Basic Energy Sciences
Research Priorities for Clean Energy

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Office of Basic Energy Sciences
Office of Science, Department of Energy

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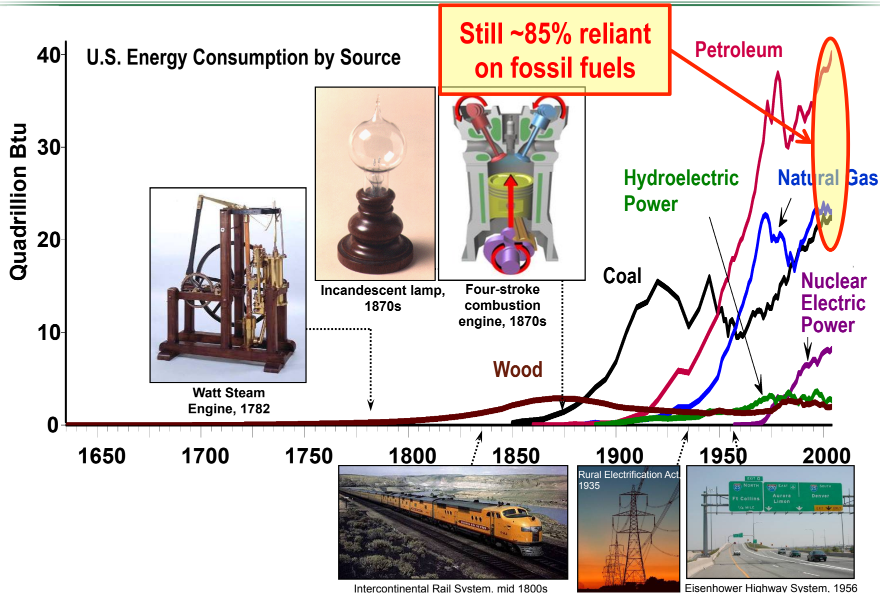
National Institute of Standards and Technology

Our Energy Challenges

For way more information, see any of Pat Dehmer's energy talks:
http://science.energy.gov/sc-2/presentations-and-testimony/

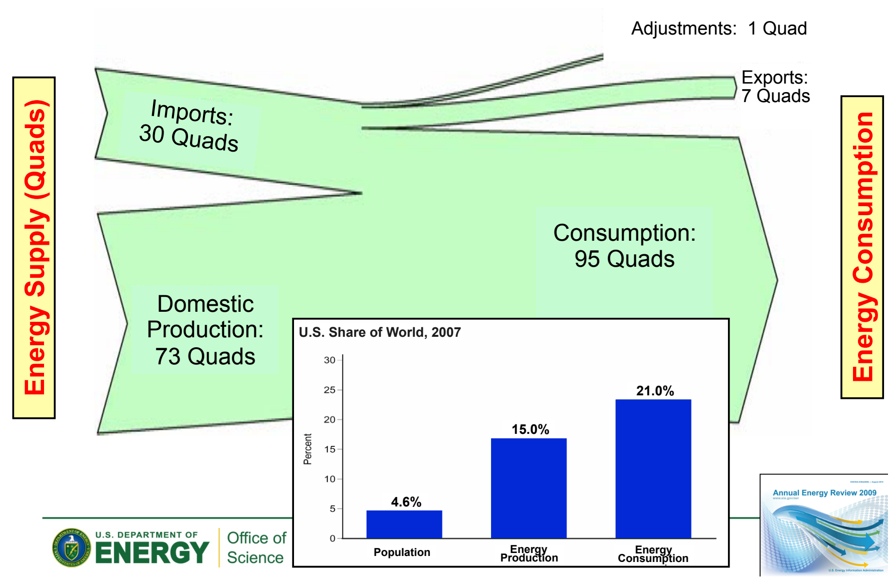
400 Years of Energy Use in the U.S.

19th C discoveries and 20th C technologies are very much part of today's infrastructure



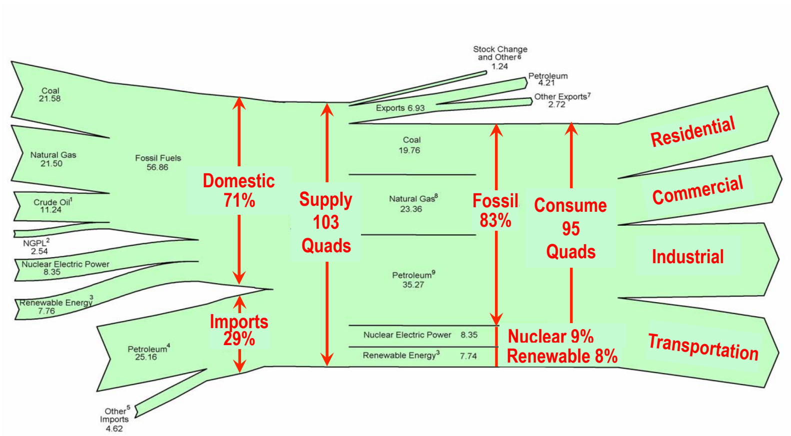
U.S. Energy Flow, 2009

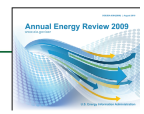
About 1/3 of U.S. primary energy is imported



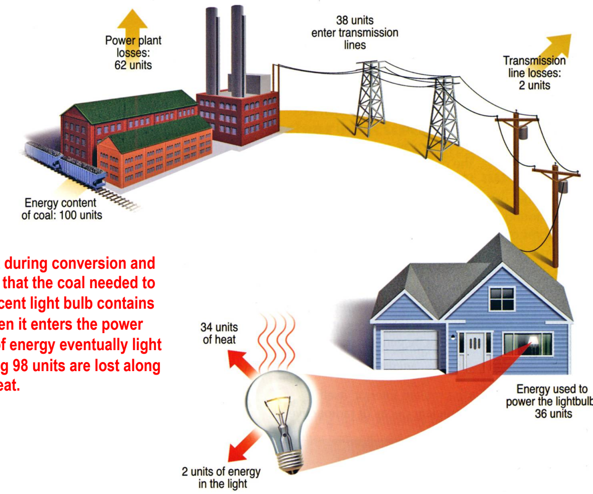
U.S. Energy Flow, 2009 (Quads)

>80% of primary energy is from fossil fuels

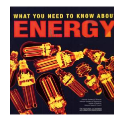




Overall Efficiency of an Incandescent Bulb ≅ 2%

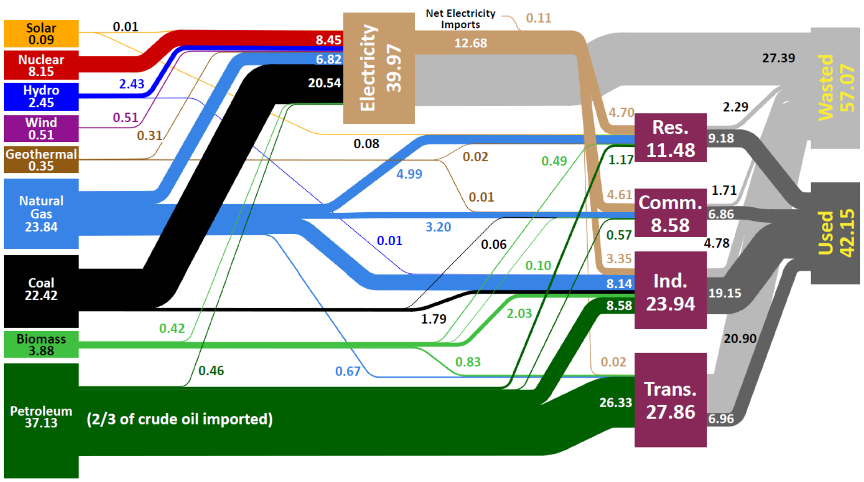


Example of energy lost during conversion and transmission. Imagine that the coal needed to illuminate an incandescent light bulb contains 100 units of energy when it enters the power plant. Only two units of energy eventually light the bulb. The remaining 98 units are lost along the way, primarily as heat.



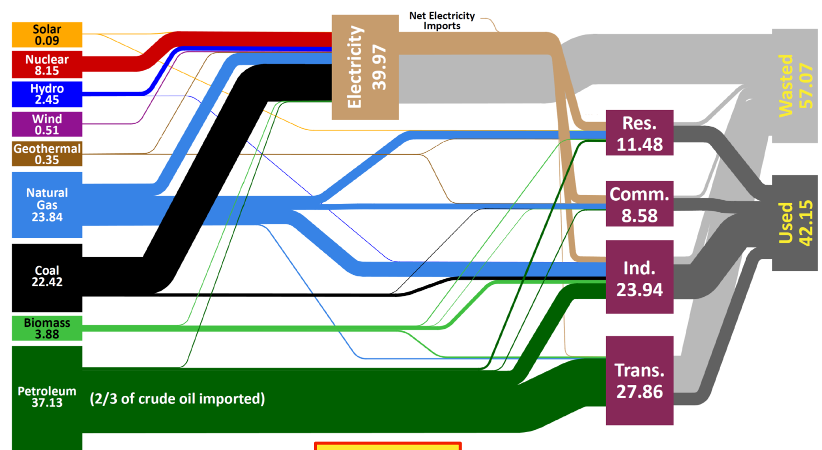
U.S. Energy Production and Usage in 2008

Units in Quadrillion BTUs (Quads)



Source: Lawrence Livermore National Laboratory and the Department of Energy, Energy Information Administration, 2009 (based on data from DOE/EIA-0384(2008), June 2009).

A National Strategy for a Clean Energy Economy



Climate Science

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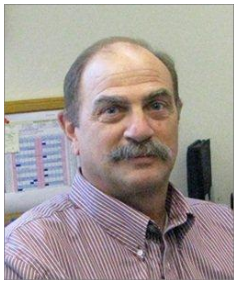
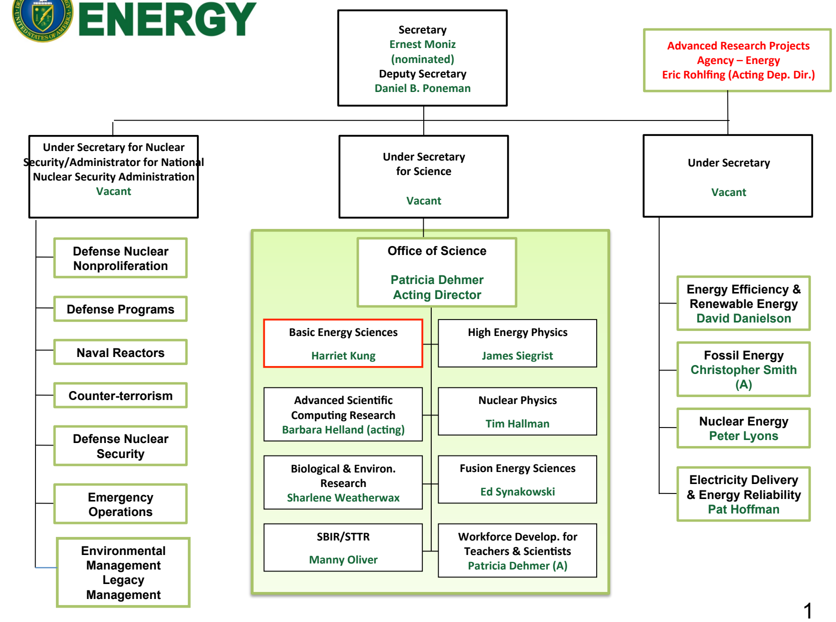
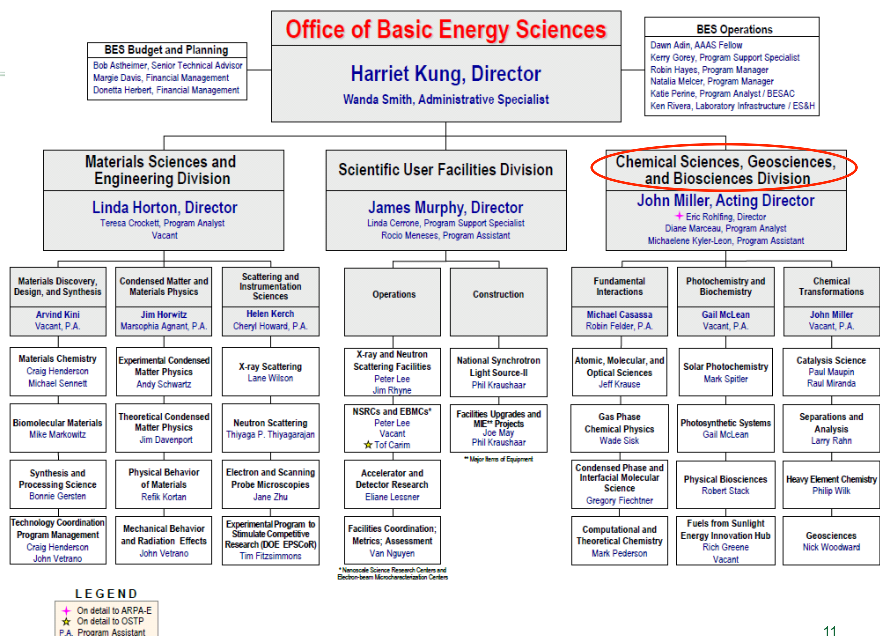
Basic Energy Sciences Overview







April 2013

BES Research — Science for Discovery & National Needs Three Major Types of Funding Modality

- **Core Research**
  Single-investigator, small groups, and targeted larger programs
  - Enable seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, and aspects of geosciences and biosciences. Scientific discoveries at the frontiers of these disciplines establish the knowledge foundation to spur future innovations and inventions.
- **Energy Frontier Research Centers**
  $2-5 million-per-year research centers; multi-investigator and multi-disciplinary
  - Harness the most basic and advanced discovery research in a concerted effort to accelerate the scientific breakthroughs needed to create advanced energy technologies. Bring together critical masses of researchers to conduct fundamental energy research in a new era of grand challenge science and use-inspired energy research.

  Started in FY 2009
- **Energy Innovation Hubs**
  $25 million-per-year research centers focus on co-locating and integrating multi-components, multi-disciplinary research with technology development to enable transformational energy applications.

  Started in FY 2010

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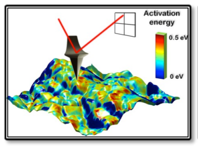
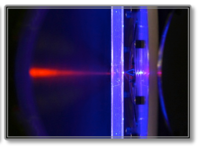
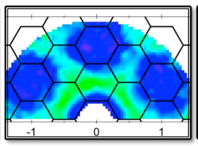
Basic Energy Sciences

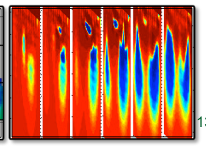
Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels

FY 2014 Budget Highlights:

- Energy Frontier Research Centers (EFRCs) are recompeted (both existing and new)
- Energy Innovation Hubs
  - Fuels from Sunlight Hub: Joint Center for Artificial Photosynthesis (JCAP) will be in its fourth project year.
  - Batteries and Energy Storage: Joint Center for Energy Storage Research (JCESR) will be in its second year.
- Core research
  - Research, approximately flat at the FY 2012 level, increases work at the mesocale (2012 BESAC report *From Quanta to the Continuum: Opportunities for Mesoscale Science).*
- Scientific user facilities are funded at optimum operations
- Construction projects
  - National Synchrotron Light Source-II
  - Linac Coherent Light Source-II
- Major Items of Equipment
  - Advanced Photon Source Upgrade
  - NSLS-II Experimental Tools

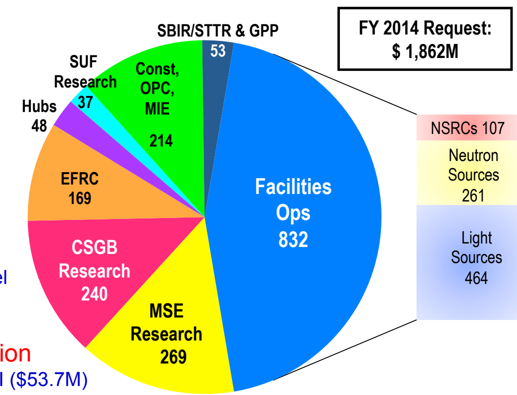




FY 2014 BES Budget Request

- **Research programs**
  - Core Research
  - Energy Innovation Hubs
  - Energy Frontier Research Centers
    - Open competition for new and renewal EFRCs ($100M + one-time $68.7M)
- **Scientific user facilities operations**
  - All facilities operate at optimum level
  - Early operations at NSLS-II ($69M)
- **Construction and instrumentation**
  - National Synchrotron Light Source-II ($53.7M)
  - NEXT instrumentation ($25M)
  - Advanced Photon Source Upgrade ($39.2M)
  - Linac Coherent Light Source-II ($95.7M)

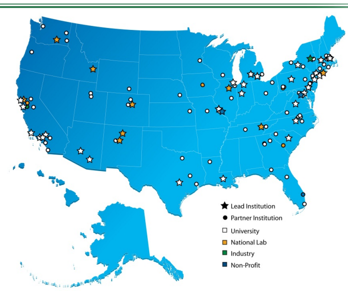


Energy Frontier Research Centers

46 EFRCs were launched in late FY 2009; $777M for 5 Years

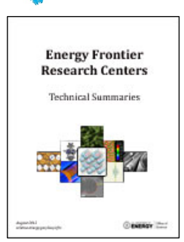
Participants:

- **46** EFRCs in **35** States + Washington D.C.
- ~**850** senior investigators and ~**2,000** students, postdoctoral fellows, and technical staff at ~**115** institutions
- > **250** scientific advisory board members from **13** countries and > **40** companies



Progress to-date (~3.5 years funding):

- >**3,400** peer-reviewed papers including >**110** publications in *Science* and *Nature*
- **18** PECASE and **11** DOE Early Career Awards
- > **200** patent/patent applications, plus an additional >**60** invention disclosures, and at least **30** licenses
- at least **60** companies have benefited from EFRC research
- EFRC students and staff now work in : > **195** university faculty and staff positions; > **290** industrial positions; > **115** national labs, government, and non-profit positions



http://science.energy.gov/bes/efrc/

Energy Frontier Research Centers Recompetition in FY2014

- The initial 46 EFRCs were funded for 5-years beginning in FY 2009: 30 EFRCs were funded annually at about $100M; 16 were fully funded by Recovery Act support
- For FY 2014, funding continues at $100M plus one-time funding of $68.7M
- Solicitation will request both renewal and new EFRC applications including:
  - Areas of energy-relevant research identified by recent BES and BESAC workshops
  - Research to advance the rate of materials and chemical discovery
  - Mesoscale science
- Selection of awards will be based on rigorous peer review of applications of the proposed research
  - Renewal awards will include assessment of the progress during the first 5-year award
- Renewal and new awards will maintain a balanced EFRC portfolio for grand challenge and use-inspired energy research

Current Energy Innovation Hubs

- Three initial Hubs were funded with Fiscal Year 2010 appropriations

Fuels from Sunlight – Joint Center for Artificial Photosynthesis (JCAP)
Lead Institution: California Institute for Technology
Oversight: Office of Science, Basic Energy Sciences

Nuclear Energy Modeling and Simulation – Consortium for Advanced Simulation of Light Water Reactors (CASL)
Lead Institution: Oak Ridge National Laboratory
Oversight: Office of Nuclear Energy

Energy Efficient Buildings System Design – Energy Efficient Buildings (EEBHub)
Lead Institution: Pennsylvania State University
Oversight: Energy Efficiency and Renewable Energy

- Two additional Hubs were funded with Fiscal Year 2012 appropriations

Batteries and Energy Storage – Joint Center for Energy Storage Research (JCESR)
Lead Institution: Argonne National Laboratory
Oversight: Office of Science, Basic Energy Sciences

Critical Materials – Critical Materials Institute (CMI)
Lead Institution: Ames National Laboratory
Ov ciency and Renewable Energy

Fuels from Sunlight Hub
Joint Center for Artificial Photosynthesis (JCAP)

Mission
Develop a solar-fuels generator scalable to manufacture, from earth-abundant elements, that uses only sunlight, water, and carbon dioxide in the robust production of fuels

JCAP Team
Carl Koval, Director (CalTech); Nate Lewis, Founding Director and Chief Scientist (CalTech); two Assistant Directors; about 150 staff

Space
- JCAP North at LBNL: 14,000 sq. ft. leased space
- JCAP South at Caltech: 18,500 sq. ft. in renovated Jorgensen Lab Building (by Caltech & initial startup funds from DOE)

Funding & Oversight
- Up to $122 million over five years
- External reviews in 2011, 2012; scheduled at both sites for April 2013

Goals & Lasting Legacies
- Produce fuel from the sun 10x more efficiently than crops
- Library of fundamental knowledge
- Research prototype solar-fuels generator
- Develop the science and the critical expertise for a solar fuels industry

Milestones

2013: Establish benchmarking capabilities to compare large quantities of catalysts and light absorbers under standard conditions. Progress:
- Benchmarking protocols established for thin films, plan to benchmark over 40 catalytic thin films.
- As of March 2013, more than 20 films evaluated

2014: Design the first prototypic devices for testing components (catalysts, light harvesters, membranes, interfaces, etc.) as an integrated system

Jorgensen Laboratory Building

Batteries and Energy Storage Hub
Joint Center for Energy Storage Research (JCESR)

Mission
Science to enable next generation batteries—beyond lithium ion—and energy storage for the grid and for transportation

JCESR Team
George Crabtree, Director (ANL); 5 national labs, 5 universities, 4 industry partners, and 2 individual members' institutions

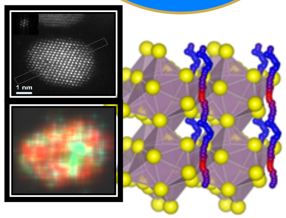
Space
- ANL Electrochemical Discovery Laboratory will provide lab and office space for use by all JCESR Institutions.
- State of Illinois has provided $5M for a new JCESR building with state-of-the-art laboratory and meeting space

Funding & Oversight
- Up to $120 million over five years
- Management review (PY1), Annual external S&T reviews (PY2-5)

Goals & Lasting Legacies
- 5x Energy Density, 1/5 Cost, within 5 Years
- Library of fundamental knowledge
- Research prototype batteries for grid and transportation
- New paradigm for battery development

Initial Milestones

2013-2014:
- Bring suite of experimental tools to full operation.
- Design new architectures of electrode/working ion combinations
- Begin the development of an electrolyte database to predict the design of new electrolytes



JCESR will use nanoscience tools and theoretical approaches to enable next generation energy storage

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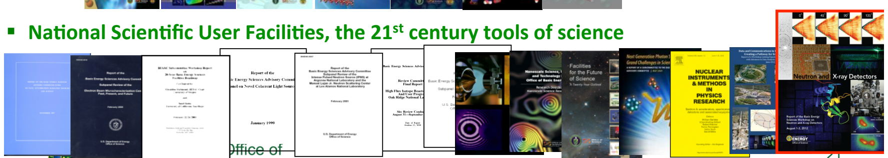
Strategic Planning in BES

BES Strategic Planning Activities

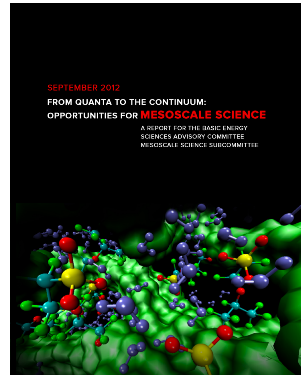
- **Science for Discovery**

- **Science for National Needs**

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



Why Mesoscale Science?



September 2012
http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS_rpt.pdf

"The great scientific advances of the last decade and more, especially at the nanoscale, are ripe for exploitation.

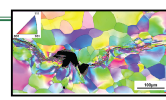
Seizing this opportunity requires mastering the mesoscale, where classical, quantum, and nanoscale science meet.

The functionality that is critical to macroscopic behavior begins to manifest itself not at the atomic or nanoscale but at the mesoscale, where defects, interfaces, and non-equilibrium structures are the norm.

The reward for breakthroughs in our understanding at the mesoscale is the emergence of previously unrealized functionality."

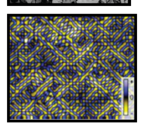
Mesoscale Science - From Quanta to the Continuum

- Mastering Defect Mesostructure and its Evolution
  Tracking, modeling and controlling the dynamic evolution of mesoscale defect patterns from their atomic origins to their macroscale impact is critical for extending materials lifetime, designing new generations of functional materials, and creating less expensive, more efficient advanced manufacturing.
- Regulating Coupled Reactions and Pathway-dependent Chemical Processes
  Characterizing and controlling fluid flow and chemical reactions in mesoscale pathways are central to solving energy and environmental challenges such as carbon sequestration, groundwater contamination and cleanup, shale gas extraction, energy storage, separation membranes for fluid and gas purification, and subsurface geological processes.
- Optimizing Transport and Response Properties by Design and Control of Mesoscale Structure
  Controlling the size and geometry of mesoscale architectures that mediate the interaction of electrons, photons and lattices allows new horizons in materials functionalities spanning thermoelectricity, light absorption and emission, spintronics, and multiferroics, building blocks for innovating next generation energy conversion and information technology.
- Elucidating Non-equilibrium and Many-Body Physics of Electrons
  Controlling electronic correlation in artificial mesoscale architectures such as quantum dots and nanoparticle arrays adds new dimensions to exploiting functional behaviors from metal-insulator transitions to magnetism and high temperature superconductivity to produce entirely new levels of macroscopic functionality and advanced technology.
- Harnessing Fluctuations, Dynamics, and Degradation for Control of Metastable Mesoscale
  The inherent metastability of complex behaviors in mesoscale biological and human-engineered systems appears on multiple length and time scales that can be exploited to introduce smart, real-time responses to environmental cues, mitigate materials degradation due to defect accumulation, and dramatically extend useful technology life.
- Directing Assembly of Hierarchical Functional Materials
  Directed assembly of functional materials in hierarchical mesoscale architectures requires the ability to model, synthesize, and assemble building blocks with motifs that embed information and behavior via anisotropies in chemical make-up, shape, and bonding strength. The integration of disparate material motifs by "top-down" design and "bottom-up" assembly creates a new paradigm in materials synthesis and advanced manufacturing.

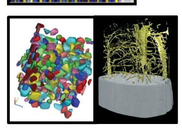


Scanning electron microscope image of pore coalescence in dynamically loaded Tantalum, showing defect evolution

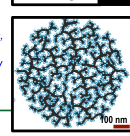
Pores in sandstone, a sedimentary rock formed by accumulation of many sizes and shapes of mineral and organic grains, may significantly influence transport properties.



Spectroscopic scanning tunneling microscope image of the electronic modulation in BSCCO superconductors – a correlated electron material that exhibits self-organized meoscale structure.



X-ray tomography (left) and 3-D coherent imaging (right) are critical tools for mesoscale structural characterization.



Self-assembly of silicon coated carbon fibers for battery electrodes as an energy efficient synthesis approach with organized instead of random mesostructure.

Materials Genome Initiative

- *The Materials Genome Initiative will create a new era of materials innovation that will serve as a foundation for strengthening domestic industries… and offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.*
- Multiagency Initiative led by the Office of Science and Technology Policy
- DOE role:
  - Software development, building on theory and partnering (BES)
    - Robust, accurate and multiscale in both size and time
  - Validation of software and theory
    - User facilities and broad experimental materials science portfolio
  - Application specific R&D for manufacturing and to develop lightweight, high-strength alloys for automotive (EERE)
- Technical emphasis includes materials for clean energy

Thank You!