



Moving Towards a More Secure Energy Future – Fundamental Research at the US-DOE

EERE's Venture Capital Day DOE Headquarters August 21, 2007

John S. Vetrano

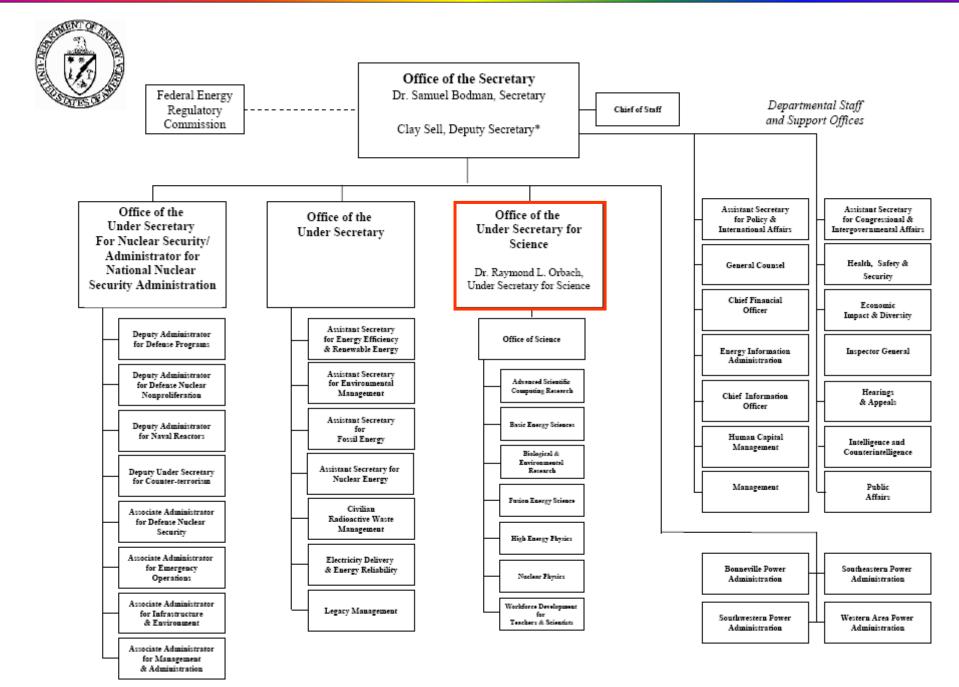
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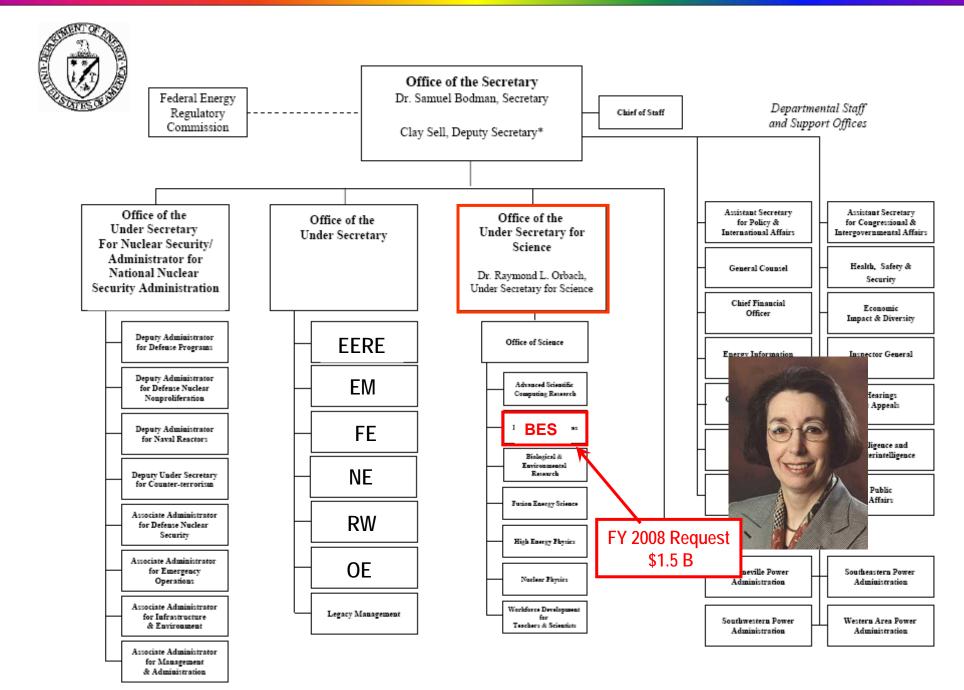
BASIC ENERGY SCIENCES Serving the Present, Shaping the Future

http://www.science.doe.gov/bes/

Department of Energy



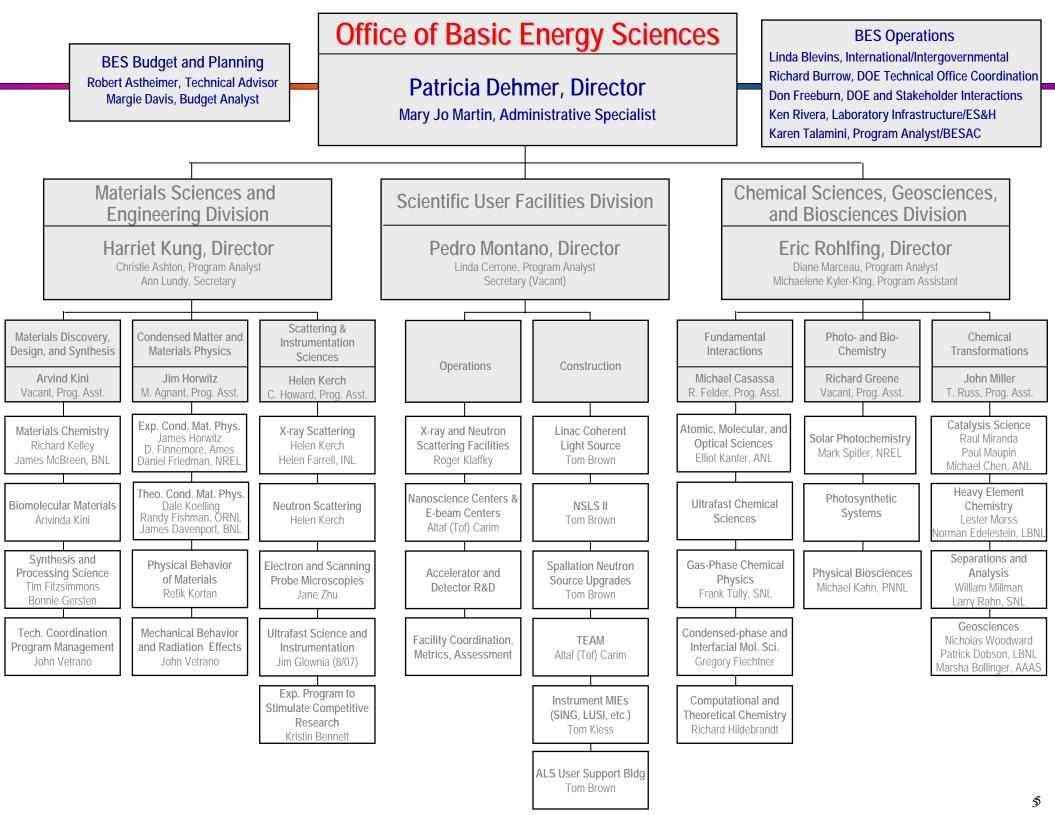
Department of Energy

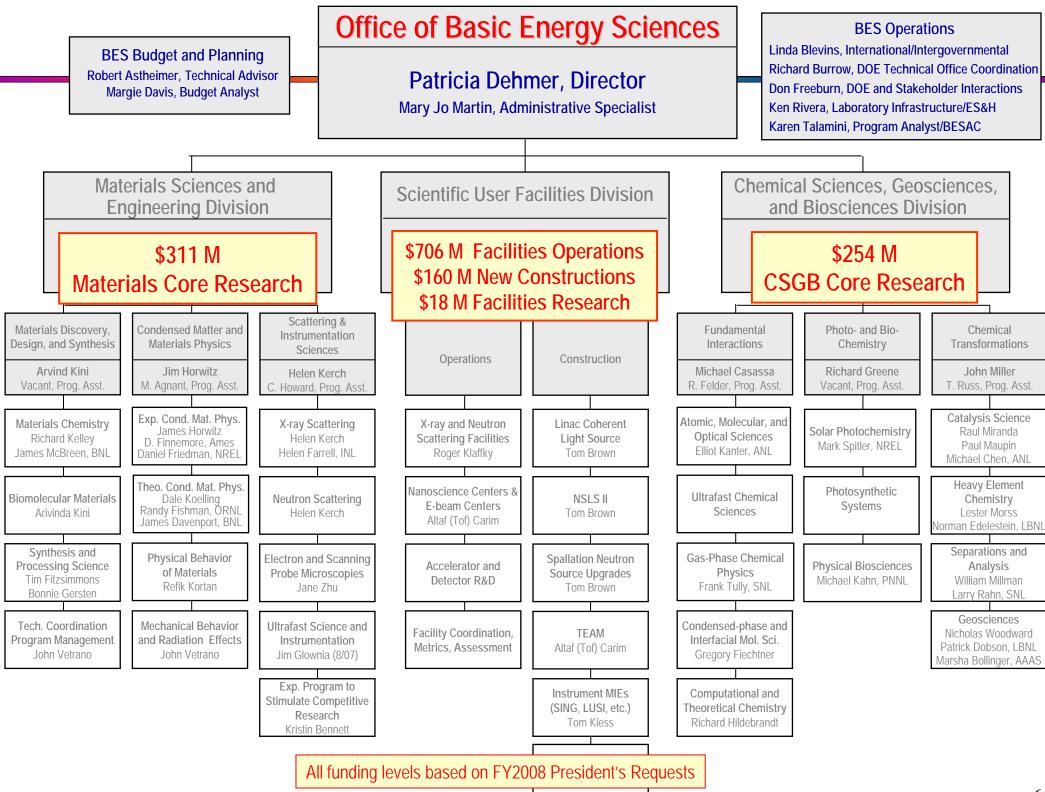


Our Mission:

- Foster and support <u>fundamental research programs</u> 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 <u>major scientific user facilities</u> for "materials sciences and related disciplines" to serve researchers at universities, federal laboratories, and industrial laboratories



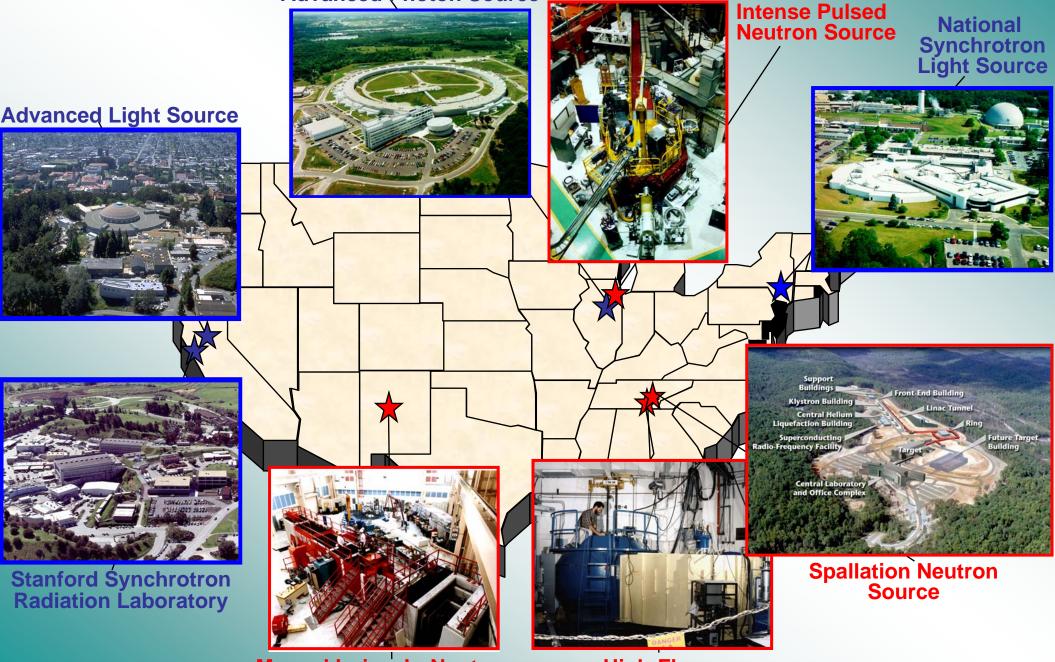




BES Neutron and X-ray Scattering User Facilities

Characterizing Nanoscale Materials for Energy Applications

Advanced Photon Source



Manuel Lujan Jr. Neutron Scattering Center High-Flux Isotope Reactor

DOE Nanoscale Science Research Centers



BES Research Portfolio

Distinguishing Features:

- Idea-driven fundamental research
- Underpin broadly-defined energy missions
- Addressing long-range grand challenges
- Scientific excellence and innovation
- Revolutionary and high risk-high payoff approaches
- Strive for flexibility and stability
- Competitive and peer review process

Deliverables:

- Knowledge broadly disseminated
- High impact results/publications
- New concepts/design for instrumentation
- Important discoveries impacting others' research

Serving the Present, Shaping the Future

impacting directions in basic and applied research and technology development

Relationships Between the Science and the Technology Offices in DOE

Discovery Research

Use-inspired Basic Research

Applied Research

- Research with the goal of meeting <u>technical milestones</u>, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
 - Proof of technology concepts

Technology Maturation & Deployment

- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

- Basic research for fundamental new understanding (i.e., science grand challenges) on materials or systems that may be only peripherally connected or even unconnected to today's problems in energy technologies
- Development of new tools, techniques, and facilities, including those for advanced modeling and computation
- Basic research for fundamental new understanding, with the goal of addressing short-term showstoppers on real-world applications in the energy technologies

Office of Science BES

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

Applied Energy Offices EERE, NE, FE, TD, EM, RW, ...

Goal: practical targets Mandate: restricted to target Focus: performance Metric: milestone achievement

American Competitiveness Initiative

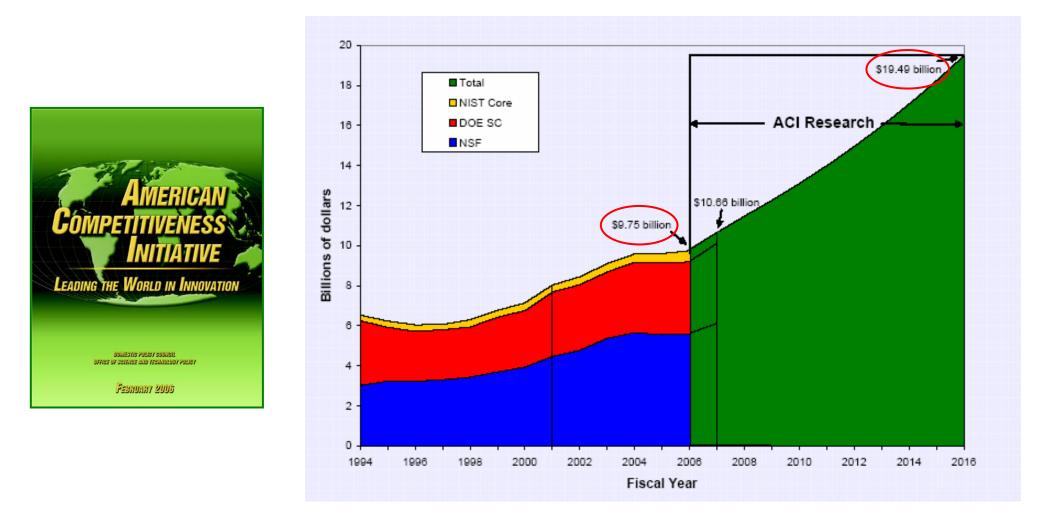


"We must continue to lead the world in human talent and creativity. Our greatest advantage in the world has always been our educated, hardworking, ambitious people – and we're going to keep that edge. Tonight I announce an American Competitiveness Initiative, to encourage innovation throughout our economy, and to give our nation's children a firm grounding in math and science."

"I propose to double the federal commitment to the most critical basic research programs in the physical sciences over the next 10 years. This funding will support the work of America's most creative minds as they explore promising areas such as nanotechnology, supercomputing, and alternative energy sources."

> President George W. Bush State of the Union Message January 31, 2006

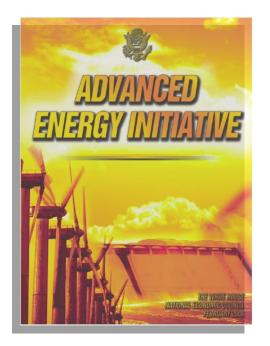
The President's American Competitiveness Initiative



Doubles, over 10 years, funding for innovation-enabling research at key Federal agencies that support high-leverage fields of physical science and engineering: the NSF, the DOE's Office of Science, and NIST.

The President's Advanced Energy Initiative

Accelerating Future Technologies



"....we must reduce our dependence on foreign sources of energy ... "

Changing the way we fuel our vehicles





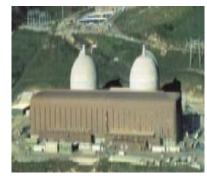


Cellulosic Ethanol

Hydrogen

Batteries

Changing the way we power our homes and businesses







Wind Solar Energy

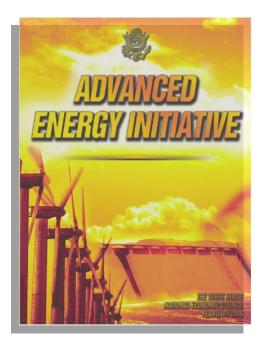


Clean Coal

BES related basic research activities

The President's Advanced Energy Initiative

Accelerating Future Technologies



"....we must reduce our dependence on foreign sources of energy ... "

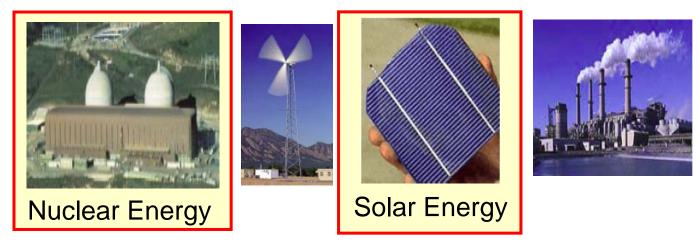
Changing the way we fuel our vehicles



Hydrogen

Batteries

Changing the way we power our homes and businesses



BES related basic research activities

Overview of Relationships between BES Activities and the ACI & AEI

Grand Challenges	Discovery Research	Use-Inspired Basic Research	Applied Research	Technology Maturation
 Basic research to address fundamental limitations of current theories and descriptions of matter in the energy range important to everyday life – typically energies up to those required to break chemical bonds. Particularly challenging are the failures to understand systems that are ultrasmall or isolated or that display emergent phenomena of many kinds. 	 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 advanced modeling and computation 	 Basic research for fundamental new understanding, usually with the goal of addressing showstoppers on real- world applications in the energy technologies 	 Research with the goa of meeting <u>technical</u> <u>milestones</u>, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes Proof of technology concepts 	 At-scale demonstration Cost reduction Prototyping Manufacturing R&D Deployment support
∕∟	Challenges Panel	Research Needs Workshops	DOE Technology Office	/Industry Roadmaps
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BES Energy Security Plan

Basic Research Needs To Assure A Secure Energy Future

A Report from the Basic Energy Sciences Advisory Committee "Considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, <u>BESAC* believes that a new national energy</u> <u>research program is essential and must be</u> <u>initiated with the intensity and commitment</u> <u>of the Manhattan Project, and sustained</u> <u>until this problem is solved."</u>

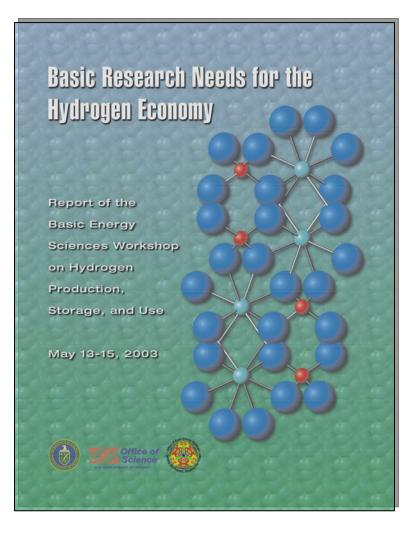
- Eliminate Environmental Concerns
 Diversify Energy Sources
- Increase Energy Efficiency
- Improve Distribution System

*BESAC: Basic Energy Sciences Advisory Committee, http://www.sc.doe.gov/bes/BESAC/BESAC.htm

"Basic Research Needs" Workshops



- Basic Research Needs to Assure a Secure Energy Future BESAC Workshop, October 21-25, 2002 The foundation workshop that set the model for the focused workshops that follow.
- Basic Research Needs for the Hydrogen Economy BES Workshop, May 13-15, 2003
- Nanoscience Research for Energy Needs BES and the National Nanotechnology Initiative, March 16-18, 2004
- Basic Research Needs for Solar Energy Utilization BES Workshop, April 18-21, 2005
- Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors BES, ASCR, FES, and NE Workshop, March 31-April 2, 2004
- The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycles BES, NP, and ASCR Workshop, September 2005
- Basic Research Needs for Superconductivity BES Workshop, May 8-10, 2006
- Basic Research Needs for Solid-state Lighting BES Workshop, May 22-24, 2006
- Basic Research Needs for Advanced Nuclear Energy Systems BES Workshop, July 31-August 3, 2006
- Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels BES Workshop, October 30-November 1, 2006
- Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems BES Workshop, February 21-23, 2007
- Basic Research Needs for Electrical Energy Storage BES Workshop, April 2-5, 2007
- Basic Research Needs for Materials under Extreme Environments BES Workshop, June 10-14, 2007
- Basic Research Needs for Catalysis for Energy BES Workshop, August 5-10, 2007

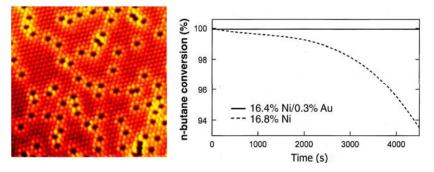


"Bridging the gaps that separate the hydrogenand fossil-fuel based economies in cost, performance, and reliability goes far beyond incremental advances in the present state of the art. Rather, fundamental breakthroughs are needed in the understanding and control of chemical and physical processes involved in the production, storage, and use of hydrogen. Of particular importance is the need to understand the atomic and molecular processes that occur at the interface of hydrogen with materials in order to develop new materials suitable for use in a hydrogen economy. New materials are needed for membranes, catalysts, and fuel cell assemblies that perform at much higher levels, at much lower cost, and with much longer lifetimes. Such breakthroughs will require revolutionary, not evolutionary, advances. Discovery of new materials, new chemical processes, and new synthesis techniques that leapfrog technical barriers is required. This kind of progress can be achieved only with highly innovative, basic research."

Priority Research Areas in Hydrogen Production

Fossil Fuel Reforming

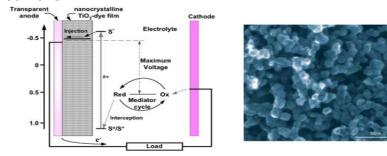
Catalysis; membranes; theory and modeling; nanoscience



Ni surface-alloyed with Au to reduce carbon poisoning

Solar Photoelectrochemistry/Photocatalysis

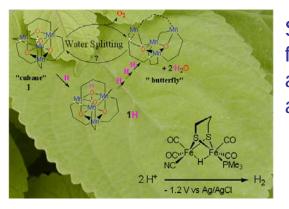
Understanding physical mechanisms; novel materials; theory and modeling; stability of materials



Dye-Sensitized solar cells

Bio- and Bio-inspired H₂ Production

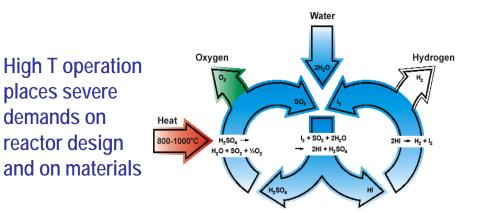
Biological enzyme catalysis; nanoassemblies; bio-inspired materials and processes



Synthetic catalysts for water oxidation and hydrogen activation

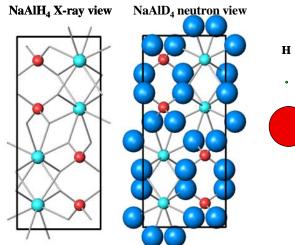
Nuclear and Solar Thermal Hydrogen

Thermodynamic data and modeling; novel materials; membranes and catalysts

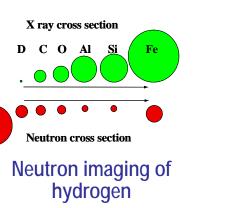


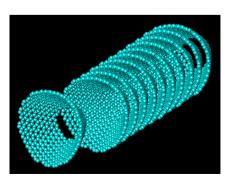
Priority Research Areas in Hydrogen Storage

Novel and Nanoscale Materials



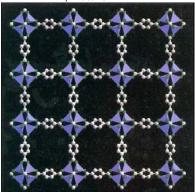
Complex metal hydrides can be recharged on board the vehicles





Cup-stacked carbon Nanofiber

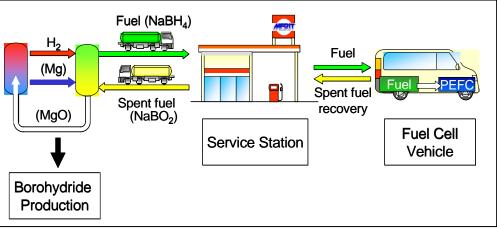
Li, Nature 1999



Nanoporous inorganicorganic compounds

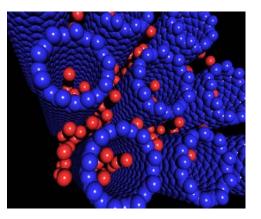
Theory and Modeling

To Understand Mechanisms, Predict Property Trends, Guide Discovery of New Materials



Chemical hydrides will need off-board regeneration

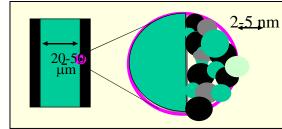
H Adsorption in nanotube array



Priority Research Areas in Fuel Cells

Electrocatalysts and Membranes

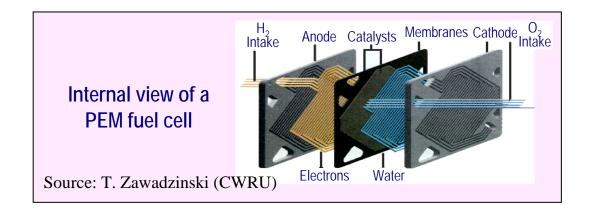
Non-noble metal catalysts; designed triple-percolation electrodes



Controlled design of triple percolation nanoscale networks: ions, electrons, and porosity for gases

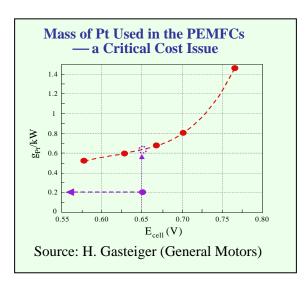
Low temperature fuel cells

'Higher' temperature membranes; degradation mechanisms; tailored nanostructures



Solid Oxide Fuel Cells

Theory, modeling, and simulation; new materials; novel synthesis; in-situ diagnostics



YSZ Electrolyte for SOFCs



Tailored PorositySource: R. Gorte (U. Penn)

Potentials of Renewable Energy Sources



Solar 120,000 TW at Earth surface 600 TW practical

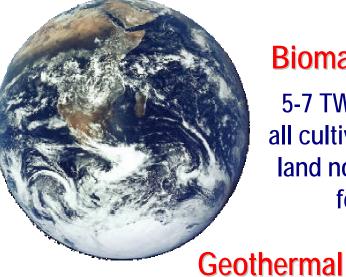


Wind

2-4 TW extractable



Tide Ocean Currents 2 TW gross



Biomass 5-7 TW gross all cultivatable land not used for food





Hydroelectric

4.6 TW gross 1.6 TW technically feasible 0.6 TW installed capacity

12 TW gross over land small fraction recoverable



Basic Research Needs for Solar Energy Utilization

The Sun is a singular solution to our future energy needs

- capacity dwarfs fossil, nuclear, wind . . .
- sunlight delivers more energy in one hour than the earth uses in one year
- free of greenhouse gases and pollutants
- secure from geo-political constraints

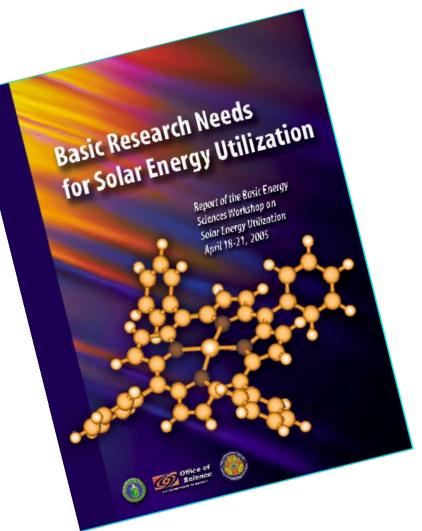
• Enormous gap between our tiny use of solar energy and its immense potential

- Incremental advances in today's technology will not bridge the gap

- Conceptual breakthroughs are needed that come only from high risk-high payoff basic research

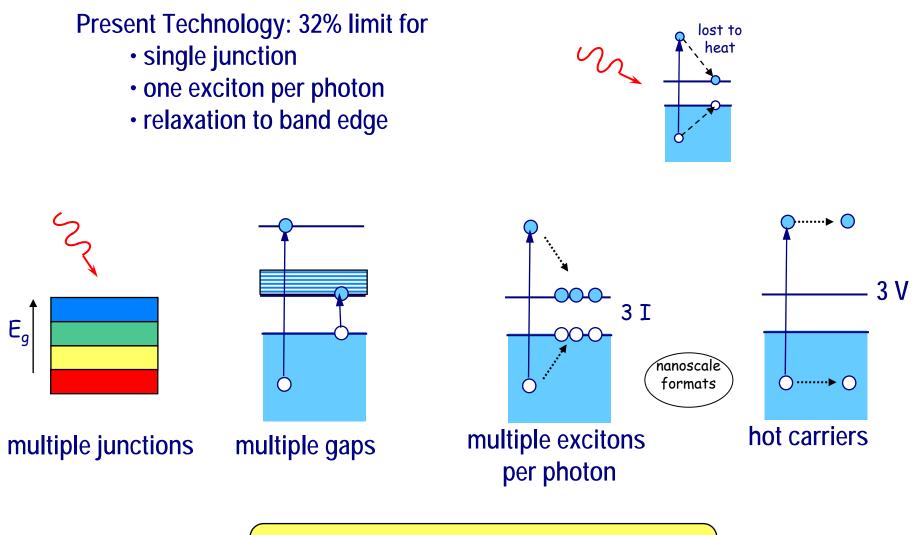
• *Interdisciplinary research is required* physics, chemistry, biology, materials, nanoscience

Basic and applied science should couple seamlessly



http://www.sc.doe.gov/bes/reports/abstracts.html#SEU

Revolutionary Photovoltaics: 50% Efficient Solar Cells

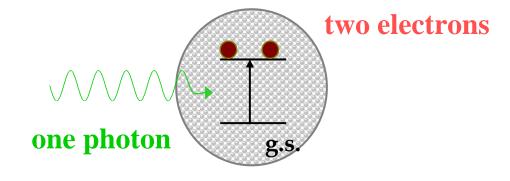


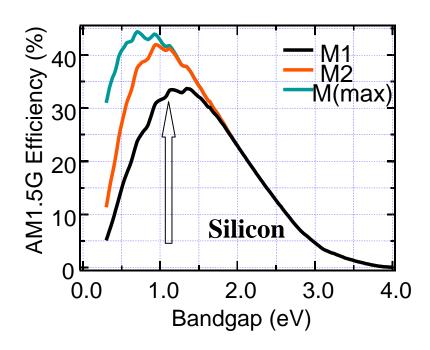
Rich Variety of New Physical Phenomena Challenge: Understand and Implement

Next Generation Photovoltaic Cells:

Exceeding Today's Thermodynamic Limits through Multi-Exciton Generation (MEG)

MEG in Si, PbSe quantum dots multiplies one photon into two, three, four, or more electrons.



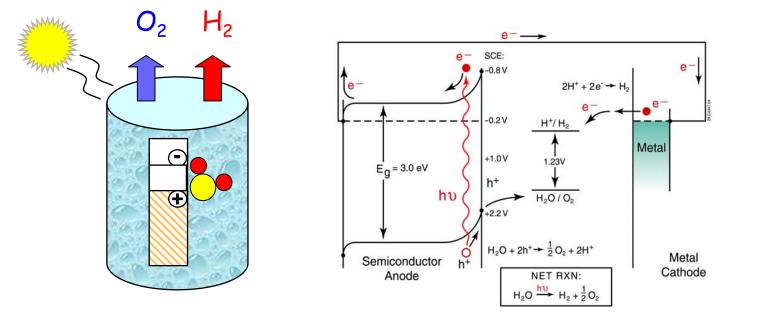


A multiplier M of only 2 increases efficiency of silicon solar cell from 32% to 42%

> BES research continues into: -mechanism of multiplication -materials that exhibit effect -method of electron extraction

A. Nozik, NREL anozik@nrel.gov V. Klimov, LANL, klimov@lanl.gov

Efficient Solar Water Splitting





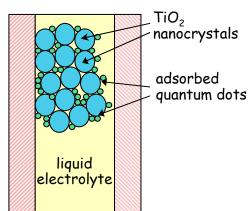
Demonstrated 10% Efficiencies in Laboratory

Scientific Challenges

- Cheap materials that are robust in water
- Catalysts for the redox reactions at each electrode
- Nanoscale architecture for electron excitation \Rightarrow transfer \Rightarrow reaction

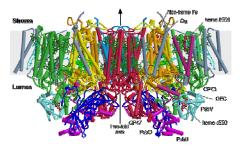
Nanoscience as a Cross-cutting Theme

Manipulation of Photons, Electrons, and Molecules



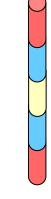
quantum dot solar cells

>-8-0360 -2007



artificial photosynthesis

natural photosynthesis



nanostructured thermoelectrics

Nanoscale Architectures

top-down lithography bottom-up self-assembly multi-scale integration

Characterization

scanning probes electrons, neutrons, x-rays smaller length and time scales Theory and Modeling multi-node computer clusters density functional theory 10 000 atom assemblies

Interdisciplinary research is required to enable transformational breakthroughs in solar energy utilization

Basic Research Needs for Solid State Lighting Workshop May 22-24, 2006



Workshop Chairs: Julia Phillips (Sandia National Labs) Paul Burrows (Pacific Northwest National Lab)

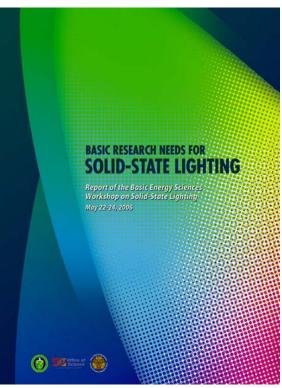
Panels and Leads:

LED Science: Jerry Simmons (SNL); Bob Davis (Carnegie Mellon) OLED Science: Franky So (U of Florida); George Malliaras (Cornell) Cross-Cutting Science: J. Misewich (BNL); A. Nurmikko (Brown); D. Smith (LANL)

Plenary Speakers:

Fred Schubert (RPI), George Craford (Lumileds); Alan Heeger (UCSB), Eli Yablonovitch (UCLA)

Workshop Charge: To identify basic research needs and opportunities underlying light emitting diode and related technologies, with a focus on new or emerging science challenges with potential for significant long-term impact on energy-efficient and productivity-enhancing solid state lighting. Highlighted areas will include organic and inorganic materials and nanostructure physics and chemistry, photon manipulation, and cross-cutting science grand challenges.



Solid State Lighting

		<u> </u>	
Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
 Rational design of SSL lighting structures Control of radiative & non-radiative processes in light-emitting materials New functionalities through heterogeneous nanostructures Innovative photon management Enhanced light-matter interactions Precision nanoscale characterization, synthesis, and assembly Multi-scale modeling – quantum excitations to light extraction 	 Polar materials and heterostructures for SSL Luminescence efficiency of InGaN Managing and exploiting disorder in OLEDs Understanding degradation in OLEDs 	 Fechnology Milestones: By 2025, develop advanced solid state lighting technologies with a product system efficiency of 50 percent with lighting that accurately reproduces sunlight spectrum. Materials and components for inorganic and organic light-emitting diodes research for improved efficiency and cost reduction Strategies for improved device light extraction Low-cost fabrication and patterning techniques and tools & manufacturing R&D Product degradation and reliability issues 	 Developing national standards and rating systems for new products Commercial adoption and support Industrial partnership Legal, health, market, and safety issues Cost reduction Prototyping
	of Science BES	Technology Offic EERE	es

Basic Research Needs for Electrical Energy Storage April 2-4, 2007

Chair: Co- Chairs:

John Goodenough(UT-Austin)Hector Abruna(Cornell)Michelle Buchanan(ORNL)



Breakout Session Panel and Leaders: Chemical Storage Science Stan Whittingham, SUNY-Binghamton Steven Visco, LBNL Capacitive Storage Science Bruce Dunn, UCLA Yury Gogotsi, Drexel Cross-Cutting Daniel Nocera, MIT Andy Gewirth, U Illinois CHARGE: To identify basic research needs and opportunities underlying batteries, capacitors and related technologies, with a focus on new or emerging science challenges with potential for significant long-term impact on the efficient storage and release of electrical energy. Highlighted areas will include coupled ionic and charge transport, electrolyte physics, theory and modeling, and novel materials and approaches.

Electrical Energy Storage

Discovery Research

Use-inspired Basic Research

Applied Research

Technology Maturation & Deployment

- Understand and predict interfacial charge transfer and multi-body effects
- Predict and control dynamics of phase transitions
- Control of chemistry and its dynamics at electrified interfaces
- Determine consequences of dimensionality
- Physicochemical consequences of nanodimensions
- Fundamentals of solvation dynamics and ionic transport
- Revolutionary tools for *in situ* structural and dynamic studies over broad spatial / temporal regimes

- Retrosynthetic approaches to high performance new materials
- Design of new materials capable of multi-electron storage per redox center
- Understand design criteria for electrolytes that enable higher voltages
- Tailor nanoscale electrode architectures for optimal transport
- Novel chemistries for scavenging impurities and self-healing
- Generation of knowledge and computational and experimental tools to predict properties, performance evolution, and lifetime of materials

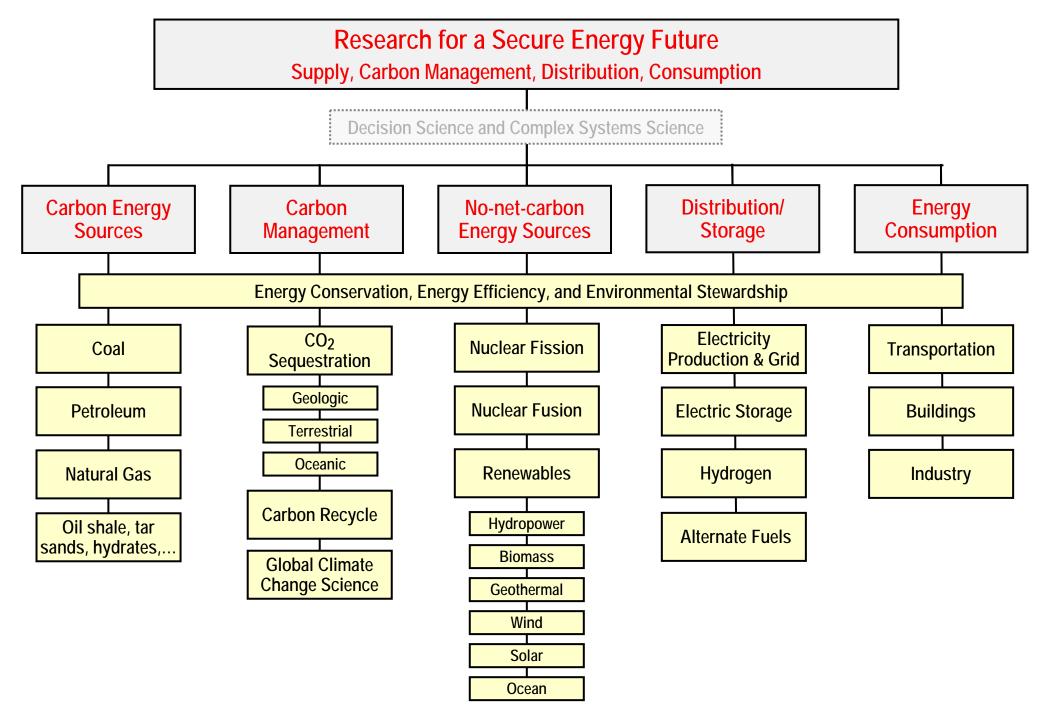
- Develop and apply material models and computational tools for component and system design and diagnostics
- Identify, develop, evaluate materials, electrodes, cells, and advanced electrochemical systems
- Develop and apply novel material processing technologies
- Design and develop device and system architectures
- Assemble/test devices with respect to energy storage system requirements—high power, high energy density, long lifetime, rapid recharge, deep discharge, reliability, safety, low cost.

- Demonstrate energy storage systems in advanced vehicle applications.
- Support the establishment of domestic manufacturing capabilities for components and systems
- Assist development and deployment of high capacity storage systems for centralized and distributed power sources
- Develop long-life, low cost, reliable, environmentally friendly, recyclable energy storage for portable and stationary energy storage

Office of Science BES

Technology Offices EERE and OE

Past and Future BRN Workshops Address Many Elements Required for a Decades-to-Century Energy Security Strategy



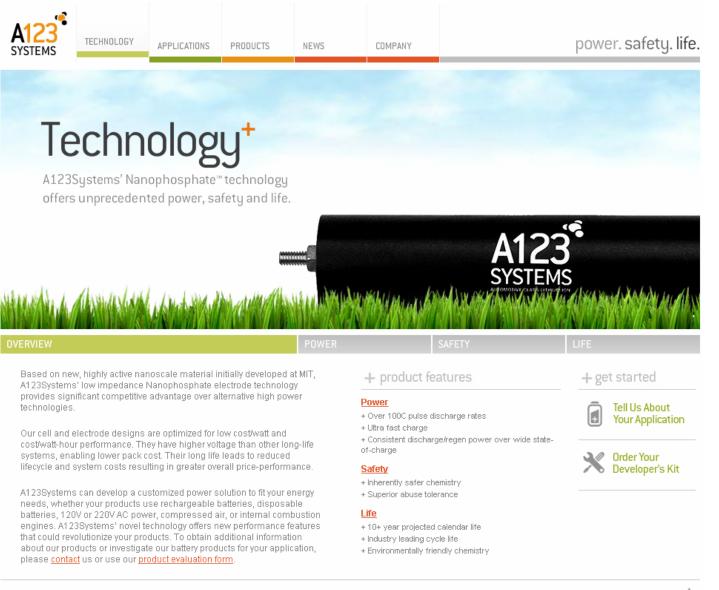
Grand Challenge Research Areas Emerged from the Workshops

- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- Science at the nanoscale, especially low-dimensional systems that promise materials with new and novel properties
- Methods to "control" photon, electron, ion, and phonon transport in materials for next-generation energy technologies
- Structure-function relationships in both living and non-living systems
- Designer catalysts
- Interfacial science and designer membranes
- Bio-materials and bio-interfaces, especially at the nanoscale where soft matter and hard matter can be joined
- New tools for:
 - Spatial characterization, especially at the atomic and nanoscales and especially for in-situ studies
 - Temporal characterization for studying the time evolution of processes
 - Theory and computation

- \$15 million FY06 biomass crosscut (93% at universities)
 - \$3 million in microbial biochemistry
 - Ingram at Florida Multiple substrate fermentation (Celunol)
 - Lynd at Dartmouth Cellulase Complex (Mascoma)
 - \$12 million in plant growth & development/biochemistry (training as well)
 - ~ \$1.5 million at Complex Carbohydrate Research Center (CCRC), University of Georgia
 - ~ \$4.4 million at Plant Research Laboratory (PRL), Michigan State
 - Somerville at Carnegie Biocatalyst Fatty Acyl-CoA Reductase (Newco LS9)

A123 Systems

Yet-Ming Chiang, MIT

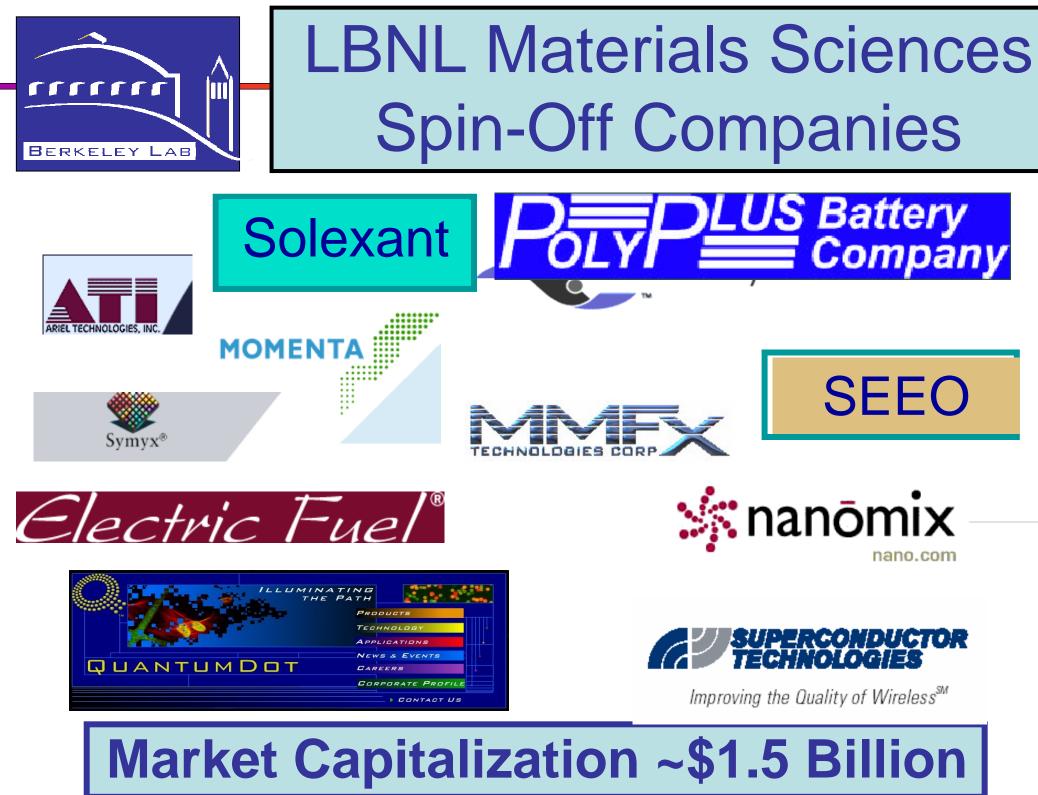


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Symyx

Peter Schultz, LBNL (now at Scripps Research Institute)

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About the Company Licensed Discoveries News Releases Investors Careers	<section-header><section-header>Supremention<</section-header></section-header>	entists and see our labs iyx 2006



Thank You!

http://www.sc.doe.gov/bes/bes.html