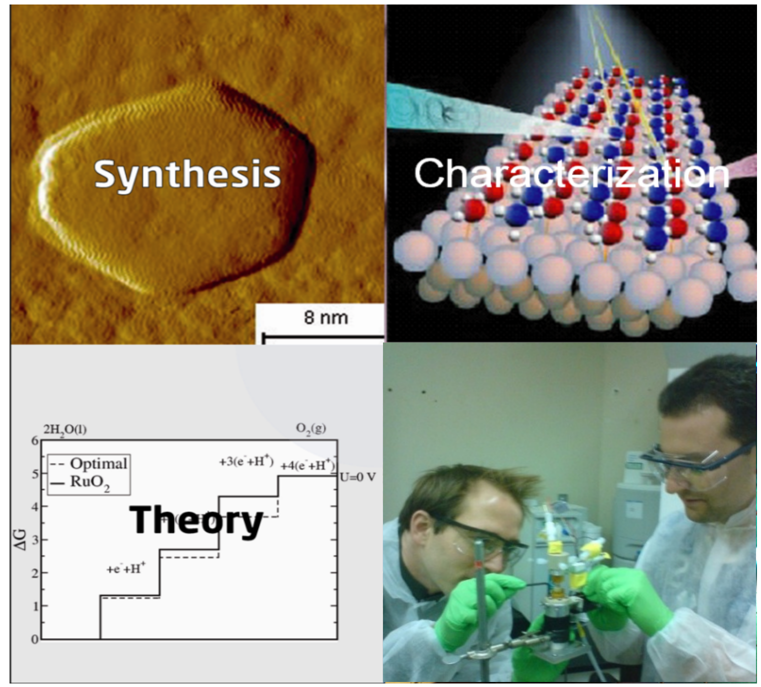
- **Elucidate the mechanisms that control superconductivity and other phenomena in correlated electron systems**
  - Use scattering probes to determine important correlations (spin, lattice, charge, orbital) that govern superconductivity, magnetism, and other phenomena.
- **Develop a structural, dynamical, and functional understanding of materials**
  - Understand the interplay between properties and structure spanning multiple energy, length, and time scales and develop new tools that interrogate atomic to mesoscale.
- **Understand the behavior of materials using Ultrafast Diffraction, Spectroscopy and Imaging Techniques**
  - Understand how entities form, grow, and move under the influence of external fields, and understand functionality.
- **Unify the complementary information obtained through multiple techniques**
  - Develop the capability to analyze, visualize, and understand data from different experimental probes.

Chemical Sciences, Geosciences and Biosciences

…supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use

- Quantum mechanical understanding of matter
- Atomistic & molecular level tailoring/control of chemical reactions
- Nanoscale revolution

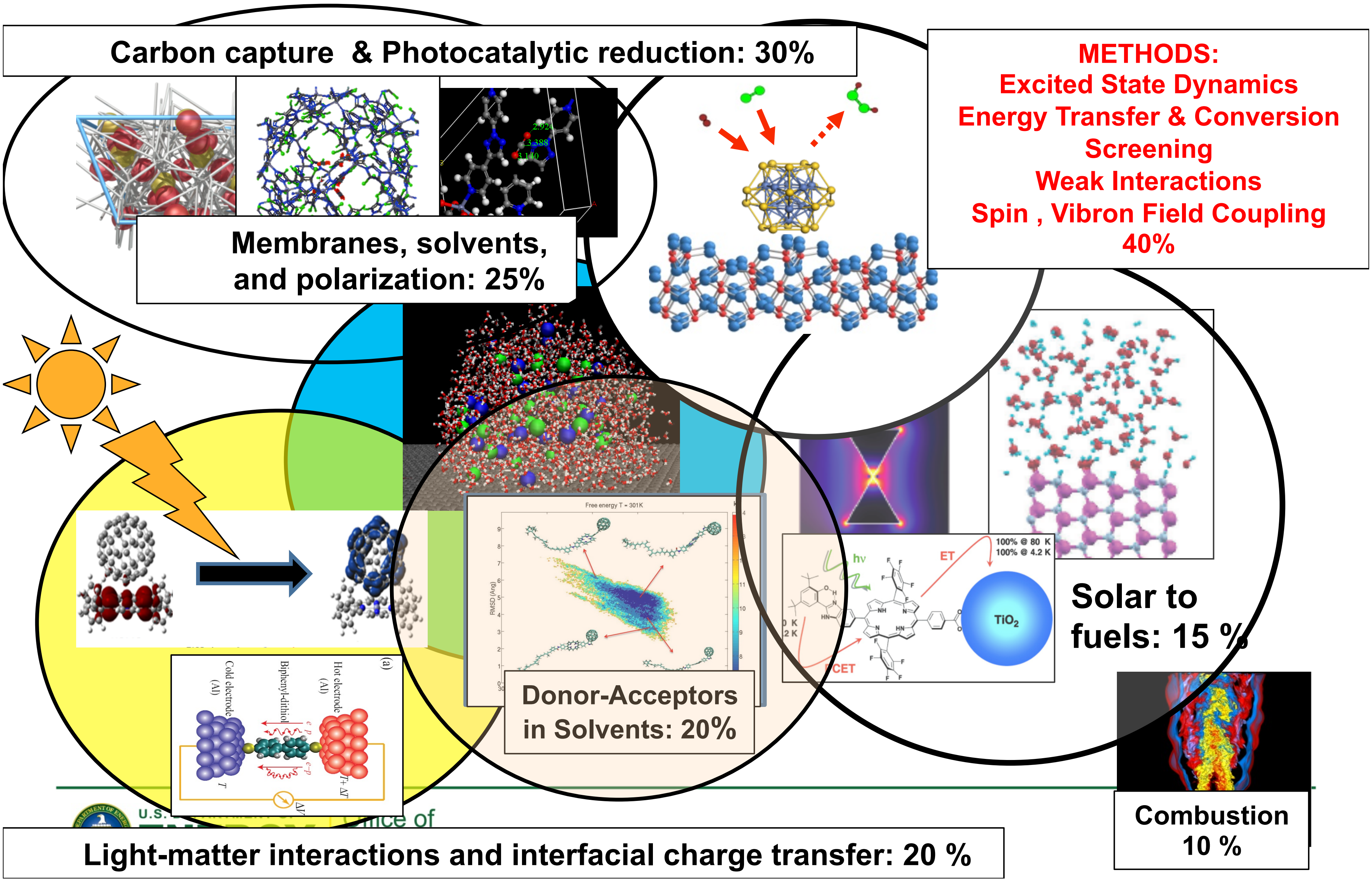
- Efficient & clean combustion
- New & improved photo-conversion processes
- Improved catalysts for production of new fuels and chemicals
- Better separation processes
    - Energy processes
    - Environmental Remediation
    - Waste Management



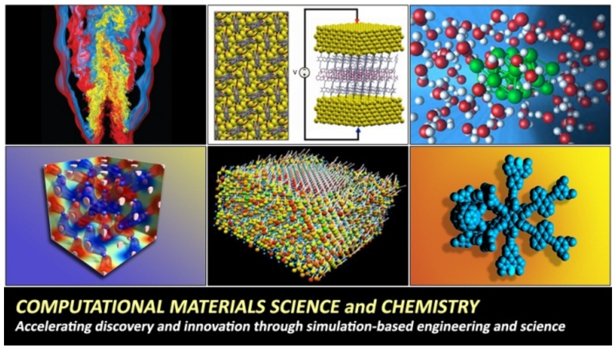
A Snapshot of the Computational and Theoretical Chemistry program

For more information see: http://science.energy.gov/bes/csgb/research-areas/computational-and-theoretical-chemistry/

(PM: M.R. Pederson)



…understanding the quantum mechanical behavior of electrons, atoms, and molecules in the 20th century allows for control of molec & chem processes…



New Computational Architectures

$$H\Psi=\lambda\Psi$$

$$F=MA$$

New Techniques

- Applied Math
- Computational Techniques
- Scientific Knowledge
- Experimental Verification

- Magnetism
- Superconductivity
- Separations
- Photovoltaics
- Energy Storage
- Combustion
- Catalysis
- Biomolecular Materials
- Light Sources
- Structural Materials
- Functional Materials
- Interfacial Transport
- Carbon Capture
- Geophysics/chemistry

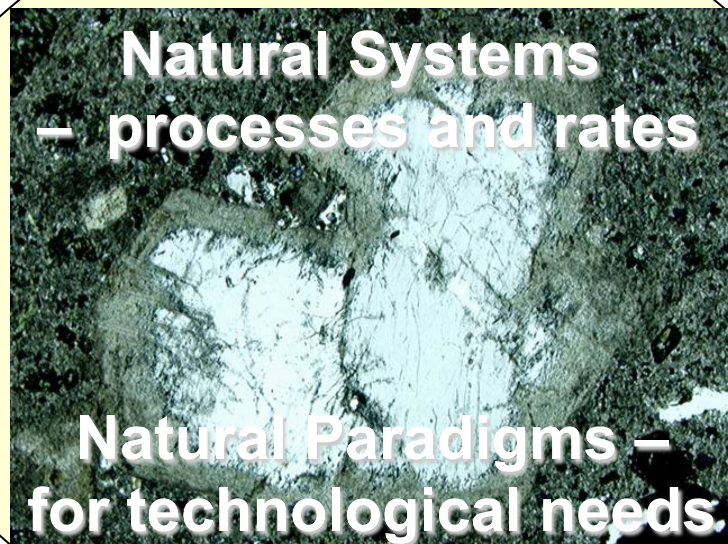
Geosciences Research Program

Rock Physics ($3.2 M)

Electrical properties
Nonlinear elasticity
Fracturing and imaging
Signatures of fluids
Attenuation and scattering
Electromagnetic inversions
Time-lapse imaging
Imaging permeability

Flow and Transport ($2.9 M)

Channelization
Fractures
Porosity evolution
Large scale transport
Coupled processes
Reactive transport
Thermal-chemical-mechanical feedbacks



Analytical Geochemistry ($3.5 M)

Synchrotron science
Mass spectrometry
Isotope geochemistry
Neutron science

Theoretical & Experimental Geochemistry $10 M)

Computational modeling
Thermodynamics
Surface geochemistry
Reactivity
Interfacial processes
Microbe-mineral interactions
Chemical imaging
Nanogeosciences

5 Energy Frontier Research Centers are based in the Geosciences Community – LBNL (DePaolo), Texas/Sandia (Pope), ORNL (Wesolowski), Carnegie Institution (Mao), Notre Dame (Burns).

Geosciences

Society, Industry and DOE all rely on the Earth to provide energy resources, or the materials to synthesize energy systems, and to be the ultimate repository of energy wastes. <u>SAFE</u> and <u>COST-EFFECTIVE.</u>

Performance assessments of energy and environmental systems can't be tested with any usual engineering approach. They have to rely upon conceptual and <u>computational predictions of those systems over long distances and geological periods of time</u> (decades to centuries to millennia) based on geological observations.

The Geosciences activity in BES focuses on:

- Developing the ability to make **critical geochemical and geophysical measurements** including improved techniques or technology
- Understanding what individual observations mean at the system scale, i.e. how to handle **spatial and temporal scaling and heterogeneity**
- Making observations of **natural systems that provide unique perspectives** on long-time-scale or long-length-scale processes

Because targeted topical research in Geosciences is funded by a number of applied programs across the Department Basic Energy Sciences funding emphasizes research that has multiple potential application areas Office of Science Broad Agency Announcement.   http://science.doe.gov/grants/pdf/SC_FOA_0000600.pdf

ASCR Subsurface Sciences Workshop

Within Geosciences Related Efforts - Models with enhanced physical realism and fewer simplifying approximations.

Conceptual Infrastructure – verification, validation, "convergence" metrics, measures for stochastic processes, benchmarks

- Uncertainty Analysis – complex, large, multi-physics, multiscale systems.
- New Algorithms for Coupled Phenomena- heterogeneities in phases, components, interactions, mixtures, better discretization, better solvers

Practical Infrastructure- data storage, programming interfaces, tools for handling large simulations and large datasets.

HPC Data Management – integration dispersed data sources, new parallel computational algorithms.

Improved Multi-Phase Flow Simulators – linkages among processes

Protocols for "Soft" Data – better assimilate "soft" data in models

New Multi-Scale Computational Tools – link scales, represent processes beyond initial parameterizations, link pore scale processes to bulk responses.

Performance Assessment-

Risk Analysis – higher-resolution analytical methods, coupling processes models, monitoring observations and risk assessment methods (Averages vs Thresholds?).

Integrated Site Characterization – conceptual model formulation, calibration, engineering design, management and decision making.

Basic Energy Sciences: Scientific User Facilities

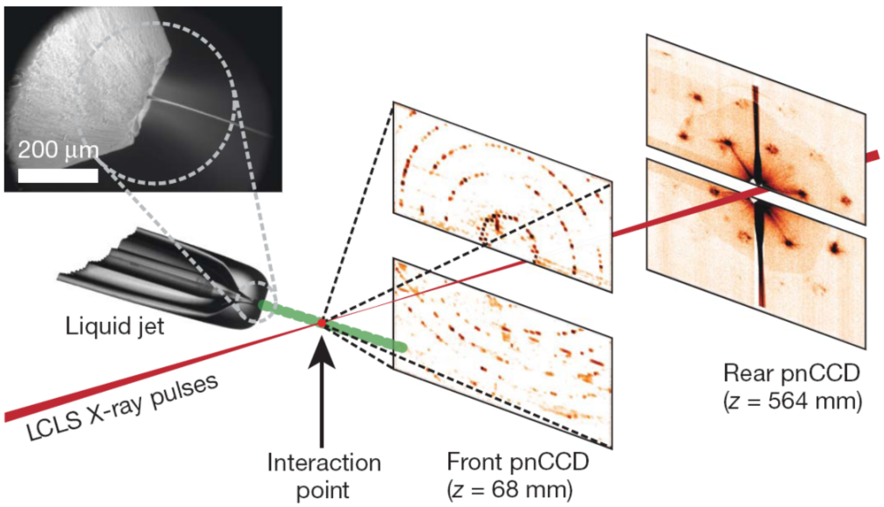
http://www.science.doe.gov/bes/suf/user-facilities

- 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

- **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)*
- **Electron-Beam Microcharacterization Centers**
  - *Electron Microscopy Center for Materials Research (ANL)*
  - *National Center for Electron Microscopy (LBNL)*
  - *Shared Research Equipment Program (ORNL)*

- **Light Sources**
  - *Advanced Light Source (LBNL)*
  - *Advanced Photon Source (ANL)*
  - *Linac Coherent Light Source (SLAC)*
  - *National Synchrotron Light Source (BNL)*
    National Synchrotron Light Source II (under construction)
  - *Stanford Synchrotron Radiation Laboratory (SLAC)*
- **Neutron Sources**
  - *High Flux Isotope Reactor (ORNL)*
  - *Manuel Lujan, Jr. Neutron Scattering Center (LANL)*
  - *Spallation Neutron Source (ORNL)*

LCLS : Femtosecond Crystallography



❖ **Low resolution structure of Photosystem I determined from ~15,000 nanocrystals**

❖ **Each crystal was illuminated sequentially and destroyed by the LCLS beam**

❖ **Dose >30 times larger than classical damage limit**

❖ **Unfortunately, low photon energy at AMO limited resolution and chance for new biology**

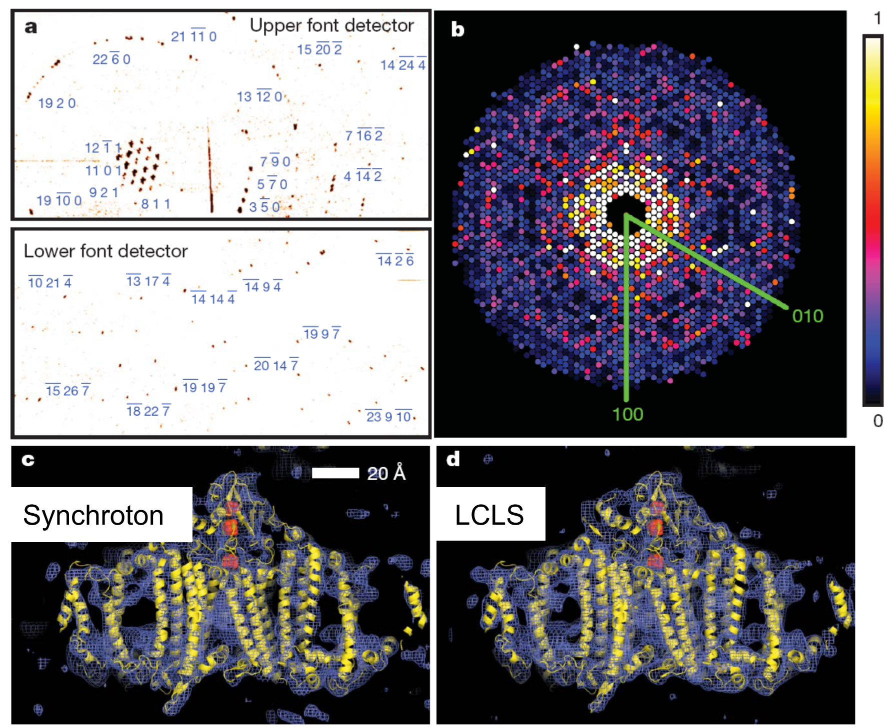
❖ **Recent experiment**
~ 18 Terabytes collected in 8 hours!

LETTER

doi:10.1038/nature09750

Femtosecond X-ray protein nanocrystallography

Henry N. Chapman[1,2], Petra Fromme[3], Anton Barty[1], Thomas A. White[1], Richard A. Kirian[4], Andrew Aquila[1], Mark S. Hunter[3], Joachim Schulz[1], Daniel P. DePonte[1], Uwe Weierstall[4], R. Bruce Doak[4], Filipe R. N. C. Maia[5], Andrew V. Martin[1], Ilme Schlichting[6,7], Lukas Lomb[7], Nicola Coppola[1]†, Robert L. Shoeman[7], Sascha W. Epp[6,8], Robert Hartmann[9], Daniel Rolles[6,7], Artem Rudenko[6,8], Lutz Foucar[6,7], Nils Kimmel[10], Georg Weidenspointner[11,10], Peter Holl[9], Mengning Liang[1], Miriam Barthelmess[12], Carl Caleman[1], Sébastien Boutet[13], Michael J. Bogan[14], Jacek Krzywinski[13], Christoph Bostedt[13], Saša Bajt[12], Lars Gumprecht[1], Benedikt Rudek[6,8], Benjamin Erk[6,8], Carlo Schmidt[6,8], André Hömke[6,8], Christian Reich[9], Daniel Pietschner[10], Lothar Strüder[6,10], Günter Hauser[10], Hubert Gorke[15], Joachim Ullrich[6,8], Sven Herrmann[10], Gerhard Schaller[10], Florian Schopper[10], Heike Soltau[9], Kai-Uwe Kühnel[8], Marc Messerschmidt[13], John D. Bozek[13], Stefan P. Hau-Riege[16], Matthias Frank[16], Christina Y. Hampton[14], Raymond G. Sierra[14], Dmitri Starodub[14], Garth J. Williams[13], Janos Hajdu[5], Nicusor Timneanu[5], M. Marvin Seibert[5]†, Jakob Andreasson[5], Andrea Rocker[5], Olof Jönsson[5], Martin Svenda[5], Stephan Stern[1], Karol Nass[2], Robert Andritschke[10], Claus-Dieter Schröter[8], Faton Krasniqi[6,7], Mario Bott[7], Kevin E. Schmidt[4], Xiaoyu Wang[4], Ingo Grotjohann[3], James M. Holton[17], Thomas R. M. Barends[7], Richard Neutze[18], Stefano Marchesini[17], Raimund Fromme[3], Sebastian Schorb[19], Daniela Rupp[19], Marcus Adolph[19], Tais Gorkhover[19], Inger Andersson[20], Helmut Hirsemann[12], Guillaume Potdevin[12], Heinz Graafsma[12], Björn Nilsson[12] & John C. H. Spence[4]



Accelerator and Detector Research

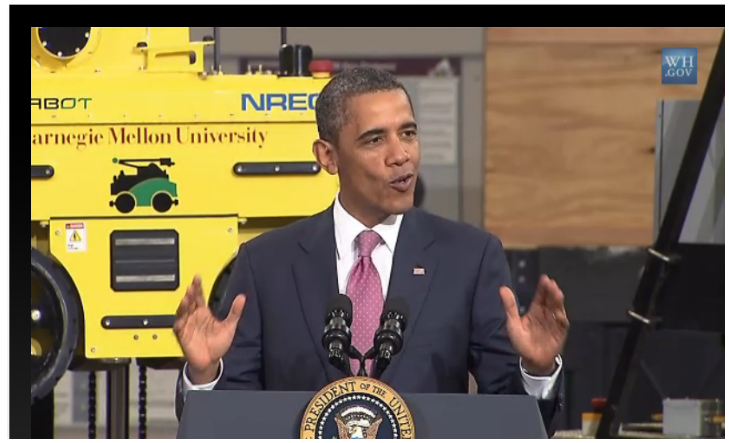
- **Accelerator and Detector Research activities include:**
  - support of existing facilities to guarantee their continued performance excellence and provide improved operating capabilities.
  - support of future light sources and neutron sources through innovative concepts, modeling, and design and testing of accelerator component prototypes.
  - support of detectors capable of acquiring x-ray and neutron scattering data that will match the requirements of the fast advancement of x-ray and neutron sources.
  - support of next generation of x-ray optics instruments to advance photon-based science.

Announcement of Materials Genome Initiative

National Science and Technology Council Office of Science and Technology Policy

http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

A Renaissance in American Manufacturing President Obama Speech on June 24, 2011



*President Obama kicks off the **Advanced Manufacturing Partnership** (AMP), a national collaboration between the government, industries, and universities to invest in cutting-edge technologies, create new jobs and bring about a renaissance in American manufacturing. As part of his new AMP, the President is announcing an ambitious plan, the **Materials Genome Initiative**, to <u>double the speed with which we discover, develop, and manufacture new materials.</u>*

FY 2012 SC Computational Materials Science Awards in Support of Materials Genome Initiative

BES Predictive Theory & Modeling ~$13.5M/year, 3 - 5 year awards, + ~ $4 million for equipment

- **5 Software Innovation Centers, 2 glue, 12 small group – single investigator awards**
  - Next generation electronic structure
  - Excited states, electron correlation
  - High throughput computational techniques, data management
  - Optical, thermoelectric properties of oxides, multi-phase materials, grain boundaries, self-assembly
  - Reaction pathways, catalysis, combustion

BES/ASCR SciDAC

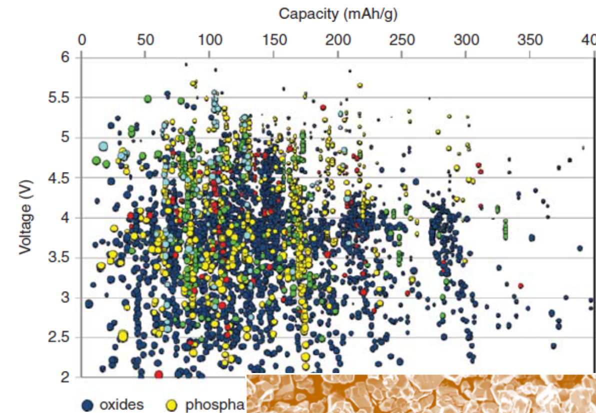
- **7 Awards, ~$6M/year, 5 years (split with ASCR)**
  - Improved quantum chemistry, quantum Monte Carlo and molecular dynamics, photovoltaic & photocatalytic materials, solvated ions, Li-ion batteries, superconductor transport

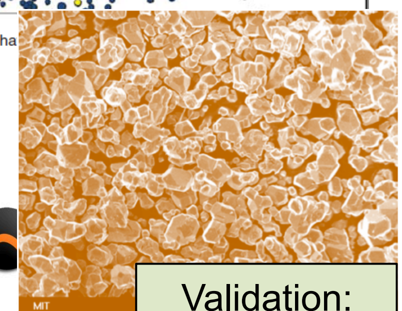
Materials and Chemistry by Design

Accelerating Discovery for Global Competitiveness

- Research to establish design rules to launch an era of predictive modeling, changing the paradigm of materials discovery to rational design.
    - New software tools and data standards to catalyze a fully integrated approach from material discovery to applications
- Discovery of new materials has been the engine driving science frontiers and fueling technology innovations. Research would utilize the powerful suite of tools for materials synthesis, characterization, and simulation at DOE's world-leading user facilities
- Integrated teams to focus on key scientific knowledge gaps to develop new theoretical models
    - Long-term: realization in reusable and broadly-disseminated software
    - Collection of validated experimental and modeling data for broader community use

Prediction: New battery materials starting from first principles theory





Validation: Materials fabrication

MATERIALS PROJECT

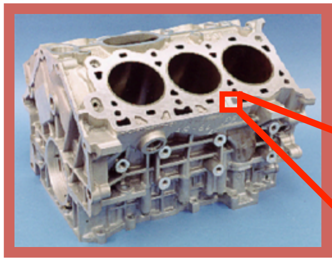
http://materialsproject.org/

End Use: Software on-line for general community use

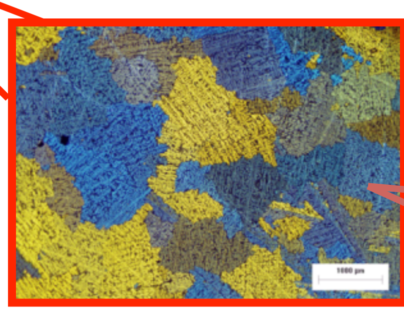
Theory, Modeling and Simulation: From Atoms to Components

Ford Virtual Aluminum Castings had to treat all these scales

Research and Advanced Engineering



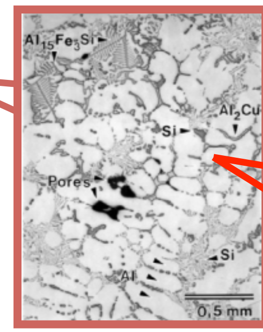
1 m
Engine Block



1 – 10 mm

Macrostructure
- Grains
- Macroporosity

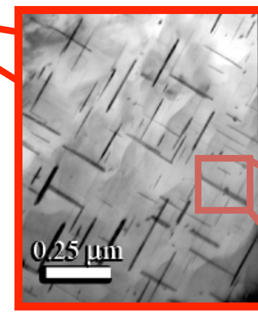
Properties
- High cycle fatigue
- Ductility



10 – 500um

Microstructure
- Eutectic Phases
- Dendrites
- Microporosity
- Intermetallics

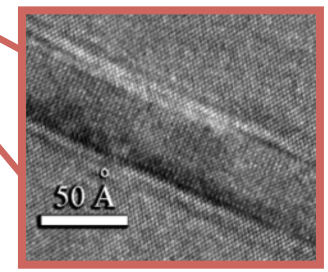
Properties
- Yield strength
- Tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility



1-100 nm

Nanostructure
- Precipitates

Properties
- Yield strength
- Thermal Growth
- Tensile strength
- Low cycle fatigue
- Ductility



0.1-1 nm

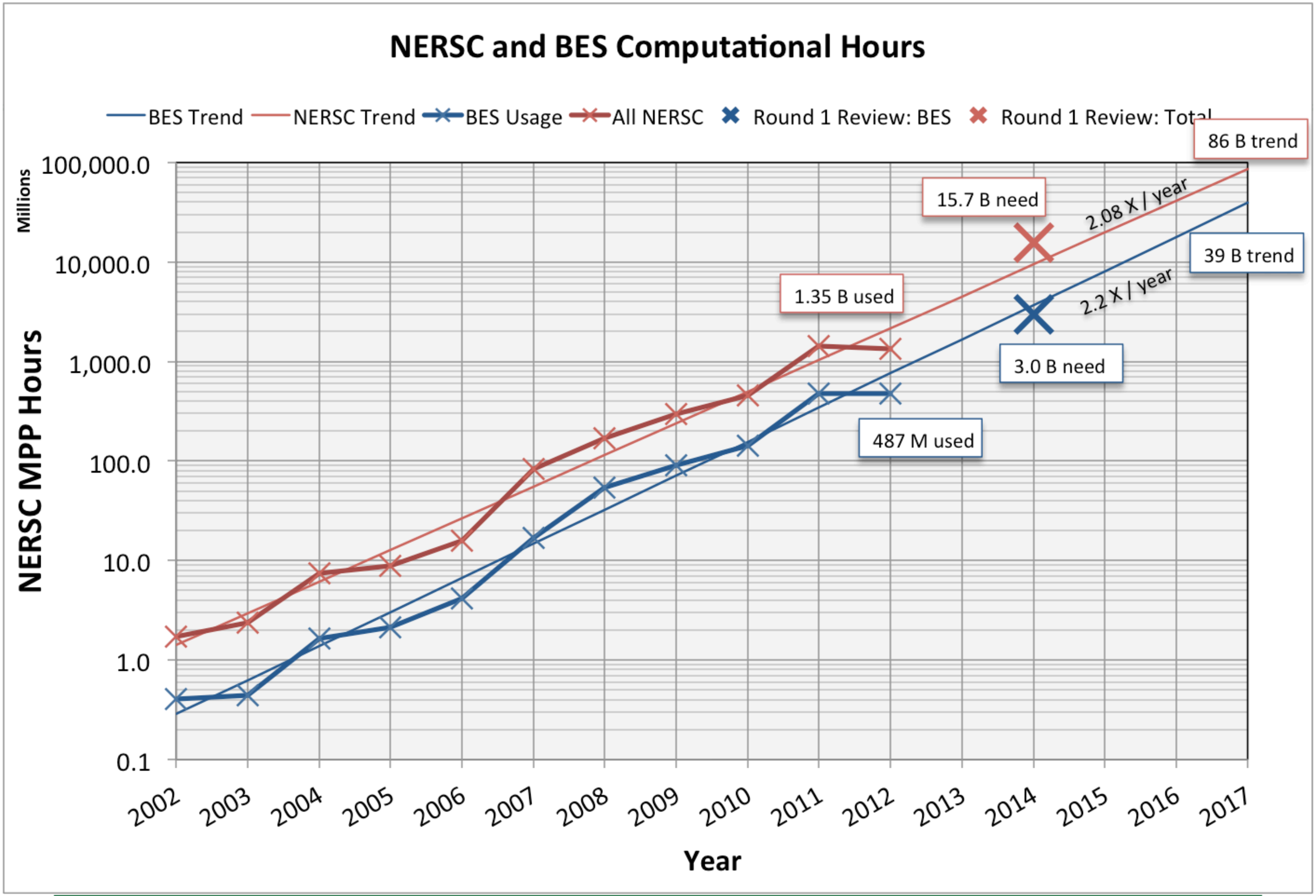
Atomic Structure
- Crystal Structure
- Interface Structure

Properties
- Thermal Growth
- Yield Strength

Key materials processes occur at many length scales – and all can be influenced by manufacturing history

U.S. DEPARTMENT OF ENERGY | Office of Science

Courtesy: John Allison, U Michigan



NERSC and BES Computational Hours
BES Trend
NERSC Trend
BES Usage
All NERSC
Round 1 Review: BES
Round 1 Review: Total
86 B trend
15.7 B need
2.08 X / year
39 B trend
1.35 B used
2.2 X / year
3.0 B need
487 M used
Millions
NERSC MPP Hours
100,000.0
10,000.0
1,000.0
100.0
10.0
1.0
0.1
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
Year

Conclusion

- **Welcome**
- **We appreciate the time you are putting into this**
- **Computing is important to our mission**
  - High end: capability computing
  - High throughput: capacity computing
  - Big Data
- **Impacts**
  - Core Programs
  - MGI: Predictive Theory and Modeling
  - SciDAC
- **We appreciate your help in thinking through all this**