# DOE goals and challenges in Energy Security

Presentation to the NNSA
Laboratory Directed Research & Development
2008 Symposium
Focus on Energy Security

**Dr. Raymond L. Orbach**
Under Secretary for Science
U.S. Department of Energy
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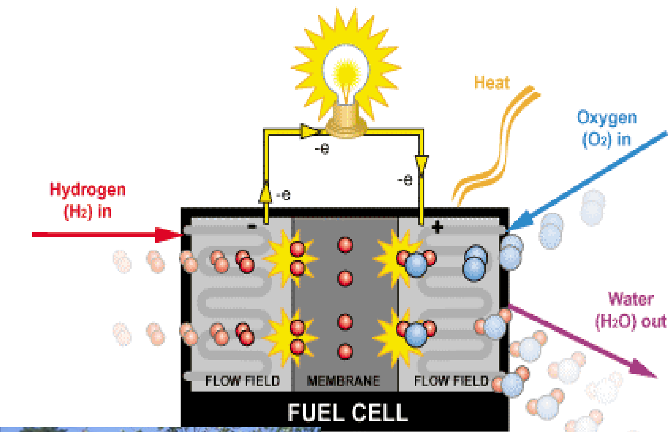
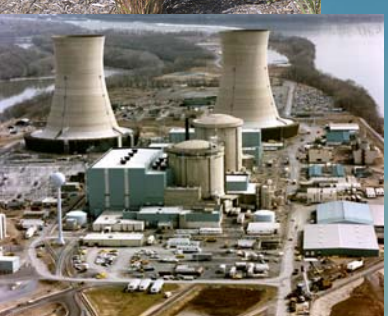
# Energy Science Challenges

*Five Areas Where Science and Imagination Can Impact Energy Security*







- Solar energy utilization
- Electrical energy storage
- Bioenergy
- Nuclear energy
  - Fission
  - Fusion
- Hydrogen: production, storage, and use

# Institutional Challenges – *Vision, Leadership, Business Acumen*

- *Vision* – know what is important
  - **Significant opportunities exist for science to make an impact**

- *Leadership* – focus on what is important
  - **Nurture and develop core competencies**
  - **Choose Relevant projects**
  - **Operate at “scale”**

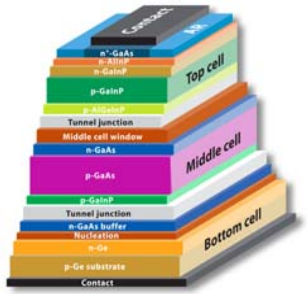
- *Business acumen* – know and meet the competition
  - **SC laboratories are significantly engaged**
  - **Universities are very active in this area**
  - **Connections to industries are important**
  - **Need to be nimble, cost effective, …**

# Solar Energy

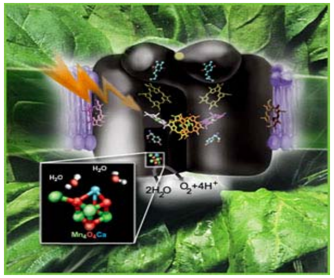
## Science Transforming Energy Technologies

**Imagine:**
- Solar photovoltaics exceeding thermodynamic efficiency limits
- Direct conversion sunlight to chemical fuels

- Sunlight provides by far the largest of all carbon-neutral energy sources – more energy from sunlight strikes the Earth in one hour (4.6 x $10^{20}$ joules) than all the energy consumed on the planet in a year.
- Despite the abundance, less than 0.1% of our primary energy derives from sunlight.
- The three routes for using solar energy – conversion to electricity, fuels, or thermal heat – exploit the functional steps of capture, conversion, and storage. They also exploit many of the same electronic and molecular mechanisms.
- The challenge: reducing the costs and increasing the capacity of converting sunlight into electricity or fuels that can be stored or transported (solar electricity, solar fuels, solar thermal systems).
- Silicon: The top commercial solar cells (single crystal silicon) have reached conversion efficiencies of 18%; triple-junction cells with Fresnel lens concentrator technology are approaching efficiencies of 40%. Cost-effective improvements in efficiency dependent on our ability to understand and control phenomena at the nanoscale.
- Photosynthesis: Borrowing nature's design for capturing sunlight – bio-inspired nanoscale assemblies to produce fuels from water and $CO_2$.

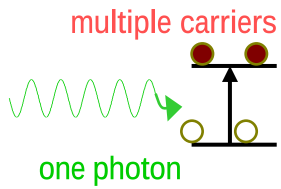


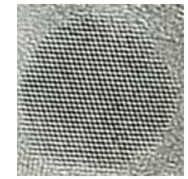
A multi-layered triple-junction solar cell designed to absorb different solar photons.


Photosystem II uses solar energy to break two molecules of water into one oxygen molecule plus four hydrogen ions, meanwhile freeing electrons to drive other reactions.

# Basic Research Needs for Solar Energy Utilization

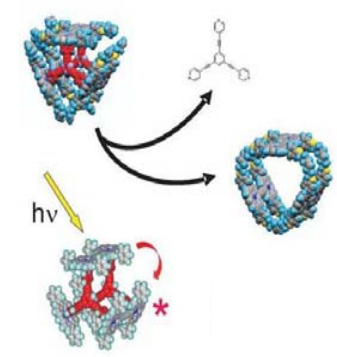
The physical, chemical, and biological pathways of solar energy conversion meet at the nanoscale. The ability to create nanoscale structures coupled with advanced characterization, theory, and computational tools suggest that understanding and control of efficient solar energy conversion are within reach.



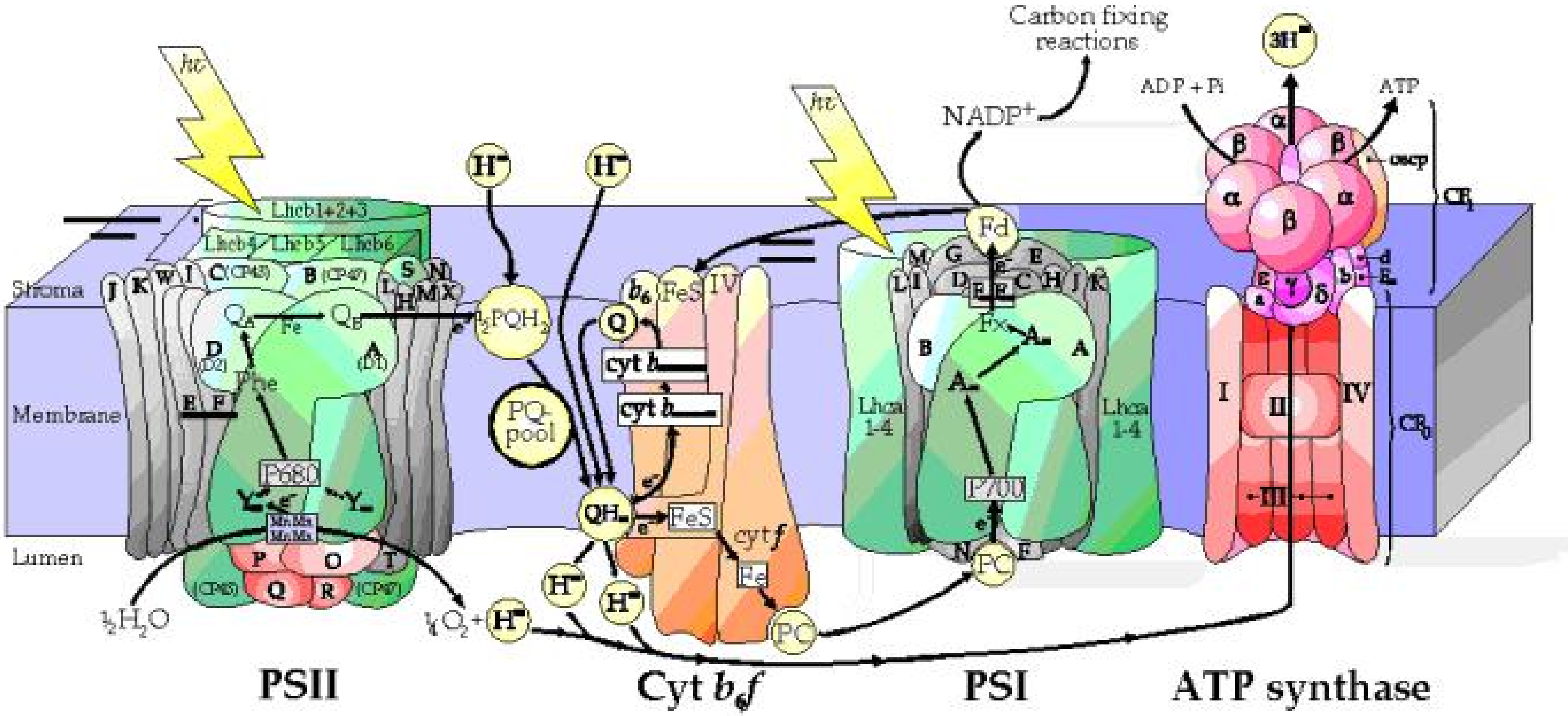
Si nanocrystals (7 nm diameter)

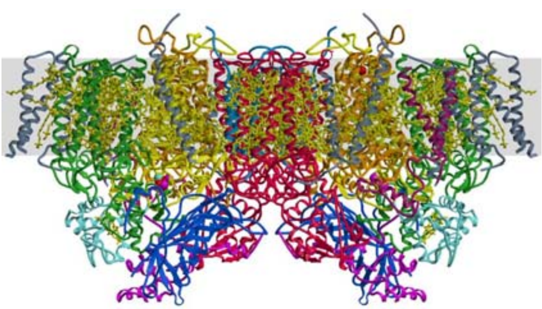
- **Photovoltaics exceeding thermodynamic efficiency limits**
  New concepts, structures, and methods of capturing the energy from sunlight without thermalization of carriers are required to break through the Shockley-Queisser efficiency barrier (32%). Multiple-exciton generation from a single photon is a prime example.
- **Easily manufactured, low-cost polymer and nanoparticle photovoltaic structures**
  "Plastic" solar cells made from molecular, polymeric, or nanoparticle-based structures could provide flexible, inexpensive, conformal solar electricity systems.
- **Efficient photoelectrolysis**
  Solar fuels generation involves coupling photo-driven single electron steps with fuel-forming, multi-electron processes. No man-made systems approach the performance of naturally found enzymes. Practical solar fuel formation requires construction of new catalyst systems to form hydrogen and oxygen from water and to efficiently reduce carbon dioxide from the air.
- **Defect-tolerant and self-repairing systems**
  Understanding the defect formation in photovoltaic materials and self-repair mechanisms in photosynthesis will lead to defect tolerance and active self-repair in solar energy conversion devices, enabling 20+ years operation.
- **Bio-inspired molecular assemblies systems**
  The design and development of light-harvesting, photoconversion, and catalytic modules capable of self-ordering and self-assembling into an integrated functional unit to realize an efficient artificial photosynthetic system for solar fuels.
- **New experimental and theoretical tools**
  Development of experimental and theoretical tools that could enable the theoretical prediction of optimally performing structures.




A prism-shaped assembly of three porphyrin molecules that displays enhanced light harvesting capability

# Photon Capture in Nature

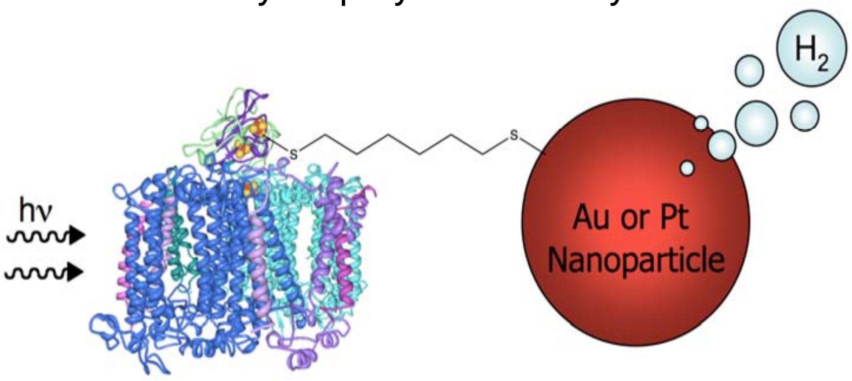


# Efficient Solar Hydrogen Production by a Hybrid Photo-catalyst System

## Molecular Wire

Delivers the highly reducing electrons to the catalyst rapidly and efficiently




**Photosystem I**

Efficient solar absorber which generates a stable charge-separated state, a source of highly reducing electrons.

**Catalyst**

Uses the photo-generated electrons to reduce protons from solution into hydrogen ($H_2$).

- Solar energy is an attractive source for large scale hydrogen production. Robust, inorganic catalyst systems such as platinized $TiO_2$ have been used to generate hydrogen from sunlight, but efficiency is low because they can only use the UV portion of the solar radiation. Natural photosynthetic systems such as Photosystem I (PS I) can absorb ~45% of solar spectrum, but are coupled indirectly and inefficiently to a non-robust, oxygen-sensitive hydrogenase to generate hydrogen.
- In a novel strategy that combines the best of both worlds, a synthetic molecular wire, consisting of a $Fe_4$-$S_4$ cluster and an organic dithiol, is used to covalently link PS I with the Au or Pt nanoparticles. This provides a rapid, efficient pathway for shuttling photo-generated electrons to the inorganic nanocatalyst.
- Upon illumination, the PS I-Molecular Wire-Nanocatalyst hybrid system generates 8 $H_2$ per PS I per second over a period of 12-16 hours (with cytochrome $c_6$ as electron donor).
- This represents a new benchmark in the efficiency of hydrogen production by use of modified or hybrid photosynthetic systems. To compare, a genetically engineered PS I-hydrogenase gene fusion generates 0.0045 $H_2$ per PS I per second, and platinized chloroplasts generate 0.045 $H_2$ per PS I per second.

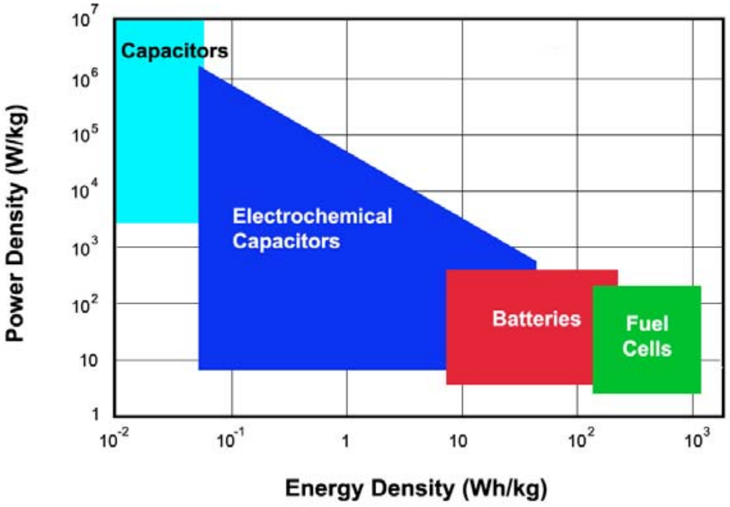
R. A. Grimme, C. E. Lubner, D. A. Bryant and J. H. Golbeck, *J. Am. Chem. Soc.*, 2008, *130*, 6308-6309

# Electrical Energy Storage

Science Transforming Energy Technologies

**Imagine:**
- Solar and wind providing over 30% of electricity consumed in U.S.
- The number of all-electric/plug-in hybrid vehicles on the road exceeding gasoline-powered vehicles

- Many renewable energy sources such as wind and solar are *intermittent* — To make these energy sources truly effective and integrate them into the electrical grid, we need significant breakthroughs in electrical energy *storage* technologies.
- Electrical energy storage (EES) devices with substantially higher energy and power densities and faster recharge times are needed if all-electric/plug-in hybrid vehicles are to be deployed broadly.
- EES devices: batteries—store energy in chemical reactants capable of generating charge; electrochemical capacitors—store energy directly as charge.
- Fundamental gaps exist in understanding the atomic- and molecular-level processes that govern operation, performance limitations, and failure of these devices.

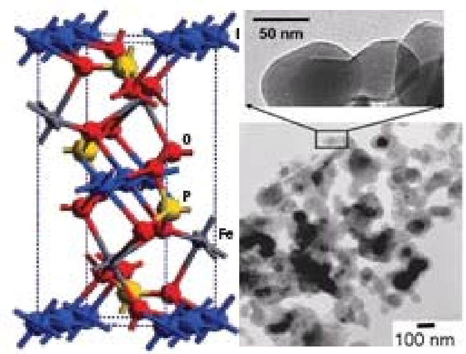



Energy and power densities of various energy storage devices. Electrochemical capacitors bridge between batteries and conventional capacitors.

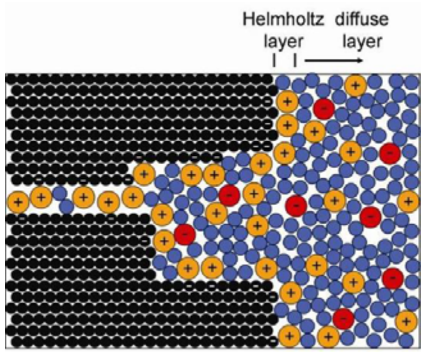
# Basic Research Needs for Electrical Energy Storage

Knowledge gained from basic research in chemical and materials sciences is needed to surmount the significant challenges of creating radical improvements for electrical energy storage devices for transportation use, and to take advantage of large but transient energy sources such as solar and wind.

- **Nanostructured electrodes with tailored architectures**
  Fundamental studies of the electronic conductivity of $LiFePO_4$ led to the discovery of doping-induced conductivity increases of eight orders of magnitude. This research discovery led to the development of high power-density Li-ion batteries by A123 Systems to power electric vehicles such as the Chevy Volt and the Th!nk.
- **The promise of higher battery power via conversion reactions**
  Current batteries operate with slightly less than one electron per redox center with typical electrode materials. New research on conversion reactions is looking at advanced materials to yield up to six electrons per redox center, allowing a large increase in battery power density. An example of such a reaction using cobalt is: $CoO_2 + 2\,e^- + 2\,Li^+ \leftrightarrows CoO + Li_2O$. Other reactions using sulfides, phosphides and flourides are being investigated.
- **Multifunctional material architectures for ultracapacitors:**
  Basic research in materials for capacitors is enabling the development of multi-functional nanoporous structures and facilitating the understanding of charge storage mechanisms at surfaces. Ultracapacitors complement battery power by allowing very rapid charge and discharge cycles and the high surface area of nanostructures yields high charge storage capacity.
- **Understanding behavior in confined spaces:**
  The behavior of electrolytes as a function of pore size in electric double layer capacitors is not well understood but crucial to enabling higher charge densities. Nanometer-scale pores offer high surface areas but create an increased importance of the Helmholz layer in the overall capacitance and affect the dynamics of the charge cycle.




$LiFePO_4$ structural model and nanostructure




Ion solvation changes with pore size during electric double layer charging (electrode, black; solvent, blue; cation, orange; anion, red)

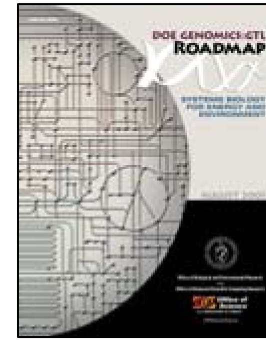
# Bioenergy

## Science Transforming Energy Technologies

**Imagine:**
- A sustainable, carbon-neutral biofuels economy that meets over 30% of U.S. transportation fuel needs (cars and trucks) without competing with food, feed, or export demands.

- The development of biofuels—especially lignocellulose biofuels—represents a major scientific opportunity that can strengthen U.S. energy security and protect the global environment.
- Biofuels can be essentially carbon-neutral or even carbon-negative – as plant feedstocks grow, they reabsorb the carbon dioxide emitted when biofuels are burned, and they can store carbon dioxide in their roots.
- To produce lignocellulosic biofuels, or biofuels from plant fiber, cost-effectively on a commercial scale will require transformational breakthroughs in basic science focused on both plants and microorganisms and processing methods.
- The challenge is the recalcitrance of the plant cell wall – plant fiber has evolved over the millennia to be extremely resistant to breakdown by biological or natural forces.
- Many scientists believe we are within reach of major breakthroughs in developing cost-effective methods of producing liquid fuels from lignocellulose in the near- to mid- term.
- The environmental sustainability aspects associated with bioenergy derived from feedstock crops – water, soil quality, land-use changes, genetically altered plants, carbon balance – must be addressed proactively.

# DOE Bioenergy Research Centers

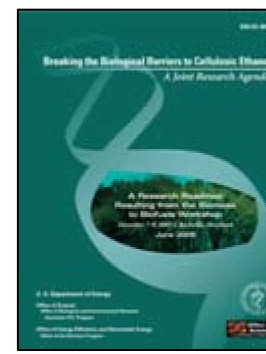



## Grand Science Challenges:

- Using a systems biology approach, understand the principles underlying the structural and functional design of living systems — plants and microorganisms.
- Develop the capability to model, predict, and engineer optimized enzymes, microorganisms, and plants — bioenergy and environmental applications.

## “Basic Research Needs” for cellulosic ethanol (and other biofuels) production:

The emerging tools of systems biology are being used to help to overcome current obstacles to bioprocessing cellulosic feedstocks to ethanol and other biofuels– metagenomics, synthetic biology, high-throughput screening, advanced imaging, high-end computational modeling.



- **DOE BioEnergy Science Center** – led by Oak Ridge National Laboratory, includes 9 partnering institutions. This center focuses on the resistance of plant fiber to breakdown into sugars and is studying the potential energy crops poplar and switchgrass.
- **DOE Great Lakes Bioenergy Research Center** – led by University of Wisconsin-Madison in partnership with Michigan State University, includes 6 other partnering institutions. This center is studying a range of plants and is exploring plant fiber breakdown and how to increase plant production of starches and oils, which are more easily converted to fuels. This Center also focuses on sustainability, examining the environmental and socioeconomic implications of moving to a biofuels economy.
- **DOE Joint BioEnergy Institute** – led by Lawrence Berkeley National Laboratory, includes 5 other partnering institutions. This center focuses on “model” crops of rice and *Arabidopsis thaliana* in the search for breakthroughs in basic science and is exploring microbial-based synthesis of fuels beyond ethanol.

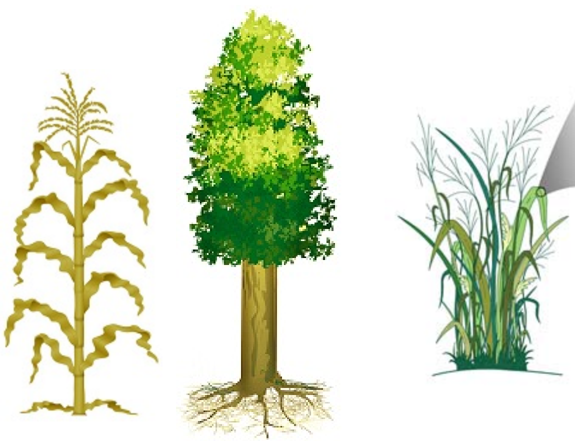
# DOE Bioenergy Research Centers –
## *A New Model for Accelerated Advances*

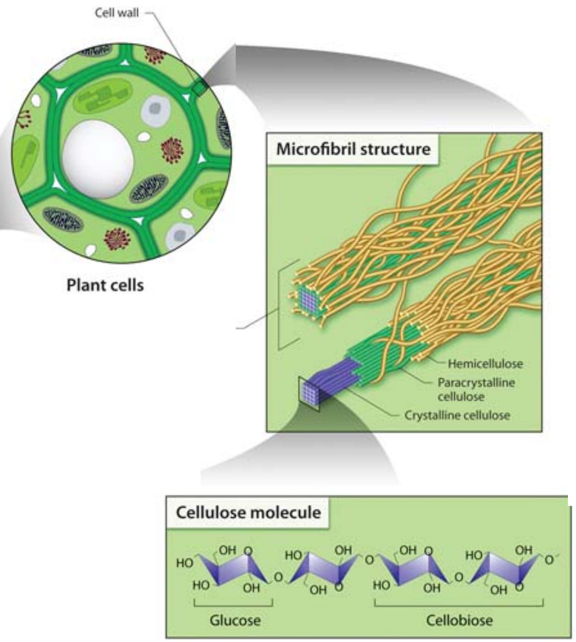
- Three centers established in FY 2008
  - **Oak Ridge National Laboratory**
  - **U. Wisconsin Madison**
  - **Lawrence Berkeley Laboratory**
- Each center funded at $25 million per year for up to five years starting in FY 2008
  - **Centers were chosen competitively**
  - Housed in existing buildings or leased space, and
  - Are fully staffed
- Management model involves high degree of cooperation between DOE federal staff and Centers' leadership
- Significant results already are forthcoming

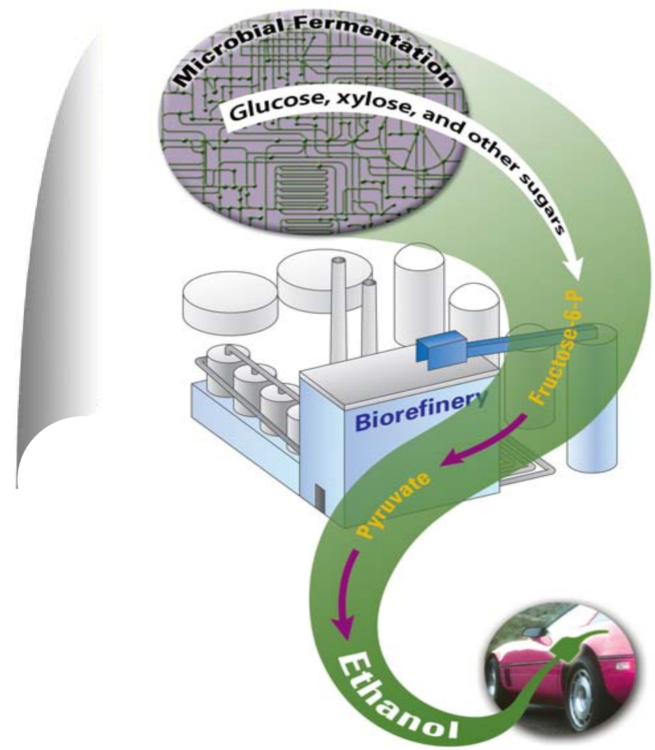
# Opportunities for Local Transportation Fuels

**Imagine:** Development of local biofuels infrastructure from regional plants and feedstock crops

*Lignocellulose* → *Sugars/Metabolites* → *Biofuels*






- Local agricultural waste and regional feedstock crops optimized to climate and minimal inputs

- Biochemical, thermochemical, and/or catalytic processing of plants to sugars, lipids, and other metabolites

- Biological, thermochemical, and/or catalytic synthesis of biofuels that meet national standards.

# Nuclear Energy

## Science Transforming Energy Technologies

| | |
|---|---|
| **Imagine:** | • Abundant fossil-free power with zero greenhouse gas emissions<br>• A closed fuel cycle |

- Good for both energy security and the environment:
  - Reduces Nation's dependence on fossil fuels and imports
  - No carbon dioxide or toxic emissions
- Currently provides 20% of nation's electricity and could provide much more
- Key challenge is handling spent fuel – and related problem of proliferation
- Advances in science and engineering can provide major reduction in spent fuel by "closing" fuel cycle:
  - Recycling spent fuel and burning it in fission reactors
  - Reducing storage requirements by up to 90%
  - Can extend fuel supplies 100X; energy remaining in "spent" fuel
  - New recycling technologies could reduce nuclear materials proliferation concern

**Performance of materials and chemical processes under extreme conditions is a limiting factor in all areas of advanced nuclear energy systems**

# Basic Science for Advanced Nuclear Energy Systems

**Fundamental Challenge:** To understand and control chemical and physical phenomena in complex systems from femto-seconds to millennia, at temperatures to 1000 $^{o}$C and for radiation doses to hundreds of displacements per atom.

## Basic Science:

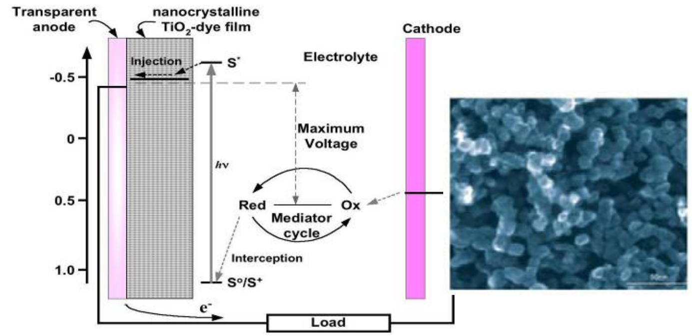
- Research in Basic Energy Sciences
  - Materials and chemistry under extreme temperature, pressure, corrosive, and radiative environments; chemistry at interfaces and in complex solutions; separations science; advanced actinide fuels; nanoscale synthesis and characterization for design of materials and interfaces with radiation, temperature and corrosion resistence; predictive modeling and simulation
  - Workshop: Basic Research Needs for Advanced Nuclear Energy Systems, July 31-August 2, 2006.
- Research in Nuclear Physics
  - Nuclear measurements (neutron and charged particle beam accelerator experiments, cross-section measurements), nuclear data (cross-section evaluation, actinide nuclear data), nuclear theory and computation
  - Nuclear Physics and Related Computational Science R&D for Advanced Fuels Cycles Workshop, August 10-11, 2006.
- Research in Advanced Scientific Computing
  - Developing and scaling next-generation multiscale and multiphysics codes; advanced modeling and simulation to improve future reactor designs; reactor core simulations; fluid flow and heat transfer; and radiation induced microstructural evolution of defects.
  - Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems, August 15-17, 2006.

# Hydrogen Economy

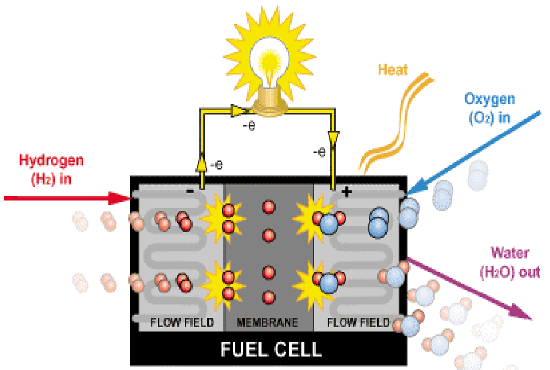
## Science Transforming Energy Technologies

**Imagine:**
- A hydrogen economy that provides ample and sustainable energy, flexible interchange with existing energy technologies, and a diversity of end uses to produce electricity through fuel cells.

- The hydrogen economy is a compelling vision, as it provides an abundant, clean, secure and flexible energy carrier. However, it does not operate as an integrated network, and it is not yet competitive with the fossil fuel economy in cost, performance, or reliability.
- There have been significant accomplishments in basic and applied hydrogen research in the past years leading to major advances in hydrogen production, storage, and fuel cell technologies.
- Specifically, hydrogen production from natural gas has met its 2010 target of $3/gge (gallon of gasoline equivalent); hydrogen storage capacities have been increased by 50%; and fuel cells costs have been decreased by 60%.
- But fundamental science breakthroughs are needed in order to meet the longer-term (2015 and beyond) technological readiness requirements.




Dye-Sensitized photoelectrochemical cells for solar hydrogen production via water electrolysis. The cell consists of a highly porous thin layer of titanium dioxide nanocrystal aggregates.

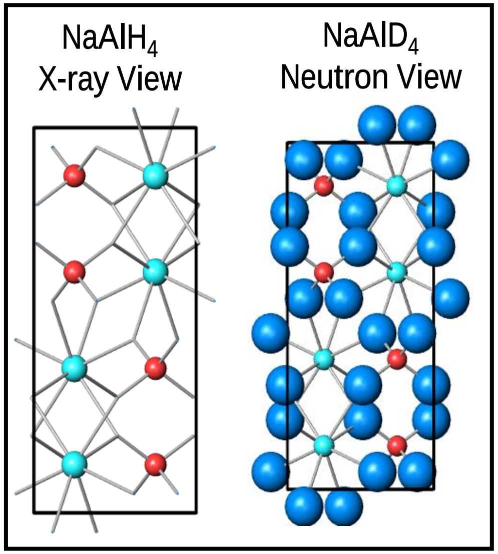


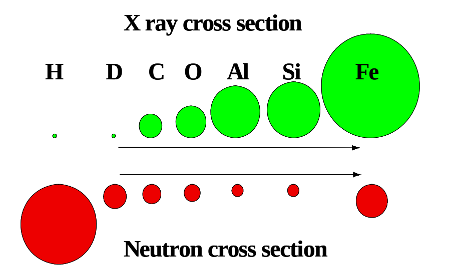

$2H_2 + O_2 \rightarrow 2H_2O$ + electrical power + heat

# Basic Research Needs for Hydrogen Production, Storage and Use

The hydrogen economy offers a vision for energy management in the future.  Research needs are quintessentially *nano*: catalysis, hydrogen storage materials, and electrode assemblies for fuel cells all depend on nanoscale processes and architecture to achieve high performance.

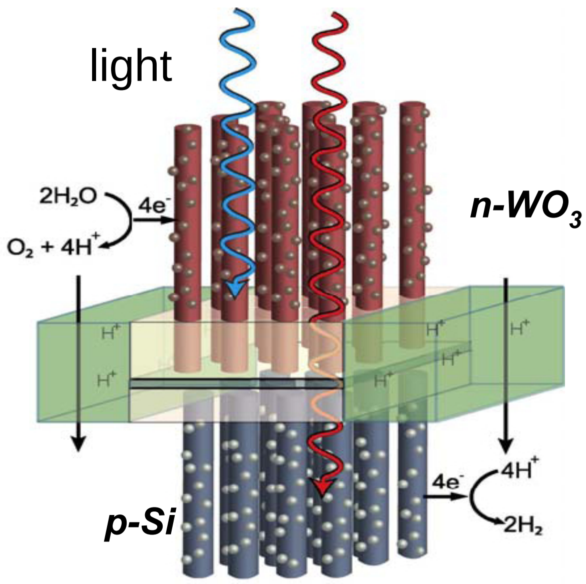
- Hydrogen Production
  - **Fossil Fuel Reforming:** Catalytic mechanisms and design, high temperature gas separation
  - **Solar Photoelectrochemistry/Photocatalysis:** Light harvesting, charge transport, chemical assemblies, bandgap engineering, interfacial chemistry, catalysis, organic semiconductors, theory and modeling
  - **Bio- and Bio-inspired $H_2$ Production:** Microbes & component redox enzymes, nanostructured 2D & 3D hydrogen/oxygen catalysis, sensing, energy transduction, biological and biomimetic $H_2$ production systems
  - **Nuclear and Solar Thermal Hydrogen:** Thermodynamic data and modeling for thermochemical cycle (TC), high temperature materials: membranes, TC heat exchanger materials, gas separation, improved catalysts
- Hydrogen Storage
  - **Metal Hydrides and Complex Hydrides:** Degradation, thermophysical properties, effects of surfaces, processing, dopants, and catalysts in improving kinetics, nanostructured composites
  - **Nanoscale/Novel Materials:** Finite size, shape, and curvature effects on electronic states, thermodynamics, and bonding, heterogeneous compositions and structures, catalyzed dissociation and interior storage phase
  - **Theory and Modeling:** Model systems for benchmarking against calculations at all length scales, integrating disparate time & length scales, first principles methods applicable to condensed phases
- Fuel Cells
  - **Electrocatalysts and Membranes:** Oxygen reduction cathodes, minimize rare metal usage in cathodes and anodes, synthesis and processing of designed triple percolation electrodes
  - **Low Temperature Fuel Cells**: 'Higher' temperature proton conducting membranes, degradation mechanisms, functionalizing materials with tailored nano-structures
  - **Solid Oxide Fuel Cells:** Theory, modeling and simulation, validated by experiment, for electrochemical materials and processes, new materials-all components, novel synthesis routes for optimized architectures, advanced in-situ analytical tools




Neutron Imaging of Hydrogen

# Sunlight Driven Hydrogen Formation




Solar powered water splitting scheme incorporating two separate semiconductor rod-array photoelectrodes that sandwich an electronically and ionically conductive membrane.

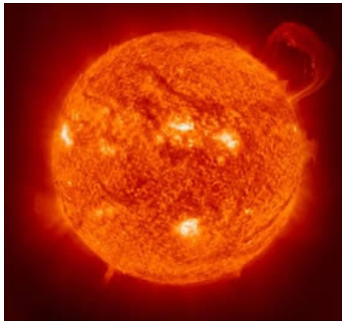
- Traditional photoelectrochemical water splitting is limited by a cumbersome planar, two electrode configuration for light absorption and $H_2$ and $O_2$ generation. Current generation of semiconductors used for absorbing visible solar spectrum are intrinsically unstable. Precious metals (Pt, Pd) are needed for $H_2$ evolution.
- One key constraint in photon absorbers for solar energy conversion is that the samples need to be thick enough for sufficient absorption, yet pure enough for high minority carrier length and photocurrent collection.
- New nanorod configuration was recently developed to orthogonalize the directions of light absorption and charge carrier collection, i.e. it separates longitudinal light absorption from transverse carrier diffusion to reactive surface.
- The short diffusion paths to reaction broadens usable materials to include earth abundant, resistive semiconductors. Opposing nanorod configuration with conductive ion membrane allows for compact device with inherent separation of $O_2$ and $H_2$ gas.
- High surface-to-volume ratio of nanostructure decreases current density and permits use of broad range of new metals as sites for $H_2$ and $O_2$ evolution.

Spurgeon JM, Atwater HA, Lewis NS, *Journal of Physical Chemistry C,* 112, 6186-6193 (2008).

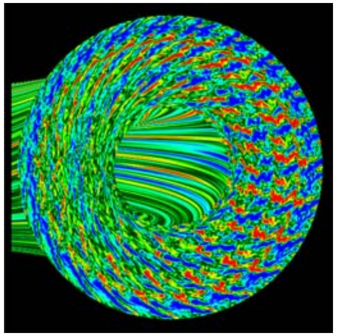
# The Promise of Fusion

Science Transforming Energy Technologies

**Imagine:** • Bringing the power of the sun and the stars to Earth



- Fusion – harnessing the sun’s and stars’ own method of energy production
- Uses abundant fuel, available to all nations - deuterium and lithium are easily available for millions of years
- No carbon emissions, short-lived radioactivity
- Low risk of nuclear materials proliferation
- Cost of power estimated similar to coal, fission
- Can produce electricity and hydrogen for fuel



Computer simulation of plasma turbulence in a tokamak

## Basic Science:

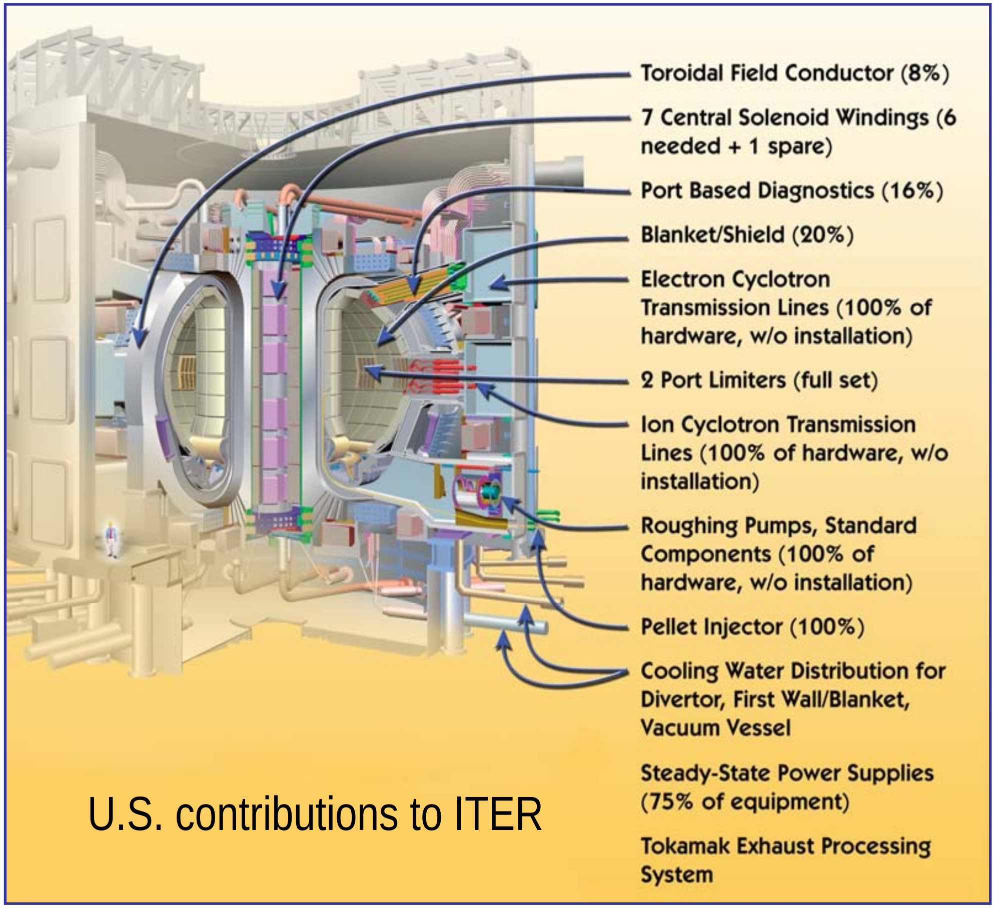
- Fundamental understanding of plasma science necessary to explore innovative, improved pathways to plasma confinement
- Materials for the extreme thermochemical environments and high neutron flux conditions
- Predictive capability of plasma confinement and stability for optimum experimental reactor design

# ITER

## Unprecedented International Cooperation on Fusion

**ITER:** Experimental fusion reactor designed to be the penultimate step to development of commercial fusion energy

- ITER is based on the tokamak concept in which a hot gas is confined in a torus-shaped vessel using a magnetic field. The gas is heated to over 100 million degrees and will produce 500 MW of fusion power.
- ITER will demonstrate the technical and scientific feasibility of a sustained fusion burning plasma—for power out/in (Q) up to 10. (A power reactor has a Q of ~30)
- Sited in Cadarache, France, ITER is a international partnership of the U.S., the European Union, Japan, Russia, China, Republic of Korea, and India.
- Historic international agreement signed on November 21, 2006. The first ITER Council Meeting was held November 27-28, 2007.




U.S. contributions to ITER

# Energy Frontier Research Centers

## Engaging the Nation's Intellectual and Creative Talent

### Innovative basic research to accelerate scientific breakthroughs needed to create advanced energy technologies for the 21st century

The DOE Office of Science announced the Energy Frontier Research Centers (EFRCs) program. EFRC awards are $2–5 million/year for an initial 5-year period. Universities, labs, and other institutions are eligible to apply.

**Energy Frontier Research Centers** will pursue fundamental basic research in areas such as:

- Solar Energy Utilization
- Catalysis for Energy
- Electrical Energy Storage
- Solid State Lighting
- Superconductivity
- Biofuels
- Geosciences for Nuclear Waste and CO2 Storage
- Advanced Nuclear Energy Systems
- Combustion of 21st Century Transportation Fuels
- Hydrogen Production, Storage, and Use
- Materials Under Extreme Environments

# Institutional Challenges – *Vision, Leadership, Business Acumen*

- *Vision* – know what is important
  - **Significant opportunities exist for science to make an impact**

- *Leadership* – focus on what is important
  - **Relevant projects**
  - **At “scale”**
  - **Nontraditional competencies**

- *Business acumen* – know and meet the competition
  - **Universities are very active in this area**
  - **SC laboratories significantly engaged**
  - **Connections to industries are important**
  - **Nimble, cost effective, …**