Office of Science
Basic Energy Sciences

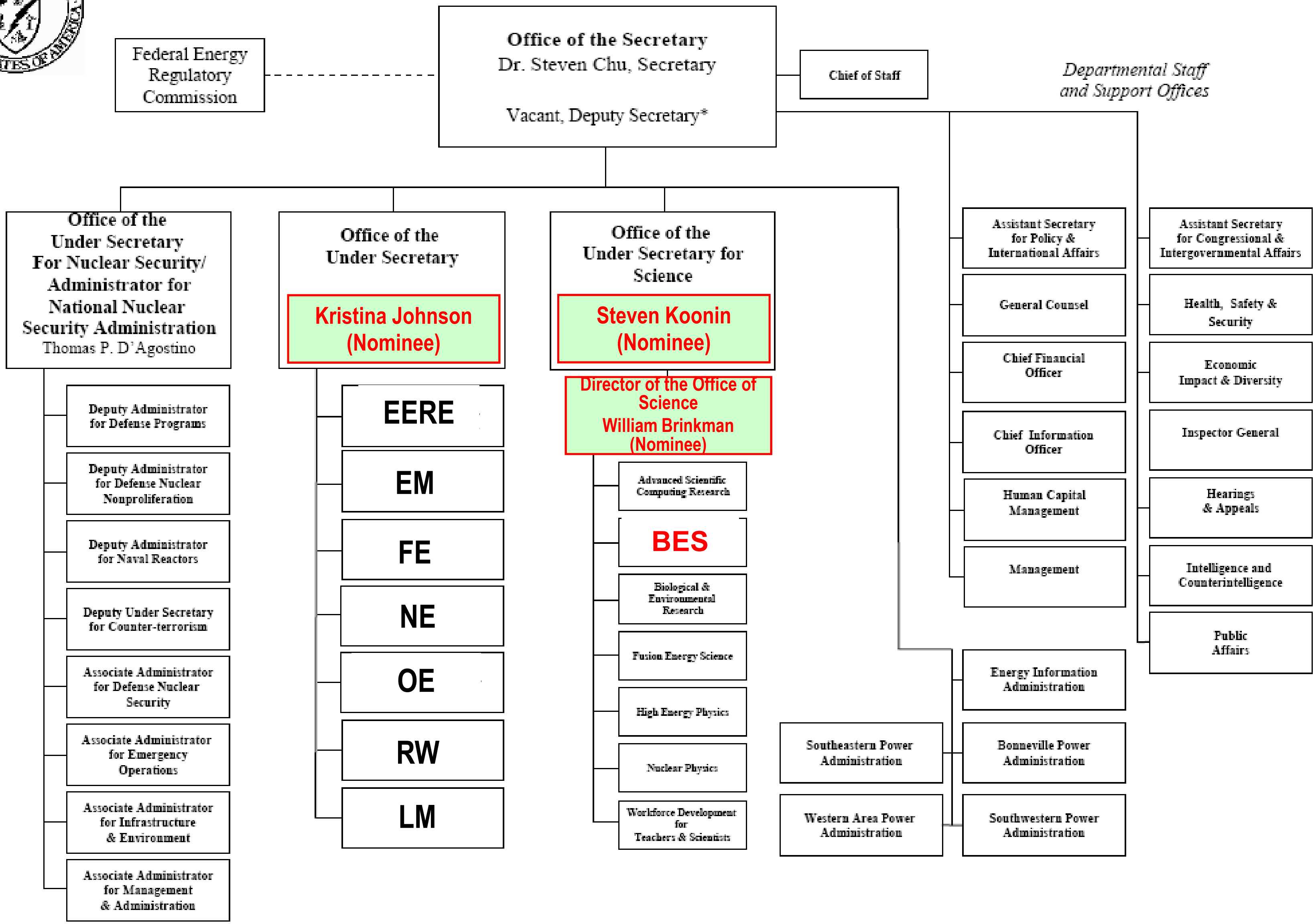
Harriet Kung

Office of Basic Energy Sciences

2009 DOE Hydrogen & Vehicle Technologies
Merit Review and Peer Evaluation Meeting

May 18, 2009

DEPARTMENT OF ENERGY



* The Deputy Secretary also serves as the Chief Operating Officer

21 Jan 09

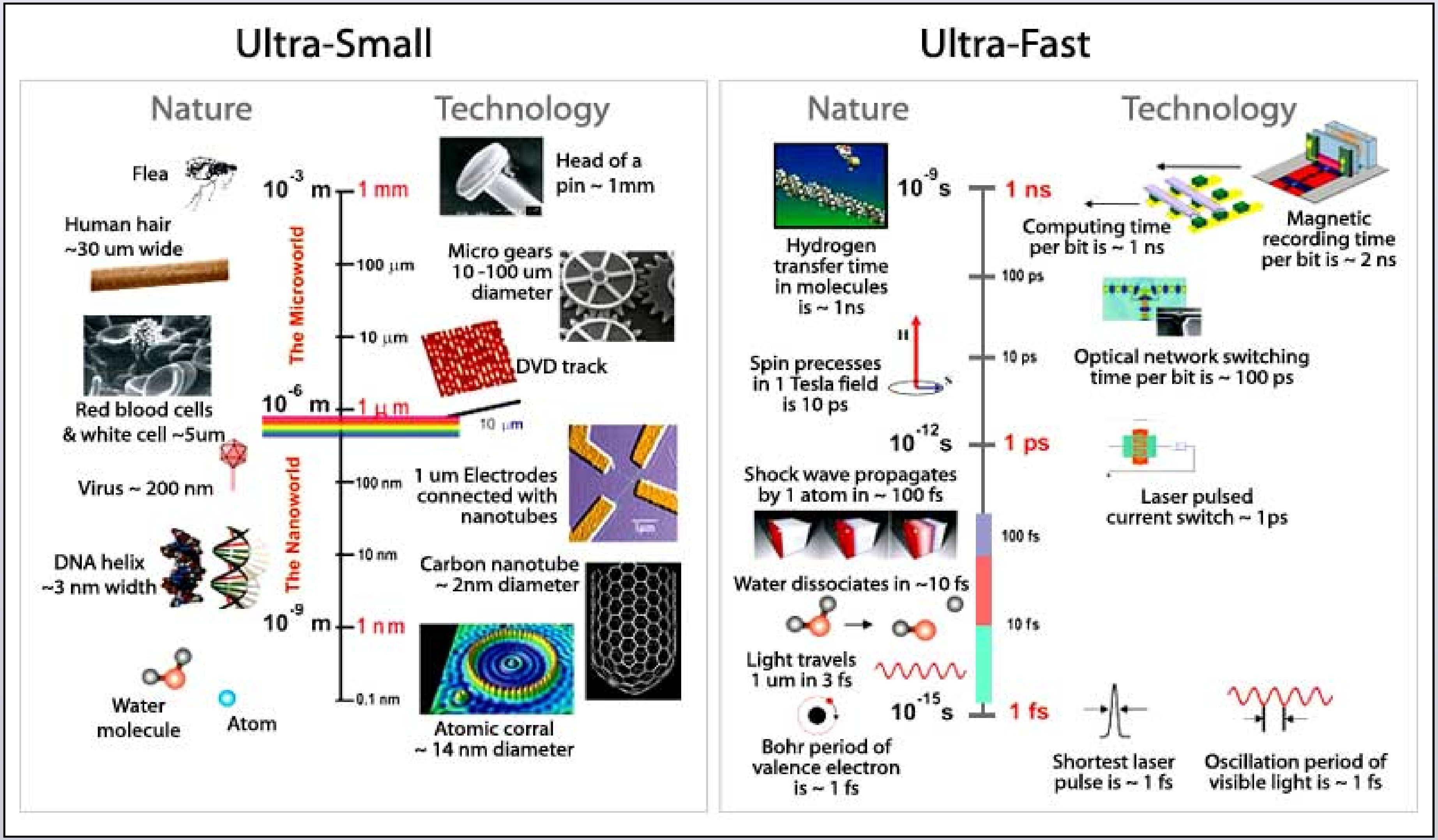
Office of Basic Energy Sciences

Our Mission:

- **Foster and support *fundamental research programs* to expand the scientific foundation for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use**

- **Plan, construct, and operate *major scientific user facilities* for "materials sciences and related disciplines" to serve researchers at universities, federal laboratories, and industrial laboratories**

Ultra-small and Ultra-fast:
Frontiers in Science & Technology



The Scientific Opportunities in BES

Identified in The "Basic Research Needs …" Workshop Series

Identifying Basic Research Directions for Today's and Tomorrow's Energy Technologies

Basic Research Needs for a Secure Energy Future (BESAC)

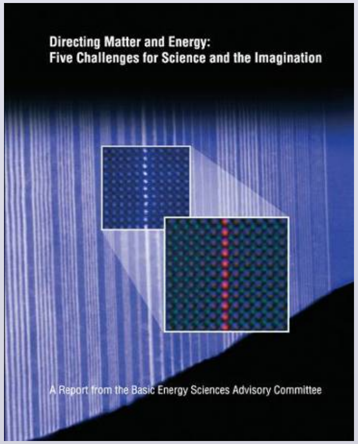
http://www.sc.doe.gov/bes/reports/files/SEF_rpt.pdf

- **Basic Research Needs for the Hydrogen Economy**
- **Basic Research Needs for Solar Energy Utilization**
- Basic Research Needs for Superconductivity
- Basic Research Needs for Solid State Lighting
- Basic Research Needs for Advanced Nuclear Energy Systems
- **Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels**
- Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems
- **Basic Research Needs for Electrical Energy Storage**
- Basic Research Needs for Catalysis for Energy Applications
- **Basic Research Needs for Materials under Extreme Environments**

Science Grand Challenges

How does nature execute electronic and atomic design? How can we?

Directing Matter and Energy: Five Challenges for Science and the Imagination



http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf

- **Control the quantum behavior of electrons in materials**
  Imagine: Direct manipulation of the charge, spin and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical reactions and the strength of chemical bonds, and efficient conversion of the Sun's energy into fuel through artificial photosynthesis.
- **Synthesize, atom by atom, new forms of matter with tailored properties**
  Imagine: Create and manipulate natural and synthetic systems that will enable catalysts that are 100% specific and produce no unwanted byproducts, or materials that operate at the theoretical limits of strength and fracture resistance, or that respond to their environment and repair themselves like those in living systems
- **Control emergent properties that arise from the complex correlations of atomic and electronic constituents**
  Imagine: Orchestrate the behavior of billions of electrons and atoms to create new phenomena, like superconductivity at room temperature, or new states of matter, like quantum spin liquids, or new functionality combining contradictory properties like super-strong yet highly flexible polymers, or optically transparent yet highly electrically conducting glasses, or membranes that separate CO_2 from atmospheric gases yet maintain high throughput.
- **Synthesize man-made nanoscale objects with capabilities rivaling those of living things**
  Imagine: Master energy and information on the nanoscale, leading to the development of new metabolic and self-replicating pathways in living and non-living systems, self-repairing artificial photosynthetic machinery, precision measurement tools as in molecular rulers, and defect-tolerant electronic circuits
- **Control matter very far away from equilibrium**
  Imagine: Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically-inspired molecular machines, long-term storage of spent nuclear fuel through adaptive earth chemistry, and achieving environmental sustainability by understanding and utilizing the chemistry and fluid dynamics of the atmosphere.

How Nature Works ··· to ··· Materials and Processes by Design to ··· Technologies for the 21st Century

Grand Challenges *How nature works*	Discovery and Use-Inspired Basic Research *Materials properties and functionalities by design*		Applied Research	Technology Maturation & Deployment
▪ Controlling materials processes at the level of quantum behavior of electrons ▪ Atom- and energy-efficient syntheses of new forms of matter with tailored properties ▪ Emergent properties from complex correlations of atomic and electronic constituents ▪ Man-made nanoscale objects with capabilities rivaling those of living things ▪ Controlling matter very far away from equilibrium	▪ Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies ▪ Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation	▪ Basic research, often with the goal of addressing showstoppers on real-world applications in the energy technologies	▪ Research with the goal of meeting ***technical milestones***, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes ▪ Proof of technology concepts	▪ Scale-up research ▪ At-scale demonstration ▪ Cost reduction ▪ Prototyping ▪ Manufacturing R&D ▪ Deployment support

BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Report

DOE Technology Office/Industry Roadmaps

Basic Energy Sciences
Goal: new knowledge / understanding
Mandate: open-ended
Focus: phenomena
Metric: knowledge generation

DOE Technology Offices: EERE, NE, FE, EM, RW…
Goal: practical targets
Mandate: restricted to target
Focus: performance
Metric: milestone achievement

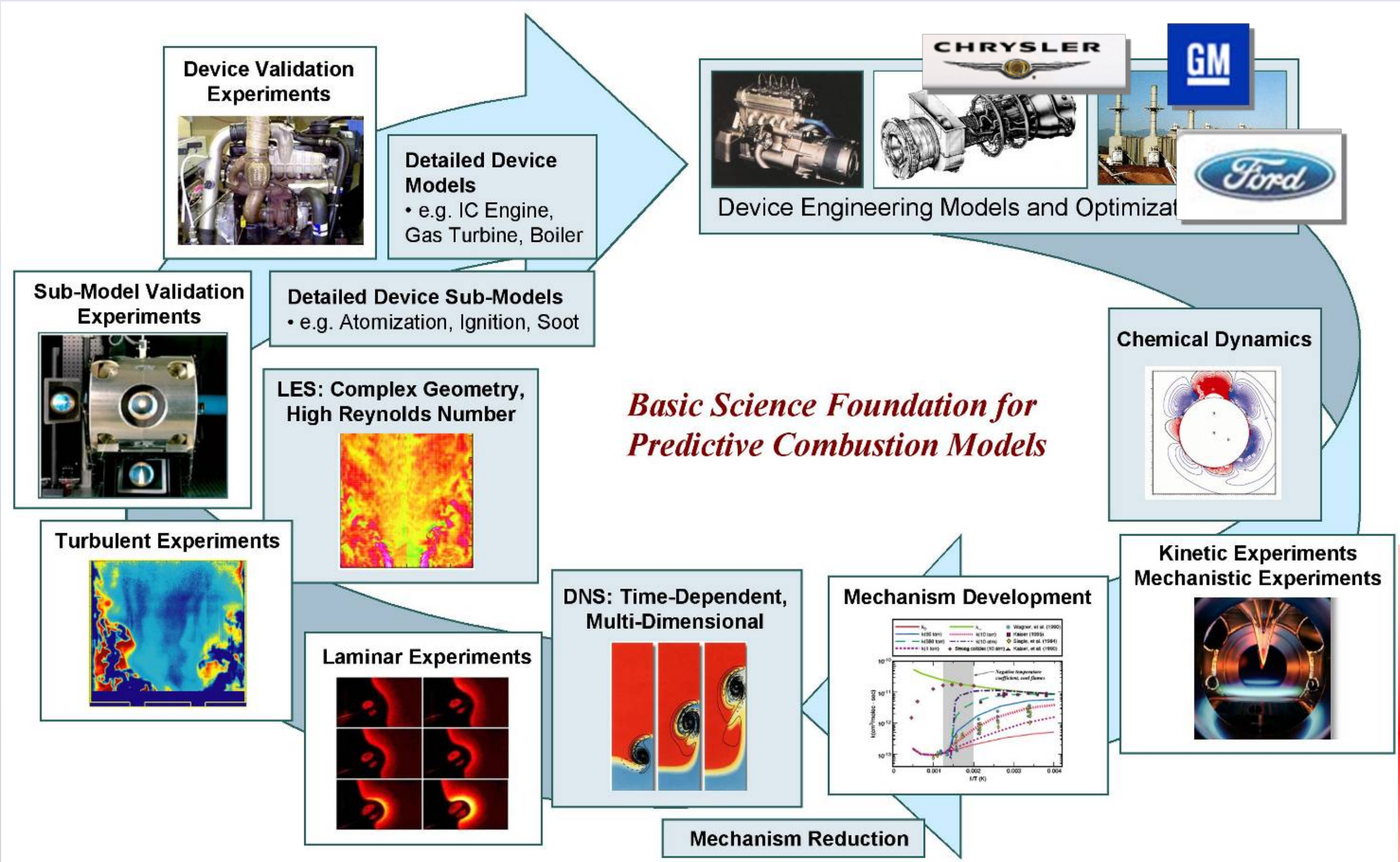
Basic Sciences Underpinning Technology

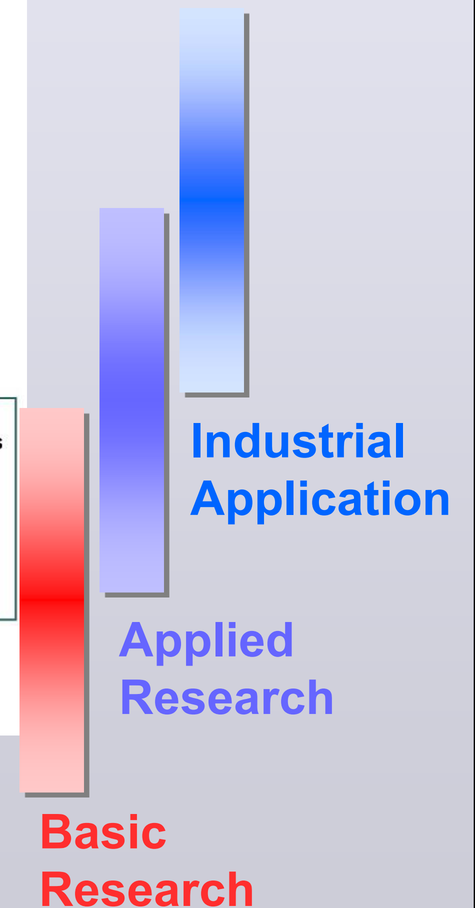
- **Coordination between basic science and applied research and technology is an important mechanism by which to translate transformational discoveries into practical devices**

- **Many activities facilitate cooperation and coordination between BES and the technology programs**
  - Joint efforts in strategic planning (e.g., 10 BRN workshops)
  - Solicitation development
  - Reciprocal staff participation in proposal review activities
  - Joint program contractors meetings
  - Joint SBIR topics

- **Co-funding and co-siting of research by BES and DOE technology programs at DOE labs or universities, has proven to be a viable approach to facilitate close integration of basic and applied research through sharing of resources, expertise, and knowledge of research breakthroughs and program needs.**

Integration of Basic & Applied Research
Example: Combustion Research Facility (SNL-CA)





- Key CRF Characteristics:
  - Common scientific purpose
  - Co-location and collaboration
  - Strong ties to application
  - Full spectrum of basic to applied

A Milestone in Science-Based Engineering

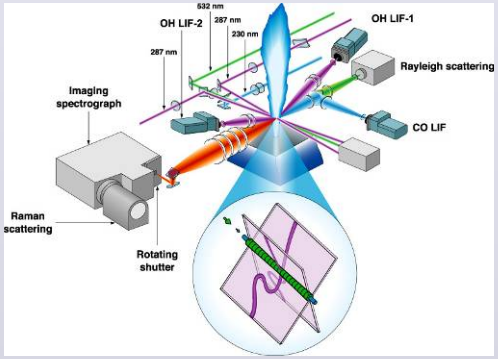
2007 ISB (6.7 liter diesel)

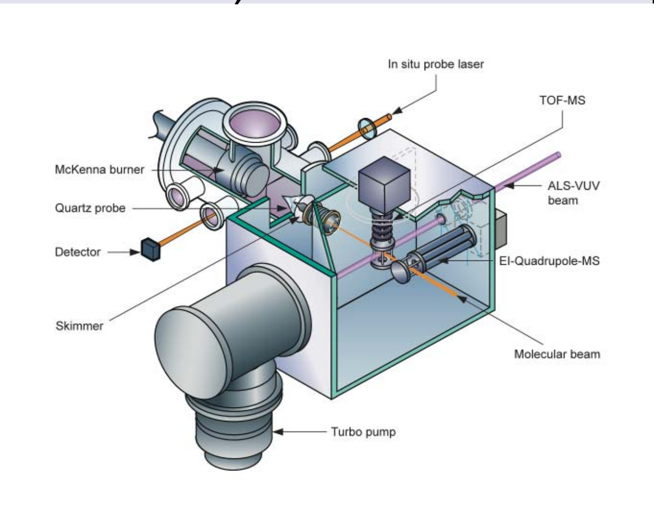
- Cummins designs 2007 diesel engine using computer modeling and analysis.
  - After-the-fact testing only.
  - Reduced development time and cost.
  - Improved tank mileage.
  - Emission compliant (new 2007 regs).
  - Customer constraints met.
  - More robust design
    - larger parameter space explored.

A key enabler was the development of a detailed, science-based understanding of diesel combustion.

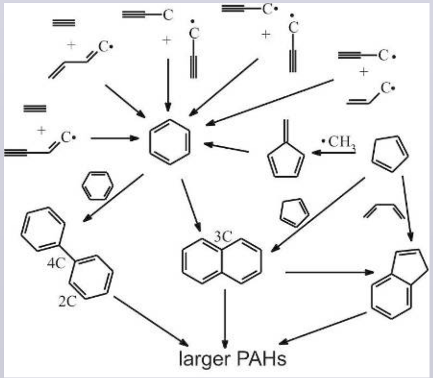
Next Generation Engine Development Enabled by Basic Research

- Advanced combustion strategies for enabling high-efficiency, low-emission engines (with potential for 4 MBD reduction in oil use).
  - Laser diagnostics
  - High pressure chemistry

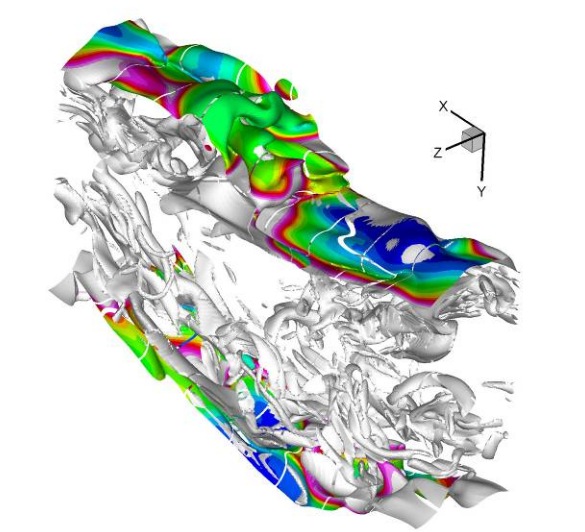




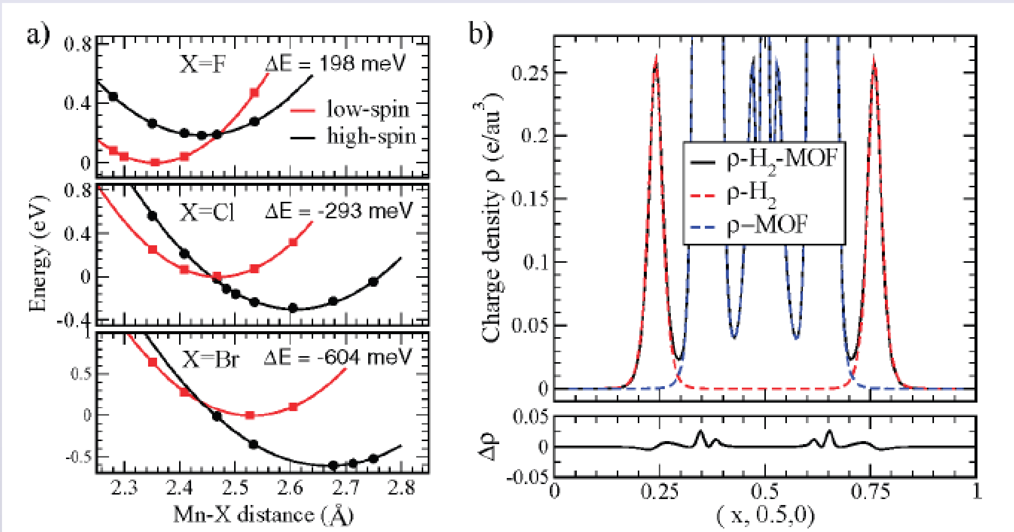
- Future fuels
  - Chemical kinetics
  - Mechanism development
  - Flame chemistry

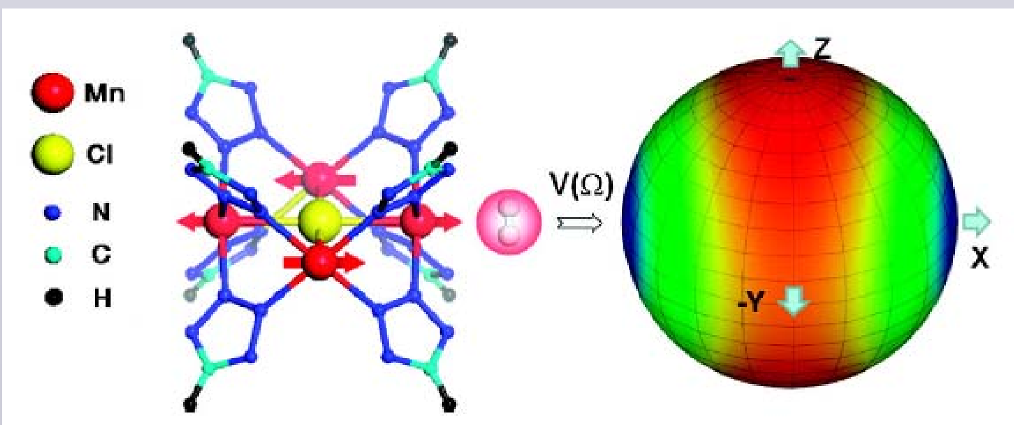


- Next generation computational tools
  - Direct Numerical Simulation
  - Large Eddy Simulation



Tunability of Hydrogen Binding in Metal-Organic Frameworks with Exposed Transition Metal Sites



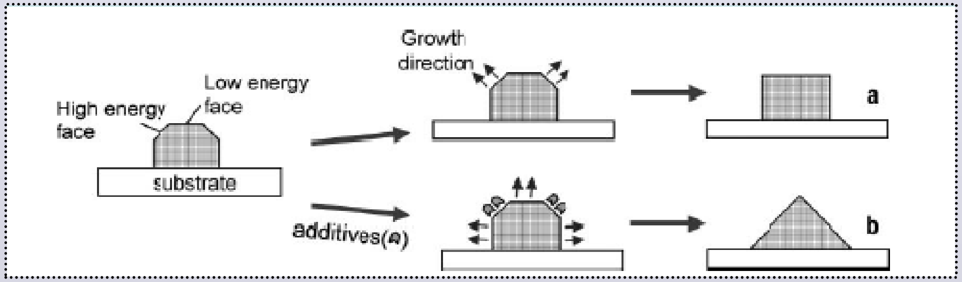


W. Zhou and T. Yildirim, *J. Phys. Chem. C* 112 (22) **2008**

- Recent results incorporating exposed transition metals (TM) sites in Mn_4Cl-MOFs have shown an increase in binding energy (BE) to a level intermediate between pure van der Waals (4 kJ/mol) and Kubas binding (30-50 kJ/mol) but the mechanism was not clear and originally attributed to a type of Kubas interaction
- BE was shown to depend on the magnetic spin state of the Mn ions and that this spin state could be influenced by exchanging Cl with either F or Br, either reducing or increasing the BE, respectively
- DFT calculations were made on these systems that showed the hydrogen-TM binding was not a Kubas-type but was rather a Coulomb interaction (no electron sharing nor bond stretching) with little hybridization of orbitals
- This Coulomb interaction is very anisotropic and to properly calculate the binding energy it is necessary to take into account the quantum nature of the H2 orientation. Here it is shown that the rotational dynamics of the H2 molecule are strongly confined to a slab-like region (red region in bottom right figure) which has been shown to influence the BE.

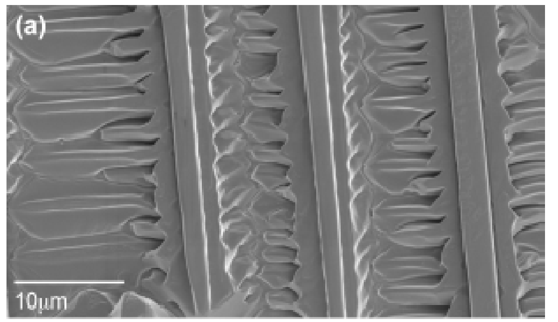
Novel Synthesis of Nanomaterials for Solar Hydrogen Production

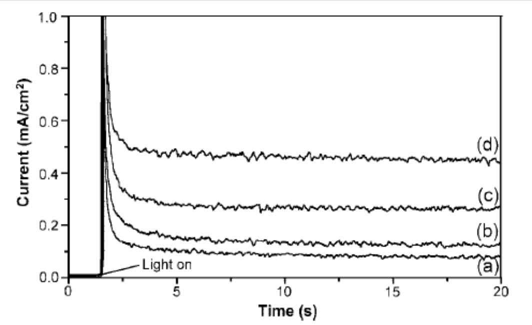
- Cu_2O is a direct-gap semiconductor and is a viable candidate to produce hydrogen by direct water photolysis using visible light with little or no external bias. The efficiency of photocurrent generation is dependent on the shape, size and interconnection of the polycrystals.
- By gaining a deeper understanding of the growth mechanisms of electrodeposited Cu_2O crystals it is possible to control the growth in such a way as to tailor the final shape and size of the crystals and therefore alter the generation of photocurrent when the crystals are illuminated.



Cu_2O →

- Two keys to branching morphology were found to be the buffering of the solution to eliminate localized changes in pH and the control of overpotential during growth; precise manipulation of these two factors allows exquisite control of dendritic branching.
- Once this was fully understood it was possible, by creating optimally branched structures, to increase the photocurrent of a thin film of Cu_2O by up to a factor of 20, thereby increasing the ability to produce hydrogen from sunlight.

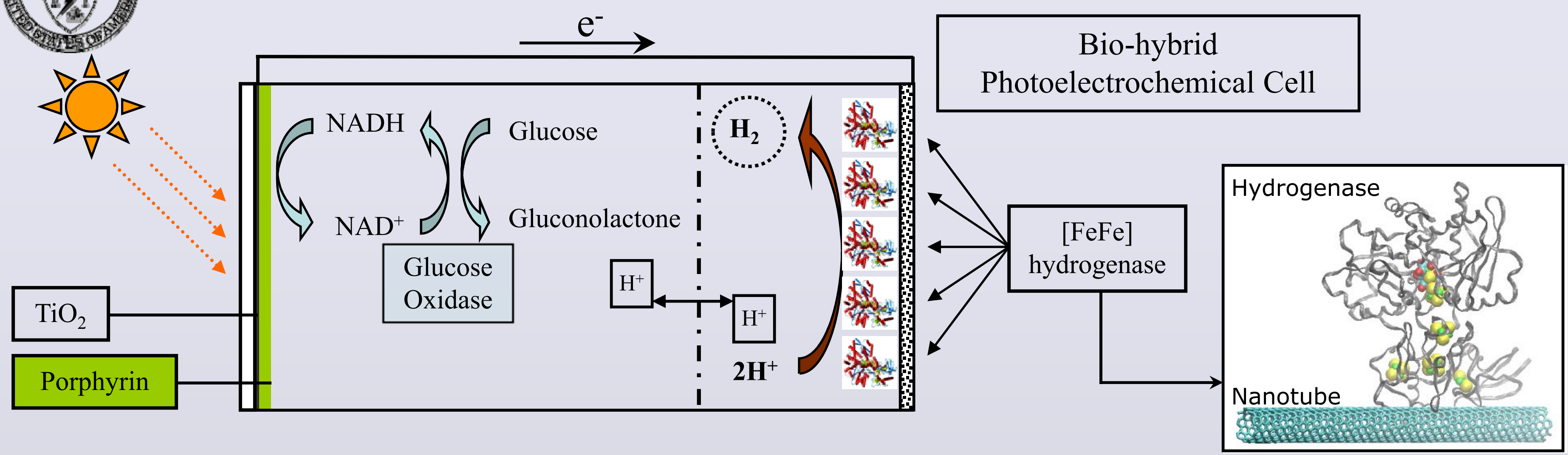




K.-S. Choi, *Dalton Trans.*, 2008, p5432

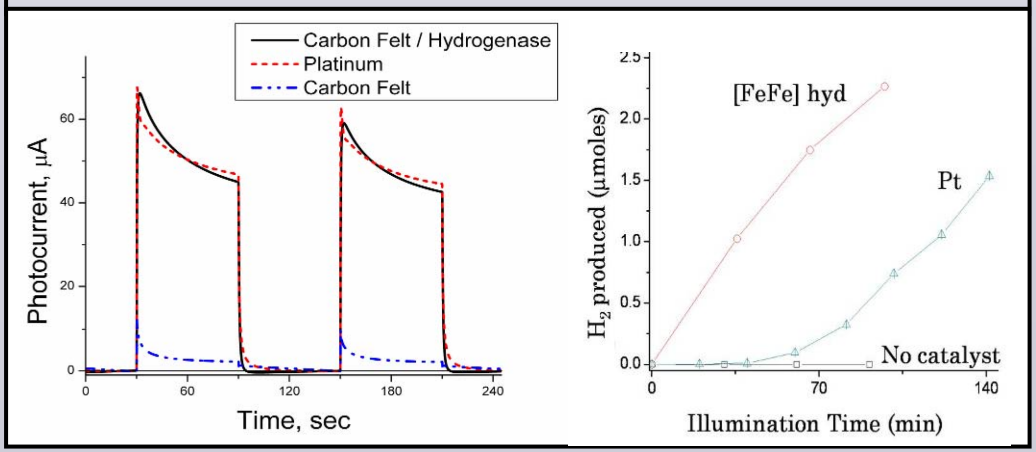
C.M. McShane and K.-S Choi, *J. Am. Chem. Soc.*, 2009, 131 (7) p. 2561

Bio-hybrid H_2-production with [FeFe] hydrogenase



- Surfactant-suspended carbon SWNTs spontaneously self-assemble with [FeFe] hydrogenases to form catalytically active biohybrids
- SWNTs act as molecular wires, making electrical contact to the biocatalytic region of the hydrogenase
- [FeFe] hydrogenase immobilized onto carbon electrodes in a PEC serves as a model Bio-hybrid, Solar-driven, H_2-production system
- H_2-production photocurrents, rates and durations with [FeFe] hydrogenase as catalyst closely match the performance values of a nanoparticulate, Pt-catalyst

Comparable performance of [FeFe] hydrogenase and Pt catalysts

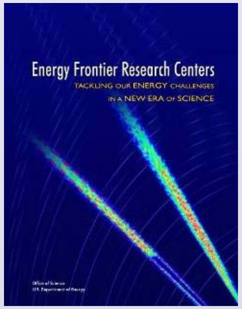


T.J. McDonald et al, NanoLetters 7 (11) 2007

M.C. Beard, J.L. Blackburn and M.J. Heben, NanoLetters 8 (12) 2008

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science



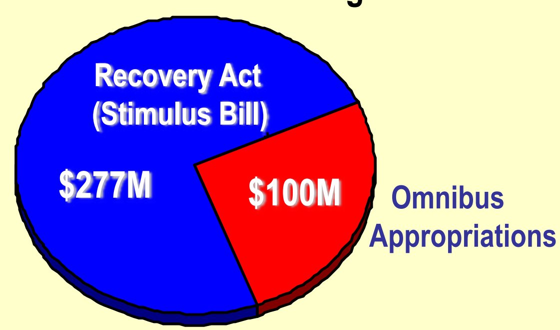
- To engage the talents of the nation's researchers for the broad energy sciences
- To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century
- To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy

EFRCs will pursue *collaborative* basic research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Bio-Fuels
- Catalysis
- Energy Storage
- Geosciences for Nuclear Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen
- Combustion
- Superconductivity
- Solid State Lighting

2003-2007	Conducted BRNs workshops
August 2007	America COMPETES Act signed
Feb. 2008	FY 2009 budget roll-out
April 2008	EFRC FOA issued
Oct. 2008	Received 261 full proposals
Oct. 2008	FY 2009 Continuing Resolution started
Feb. 2009	Recovery Act of 2009 (Stimulus) signed
March 2009	Omnibus Appropriations Act 2009 signed
April 2009	46 EFRC awards announced
Aug. 2009	EFRC projects to start

FY 2009 EFRCs Funding Status:

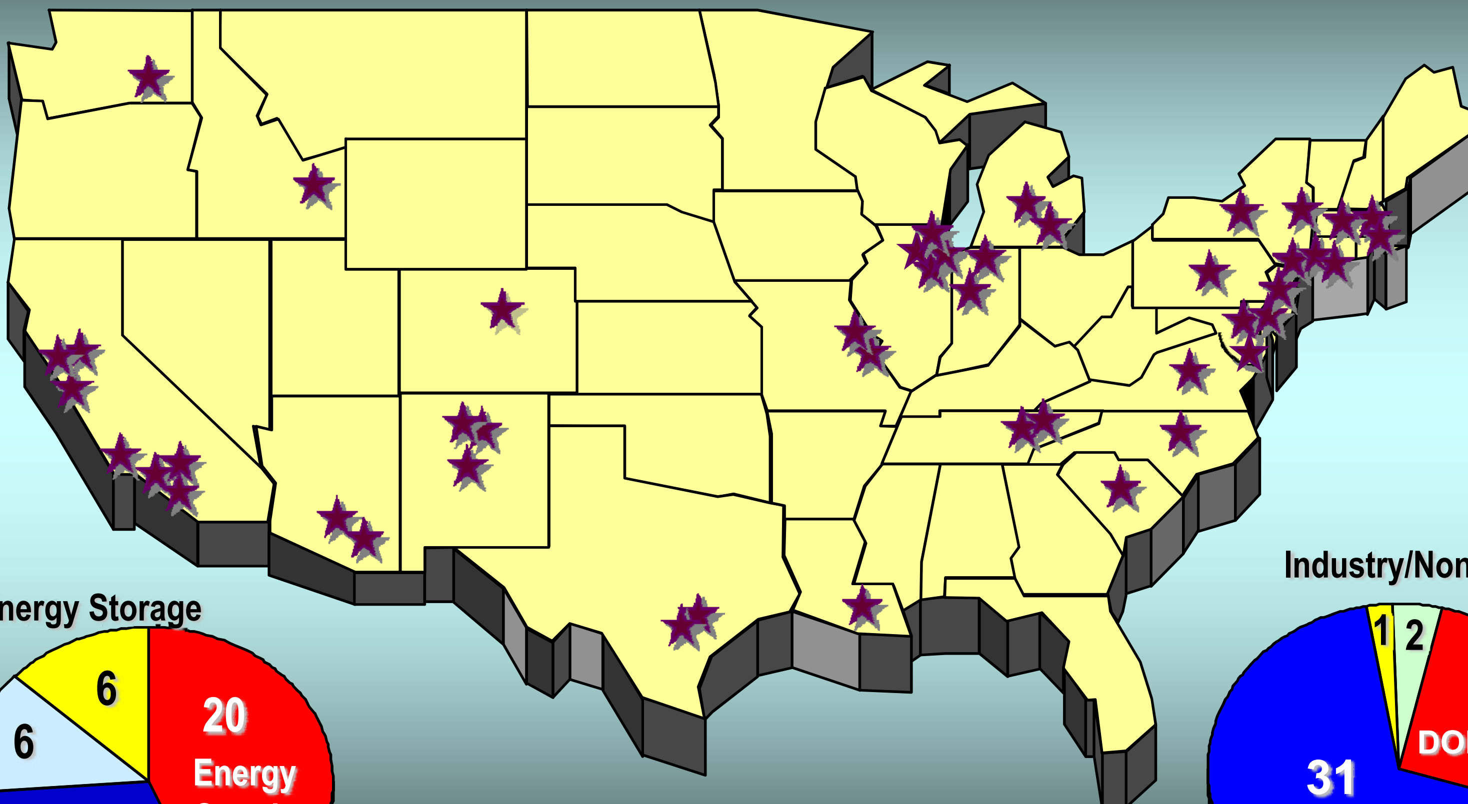


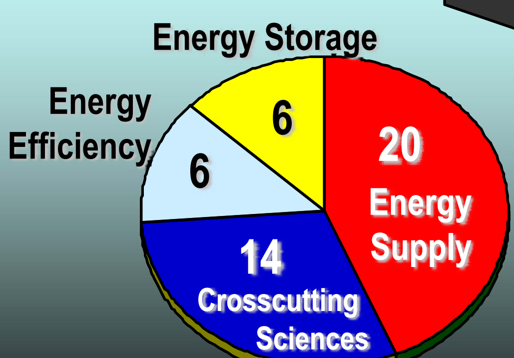
Total EFRCs = $777M over 5 years

Energy Frontier Research Centers

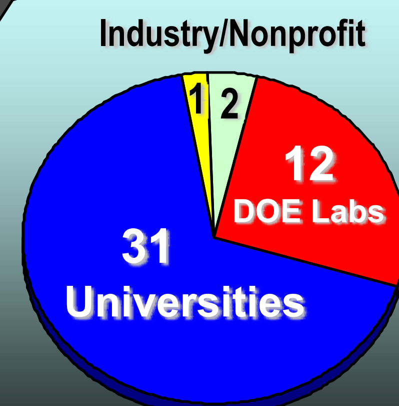
Invest in Cutting-edge Scientific Research to Achieve Transformational Discoveries

46 centers awarded in FY 2009 for five years
Representing 110 participating institutions in 36 states plus D.C.



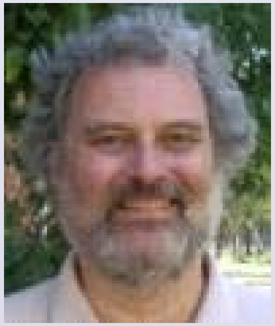


By Topical Category



By Lead Institution

Solar Energy Utilization: Solar Fuels



Robert Blankenship, Washington Univ., St. Louis MO

Photosynthetic Antenna Research Center -- Understand photosynthetic antenna system to convert sunlight into fuels.

http://news-info.wustl.edu/news/page/normal/14079.html

Tom Meyer, Univ. of North Carolina

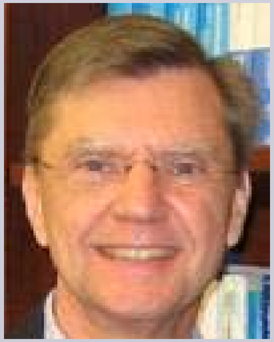
Solar Fuels and Next Generation Photovoltaics -- Nanoscale architectures for improved generation of fuels and electricity from sunlight.

http://uncnews.unc.edu/news/science-and-technology/unc-to-launch-solar-fuels-research-center-with-17.5-million-in-federal-energy-stimulus-grant.html

Devens Gust, Arizona St. Univ.

Bio-Inspired Solar Fuel Production - Adapt natural photosynthesis principles to bio-inspired approaches for solar fuels production.

http://asunews.asu.edu/20090430_EFRC



Michael Wasielewski, Northwestern Univ.

Argonne-Northwestern Solar Energy Research Center -- Revolutionize the design, synthesis, and control of molecules for solar fuels generation.

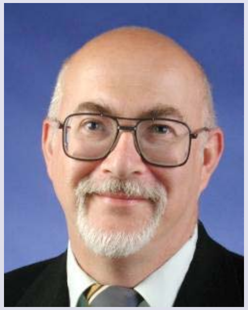
http://www.northwestern.edu/newscenter/stories/2009/04/efrc.html

Energy Storage

Michael Thackeray, ANL

Center for Electrical Energy Storage -- Understand complex phenomena in electrochemical reactions critical to advanced electrical energy storage.

http://www.anl.gov/Media_Center/News/2009/news090428.html



Grigorii Soloveichik, General Electric Global Research

Center for Innovative Energy Storage -- Explore the fundamental chemistry of electrocatalysis and ionic transport for energy storage that combines the best properties of a fuel cell and a flow battery.

Héctor Abruña, Cornell Univ.

Nanostructured Interfaces for Energy Generation, Conversion, and Storage -- Understand the nature, structure, and dynamics of reactions at electrodes.

http://www.news.cornell.edu/stories/May09/EFRC.ws.html

Clare P. Grey, Stony Brook Univ.

Northeastern Chemical Energy Storage Center -- Overcoming performance barriers of batteries through electrode designs.

http://commcgi.cc.stonybrook.edu/am2/publish/Research_20/DOE_to_Establish_Energy_Frontier_Research_Center_at_Stony_Brook_University.shtml

Gary Rubloff, Univ. of Maryland

Science of Precision Multifunctional Nanostructures for Electrical Energy Storage -- Understand and build nano-structured electrode components.

Ken Reifsnider, Univ. of South Carolina

Nano-Structure Design and Synthesis of Heterogeneous Functional Materials – Focusing on nano-structured materials functions at interfaces

http://www.sc.edu/news/newsarticle.php?nid=175

Single-Investigator and Small-Group Research

Tackling our energy challenges in a new era of science

- In FY 2009 $55M will be available for single-investigator and small-group awards.
- BES sought applications in two areas: grand challenge science and energy challenges identified in one of the Basic Research Needs workshop reports.
- Awards are planned for three years, with funding in the range of $150-300k/yr for single-investigator awards and $500-1500k/yr for small-group awards (except as noted below)
- Areas of interest include:

  Grand challenge science: ultrafast science; chemical imaging, complex & emergent behavior

  Tools for grand challenge science: midscale instrumentation; accelerator and detector research (awards capped at $5M over 3-year project duration)

  Use inspired discovery science: basic research for electrical energy storage; advanced nuclear energy systems; combustion of 21st century fuels; hydrogen production, storage, and use; other basic research areas identified in BESAC and BES workshop reports with an emphasis on nanoscale phenomena
- Full proposals were due April 24, 2009 and decisions will be made soon
- For full details see: http://www.sc.doe.gov/bes/SISGR.html

BES FY 2010 Budget Highlights

The FY 2010 BES Budget Request supports President Obama's goals for a clean energy economy, investments in science and technology—including exploratory and high-risk research, and training the next generation of scientists and engineers.

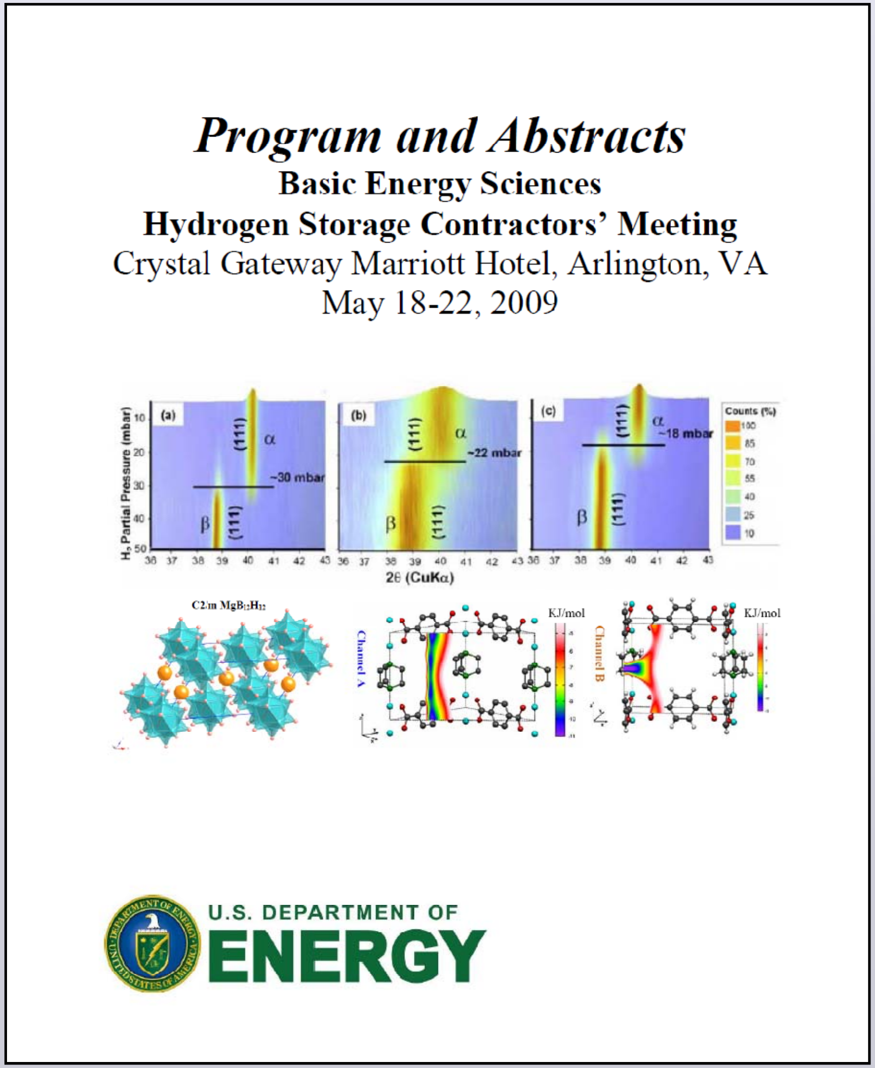
Research:

- Two **Energy Innovation Hubs** are initiated in FY 2010 in the topical areas of **Fuels from Sunlight**, and **Batteries and Energy Storage**. Each hub will assemble a multidisciplinary team to address the basic science, technology, economic, and policy issues needed to achieve a secure and sustainable energy future.
- **Energy Frontier Research Centers (EFRCs)** initiated in FY 2009 continue in FY 2010. EFRCs integrate the talents and expertise of leading scientists across multiple disciplines to conduct fundamental research to establish the scientific foundation for breakthrough energy technologies.
- **Core research**—primarily supporting single principal investigator and small group projects—will be continued and expanded to initiate promising new activities that respond to the five grand challenges identified in the BESAC Grand Challenges report: quantum control of electrons in atoms, molecules, and materials; basic architecture of matter, directed assemblies, structure, and properties; emergence of collective phenomena; energy and information on the nanoscale; and matter far beyond equilibrium.

Facilities:

- The **Linac Coherent Light Source (LCLS)** at SLAC National Accelerator Laboratory, the world's first hard x-ray coherent light source, begins operations in FY 2010. The LCLS provides laser-like x-ray radiation that is 10 billion times more intense than any existing coherent x-ray light source and will open new realms of exploration in the chemical, material, and biological sciences.
- The **National Synchrotron Light Source II** at Brookhaven National Laboratory will continue its construction phase, including the largest component of the project—the building that will house the accelerator ring.
- **Scientific User Facility Operations** are fully funded in FY 2010. The BES user facilities are visited by more than 10,000 scientists and engineers from academia, national laboratories, and industry annually and provide unique capabilities to the scientific community that are critical to maintaining U.S. leadership in the physical sciences.

2009 BES Hydrogen Storage Contractors' Meeting


Program and Abstracts
Basic Energy Sciences
Hydrogen Storage Contractors' Meeting
Crystal Gateway Marriott Hotel, Arlington, VA
May 18-22, 2009

U.S. DEPARTMENT OF
ENERGY

May 20, 2009
Crystal Gateway Marriott Hotel, Arlington, VA

- **25 Projects**
- **14 Oral Presentations**
- **11 Poster Presentations [Joint With EERE]**