U.S. DEPARTMENT OF ENERGY

OFFICE OF SCIENCE

Basic Energy Sciences

Computing and Storage Requirements for Basic Energy Sciences
An ASCR / BES / NERSC Workshop
February 9-10, 2010 9AM

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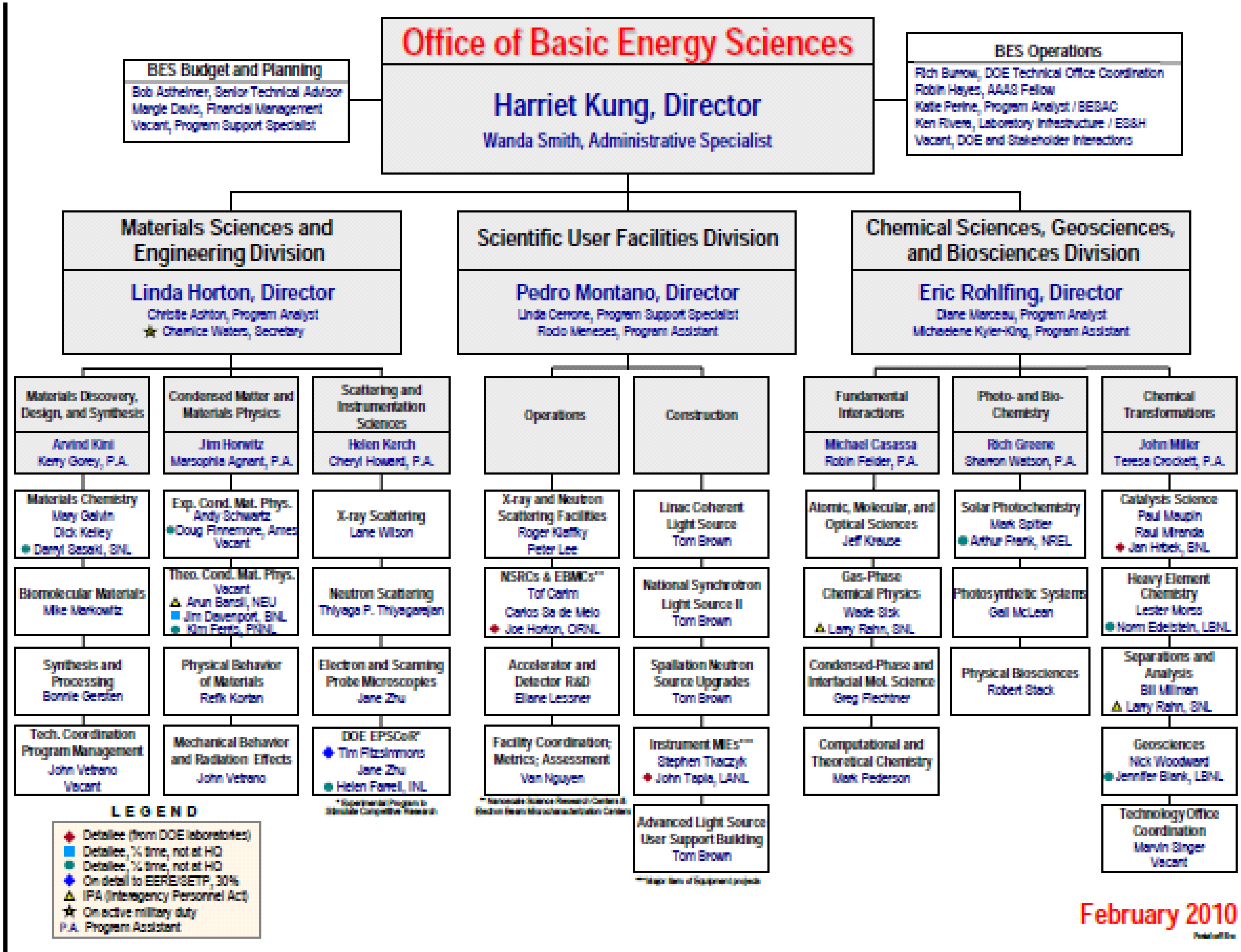


Primary: Near Future Needs of Capacity Computing?

BES has approximately 150 users requesting 50K to 4M processor hours (PU) per year.

BES users use approximately 80-100M PU per year through the NERSC allocation process

NERSC users span the BES core research areas, the energy frontier research centers and the "Basic Research Needs (BRN)" workshops.

Role/Needs of Capacity vs Capability?

Energy and Science Grand Challenges

BESAC and BES Reports

- Secure Energy Future, 2002
- Hydrogen Economy, 2003
- Solar Energy Utilization, 2005
- Superconductivity, 2006
- Solid-state Lighting, 2006
- Advanced Nuclear Energy Systems, 2006
- Clean and Efficient Combustion of Fuels, 2006
- Electrical Energy Storage, 2007
- Geosciences: Facilitating 21st Century Energy Systems, 2007
- Materials Under Extreme Environments, 2007
- Directing Matter and Energy: Five Grand Challenges for Science and the Imagination, 2007
- New Science for a Secure and Sustainable Energy Future, 2008

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

BES Basic Research Needs Workshops

Important Recurring Themes – Disruptive Technologies Require “Control”

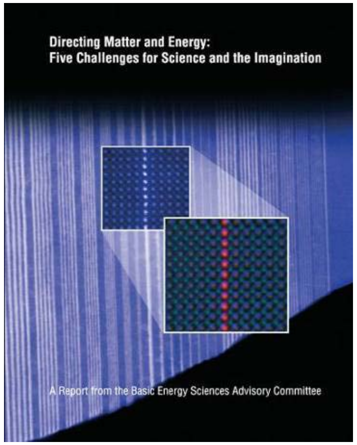
Control of materials properties and functionalities through electronic and atomic design

- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- “Control” of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems
- Designer catalysts
- Designer interfaces and membranes
- Structure-function relationships
- Bio-materials and bio-interfaces, especially at the nanoscale
- New tools for spatial characterization, temporal characterization, and for theory/modeling/computation – What does this mean to the NERSC userbase?

www.science.doe.gov/bes/reportslist.html

BESAC Subcommittee on Grand Challenges for Basic Energy Sciences

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

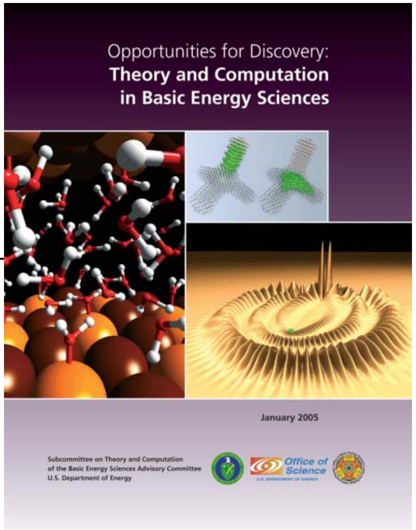


- Control the quantum behavior of electrons in materials
  Imagine: Direct manipulation of the charge, spin and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical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

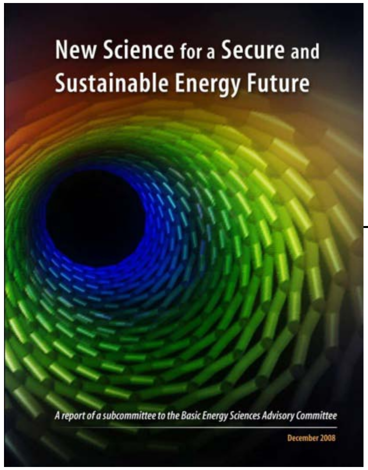
Perspectives from Past BES Studies

Enhancements in computation must be accompanied by enhancements in the rest of the theoretical endeavor. Conceptual theory and computation are not separate enterprises.

… for BES theorists to take advantage of high-end computer resources, there should also be opportunities for partnerships with applied mathematicians and computer scientists in the development of algorithms and software.



January 2005



December 2008

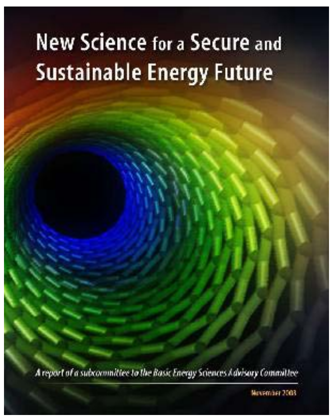
*BES must close gaps between needs and capabilities in synthesis, characterization, **theory, and computation** for advancing materials and chemistry*

What are needs of researchers who develop theory and computational implementations in parallel?

BESAC Subcommittee on Facing our Energy Challenges in a New Era of Science

Recommendations:

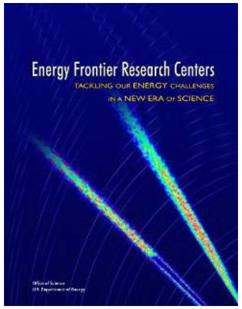
- Control science with complex functional materials.
- Increase the rate of discoveries and establish US leadership in next-generation carbon-free energy technologies.
- ‘Dream teams’ of highly educated talent, equipped with forefront tools, and focused on the most pressing challenges
- Aggressively recruit the best talent through a series of workforce development.



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

Energy Frontier Research Centers

Tackling Our Energy Challenges in a New Era of Science



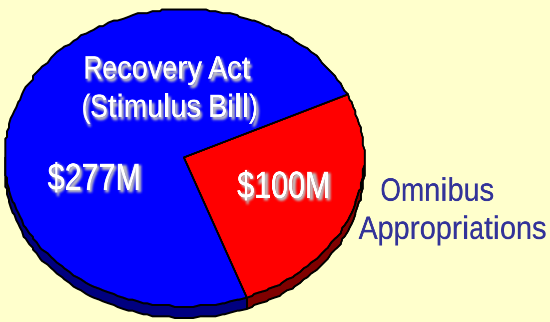
- To engage the talents of the nation's researchers for the broad energy sciences
- To accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century
- To pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical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

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

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

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

FY 2009 EFRCs Funding Status:

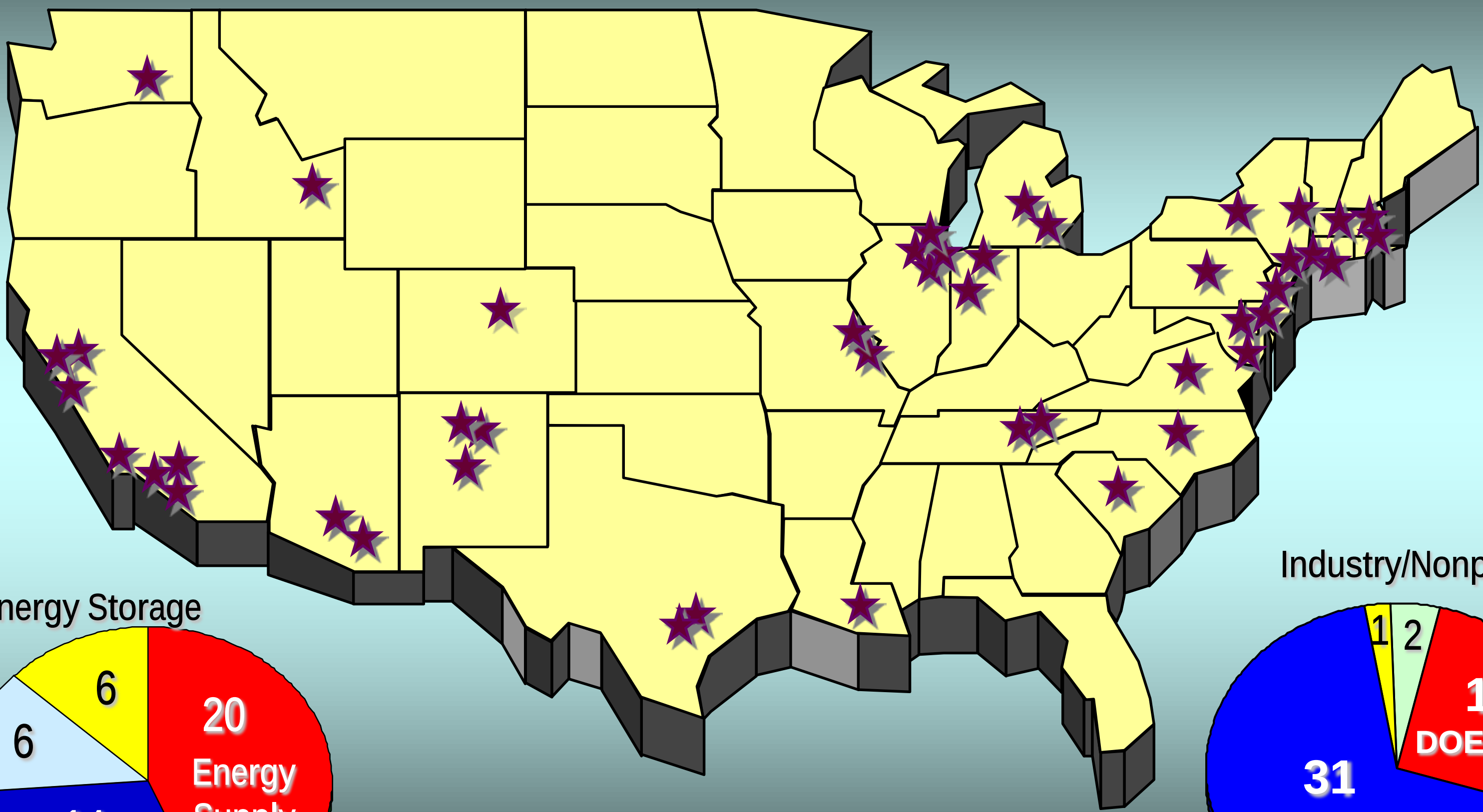


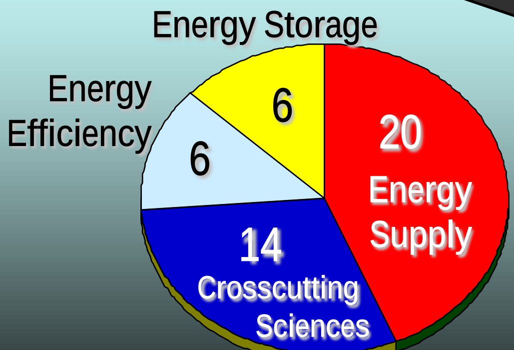
Total EFRCs = $777M over 5 years

Energy Frontier Research Centers

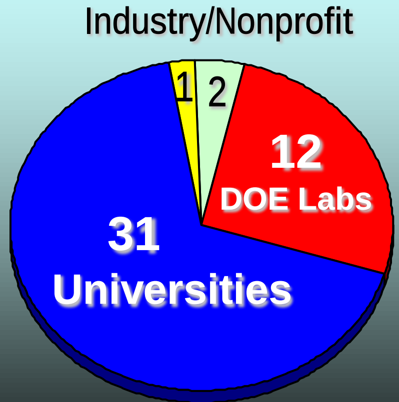
Invest in Cutting-edge Scientific Research to Achieve Transformational Discoveries

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





By Topical Category



By Lead Institution

Needs: Capacity vs Capability?

UPDATE ON: BES/ASCR Extreme Scale Workshop (Capability Needs)

12-15 August 2009

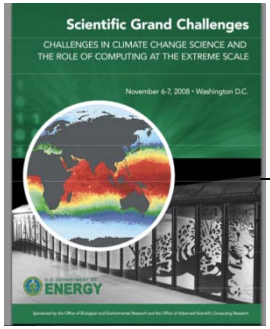
Chairs: G. Galli (UCD), T. Dunning (UIUC)

BES POC: M. Pederson & J. Davenport ASCR POC: :L. Chatterjee & P. Messina

Each workshop will produce a document outlining the DOE-relevant scientific questions that can be addressed with anticipated growth in computer power and identifying the challenges for doing so.

BES: Use BRN-series model.

Climate	Nov 6-7, 2008
High Energy	Dec 9-11, 2008
Fusion	Mar 18-20, 2009
Nuclear	May 11-12, 2009
Mat/Che/Geo	Aug 12-14, 2009
Biology	Aug 17-19, 2009



Future computing platforms provide opportunity only with increased effort on part of software and algorithms.

Briefing by: Davenport/Pederson
June 24, 2009 Germantown

Please note: the Correlation & Time Dependence breakout session will be split into 2 separate sessions on the 1st day, then together in 1 session on the 2nd day.

BREAKOUT SESSIONS

Whitepapers by all plenary/breakout participants due by June 1st, 2009. All ASCR whitepapers due by July 1st, 2009

The Plenary Talks and Speakers

- Extreme Scale Landscape — Rick Stevens
- Advanced Nuclear Geoscience & Extreme Environ: Dieter Wolf
- Catalysis: Bruce Garrett
- Combustion: Jaqueline Chen
- Superconductivity & Electrical Energy Storage (Batteries, Hydrogen and Capacitors): Warren Pickett
- Solar Energy Conversion & Solid State Lighting: Alex Zunger

Correlation & Time Dependence

M. Head -Gordon & G. Kotliar 23

- Excited States & Transition Rates
- Weak Interactions
- Correlation & Manybody Effects
- Superconductors, Oxides & Magnetism
- Advanced Spectroscopies & Facility Support
- Ultrafast Spectroscopy

Energy Storage

Michel Dupuis MY Chou 19

- Fuel Cells
- Batteries & Capacitors
- CO_2 Sequestration & H_2 Storage & Production

Photovoltaic Fundamentals

J. Grossman & K. Ming Ho 13

- Charge Separation
- Electron-Phonon Interactions & Polarons
- Transport
- Solvation & Polarization

Dynamics

C. Simmerling & M. Asta 18

- Multiscale Modeling
- Molecular Dynamics
- Entropy & Free Energy
- Energy Landscapes
- Reaction Rates & Dissipation

Cross-cutting topics

- Hardware & Systems Software IO Issues Dynamical Load Balancing
- Long Time Scale
- Rare Events & Hill Climbing
- FFTs
- Mesh Refinement
- Wavelets/Basis Sets
- Generalized Poisson Solvers
- Linear Algebra
- Data Analytics Management & Visualization

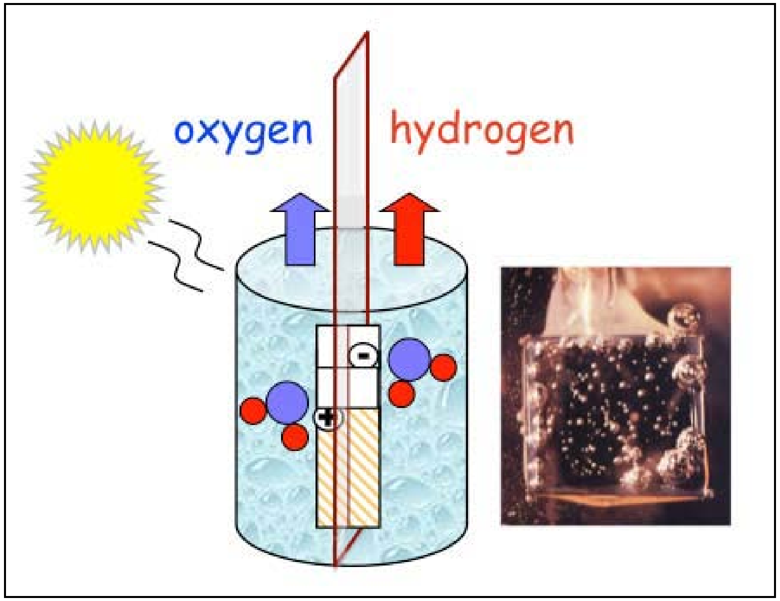
Required Resources: People & Hardware?

Energy Challenges
Grand Science Challenges
Foundational

Advanced Nuclear	Catalysis
Electrical Energy Storage	Combustion
Geosciences	Hydrogen
Extreme Environments	Solar
Solid State Lighting	Superconductivity

http://extremecomputing.labworks.org/basicenergy/index.stm

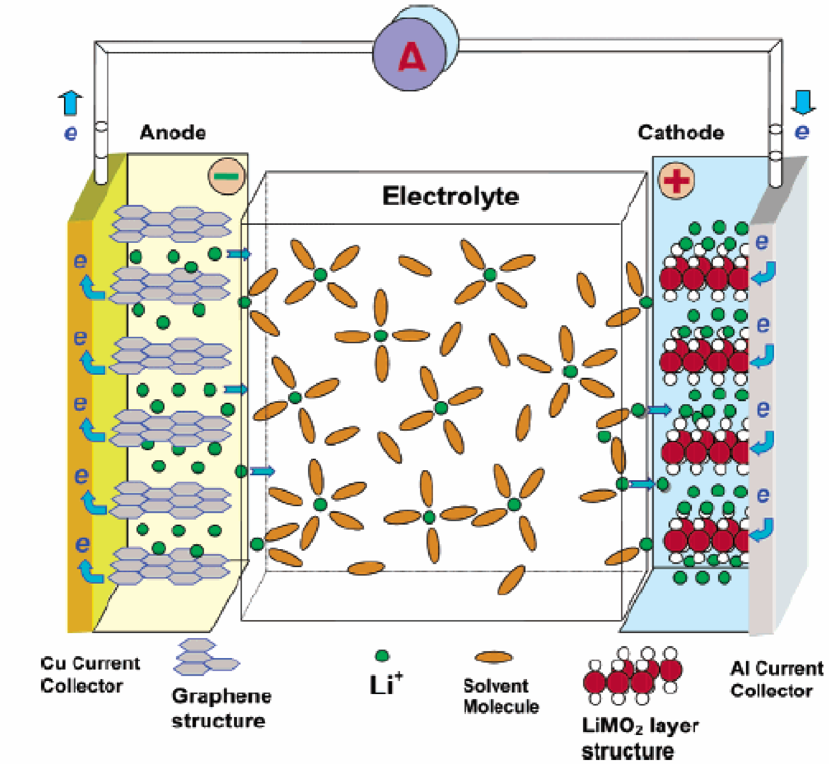
Two BRN Examples: Splitting water with sunlight? Batteries?



Light-Matter Interactions

Catalysis

Materials far from equilibrium



Transport

Electrolyte stability

Corrosion of electrodes?

Cell voltage – Chemical Reactions

Solvation effects

Weak Interactions

New Science Opportunities

Emerging Computer Simulation Techniques?

Resource Needs?

Charge for BES/NERSC Requirements Workshop

- Identify forefront scientific challenges and opportunities in basic energy sciences that could be aided by new computing platforms.

  - Memory?
  - Storage?
  - Speed?
  - Turn around time?
  - Queuing requirements / Amdahls law ?

- Provide NERSC with insights on where you are today and where you wish to be tomorrow?

BES | ASCR

- To discover and design new materials and molecular assemblies with novel structures and functions through ac
and molecule-by-mo

- To conceptualize, ca
processes underlyin
transformations.

- To probe, understan
interactions of phon
ions with matter to d
flow in materials anc

- To conceive, plan, de
scientific user facilit
and atomic propertie
fundamental limits o
resolution through x-ray, neutron, and electron
beam scattering.

- To develop mathematical descriptions, models, methods and algorithms to accurately describe and understand the behavior of complex
es that span vastly
scales.

- understanding and
use of computers at

- data from
ns into scientific

- mputational
further advance the
cience through
ships.

- nputational and
xtend the frontiers
of science.

- To develop networking and collaboration tools and facilities that enable scientists worldwide to work together.

BES/ASCR/NERSC Workshop

Assessment of scientific, technical, mathematical, hardware and software challenges at extreme scale?

Interdependencies?