Strategic Planning and Energy Initiatives in DOE Basic Energy Sciences

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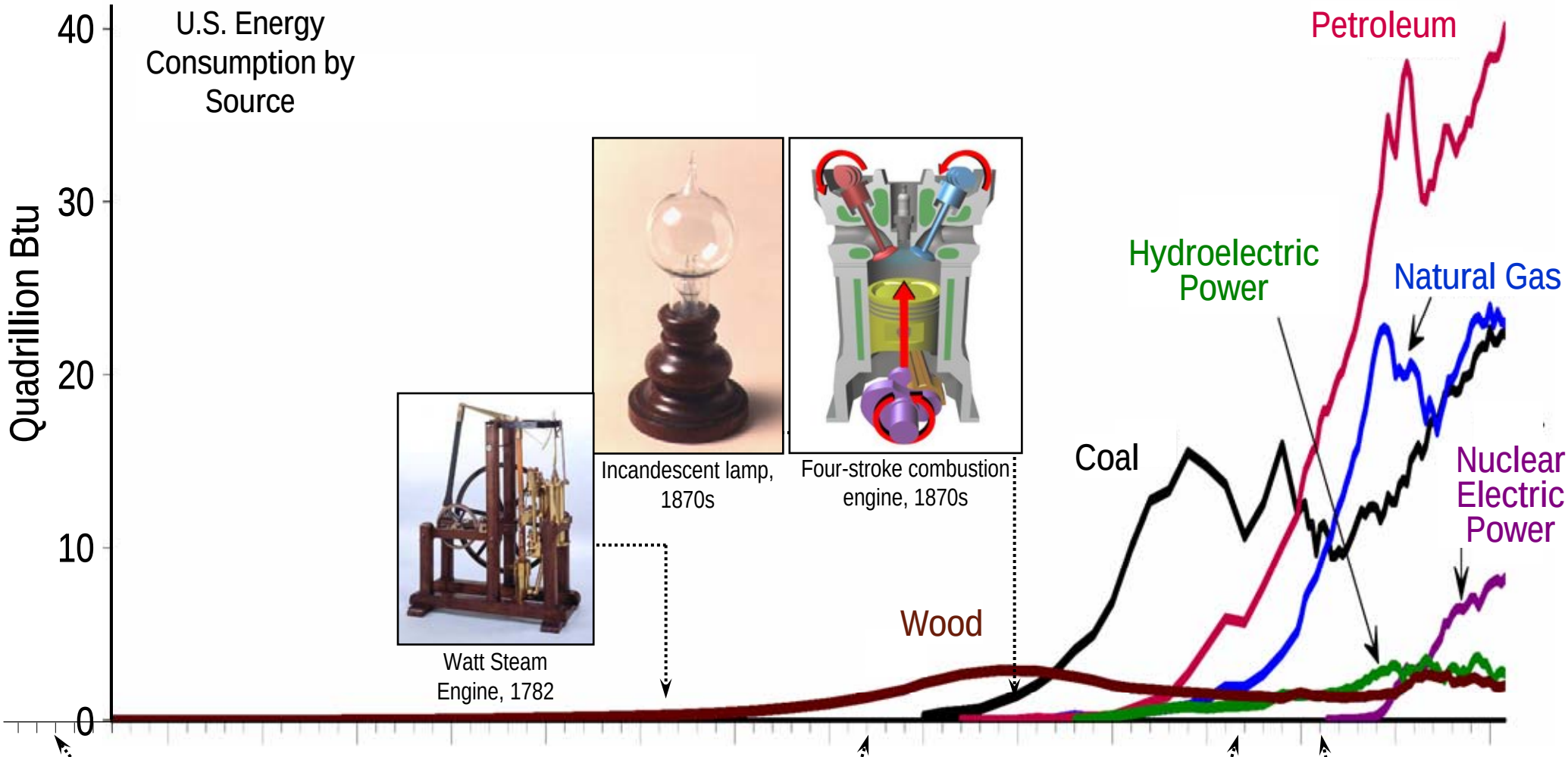
Office of Basic Energy Sciences
http://www.sc.doe.gov/bes/bes.html

EPSCoR Program Review Workshop
July 25, 2007

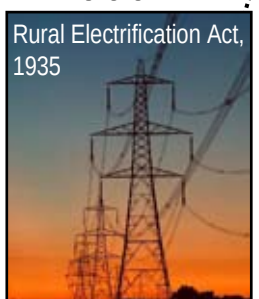
Technology, Energy, and Society are Inextricably Intertwined

Today's Energy Technologies and Infrastructures are Firmly Rooted in the 20th Century



Wind, water, wood, animals, (Mayflower,1620)

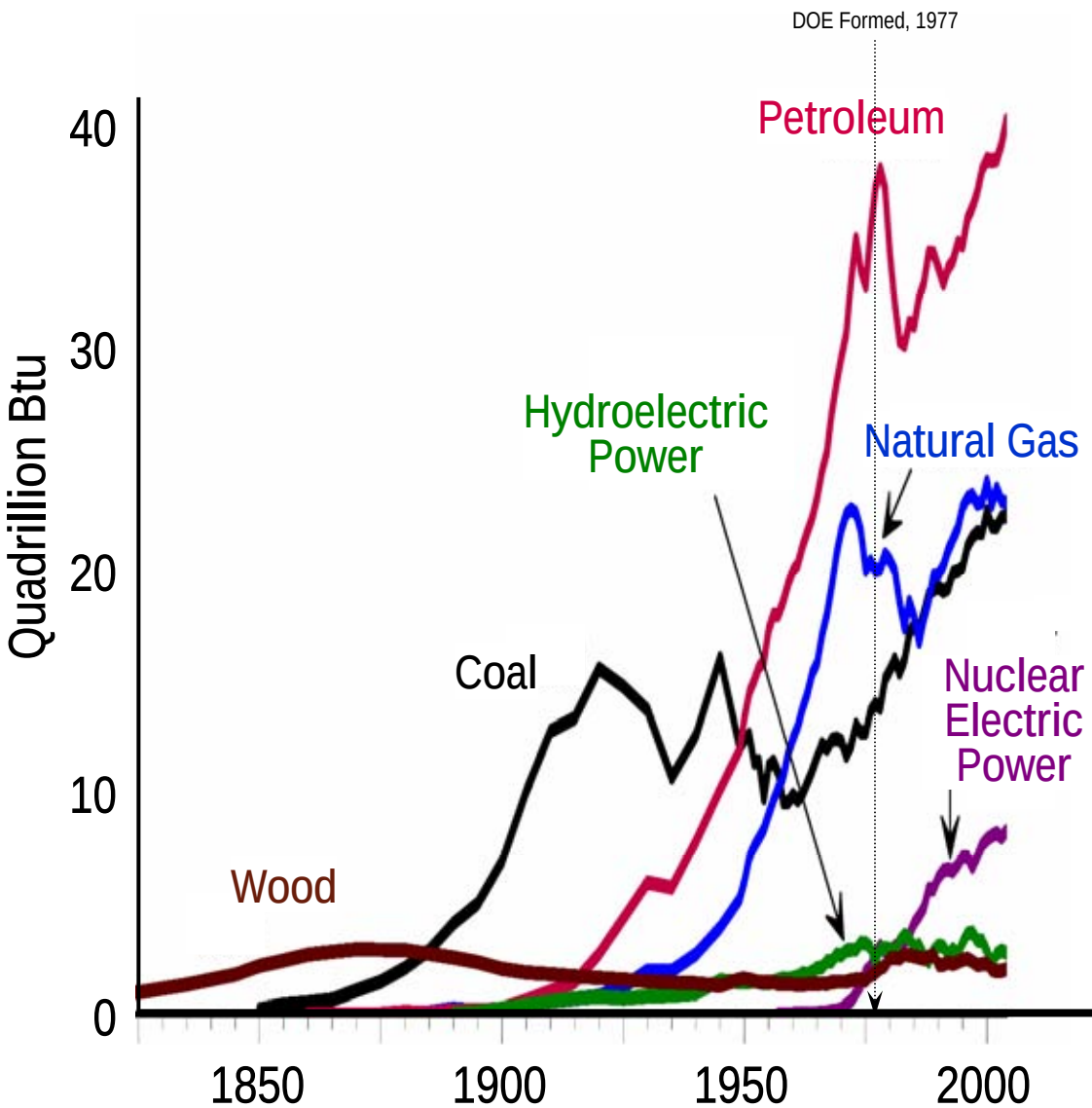
Intercontinental Rail System, mid 1800s



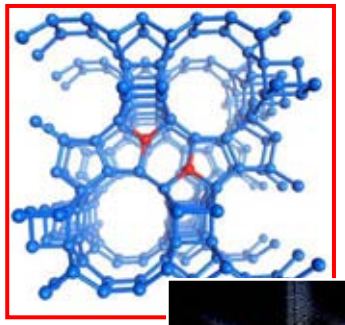
Eisenhower Highway System, 1956

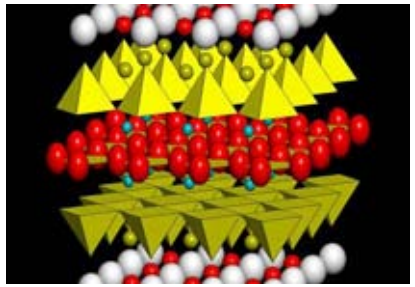
What Will the 21st Century Bring?

21st Century Science and Technology Will Exert Control at the Atomic, Molecular, and Nanoscale Levels



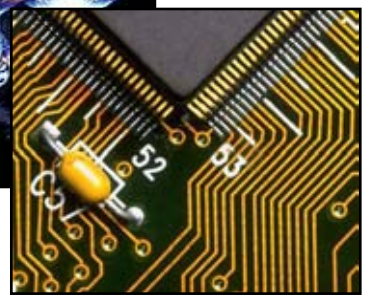
Designer molecules





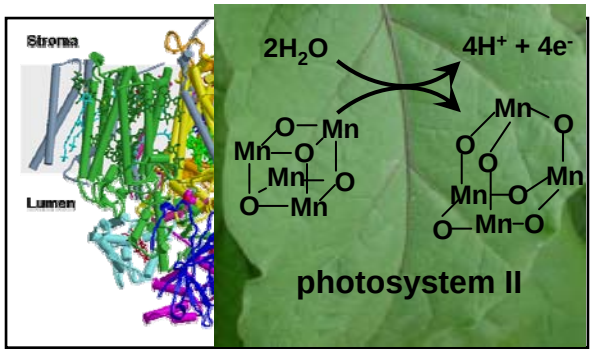
High Tc super-conductors

Solid-state lighting and many other applications of quantum confinement and low-dimensionality



Peta-scale computing

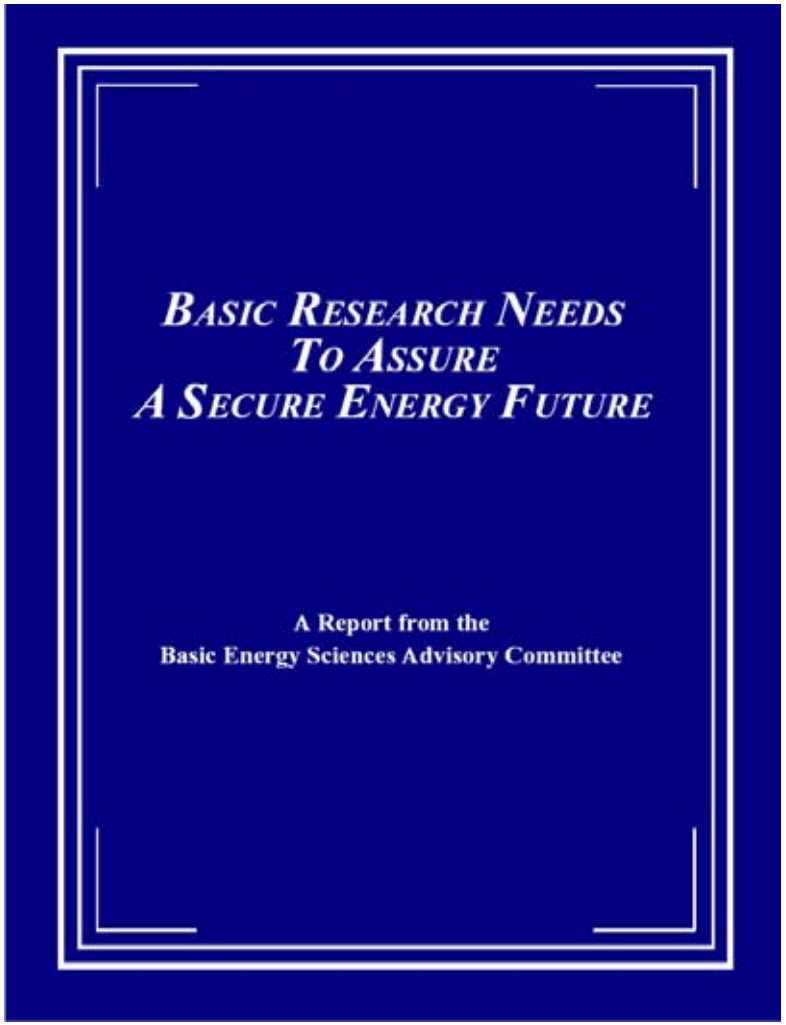
Bio-inspired nanoscale assemblies – self-repairing and defect-tolerant materials and selective and specific chemical reactivity.



Strategic Planning in BES

- Phase I: The Basic Research Need workshop series.
  - Strategic planning for BES use-inspired (energy-relevant) research in coordination with DOE technology offices.
- Phase II: BESAC Grand Challenges Report.
  - Strategic planning for BES grand-challenge/discovery research.
  - Report in preparation; update at BESAC meeting July 31; completion by fall BESAC meeting.
- Phase III: BESAC panel(s) to summarize scientific themes from Phases I and II, including “enabling tools”
  - In the early planning stages…..

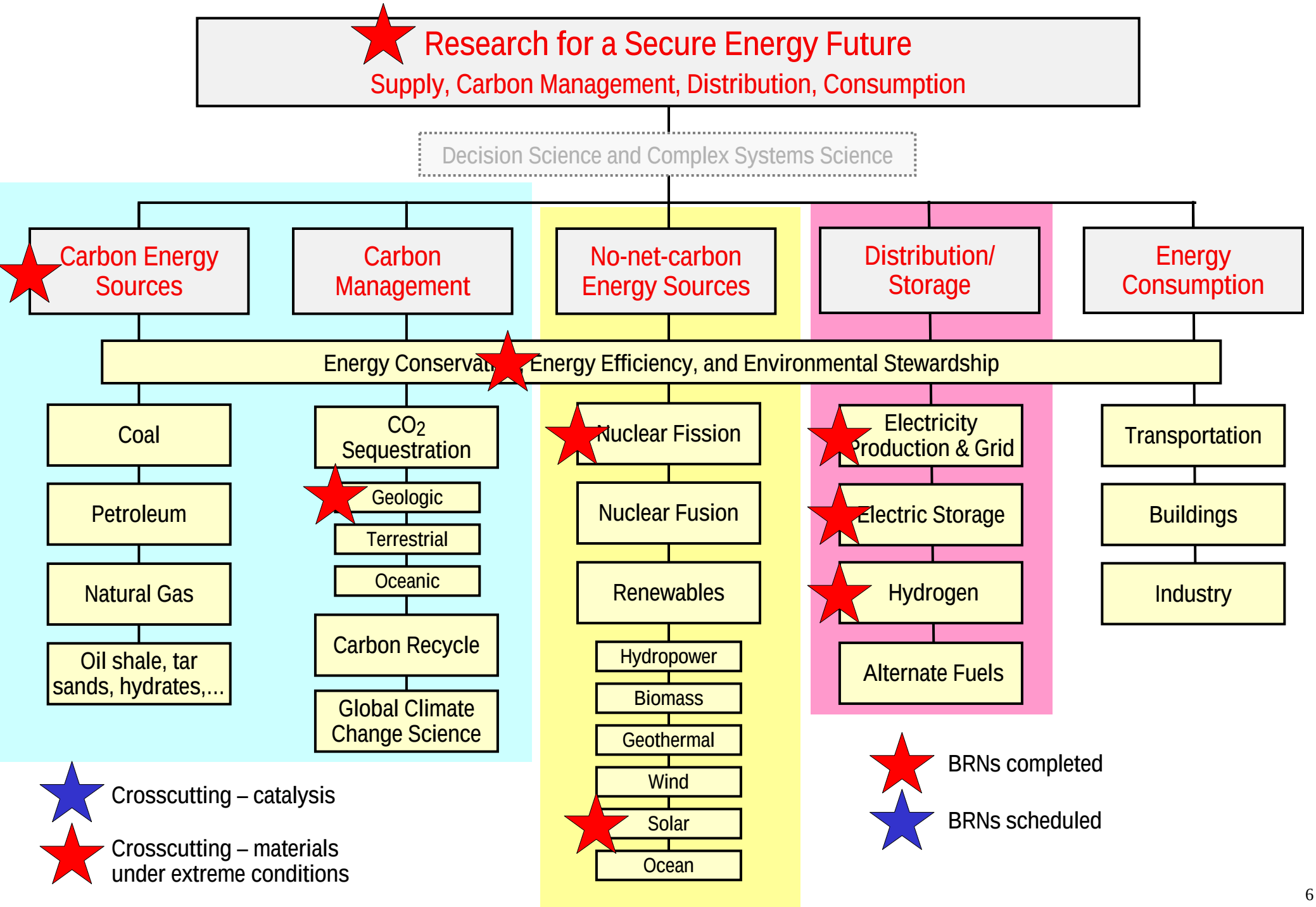
BESAC Chartered the First Basic Research Needs Workshop



RECOMMENDATION: 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, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved.

February 2003

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



Discovery and Use-Inspired Research

The "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
- **Basic Research Needs – Final Wrap-up Workshop**
  BESAC, TBD

The Continuum of Research, Development, and Deployment

Grand Challenge Research	Discovery Research	Use-Inspired Basic Research	Applied Research	Technology Maturation & Deployment
▪ 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.	▪ Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies	▪ Basic research for fundamental new understanding, usually 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

Goal: new knowledge / understanding
Focus: phenomena
Metric: knowledge generation

Goal: practical targets
Focus: performance
Metric: milestone achievement

The Continuum of Research, Development, and Deployment

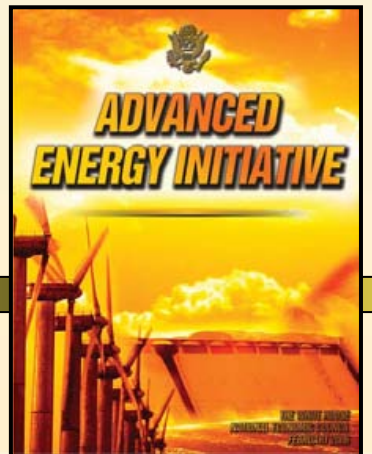
Grand Challenge Research → Discovery Research → Use-Inspired Basic Research → Applied Research → Technology Maturation & Deployment

(BESAC) Grand Challenges Panel

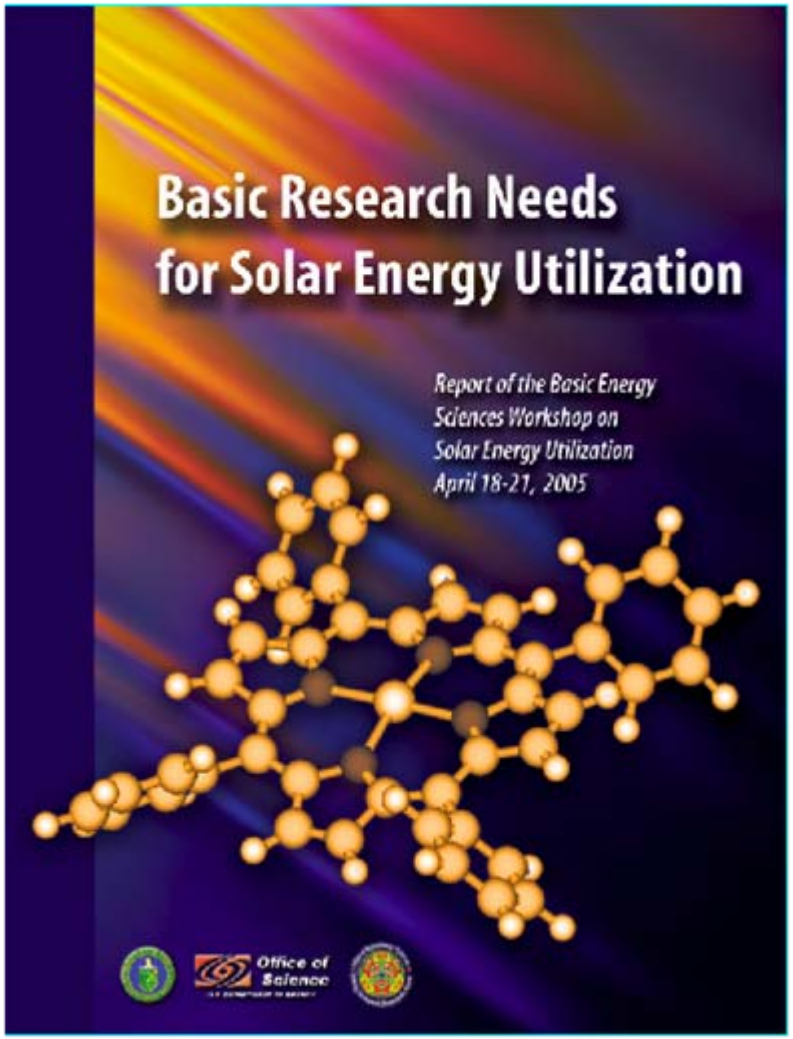
Technology Office/Industry Roadmaps

(BES) Basic Research Needs Workshops

(BES, BESAC, ...) Tools and Facilities in Support of Research



Basic Research for Solar Energy Utilization Workshop



Charge
Identify basic research needs and opportunities in solar electric, fuels, thermal and related areas, with a focus on new, emerging, and scientifically challenging areas that have the potential for significant impact in science and technologies.

Workshop Chair: Nathan Lewis, Caltech
Co-chair: George Crabtree, Argonne

- Panel Chairs
  - Arthur Nozik, NREL: Solar Electric
  - Mike Wasielewski, NU: Solar Fuel
  - Paul Alivisatos, UC-Berkeley: Solar Thermal and Crosscutting
- 200 participants
- Topics
  - *Photovoltaics*
  - *Photoelectrochemistry*
  - *Bio-inspired photochemistry*
  - *Natural photosynthetic systems*
  - *Photocatalytic reactions*
  - *Biofuels*
  - *Heat conversion and utilization*
  - *Elementary processes*
  - *Materials synthesis*
  - *New tools*
- Report

  Workshop attendees identified 13 priority research directions (PRDs) with high potential for producing scientific breakthroughs. Many of the PRDs address issues of concern to more than one approach or technology. These issues include: (1) coaxing cheap materials to perform as well as expensive materials in terms of their electrical, optical, chemical, and physical properties; (2) developing new paradigms for solar cell design that surpass traditional efficiency limits; (3) finding catalysts that enable inexpensive, efficient conversion of solar energy into chemical fuels; (4) identifying novel methods for self-assembly of molecular components into functionally integrated systems; and (5) developing materials for solar energy conversion infrastructure, such as transparent conductors and robust, inexpensive thermal management materials.

Example: Solar-to-Electric Conversion

Discovery Research

- Low-dimensionality, quantum confinement, and the control of the density of states of photons, phonons, electrons
- Defects, disorder, and tolerance to same of advanced materials
- Molecular self-assembly and self-repair
- Designer interfaces and thin films
- Photon management, including exciton creation and transport
- Control of light absorption and scattering
- Novel theoretical and experimental tools

Use-inspired Basic Research

- New or nanostructured materials for multiple-junction solar cells
- Control and extraction of energy from multiple-exciton generation
- Radiative and non-radiative processes in solar cells
- Interfacial photochemistry of dye-sensitized nanostructures
- Synthesis and processing science: Thin-film growth, templating, strain relaxation, nucleation and growth
- Enhanced coupling of solar radiation to absorber materials, e.g., by periodic dielectric or metallodielectric structures
- Energy transduction in novel molecular, polymeric, or nano-particle-based photovoltaics

Applied Research

- Technology Milestones:
  - *Decrease the cost of solar to be competitive with existing sources of electricity in 10 years*
  - *Deploy 5-10 GW of photovoltaics (PV) capacity by 2015, to power ~2 million homes.*
  - *Residential: 8-10 ¢/kWhr*
    Commercial: 6-8 ¢/kWhr
    Utility: 5-7 ¢/kWhr (2005 $s)
- Silicon solar cells – single crystal, multicrystal, ribbon, thin-layer; production methods; impurities, defects, and degradation
- Thin-film solar cells – a-Si, CuInSe, CdTe, Group III-V technologies
- High-efficiency solar cells
- Polymeric and dye-sensitized solar cells
- Assembly and fabrication R&D issues

Technology Maturation & Deployment

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

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Example: Solar-to-Fuels Conversion

Discovery Research

- Charge transfer and separation in natural and bio-inspired photosynthetic systems
- Nano-architectures for coupling light-harvesting and catalytic functions
- Self-organization and controlled-assembly of complex structures
- Robust, functional catalysts that mimic biological processes
- Ultrafast imaging of electron dynamics
- Multi-scale theoretical and computational approaches

Use-inspired Basic Research

- Novel photoelectrode materials and molecular configurations for efficient photoelectrolysis
- Biomimetic multi-electron catalysts and proton-coupled electron transfer for solar water splitting
- Photocatalytic cycles for CO_2 reduction to alcohol fuels
- Multi-scale control of reactivity in hybrid molecular materials
- Defect formation mechanisms and self-repair in solar-to-fuels pathways
- Hierarchical organization of molecular constructs for artificial photosynthesis

Applied Research

- Technology Milestones:
  - *2010 to 2012: Laboratory-scale demonstration of solar driven high-temperature thermochemical hydrogen production that projects to a cost $6.00/gge (ultimate target: $7.00/gge delivered)*
  - *2015 to 2018: Laboratory-scale photo-electrochemical water splitting system to produce hydrogen at a 10% solar-to-hydrogen efficiency. Laboratory-scale photobiological water splitting system to produce hydrogen with 5% efficiency.*
- Accelerate and expand research on the low-cost solar production of hydrogen:
  - Component development and systems integration to enable electrolyzers to operate from inherently intermittent and variable-quality power derived from solar sources
  - Solar-driven high-temperature chemical cycle water splitting
  - Photoelectrochemical systems
  - Thermochemical conversion of biomass
  - Photolytic and fermentative microorganism systems

Technology Maturation & Deployment

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

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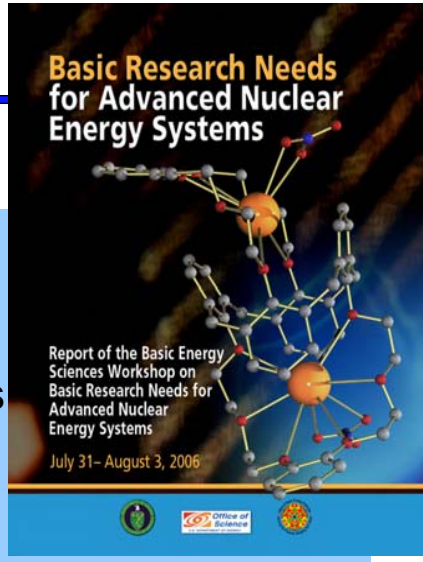
Basic Research Needs for Advanced Nuclear Energy Systems



July 31–August 2, 2006

Workshop Co-chairs

Tomas Diaz de la Rubia

Jim Roberto

Panel Topics:

- Materials under extreme conditions
- Chemistry under extreme conditions
- Separations science
- Advanced actinide fuels
- Advanced waste forms
- Predictive modeling and simulation
- Crosscutting and grand-challenge science themes

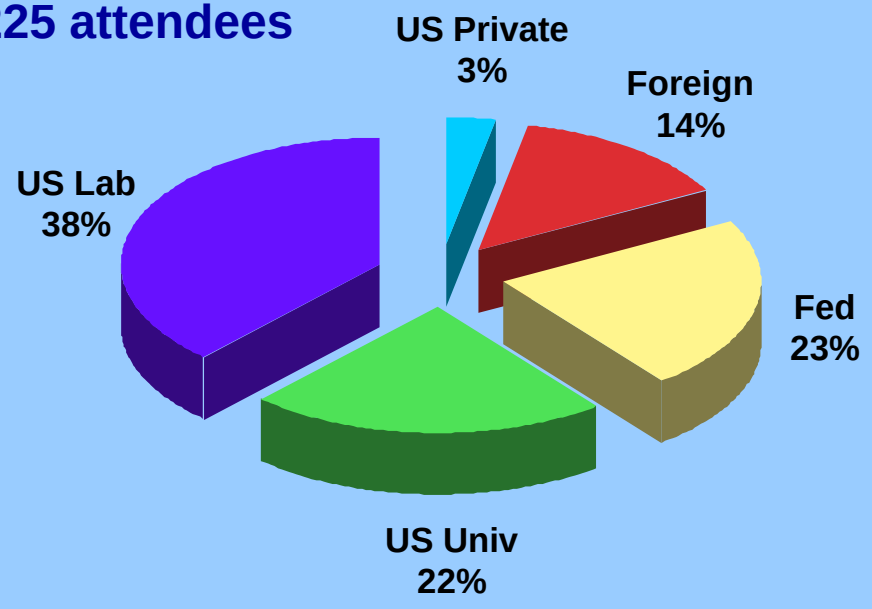
Plenary Speakers:

David Hill, Tom Mulford, Sue Ion, Vic Reis
Steve Zinkle, Carol Burns, Thom Dunning

Workshop Charge

To identify basic research needs and opportunities in advanced nuclear energy systems and related areas, with a focus on new, emerging and scientifically challenging areas that have the potential to have significant impact in science and technologies. Highlighted areas will include improved and new materials and relevant chemical processes to overcome short-term showstoppers and long-term grand challenges for the effective utilization of nuclear energy.

225 attendees



Advanced Nuclear Energy Systems

Discovery Research

- Accurate relativistic electronic structure approaches for correlated f-electron systems
- Integration of multi-physics, multi-scale computational models: atomistic to continuum
- Reactivity, dynamics, molecular speciation and kinetic mechanisms at interfaces
- Utilize microstructure control to impart radiation resistance to structural materials for ANES
- Innovative experimental methods for dynamic, *in situ* measurements of fundamental properties

Use-inspired Basic Research

- Predict microstructural and chemical evolution in actinide fuel, cladding and structural materials during irradiation
- Identify self-protective interfacial reaction mechanisms capable of providing universal stability in extreme environments
- Improve understanding of coordination geometry, covalency, oxidation state, and cooperative effects of actinides to devise next generation separation methods.
- Predict the behavior of waste forms over millennia

Applied Research

- Rational design and development of reactor fuels
- Verified and validated modules for reactor-level multi-scale simulations
- Develop 3D fuel performance code
- Laboratory-scale sample fabrication and characterization with relevant post-irradiation examination of samples
- Demonstrate new separation systems at bench scale
- Demonstrate at-scale waste-form performance in deep geologic laboratory

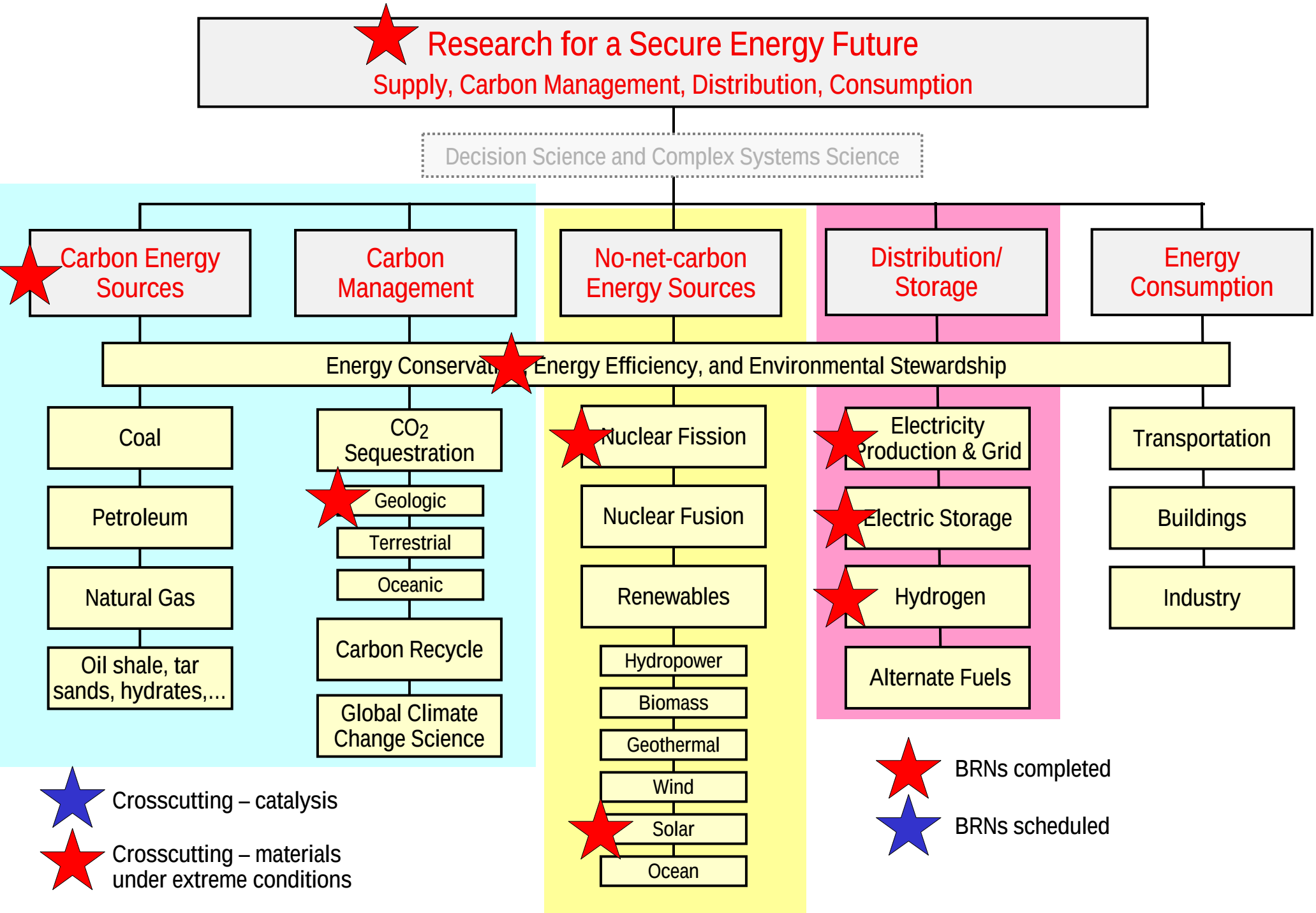
Technology Maturation & Deployment

- Demonstrate the scaling to production-scale by process prototyping
- Develop and validate fuel licensing code for design and safety basis
- Fabricate and characterize lead test assemblies (LTAs)
- Irradiate lead test assemblies in prototypic environment
- Couple waste-form performance to design and performance of a repository.

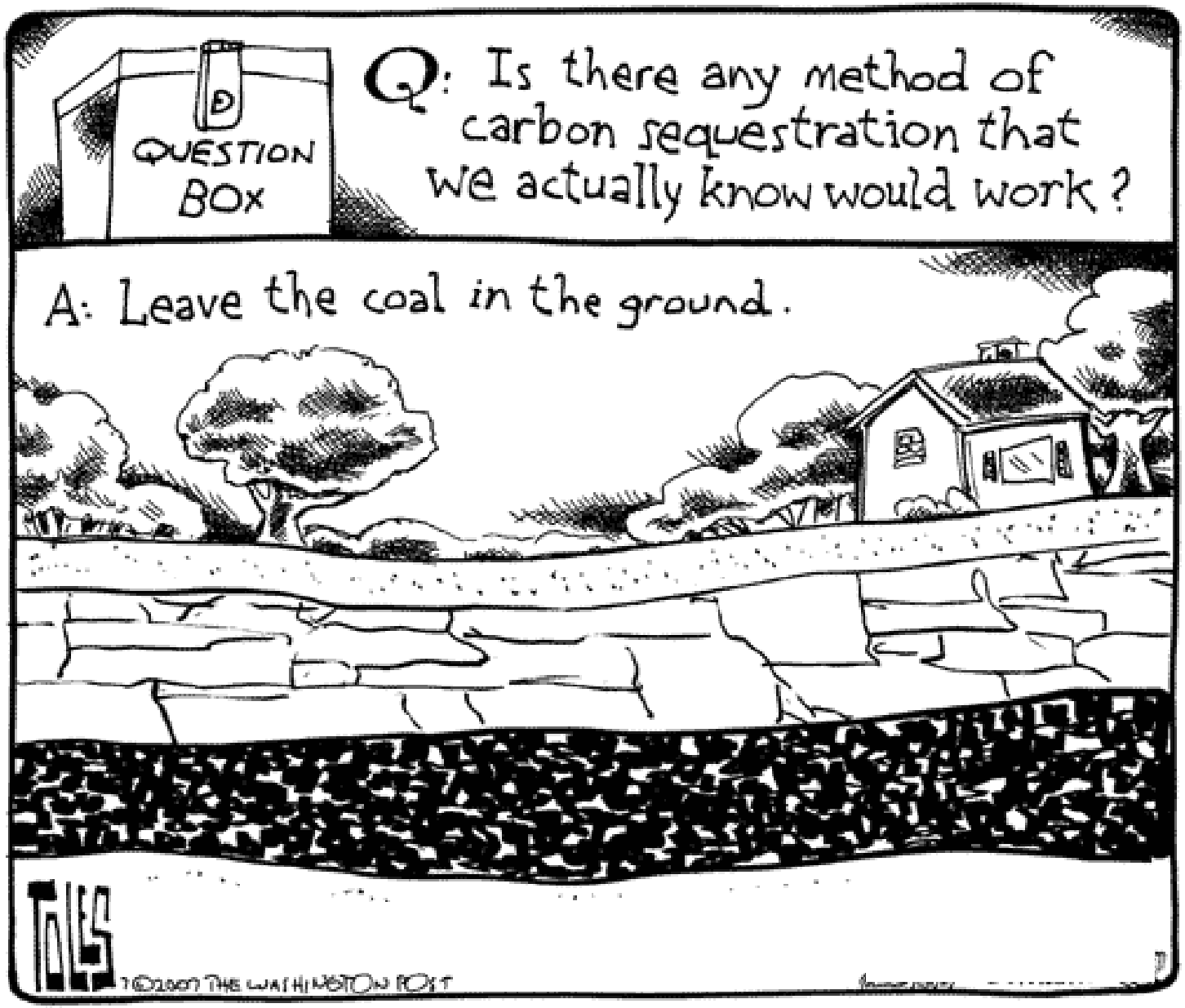
Office of Science
BES

Technology Offices
NE

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

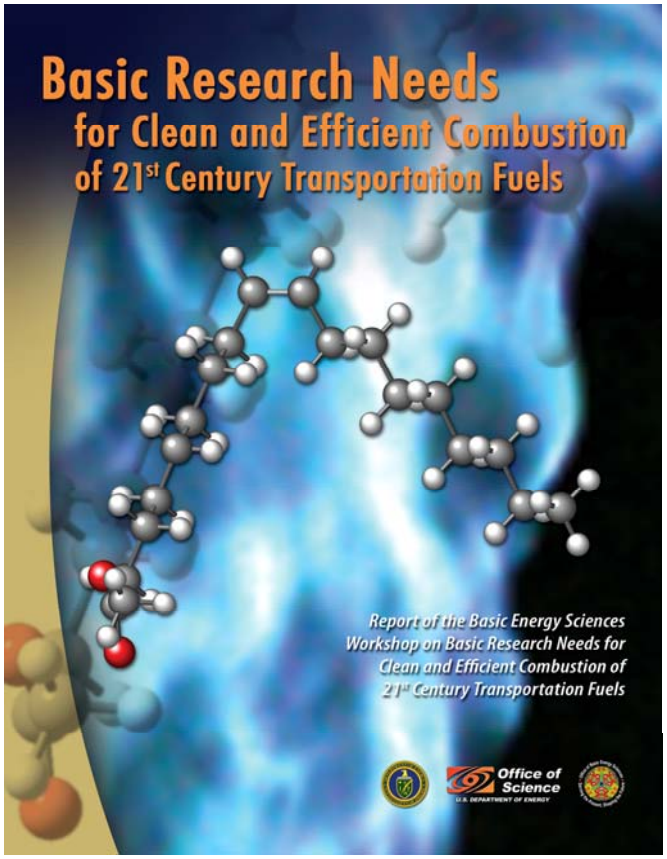


How do we deal with continued fossil fuel use...



Tom Toles, Washington Post, July 16, 2007

Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels Workshop



Organizing committee

- **Co-Chairs:**
  - Andy McIlroy, SNL
  - Greg McRae, MIT
- **Panel Leads**
  - Novel Combustion
    - Dennis Siebers, SNL
    - Volker Sick, U. Mich.
  - Fuel Utilization
    - Phil Smith, U. Utah
    - Charlie Westbrook, LLNL
  - Crosscut Science
    - Craig Taatjes, SNL
    - Arnaud Trouve, U. MD
    - Al Wagner, ANL

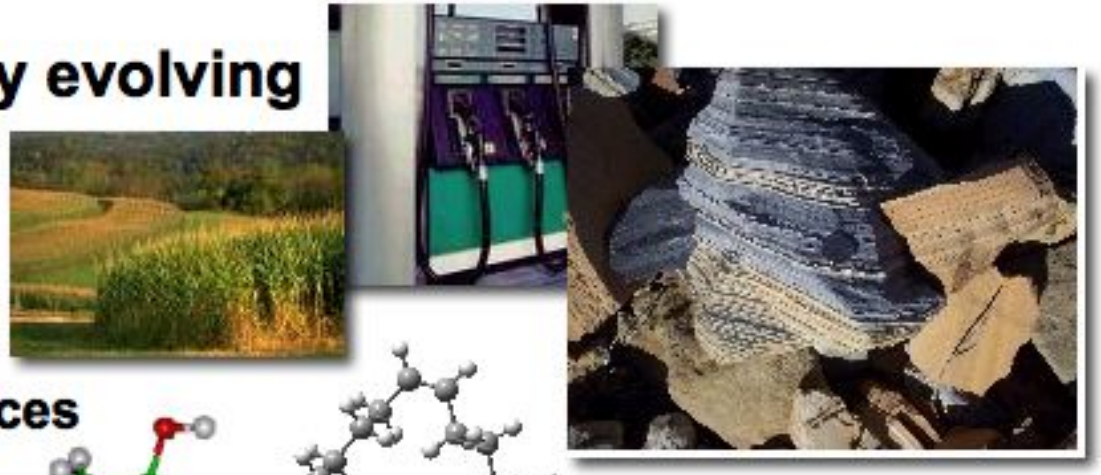
- **DOE/BES**
  - Eric Rohlfing
  - Frank Tully
  - Dick Hilderbrandt

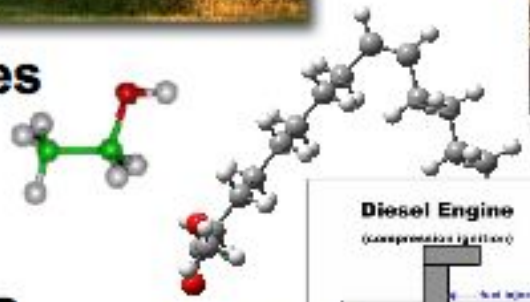
Workshop held October 30 – November 1, 2006

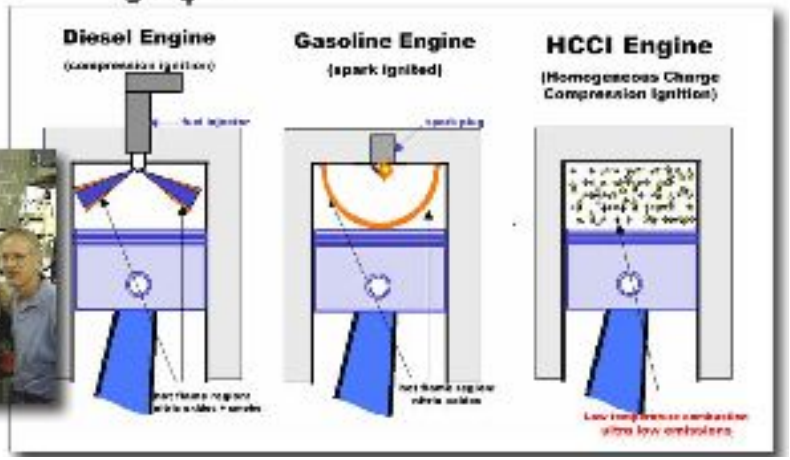
Report now available in pdf format on BES website. (Printed copies coming soon.)

Motivation:
Changing World of Fuels and Engines

- **Fuel streams are rapidly evolving**
  - Heavy hydrocarbons
    - Oil sands
    - Oil shale
    - Coal
  - New renewable fuel sources
    - Ethanol
    - Biodiesel
- **New engine technologies**
    - Direct Injection (DI)
    - Homogeneous Charge Compression Ignition (HCCI)
    - Low-temperature combustion

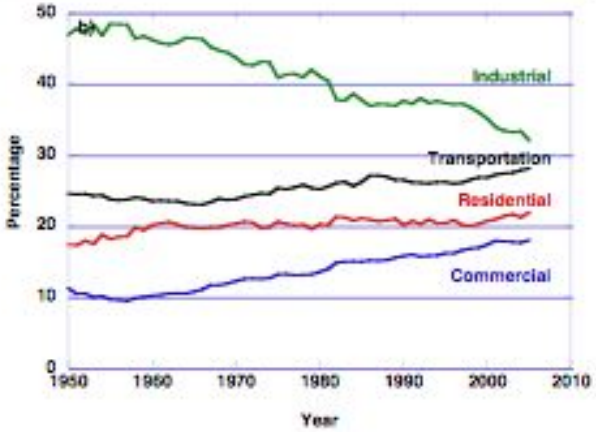


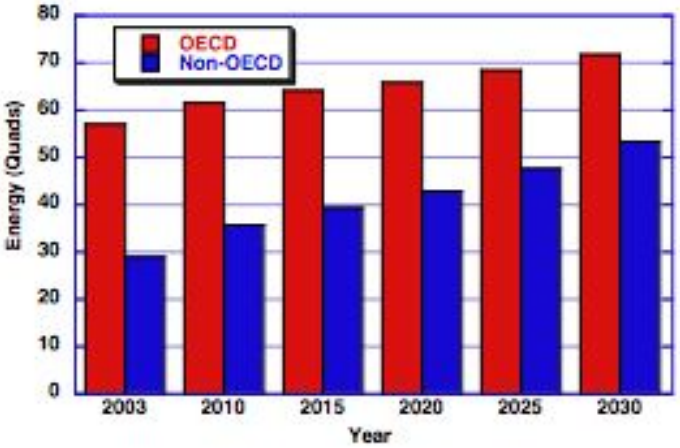




Motivation: Transportation Sector Key to Energy Use

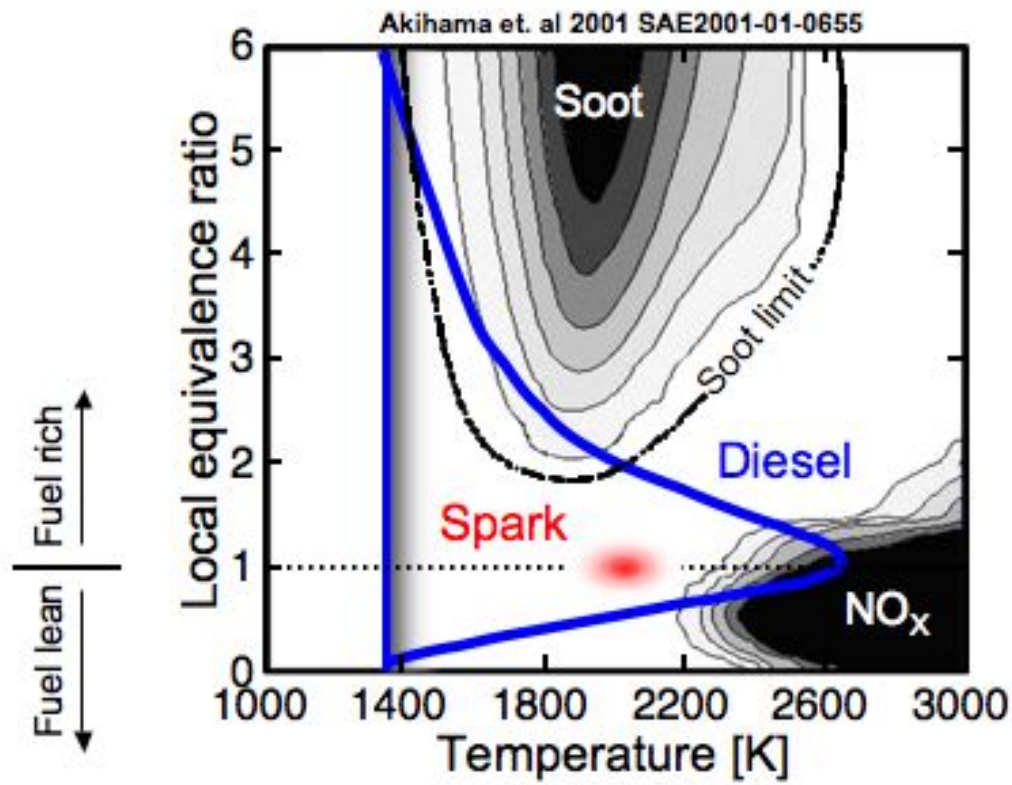
- Transportation accounts for ~1/3 of energy use
- When electricity generation factored out, transportation dominates
- Demand projected to increase
- 97% of transportation energy from petroleum
- Relatively small number of technologies employed
- Transportation sector energy use can impact national security and environmental impacts





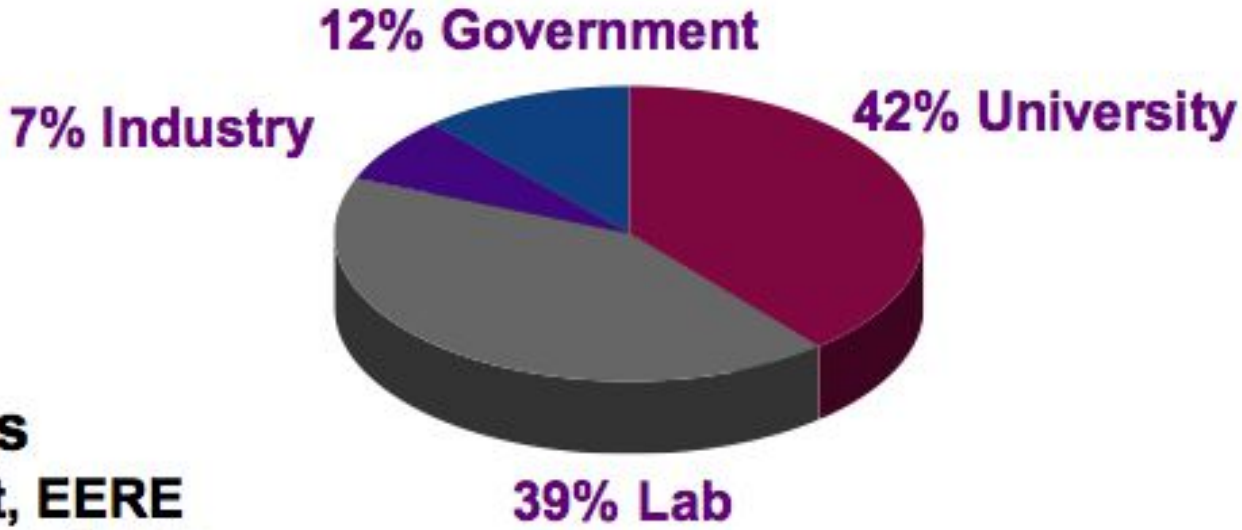
Transportation Combustion Challenges

- Efficiency & cleanliness difficult to achieve together
- Diesels are efficient, but difficult to make clean
  - No throttling losses
  - High compression ratios
  - Continuum of rich to lean
  - Soot and NOx often anti-correlated
- Spark ignited engines are 'clean', but less efficient
  - Stoichiometric burning
  - Little soot, 3-way catalyst eliminate NOx
  - Throttle losses
  - Low compression ratios



Participants

- Total of 95 participants



- Plenary Speakers
  - James Eberhardt, EERE
  - Charlie Westbrook, LLNL
  - Hukam Mongia, GE
  - David Greene, ORNL

Workshop Charge and Objectives

To explore basic research needs in the areas of gas-phase chemistry, combustion diagnostics, and combustion simulation that will enable the use of transportation fuels derived from non-traditional sources in a manner that optimizes engine efficiency and minimizes pollutant formation.

- Non traditional fuels are defined as those derived from carbon-neutral, renewable resources, such as biodiesel or ethanol, and those derived from non-traditional fossil fuel reserves, such as heavy crude oil, tar sands, oil shale, and coal.

- The output of the workshop will seek to define a set of basic, priority research directions (PRDs) that would employ and expand the current broad expertise base in gas-phase chemistry and combustion research into the realm of non-traditional fuels.

Priority Research Directions

1) Combustion under Extreme Pressure

Fundamental studies of transport and flow, and their coupling to chemistry, prevalent in fuel-flexible and efficient engines.

2) Understanding and Exploiting Surface Chemistry in Transportation Systems

New tools and theoretical methods for exploring surface chemistry on the nanoscale in the context of engines.

3) Breakthrough Discovery Tools

New tools to acquire high-fidelity, spatially and temporally resolved data on turbulent combustion processes.

4) Multiscale Modeling

New combustion models capable of spanning enormous spatial and temporal scales, ultimately capable of application as predictive tools on the device scale.

Priority Research Directions, cont'd.

4) Basic Research Needs for Smart Engines

Science and technology necessary to develop an engine that can adapt in real-time to changing fuel streams and conditions.

5) Physical and Chemical Properties for Combustion of 21st Century Transportation Fuels

Fundamental physical and chemical properties of non-traditional fuels and their affect on the combustion process.

6) Automated Discovery of Fuel Chemistry Kinetics

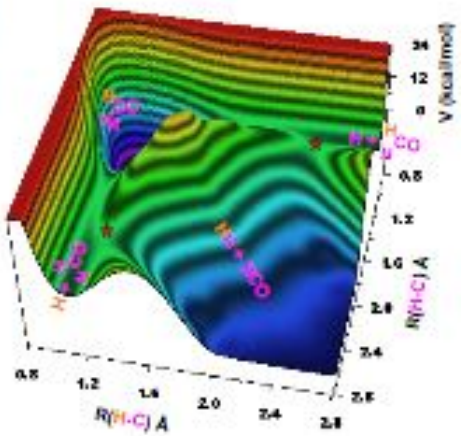
The use of theoretical chemistry techniques, validated by experiment, to automatically develop complex chemical kinetic models for combustion.

7) Spray Dynamics and Chemistry for New Fuels

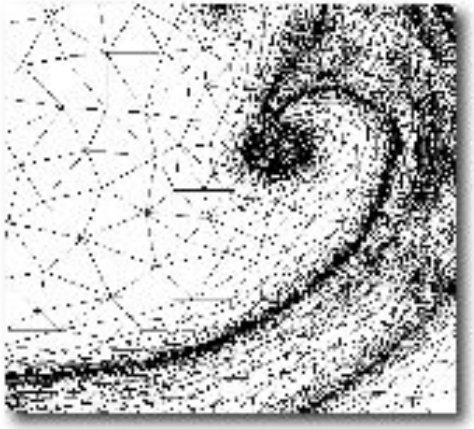
Replacement of current empirical understanding of spray dynamics with first-principles understanding of spray breakup and subsequent vaporization, mixing, and combustion chemistry.

Grand Challenge: Predictive Modeling of Combustion in a Evolving Fuel Environment

- Predictive modeling is the key to combustion optimization in a non-linear parameter space



- Challenges:
  - 9 orders of magnitude in space and time
  - Complex chemistry, varying with fuel evolution
  - Work needed in:
    - Chemical mechanism development
    - Turbulence-chemistry interaction
    - Algorithm development
    - Large dataset analysis



Combustion Science for 21st Century Fuels and Engines

Discovery Research

- Reaction chemistry of large molecules at high pressure
- Heterogeneous combustion and soot chemistry
- Turbulent reacting flows with a large range of chemical time scales
- Liquid fuel spray chemistry and dynamics
- Multi-scale modeling: from quantum to continuum
- High-fidelity computational approaches (DNS, LES)
- 4-D diagnostics at high pressure and under multi-phase conditions

Use-inspired Basic Research

- Automatic generation & reduction of chemical kinetics models of 21st Century Fuels
- Soot formation, composition, morphology, oxidation and atmospheric evolution
- High-fidelity CFD for complex and deformable engine geometries
- Elucidating combustion dynamics for control strategies
- Uncertainty quantification in multi-scale modeling
- Development of novel diagnostics for molecular characterization at high pressure
- Data and simulation framework built upon collaboratory and cyber-infrastructure tools
- Modeling of turbulent sprays and turbulent multi-mode combustion

Applied Research

- High-fidelity CFD for device scale research: Virtual Engine Simulators (VES)
- Application of VES to engine design, optimization, and real-time control
- High-resolution optical diagnostics for device scale research
- Device scale research on the impact of alternative fuel properties on novel combustion and emission processes
- Exploration of high pressure engine combustion
- Joint optimization of alternative fuel formulation and engine design
- Smart vehicle strategies and sensor development

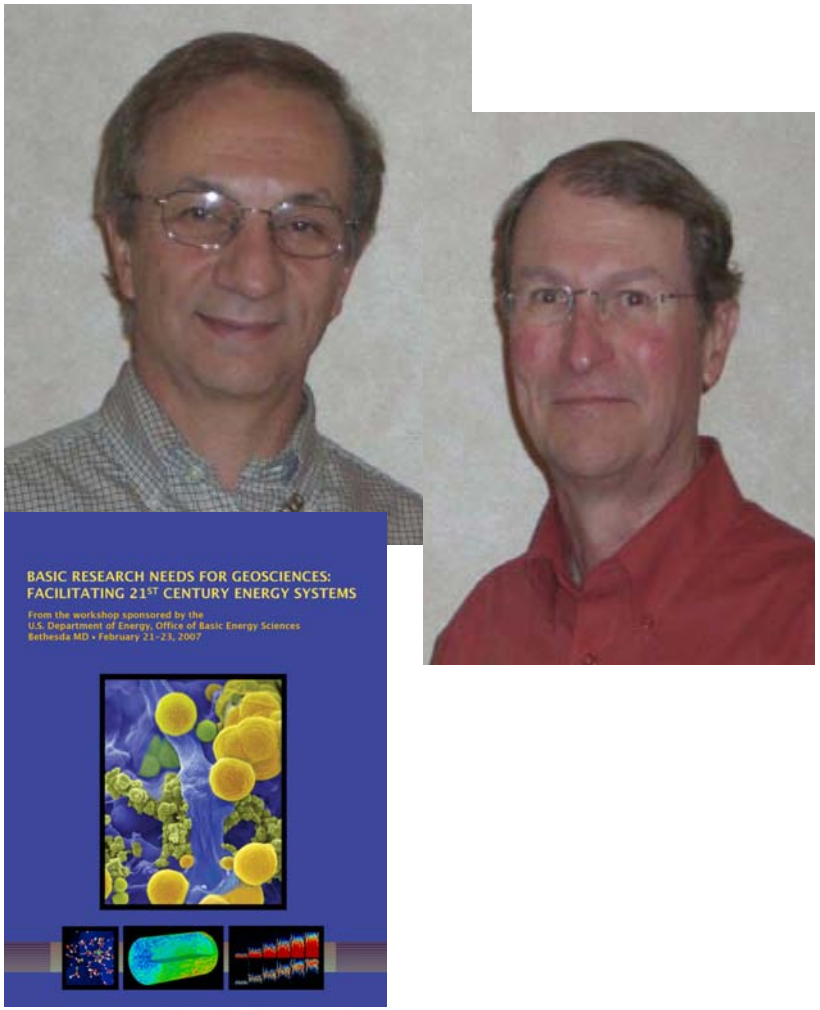
Technology Maturation & Deployment

- New generation of vehicles with alternative fuels: achieving high efficiencies with emission compliance
- Enable realization of next-generation efficiency and emissions standards
- Smart vehicles with VES-based control systems

Office of Science
BES

Applied Energy Offices
EERE

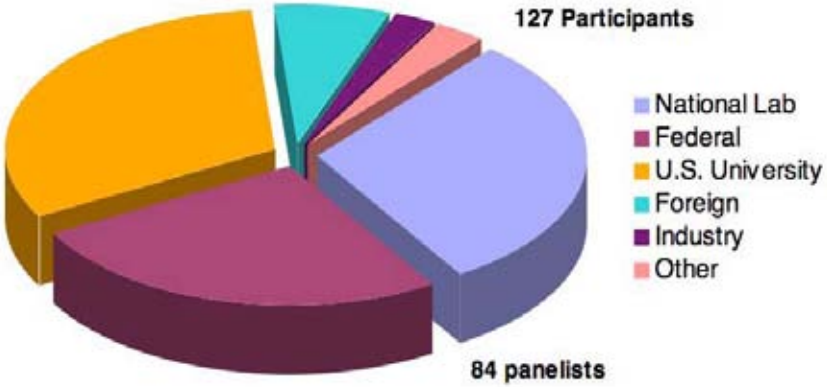
The BES Workshop on Basic Research Needs for Geosciences: Enhancing 21st Century Energy Systems 21 – 24 February 2007



Workshop Co-chairs: Don DePaulo (LBNL and UC Berkeley)
Lynn Orr (Stanford)

Organizing Committee/Panel Leads:

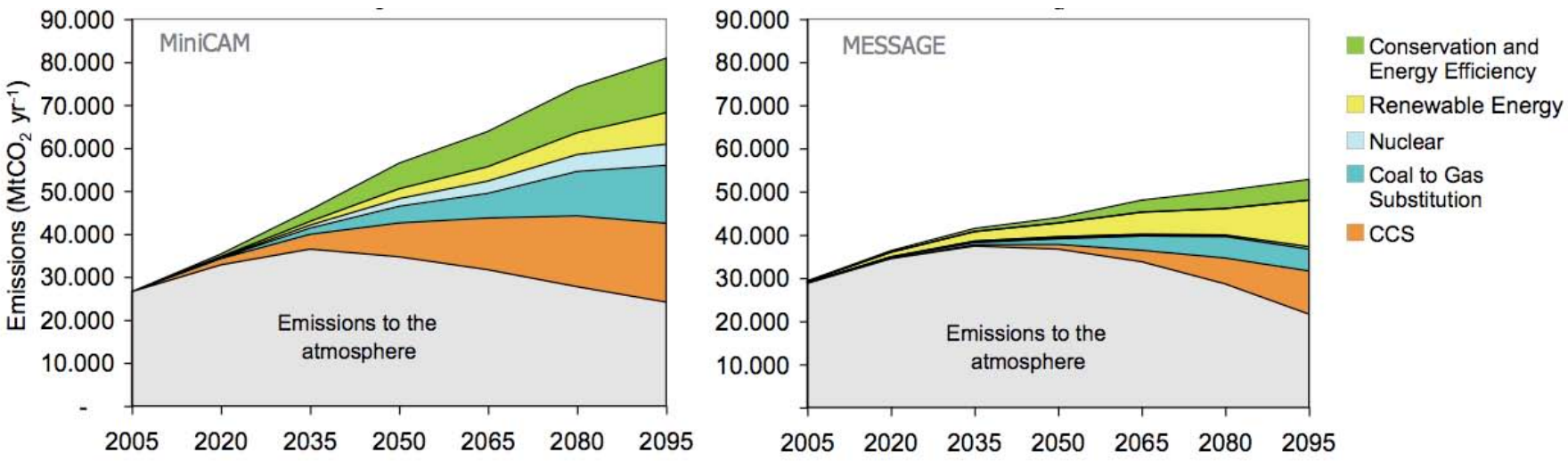
Sally Benson (LBNL - Stanford)
Michael Celia (Princeton)
Andy Felmy (PNNL)
Kathryn Nagy (U. Chicago-CC)
Roel Snieder (Colorado Sch. Mines)
Graham Fogg (U.C. Davis)
Karsten Pruess (LBNL)
James Davis (USGS)
Julio Friedmann (LLNL) (TPRD - CCS)
Mark Peters (ANL) (TPRD - NW)



Workshop Charge: "The workshop will identify the scientific challenges involved in developing better physical and chemical understanding of geological systems that can accommodate storage of energy byproducts over decadal, century and millennial time scales, and over a range of length scales. The improved understanding of the critical processes will be used to design advanced geochemical, hydrologic and geophysical measurement technologies, it will be used to enhance our ability to predict and monitor subsurface processes at a much higher resolution, and it will enable us to use our measurements and monitoring capabilities for verifying system behavior(s). "

Two Principal Motivations

- Meeting energy demand in the coming centuries
- Drastically reducing CO2 emissions



Standard Fossil Fuel ± Hydrogen Economy => Sequester 10 Gt CO_2/yr

Expand Nuclear by 10x => Sequester SNF at ≈ 1 Yucca Mtn/Yr globally

With the caveat (from the workshop report executive summary):
"Rock formations are composed of complex natural materials that were not designed by nature as storage vaults."

Geosciences Workshop Outputs

Grand Challenges

1. Computational thermodynamics of complex fluids and solids
2. Integrated Characterization, Modeling, and Monitoring of Geologic Systems
3. Simulation of complex multi-scale systems for ultra-long times

Priority Research Directions

1. Mineral-water interface complexity and dynamics
2. Nanoparticulate and colloid physics and chemistry
3. Dynamic imaging of flow and transport
4. Transport properties and *in situ* characterization of fluid trapping, isolation, and immobilization
5. Fluid-induced rock deformation
6. Biogeochemistry in extreme and perturbed environments

Cross cutting issues

1. The microscopic basis of macroscopic complexity
2. Highly reactive subsurface materials and environments
3. Thermodynamics of the solute-to-solid continuum

Basic Research Needs for Geosciences, February 21-24, 2007

Discovery Research

- Microscopic basis of macroscopic complexity - scaling
- Highly reactive subsurface materials and environments
- Thermodynamics of the solute-to-solid continuum
- Computational geochemistry of complex moving fluids within porous solids
- Integrated analysis, modeling and monitoring of geologic systems
- Simulation of multi-scale systems for ultra-long times

Use-inspired Basic Research

- Predicting impermeable interval properties and fluid trapping
- Transport properties and *in situ* characterization of fluid trapping, isolation and immobilization
- Dynamic imaging of flow and transport
- Fluid-induced rock deformation
- Mineral-fluid interface complexity and dynamics
- Multiphase flow properties of CO_2/brine systems
- Biogeochemical dynamics resulting from CO_2 sequestration

Applied Research

- Develop and test methods for assessing storage capacity and for monitoring containment of CO_2 storage
- Develop remediation methods to ensure permanent storage
- Demonstrate procedures for characterizing storage reservoirs and seals
- Integrated models for waste performance prediction and confirmation
- Radionuclide partitioning in repository environments.
- Waste form stability and release models.
- Incorporate new conceptual models into uncertainty assessments.

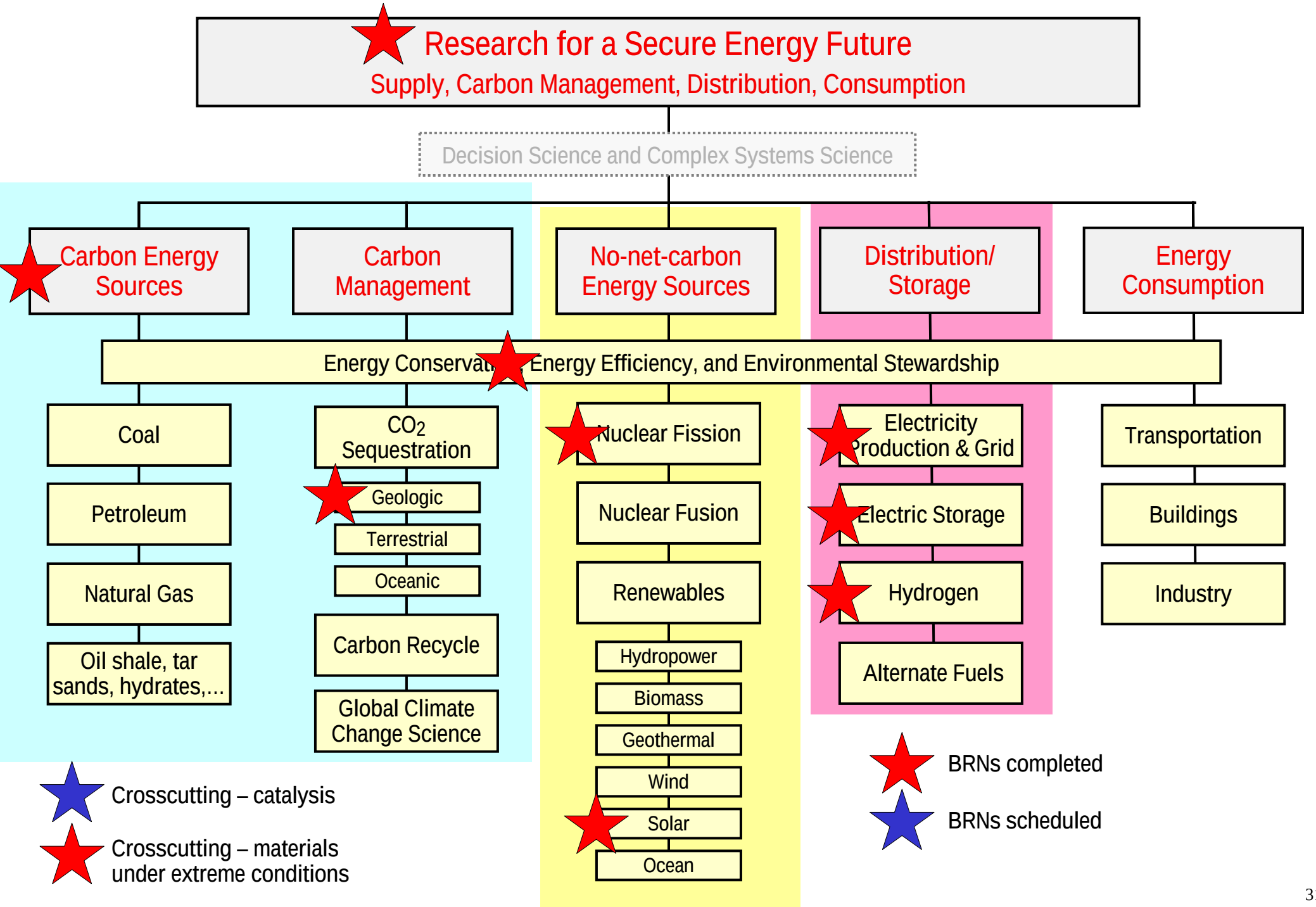
Technology Maturation & Deployment

- Develop site selection criteria
- Develop storage and operating engineering approaches
- Storage demonstrations
- Apply assessment protocols and technologies for the lifecycle of projects
- Evaluate release of radionuclide inventory from the repository
- Assess corrosion/ alteration of engineered materials
- Long-term safety/risk assessment for emplacement of energy system by-products.

Office of Science

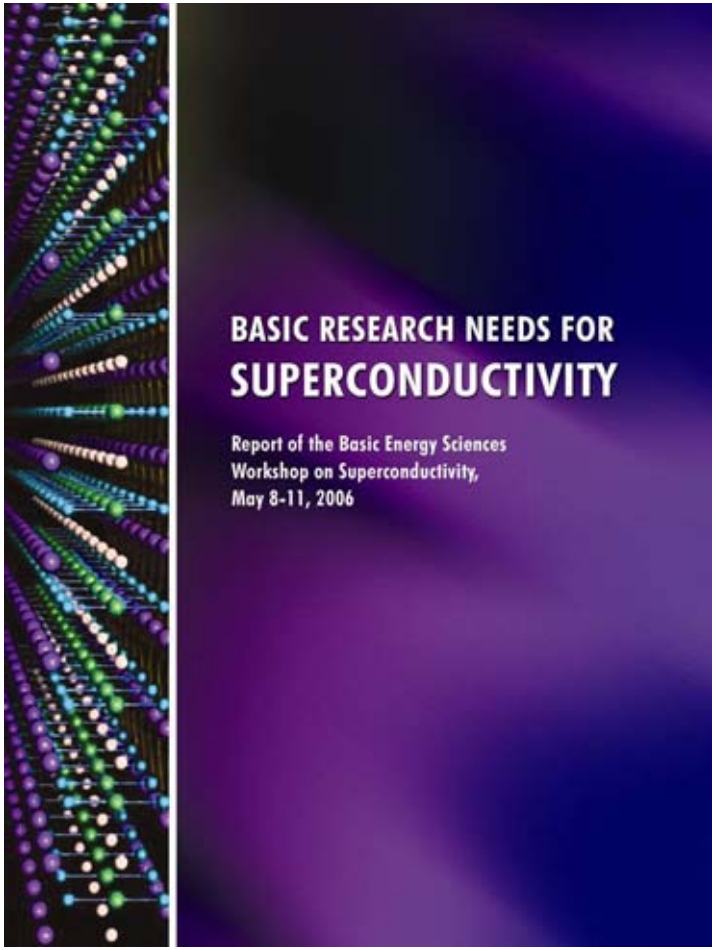
FE, RW, EM, EERE

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



The BES Workshop on Basic Research Needs for Superconductivity

8-11 May 2006



Workshop Co-chair: John Sarrao, LANL
Co-chair: Wai-Kwong Kwok, ANL

Panel Chairs:

- Materials: I. Bozovic (BNL)
- Phenomena: J. C. Davis (Cornell), L. Civale (LANL)
- Theory: I. Mazin (NRL)
- Applications: D. Christen (ORNL)

Plus 100 researchers representing 7 countries, 28 universities, and 9 national labs

Workshop Charge: "Identify basic research needs and opportunities in superconductivity with a focus on new, emerging and scientifically challenging areas that have the potential to have significant impact in science and energy relevant technologies."

Superconductivity

Discovery Research

- Complete determination of interaction functions generating HTS
- Predictive understanding of strongly correlated superconductivity
- Room-temperature superconductor
- Nano/meso-scale superconductivity
- Vortex matter
- Materials by design
- Manipulation of structure and properties on the atomic scale
- Tuning competing interactions

Use-inspired Basic Research

- 100K isotropic SC
- 3-d quantitative determination of defects and interfaces
- Intrinsic and intentional inhomogeneity
- "Pinscape engineering" in-situ manipulation of pinning centers
- Achieve theoretical limits of critical current
- Next generation SC wires

Applied Research

- Technology Milestones:
  - *2G coated conductor carrying 300 A x 100 m (2006)*
  - *In-field performance for 50 K operating temperature*
  - *Electric power equipment with ½ the energy losses and ½ the size*
  - *Wire with 100x power capacity of same size copper wires at $10/kiloamp-meter*
- Assembly and utilization R&D issues
- Materials compatibility and joining issues

Technology Maturation & Deployment

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

Office of Science
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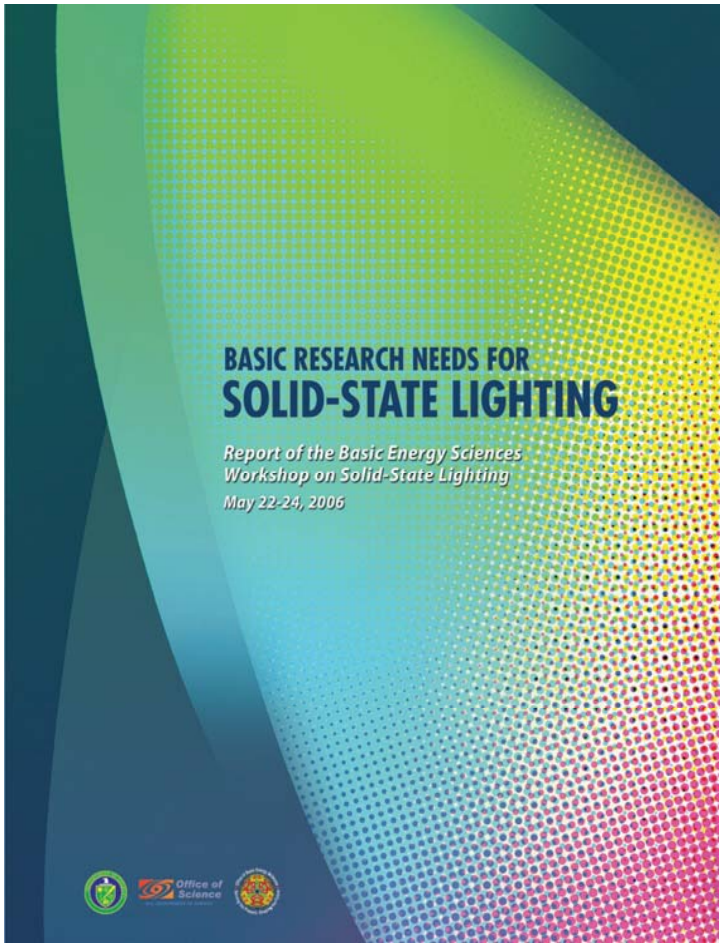
Technology Offices
EDER

The BES Workshop on Basic Research Needs for Solid-State Lighting

22-25 May 2006



Workshop Co-chair: Julia Phillips (SNL, Albuquerque)
Co-chair: Paul Burrows (PNNL)

Panel Chairs:

- LED Science: Jerry Simmons (SNL), Bob Davis (Carnegie Mellon U)
- OLED Science: Franky So (U of Florida), George Malliaras (Cornell)
- Cross-Cutting: Jim Misewich (BNL), Arto Nurmikko (Brown U), Darryl Smith (LANL)

Plus 80 researchers

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

Discovery Research

- 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

Use-inspired Basic Research

- Unconventional light-emitting semiconductors
- Photon conversion materials
- Polar materials and heterostructures for SSL
- Luminescence efficiency of InGaN
- Managing and exploiting disorder in OLEDs
- Understanding degradation in OLEDs
- Integrated approach to OLED fundamentals

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Applied Research

Technology 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

Technology Maturation & Deployment

- Developing national standards and rating systems for new products
- Commercial adoption and support
- Industrial partnership
- Legal, health, market, and safety issues
- Cost reduction
- Prototyping

Technology Offices
EERE

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

Chair: **John Goodenough (UT-Austin)**

Co- Chairs: 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.

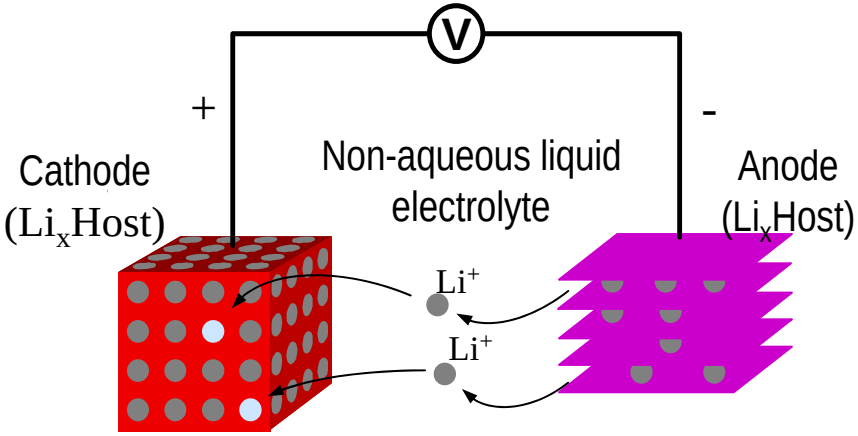
Electrical Energy Storage Vital in Two Main Areas

- Plug-in electric and all-electric vehicle place greater demands on energy storage
  - Higher energy and power densities
  - Appropriate recharge rates
  - Long life cycle
  - Reliability
  - Safety

- Effective use of renewable energy sources
  - Power quality
  - Reliability
  - Load leveling
  - Efficient use of cyclical energy sources

Limitations of Current Battery Technologies

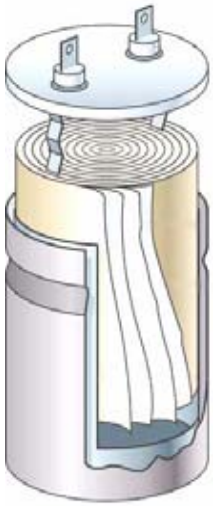
- **Increasing energy and power density without compromising safety or lifetime**
- **Advances will require**
  - Breakthroughs in materials and chemical processes
  - Understanding of solid-electrolyte interface
  - Control of charge transfer

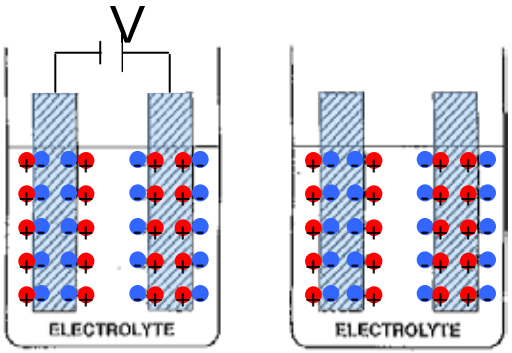


Rechargeable Li-ion battery schematic

Limitations of Current Electrochemical Capacitors

- **Increased energy densities**
- **Increased lifetimes (shelf and cycles)**
- **Advances will require**
  - Understanding of charge storage mechanisms
  - Tailored multifunctional materials
  - New electrolytes

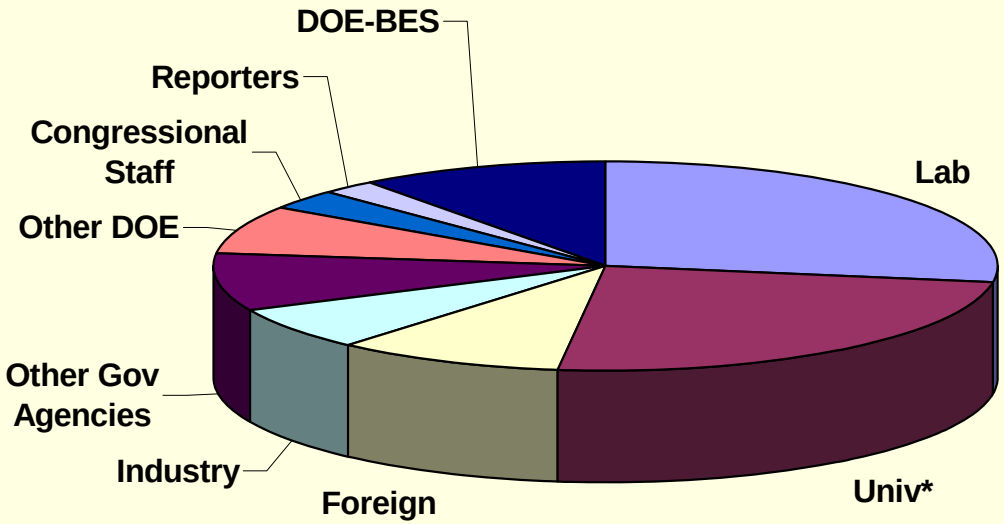




30 MJ CAPACITOR STORAGE SYSTEM

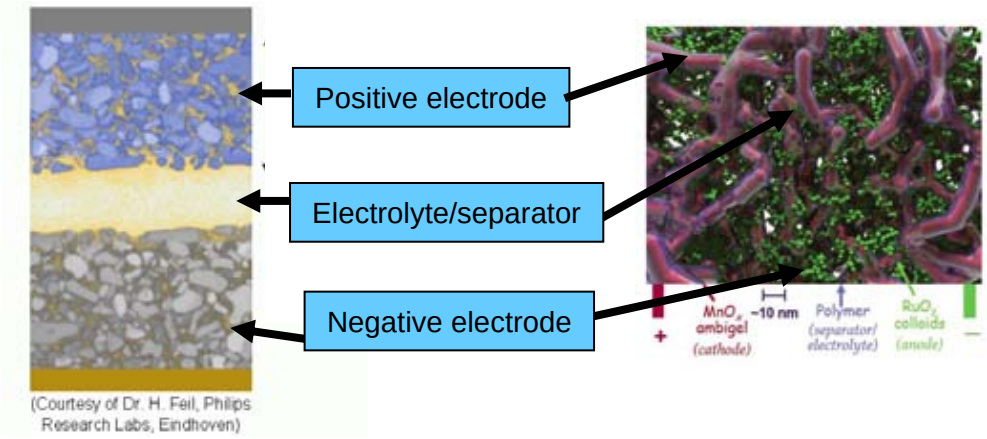
135 Participants:

- Universities
- National Laboratories
- Industries
- Foreign
- DOE: SC and Technology Program Offices
- Congressional Staff
- Reporters

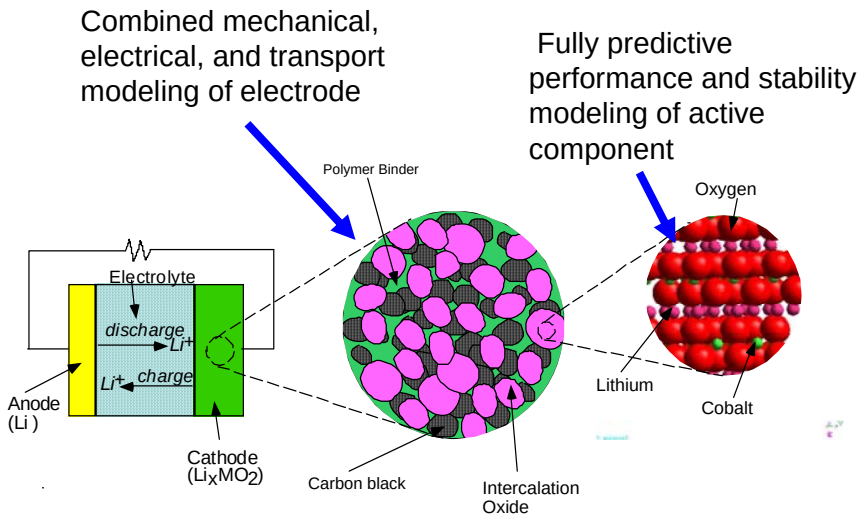


Priority research directions for chemical storage science

- **Novel system design towards performance and efficiency**
  - Design of multi-functional materials
  - Understanding physical integration of structure and charge transfer
  - Understanding of mixed conductivity and transport in electrodes
- **New materials, chemistries, and strategies**
  - Tailored nanomaterials for increased energy capacity, >1 electron transfer per redox center
  - "retrosynthetic" approaches to new high performance materials

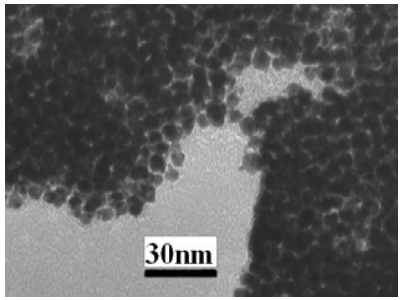


3-D Battery Self Assembled Electrochemical Cell Structures wit
Multifunctional Components.

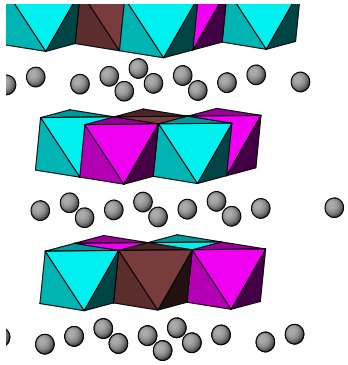


Priority research directions for chemical storage science

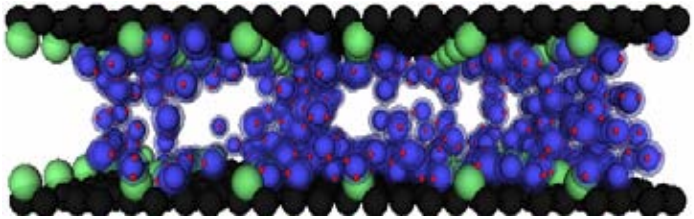
- **Rational Design of Interfaces and Interphases**
  - Understand interface/interphase dependence on electrode materials and electrolytes
  - Elucidate the role of the electrode interface in governing charge transfer to electrolytes
  - Predictive behavior of nanomaterials
  - Physicochemical consequences of dimensionality
  - Integrated kinetic modeling in multi-phase systems
  - Sensitive, multi-technique, in situ characterization methods over wide timescale (femtosec to sec)



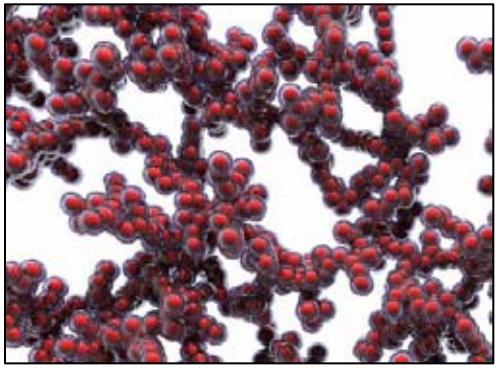
Graphite



$Li[Co_{1/3}Mn_{1/3}Ni_{1/3}]O_2$



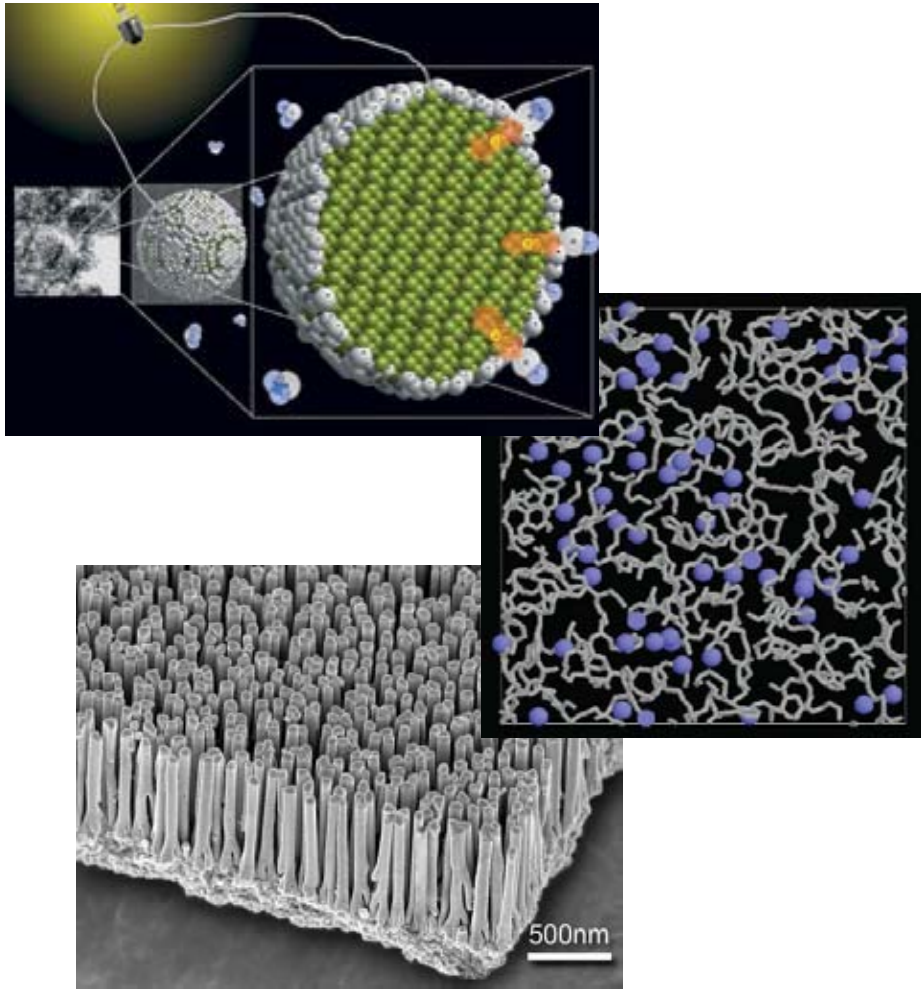
oO_2



Design of porous catalyzed 3-D nanoarchitecture as air cathode

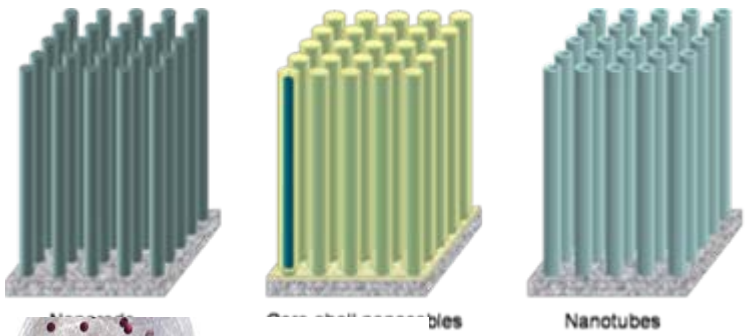
Priority research directions for capacitive storage science

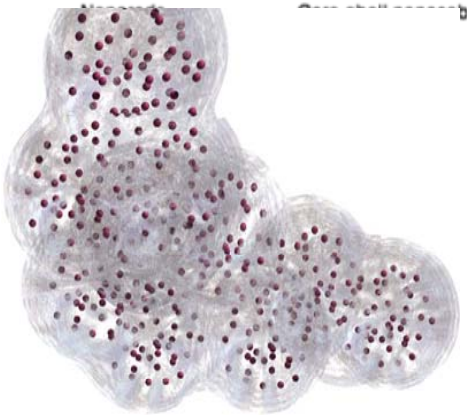
- **Charge storage materials by design**
  - Materials with tailored architectures to gain controlled high surface area
    - Surface functionality
    - Tailored porosity
    - Ordered architectures
  - Understanding pore structures and "effective" ion size
  - Predict material structure and function



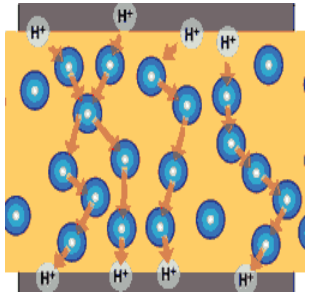
Priority research directions for capacitive storage science

- **Multifunctional Materials**
  - Materials beyond metal oxides
  - Multifunctional architectures
  - "Retrosynthetic" tailoring of functionality
  - Understanding charge-storage mechanisms
- **Novel electrolytes**
  - Understanding design criteria for electrolytes that enable higher voltages
  - Fundamentals of solvation dynamics and ionic transport
  - Design of intelligent materials that are self-healing and chemistries that scavenge impurities
  - Understanding behavior in confined spaces



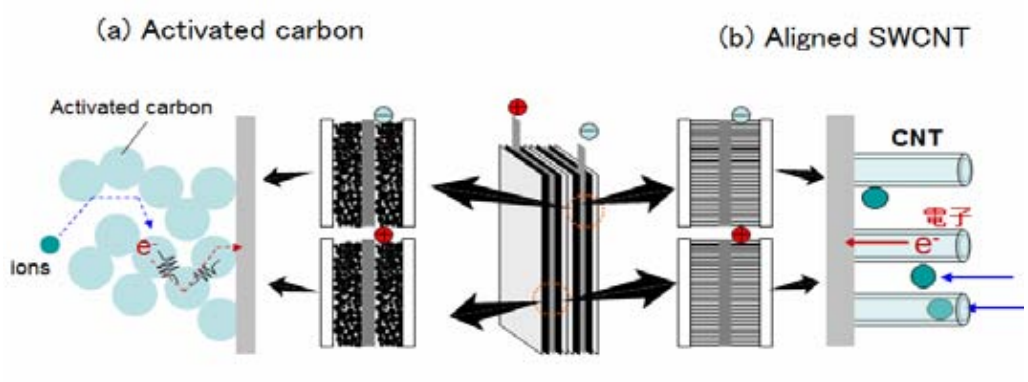


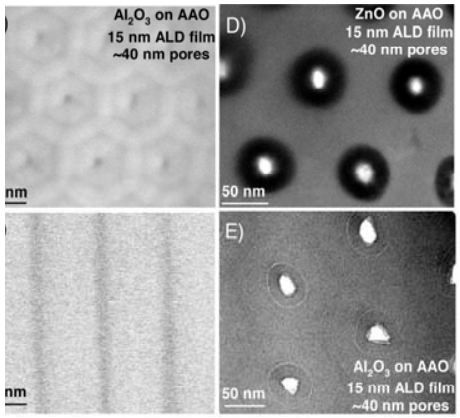
Nanodots of RuO2 particles encapsulated into graphene matrix



Cross-cutting Science

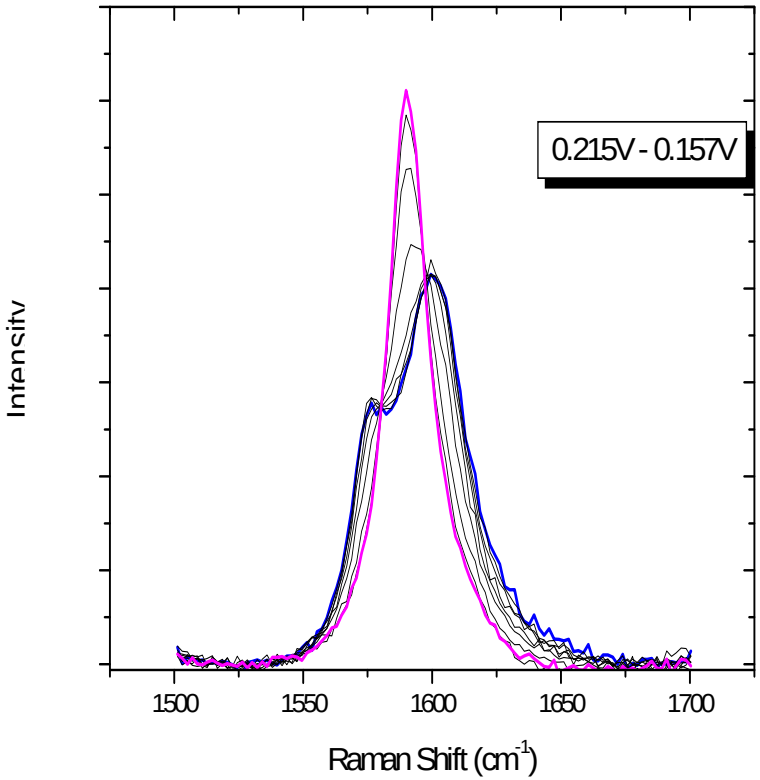
- **Efficacy of structure in energy storage**
  - Design, synthesize, and optimize architectures for improved energy storage
  - Develop multifunctional materials that are, e.g., self-healing, self-regulating, failure-tolerant, impurity-sequestering, sustainable
  - Use theory and experiment in conjunction with well-defined structures to elucidate fundamental materials properties





Cross-cutting Science

- **Charge Transfer and Transport in Energy Storage**
  - Correlation of stochastic electronic and nuclear structures and electron transfer on the nanoscale
  - Molecular scale structure/electrical potential probes
  - Electron transfer dynamics at atomically and molecularly tailored interfaces
  - Supramolecular and surfactant design for transport channels and healing interfaces

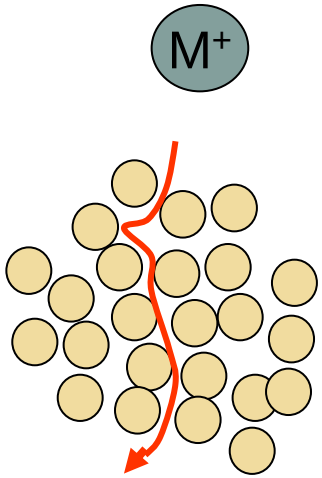


Micro-Raman spectra of single 30 μm flake of graphite vs. applied potential

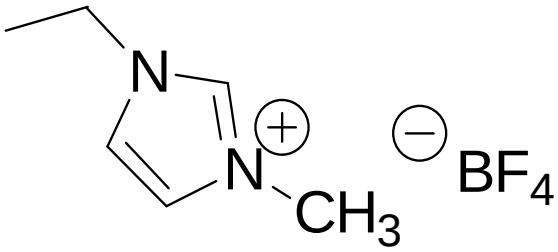
Cross-cutting Science

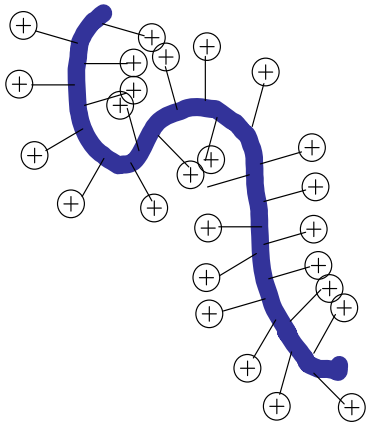
- **Innovation in Electrical Energy Storage Electrolytes**
  - Innovative design and syntheses to obtain strong ionic solvation, yet weak ion-ion inter-action, high fluidity, controlled thermodynamics
  - Ionic, multi-ionic, and redox liquids, screened anions, ions linked by conducting segments to extend the space charge region, and hard and soft additives
  - Target electrode interactions with highly concentrated ionic phases

Nanocomposites for ion transport



Molten salts

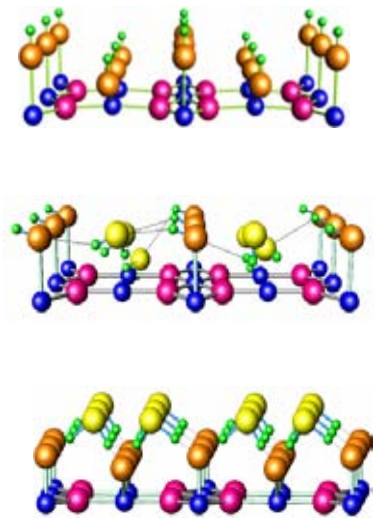




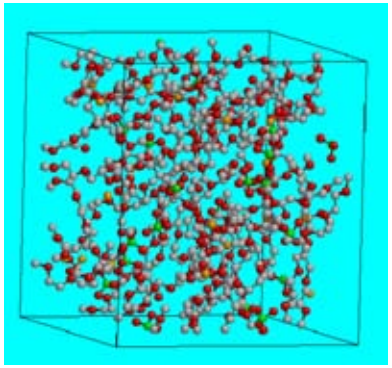
Novel molecular ions

Cross-cutting Science

- **Multi-Scale Computations for EES**
  - Multi-scale modeling: improved integration of length and time scales
  - Virtual design of materials
  - Modeling of sustainability and life cycle
  - Validation of theoretical methods with experiment on model systems



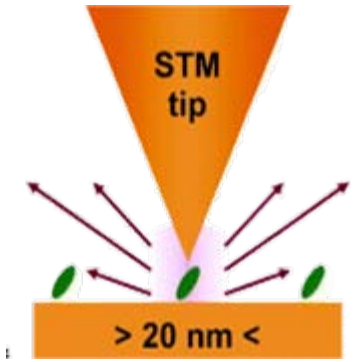
Formation and destruction of water monolayer on RuO_2 surface from theory and experiment

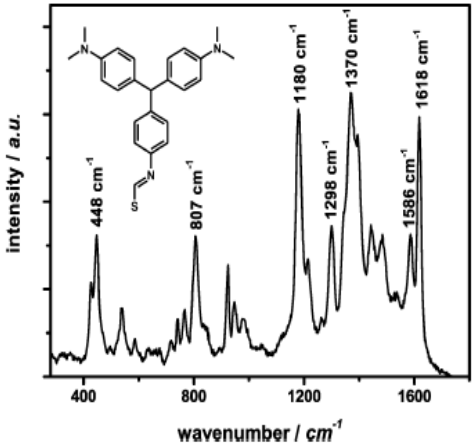


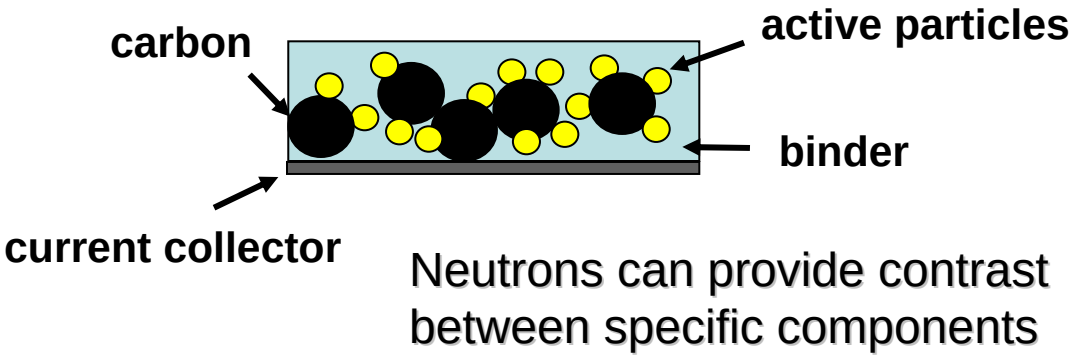
MD simulation of $LiClO_4$/PEO polymer electrolyte

Cross-cutting Science

- **Probing energy storage chemistry and physics at all time and length scales**
  - Develop and implement techniques to monitor, with spatial resolution from atomic to mesoscopic and temporal resolution down to fs, changes in structure and composition including
    - in-situ spectroscopy
    - microscopy
    - scattering







Neutrons can provide contrast between specific components

EES Workshop Conclusions

- Because of today's serious technology gaps, revolutionary breakthroughs in EES have been targeted as a crucial need for this Nation's secure energy future
  - Transportation
  - Utilization of renewable energy sources
  - Stabilization of grid

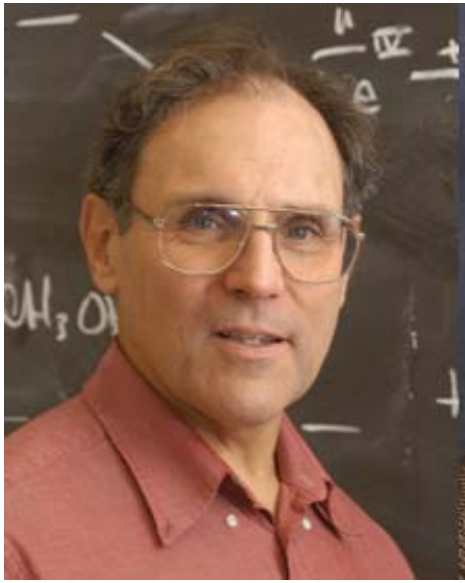
- Realizing future requirements for EES will only be achieved with basic research
  - Design of novel nanoscale materials with architectures tailored for optimum performance
  - Fundamental understanding of
    - **relationship of materials structure and function at the atomic level**
    - **dynamic chemical and physical processes at interfaces**
  - Ability to simulate and predict structure / function relationships of new materials

Workshop report, including consolidation of PRDs, science grand challenges, four-column chart, under preparation.

Basic Research Needs in Catalysis for Energy Workshop: August 6-8, 2007, N. Bethesda Marriott

Chairs:

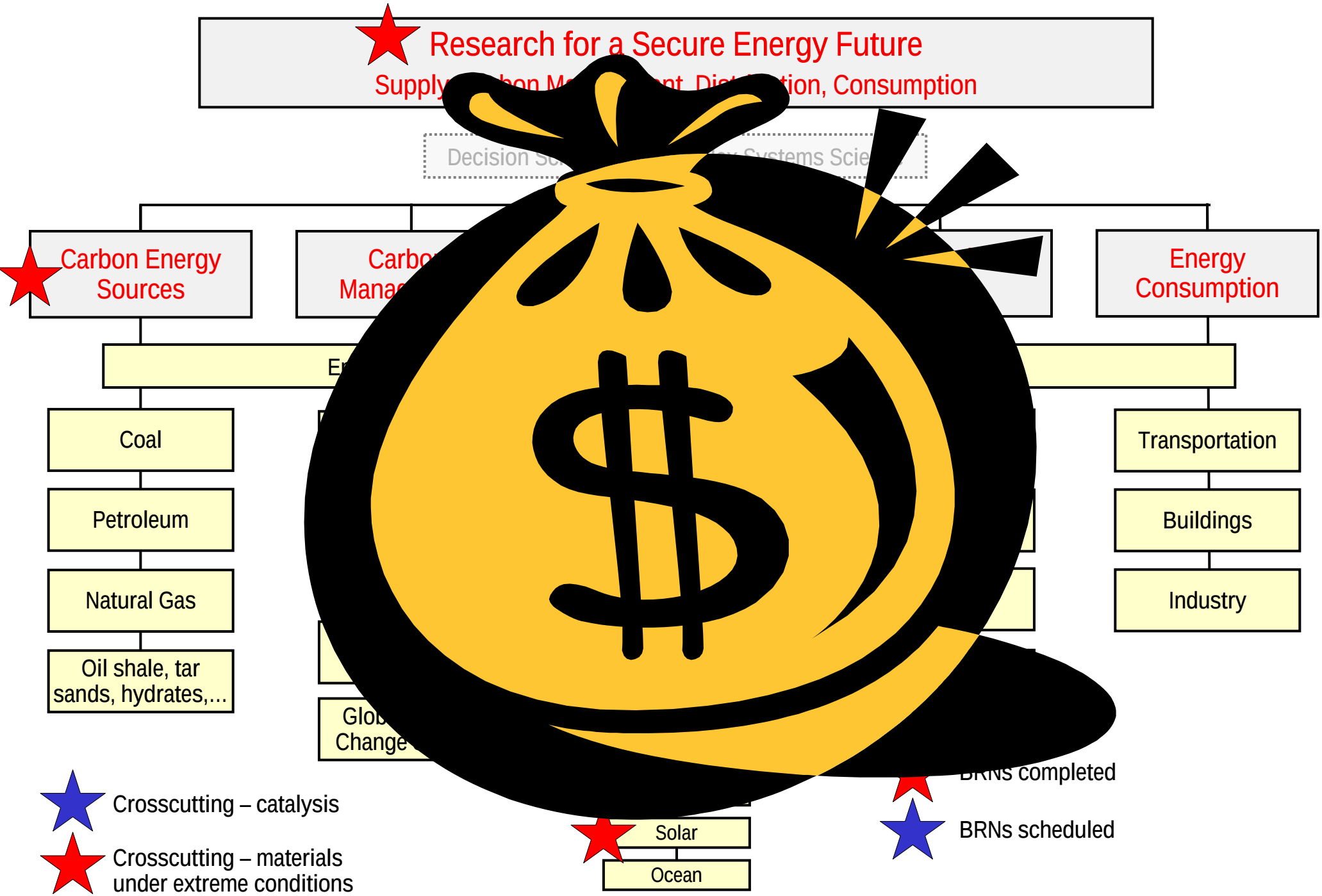
	Alexis T. Bell	**(UC Berkeley)**
	Bruce C. Gates	**(UC Davis)**
	Douglas Ray	**(PNNL)**



Charge to the Workshop:

Identify the basic research needs and opportunities in catalytic chemistry and materials that underpin energy conversion or utilization, with a focus on new, emerging and scientifically challenging areas that have the potential to significantly impact science and technology. The report ought to uncover the principal technological barriers and the underlying scientific limitations associated with efficient processing of energy resources. Highlighted areas must include the major developments in chemistry, biochemistry, materials and associated disciplines for energy processing and will point to future directions to overcome the long-term grand challenges in catalysis. A report should be published by November 2007.

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



FY2007 President's Budget

- Office of Science budget up 14.1% over FY2006 to $4.1B
- Basic Energy Sciences budget up 25% to $1.42B
  http://www.sc.doe.gov/bes/
- BES increases target several areas:

  Additional funding for basic research for the hydrogen economy +$17.5M to a total of $50M

  Basic research for solar energy utilization +$34.1M

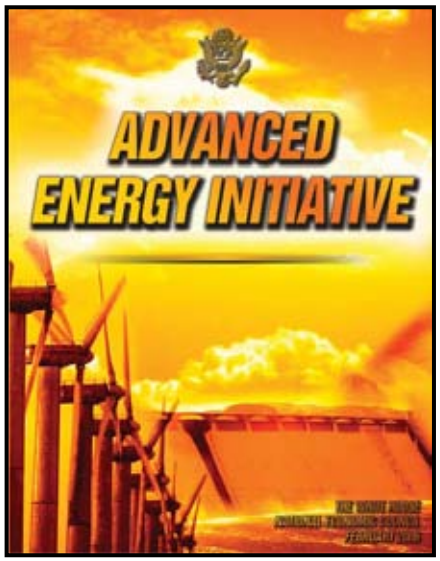
  Basic research for advanced nuclear energy systems +$12.4M

  Ultrafast science +$10M

  Mid-scale instrumentation +$10M

  Chemical Imaging +$5M

  Complex systems or emergent behavior +$5M



BES Budget under FY2007 Joint Resolution

- For SC: $200M over FY2006 level. When combined with $130M of entitlement appropriations in FY2006 gives a total of $330M above the base FY2006 budget.
- But the FY2006 base was also very poor and the bulk of the “extra” funds went to continue full operations at SC user facilities, per Congressional mandate.
- Only modest amounts were appropriated for iniatives: $8M for solare energy utilization and $4M for hydrogen fuel initiative.
- Net result: FY2007 was not a good year for BES use-inspired research.

FY2007/2008 BES Solicitations

Solicitation:	Instrumentation	Basic research for solar energy utilization	Basic research for the hydrogen fuel initiative	Basic research for advanced nuclear energy systems
Funding in FY 2007 Request	~ $20 M	$34.1 M	+ $17.5 M	$12.4 M
FY2007 Appropriation	0	$8 M	$4 M	0
Additional funding in FY 2008 Request	0	+ $5.9 M	+ $9.5 M	0
Total funding in FY2008 Request	~ $20 M	$40 M	$27 M	$12.4 M
FY 2007 Congressional Budget released	February 6, 2006			
Announcement of intent to issue solicitations	February 16, 2006			
Posting solicitation on SC website	March 7, 2006	March 21, 2006	April 20, 2006	October 12, 2006
Preproposal deadlines	May 17, 2006 106 preproposals	June 5, 2006 656 preproposals	July 6, 2006 502 preproposals	Nov. 22, 2006 209 preproposals
PIs notified of preproposal decisions	June 30, 2006 59 encouraged	August 11, 2006 346 encouraged	Sept. 12, 2006 249 encouraged	January 5, 2007 126 encouraged
Full proposal deadlines	August 30, 2006 58 received	Nov. 14, 2006 309 received	Dec. 12, 2006 229 received	March 14, 2007 117 received
FY2007 award announcements (approx)	none	27 awards May 22	13 awards May 15	none
FY2008 award announcements (pending appropriation)	???	???	???	???

Strategic Planning in BES

- Phase I: The Basic Research Need workshop series.
  - Strategic planning for BES use-inspired (energy-relevant) research in coordination with DOE technology offices.
- Phase II: BESAC Grand Challenges Report.
  - Strategic planning for BES grand-challenge/discovery research.
  - Report in preparation; update at BESAC meeting July 31; completion by fall BESAC meeting.
- Phase III: BESAC panel(s) to summarize scientific themes from Phases I and II, including “enabling tools”
  - In the early planning stages…..

BESAC Grand Challenges Sub-Panel

- **Co-Chairs: Graham Fleming (LBNL & UC Berkeley) & Mark Ratner (Northwestern)**
- **Members:**

  Paul Alivisatos (LBNL & UC Berkeley), Leon Balents (UC Santa Barbara), David Bishop (Bell Labs), Phil Bucksbaum (SLAC & Stanford), Jay Groves (LBNL & UC Berkeley), John Hemminger [ex officio] (UC Irvine)*, Michael Hochella (Virginia Tech), Walter Kohn (UC Santa Barbara), Tobin Marks (Northwestern), Paul McEuen (Cornell), Tom Moore (Arizona State), Cherry Murray (LANL), Dan Nocera (MIT), Teri Odom (Northwestern), Julia Phillips (SNL), Pete Schultz (Scripps/GNF), Robert Silbey (MIT), John Spence (Arizona State)**, Stan Williams (HP), Jun Ye (Colorado/JILA)**

*BESAC Chair
**BESAC Member

Grand Challenges Report – Connecting Themes

DRAFT

Grand Challenges Report Chapters

DRAFT

1) **Overview** **(Graham Fleming & Mark Ratner)**

2) **Control of Electrons in Atoms, Molecules, and Materials: Creating a New Language for the Behavior of Electrons** **(Phil Bucksbaum)**

3) **Basic Structure of Matter: Directed Assembly, Structure, and Properties** **(Tobin Marks)**

4) **Emergence, Complex Phenomena, and Strongly Correlated Multiparticle Systems** **(Julia Phillips/Leon Balents)**

5) **Nanoscale Communication** **(Jay Groves/Paul McEuen)**

6) **Science of Matter Beyond Equilibrium** **(Mark Ratner)**

7) **Infrastructure, Facilities, and Human Resources** **(Graham Fleming and Mark Ratner)**

Ex: Control of Electrons in Atoms, Molecules, and Materials

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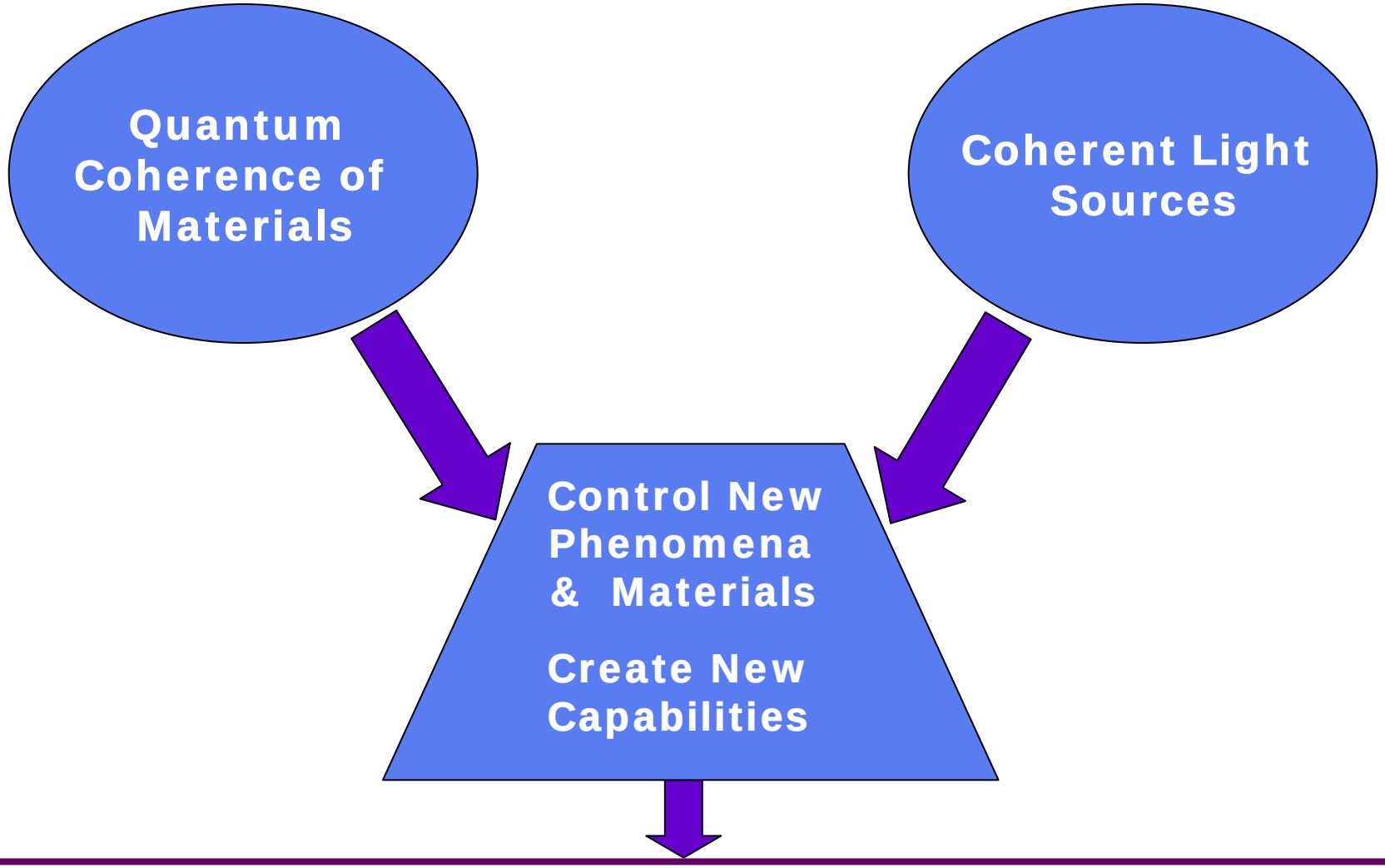

e.g. Imaging Materials in Angstroms and attoseconds

Needs: **New light sources** **Theories and language beyond the Born-Oppenheimer Approximation**