Computational Research Needs for Alternative and Renewable Energy

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National Renewable Energy Lab

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Context

- Planning started 3 years ago.
- Under a prior administration.
- Preceded IPCC 4th assessment report on climate change.

- Subsequently, green is the new black.

U.S. Department of Energy
Energy Efficiency and Renewable Energy

Computational Research Needs for Alternative and Renewable Energy

September 19-20, 2007 Rocksville, Maryland

Co-Chairs

Greg Bothun, University of Oregon
Steve Hammond, National Renewable Energy Lab
Stephen Picataggio, Synthetic Genomic Solutions

Organizing Committee

Ross Guttromson, Pacific Northwest National Lab
Mike Heben, National Renewable Energy Lab
Mike Himmel, National Renewable Energy Lab
Kai-Ming Ho, Iowa State University and Ames
Moe Khaleel, Pacific Northwest National Lab
Shawn-Yu Lin, Rensselaer Polytechnic Institute
Costas Maranas, Pennsylvania State University
Phani Nukala, Oak Ridge National Lab
Scott Schreck, National Renewable Energy Lab

DOE Contacts

Gary Johnson, Office of Science, ASCR
Sam Baldwin, Chief Technology Officer, EERE

157 workshop participants

Workshop: Five Parallel Breakout Sessions

Renewable Fuels H2:
- Dave Dixon, U. of Alabama
- Bruce Clemens, Stanford
- Mike Heben, NREL

Renewable Electricity PV:
- Victor Batista, Yale
- Jerry Bernholc, NC State
- Mark Hybertsen, BNL
- Lin-Wang Wang, LBNL
- Shengbai Zhang, RPI

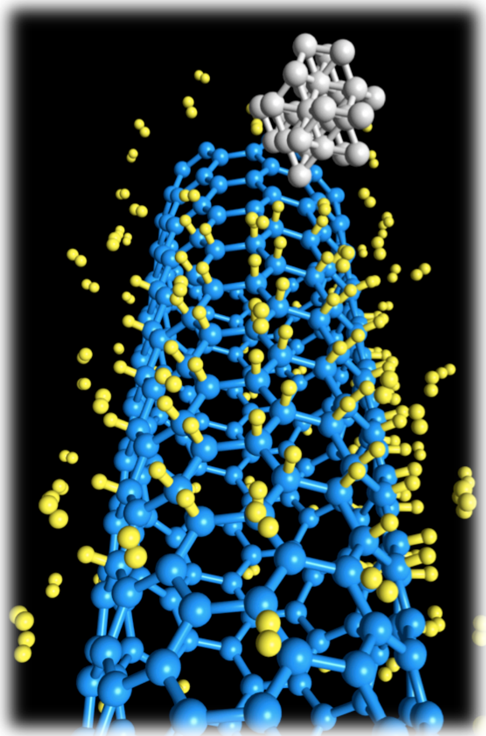
Renewable Fuels Bioenergy Conversion:
- Brian Davidson, ORNL
- Mike Himmel, NREL
- Costas Maranas, Penn State
- Jennie Reed, U. Wisc.

Renewable Electricity Wind:
- Larry Carr, US Army (retired)
- Earl Duque, Northern Ariz. University
- Scott Schreck, NREL

Grid Reliability:
- Ross Guttromson, PNNL
- Ian Hiskens, U. Wisc.
- Phani Nukala, ORNL
- Dora Yen-Nakafuji, LLNL
- Ellen Stechel, SNL

Hydrogen

- Molecular hydrogen (H_2) has tremendous promise as a potential future energy carrier, free of green house gases.
- Challenges remain in production, storage, and use.
  - Renewable generation.
  - On-board vehicle storage.
  - Platinum-free fuel cells are essential for mass market adoption.



Hydrogen: Priority Research Directions

- Rate processes in H_2 production, storage, & use.
  - New methods for treating kinetics and reactions.
  - New methods for determining reaction surfaces and predicting reaction pathways, coupled to kinetics.
  - Multiscale approaches to electronic-structure-based dynamics & atomistic approaches to large systems.
- Inverse materials and systems by design.
  - Novel optimization techniques tightly coupled with existing simulation tools to control catalysis, charge separation, spatial component arrangement…
- Synthesis of targeted material
  - Develop novel, scalable tools to calculate pathways and predict reactions in solution necessary for the fabrication of targeted materials.

Hydrogen: Priority Research Directions

- Linking models and scales – from atoms to systems
  - Cost prohibitive to simulate large systems with uniformly high levels of detail.
  - Develop novel hybrid or multiscale approaches for quantum simulation that combine approximations of different fidelity to compute quantum-level chemistry information.

Photovoltaics

- Sunlight is by far the largest of all potential carbon-neutral energy sources.
- The energy from sunlight striking the Earth in one hour exceeds annual global energy consumption.

PV Status in U.S.

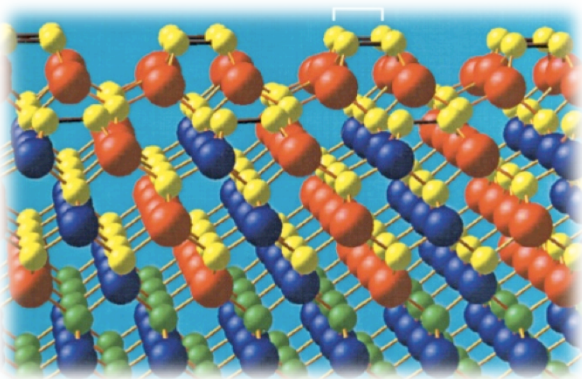
- 1,000 MW installed capacity
- Cost 18-23¢/kWh

Potential:

- 5-10 ¢/kWh by 2015
- Improve device efficiencies, reduce manufacturing costs.
- Focus on PV and thus did not address solar thermal electricity generation.

PV: Priority Research Directions

- Material properties prediction and design.
  - Improved scaling in density functional theory to model systems with +10^3 atoms.
  - Better methods for carrier transport and charge separation in organic PV.
  - New multiscale codes for predicting material properties that provide sufficient accuracy at variable scales.
  - Materials by design

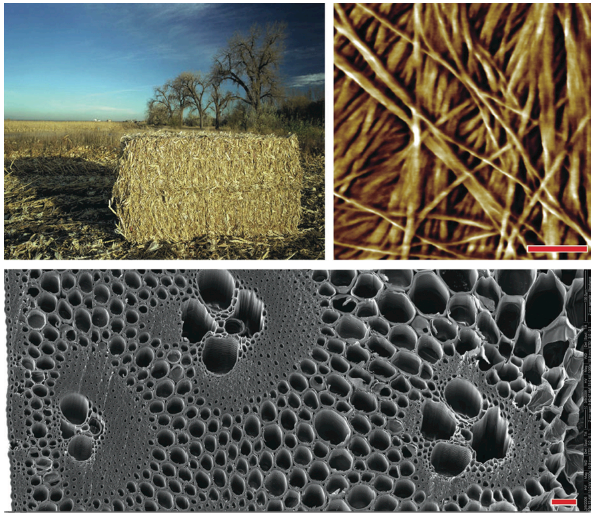


PV: Priority Research Directions

- Materials processing for industrial-scale synthesis and manufacture.
  - PV device manufacturing processes are largely developed through experimental trial and error.
  - Develop robust and scalable multi-scale, multi-physics models of materials processing.
  - Chemical vapor deposition (CVD) is used to produce thin film PV materials.
  - Numerical simulation of the CVD process will provide unique insights in the complex coupled chemistry, energy, multi-species transport, and flow patterns that determine the film characteristics.
  - Results: improved film uniformity, reduced costs and improved reliability.

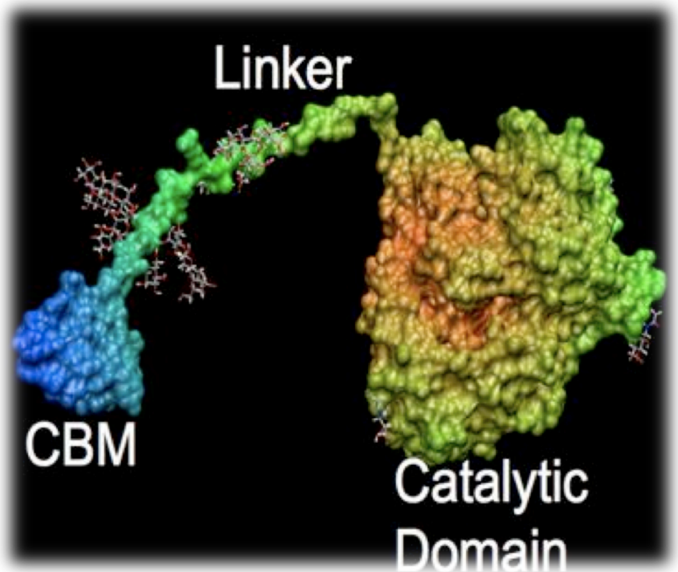
Biomass Conversion

- Cellulosic biomass offers the greatest source of renewable transportation fuel.
- A DOE and Dept. Agriculture study projected that it would be possible to displace 30% of current U.S. fuel use by 2030.
- Fundamental advances in our understanding of the structure/function relationships governing the activity of soluble enzymes on insoluble polymeric substrates is essential to make these fuels cost competitive.



Biomass: Priority Research Directions

- Biochemical conversion
  - Modeling the plant cell wall
    - Atomistic model with millions of atoms to capture the complex microfibril structure.
  - Modeling cell wall-degrading enzymes
    - Computational systems biology approaches for understanding metabolic pathways
    - Feature-rich codes such as CHARMM don't scale to large processor counts and scalable codes (AMBER, LAMMPS, NAMD) don't have the desired features.



Biomass: Priority Research Directions

- Thermochemical conversion
  - Develop integrated multiscale models to accurately simulate kinetics and thermodynamics covering pretreatment, pyrolysis, and gasification.
  - Simulate and optimize design of biomass conversion plants. This would replace the need to build numerous pilot scale facilities and traditional trial and error experimentation needed to bridge the gap between lab-scale and production.

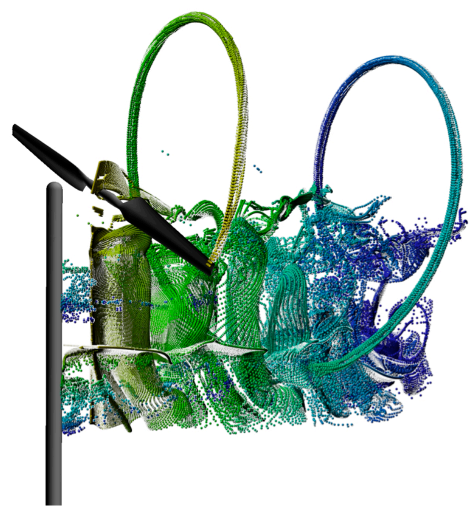
Wind

- NAS study, in the Midwest prairie states alone sufficient wind resources to supply 16x current U.S. electrical demand using existing technology.
- Presently at 2%, 2008 48% of new electrical supply from wind.
- DOE goal: 20% by 2030

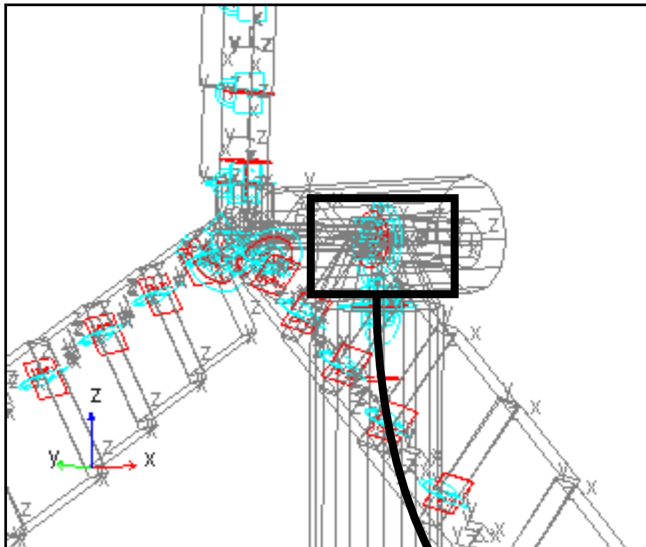
Wind: Aero-acoustics and Aero-elastics

- Developing codes to explore the complicated, unsteady, 3-D flow field is critical to cost-effective design and efficient operation.
  - Empirical methods inadequate, significant uncertainty.
  - Benefit from codes developed for rotorcraft and aerospace industry.
  - Unique flows: rapid direction changes, inflow turbulence, and flow transition & spatial scales from microns to a Km (wake extent).
  - However, need new large eddy simulation codes to account for flow separation, dynamic stall, blade loading, and broadband noise prediction.

- Current state-of-the-art tools have difficulty accurately predicting turbine rotor aerodynamics, even in ideal conditions found in a wind tunnel.

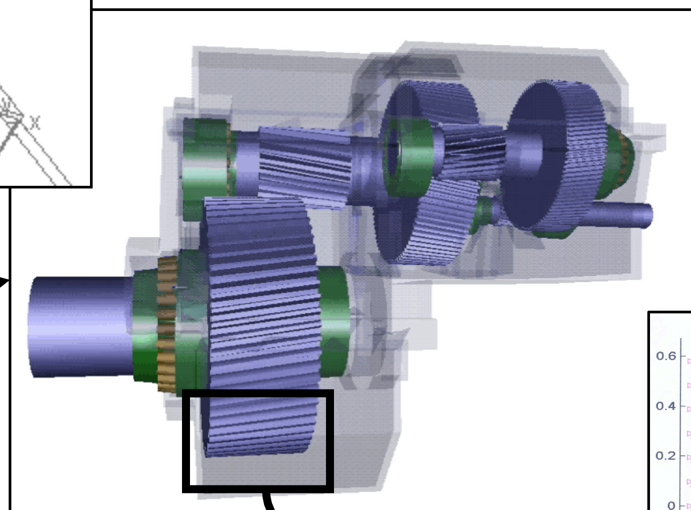


Wind: Integrated Gearbox Reliability



Gearbox

- Case flexure
- Shaft deflection
- Bearing dynamics

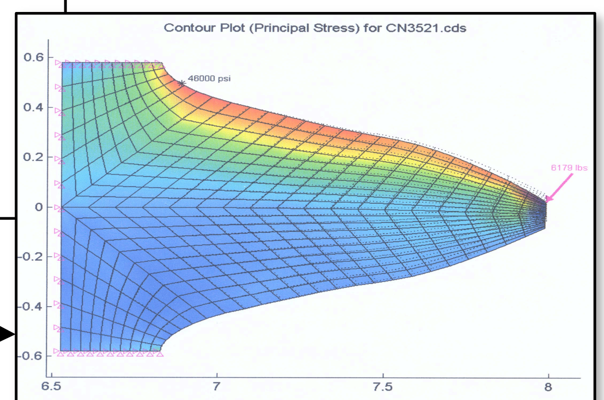


Gear teeth

- Material failure
- Surface tribology
- Lubricant rheology

Wind turbine

- Aeroelasticity
- Structural loads
- Power transmission



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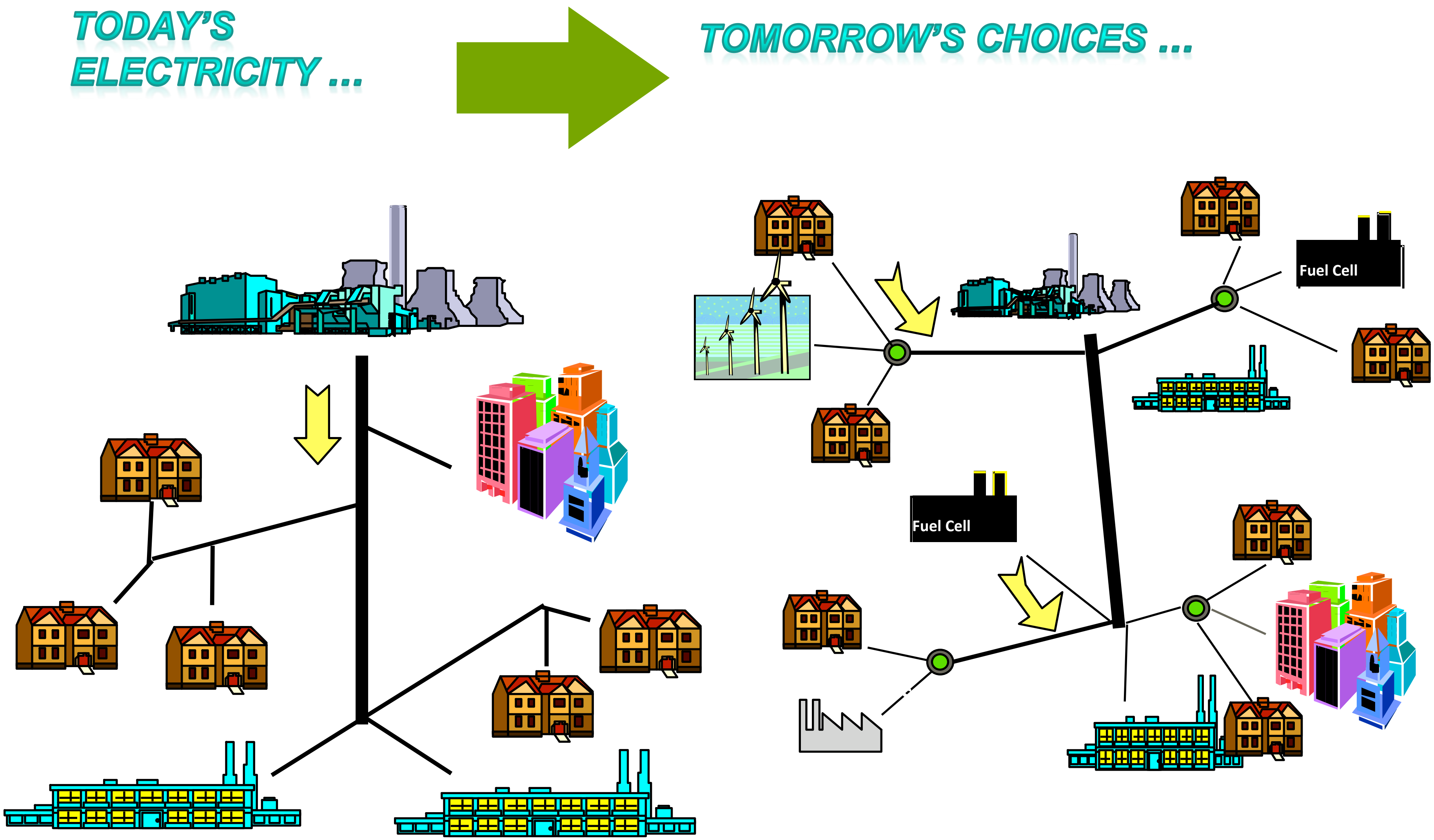
Grid Reliability



Grid Reliability: Priority Research Directions

- A national grid simulation capability could greatly improve current simulation methods. Must include:
  - Advanced contingency analysis
  - Multiple-physics effects,
  - System interdependencies,
  - Advanced control algorithms,
  - Improved model granularity, and
  - Multiple spatial and temporal scales

Grid Reliability: Priority Research Directions

- Flight simulator for the new grid
    - Scalable, real time interactive visualization
- Enhanced data streaming and analysis
- Predictive modeling with mixed digital and analog inputs
- Scalable nonlinear dynamics algorithms to describe coupled states
- Fast state estimation algorithms for real time control and operation
- Large scale application of game theory

Common Themes

- Rational design of materials, devices, and systems
- Multiscale models, from atoms to systems
- Multidisciplinary collaboration
- Additional computational resources

- In some instances simulation codes exist but they don't exploit multicore architectures or scale to large processor counts.
- Over the years ASCR has funded a significant body of work in advanced numerical libraries, adaptive and multiscale methods that can be applied to challenges of interest to EERE.

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From Science to Deployment: Renewable Energy

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
▪ Retrosynthetic approaches to high performance new materials ▪ Design of new materials capable of multi-electron storage per redox center ▪ Understand design criteria for electrolytes that enable higher voltages ▪ Tailoring nanoscale electrode architectures for optimal transport ▪ Novel chemistries for scavenging impurities and self-healing ▪ Generation of knowledge and computational and experimental tools to predict properties, performance evolution, and lifetime of materials	▪ Understand and predict interfacial charge transfer and multi-body effects ▪ Predict and control dynamics of phase transitions ▪ Control of chemistry and its dynamics at electrified interfaces ▪ Determining consequences of dimensionality ▪ Physicochemical consequences of nano-dimensions ▪ Fundamentals of solvation dynamics and ionic transport ▪ Revolutionary tools for *in situ* structural and dynamic studies over broad spatial / temporal regimes	• Evaluate and benchmark novel chemical and material systems • Define advanced electrochemical systems through advanced electrolyte modeling, anode screening and development, and electrochemical testing and diagnostics • Assemble and performance test electrical energy storage devices with respect to power fade, overcharge, deep discharge, charge rate, abuse tolerance, safety, lifetime, cost, etc.	▪ Demonstrate usage of energy storage systems in advanced vehicle applications with high power / energy density, long lifetime, appropriate charging time, deep discharge, reliability, safety and low cost. ▪ Deployment of high capacity storage for centralized and distributed power sources for power quality and load leveling ▪ Long shelf life storage devices for stand-by power ▪ Long-lived, environmentally friendly, recyclable portable energy storage for portable and stationary energy storage

Office of Science ASCR	Technology Offices EERE

U.S. Department of Energy
Energy Efficiency and Renewable Energy

From Science to Deployment: Challenge

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
▪ Retrosynthetic approaches to high performance new materials ▪ Design of new materials capable of multi-electron storage per redox center ▪ Understand design criteria for electrolytes that enable higher voltages ▪ Tailoring nanoscale electrode architectures for optimal transport ▪ Novel chemistries for scavenging impurities and self-healing ▪ Generation of knowledge and computational and experimental tools to predict properties, performance evolution, and lifetime of materials	▪ Understand and predict interfacial charge transfer and multi-body effects ▪ Predict and control dynamics of phase transitions ▪ Control of chemistry and its dynamics at electrified interfaces ▪ Determining consequences of dimensionality ▪ Physicochemical consequences of nano-dimensions ▪ Fundamentals of solvation dynamics and ionic transport ▪ Revolutionary tools for *in situ* structural and dynamic studies over broad spatial / temporal regimes	• Evaluate and benchmark novel chemical and material systems • Define advanced electrochemical systems through advanced electrolyte modeling, anode screening and development, and electrochemical testing and diagnostics • Assemble and performance test electrical energy storage devices with respect to power fade, overcharge, deep discharge, charge rate, abuse tolerance, safety, lifetime, cost, etc.	▪ Demonstrate usage of energy storage systems in advanced vehicle applications with high power / energy density, long lifetime, appropriate charging time, deep discharge, reliability, safety and low cost. ▪ Deployment of high capacity storage for centralized and distributed power sources for power quality and load leveling ▪ Long shelf life storage devices for stand-by power ▪ Long-lived, environmentally friendly, recyclable portable energy storage for portable and stationary energy storage

Office of Science ASCR

Technology Offices EERE

Final Thoughts

- Focused working groups for each area with representation from both SC/ASCR and EE to review the broad array of solicitations (ARPA-e, ARRA, EFRCs, SciDAC, ...)
- Identify gaps and prioritize areas of mutual interest to the two offices.
- Develop a SciDAC-like program around renewable energy and high performance computing where applied math, computational science, advanced algorithms, multiscale methods and petascale computing are applied to EERE priority areas.

Acknowledgments

- Gary Johnson, ASCR
- Sam Baldwin, EERE
- Co-chairs:
  - Greg Bothun, Oregon
  - Steve Picataggio, Synthetic Genomics, Inc
- Organizing Committee
- ORISE for flawless conference logistics

- Workshop Report on ASCR web site:

http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/CRNAREWorkshopReport.pdf