Alternative Energy R&D at Los Alamos

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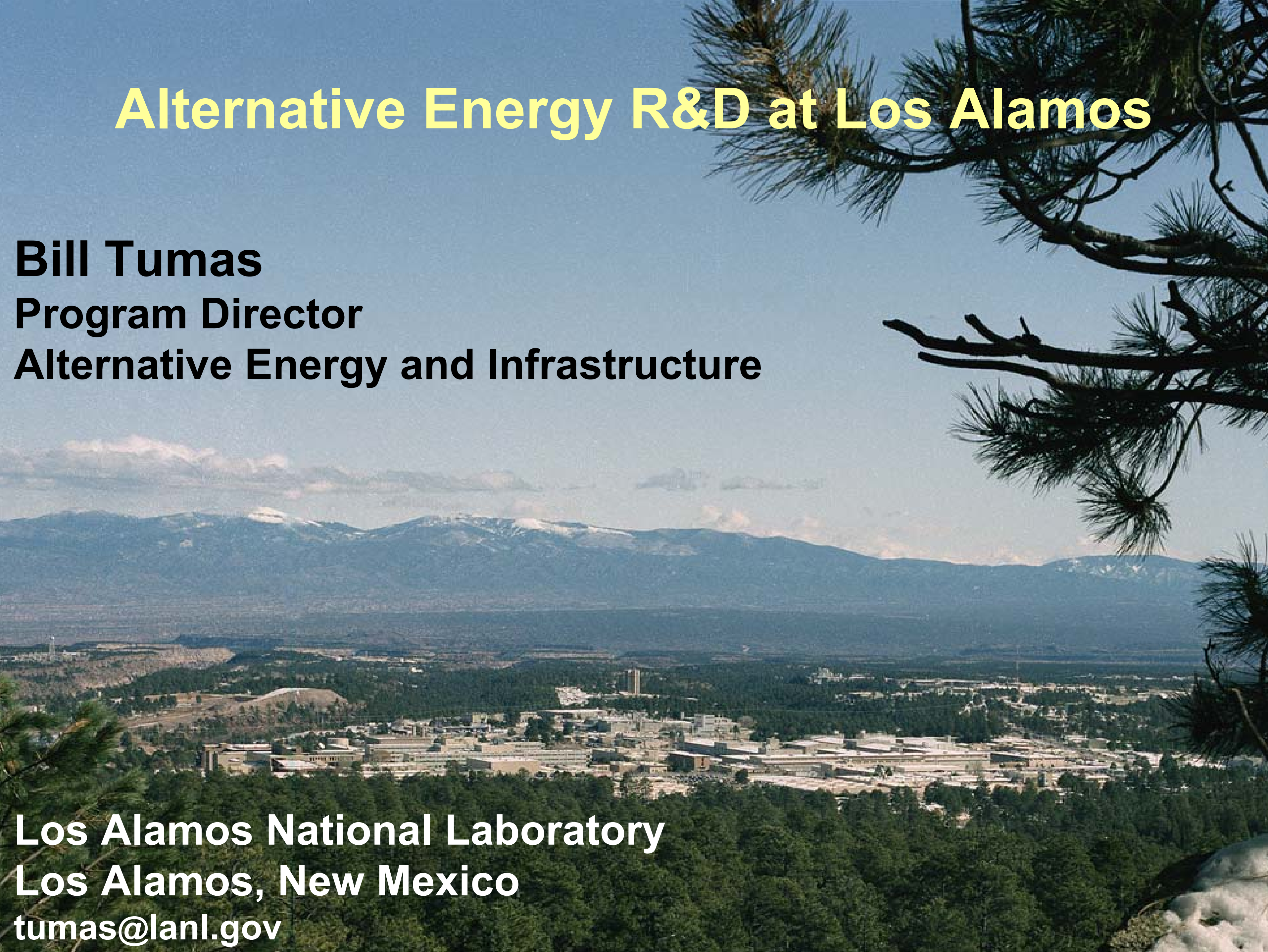

Los Alamos National Laboratory

- Our mission as a DOE national security science laboratory is to
  - Ensure the safety, security, and reliability of the U.S. nuclear deterrent
  - Reduce global threats
  - Solve other emerging national security challenges

✧ 8891 staff; 389 postdocs, 1200 students
✧ 38 square miles
✧ 54 major facilities
✧ 8.5 million square feet of space
✧ 17 nuclear facilities
✧ 150 miles of roads

Energy: The Global Need and Impact

- The impacts of energy and its use are significant
  - Economic growth and sustainability
  - Energy security: national and international
  - Environmental
- The situation and the future global need are serious
  - Additional 13-15 TW (Carbon-neutral)
- The scale is enormous; A degree of urgency is justified
- Current technology alone will not get us there
- Disruptive technologies and new materials are required for clean, sustainable, carbon-neutral energy generation, transmission, storage and use
  - Costs reduction
  - Performance and durability
  - Wide-scale application

Stationary Power **Transportation**

"Energy is the single most important challenge facing humanity today."
"We will need revolutionary breakthroughs to even get close."

- Richard Smalley, Nobel Laureate, 2004 Congressional Testimony

Why Los Alamos Conducts Energy Security R&D

- Energy security is national security
- Critical mass of scientific disciplines, facilities and equipment coupled with a collaborative culture
- Capabilities and expertise needed overcome significant technical barriers for alternative energy overlap strongly with other national security missions
- User Facilities
  - Center for Integrated Nanotechnologies
  - Los Alamos Neutron Scattering Center
  - National High Magnetic Field Laboratory
- Extensive partnering base
- Los Alamos programs have a history of strong performance and synergy with other national security missions

Theory, Computation, Modeling ⟷ Experiment/Testing

Los Alamos National Laboratory
Programs in Alternative Energy

- Hydrogen and Fuel Cells for Transportation
- Solar Energy Conversion
- Energy Efficiency
  - Solid state lighting
  - Combustion modeling
- High Temperature Superconductivity for Electricity Transmission
- Infrastructure and Grid Modeling

Los Alamos R&D for Hydrogen/Fuel Cells

- R&D for Polymer Electrolyte Membrane Fuel Cells
  - Cost
  - Durability
  - Performance
- Next Generation Fuel Cell R&D
  - New concepts, materials, theory/modeling for fuel cell membranes
  - Non-precious metal catalysts to replace platinum
- DOE Chemical Hydrogen Storage Center of Excellence
- International Codes and Standards
- Other programs
  - Clathrate science and technology
  - Biomass conversion to hydrogen
  - Hydrogen technologies for fusion energy programs
  - Advanced materials and concepts for hydrogen production and separation
  - Environmental effects of hydrogen

LANL: A Long History in Hydrogen/Fuel Cell R&D

Institute for Hydrogen & Fuel Cell Research

Hydrogen Storage Center Awarded

Objective Force Warrior Power System (Ball)

FreedomCAR & Hydrogen Fuel Initiatives

PNGV Medal, Energy 100 & Energy @ 23 Awards

2000

FES Tritium Facility

World's First Gasoline -Direct-to-Electricity Demo w/ ADL& Plug Power

GM Corporate FC Center

First Complete Methanol -Direct-to-Electricity Power System

Government/Industry Partnership for a New Generation of Vehicles (PNGV)

General Motors / LANL

CO Tolerance Established via Anode Air Bleed

1990

Staged Preferential Oxidation Developed w/ DelcoRemy

H_2/O_2 NASA tests w/ Ballard

Manufacturable Thin Film Electrodes; Pt ⇓ 20X

1980

1st DOE funded Fuel Cells for Transportation Project

2nd Oil Embargo

CH_2/O_2 Fuel Cell Golf Cart Demo

LH_2 ICE Buick Demonstration

1st Oil Embargo

1970

Hamilton Standard SPE Electrolyzers for O_2 Production on Nuclear Submarines

General Electric develops SPE fuel cell for NASA Gemini Missions

Nuclear Rocket Program (H_2 Fuel)

1960

Los Alamos defense programs develop science and engineering base for hydrogen isotope purification, storage, and materials interactions

Defense Programs

1950

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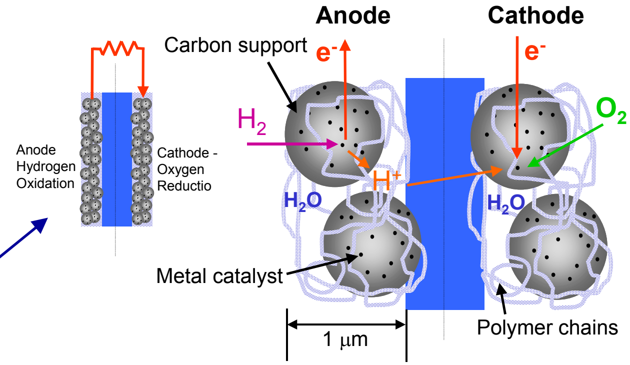
Fuel Cell R&D at Los Alamos

- One of longest running non-weapons programs at LANL (since 1977)
- Primarily polymer electrolyte membrane (PEM) technology
- Cost and durability are biggest barriers to commercialization
- Program focus is obtaining fundamental understanding to enable *"knowledge-based innovation,"* and subsequent materials and process development
- Non-precious metal catalysts, new membranes and materials

- Fuel Cells directly convert chemical energy of fuel to electricity, with byproducts of heat and water
- Scalable technology decouples power conversion and energy storage (advantage over batteries)

LANL Enabling Breakthrough Thin Film Eledctrode



An electrochemically active reaction site must have reactant access to catalyst, available electronic and ionic conduction paths, and manage water

US Patents #4,876,115, #5,211,984 and #5,234,777

Single cells are stacked to get desired voltage and the in-plane area scaled to get desired current

The Institute for Hydrogen and Fuel Cell Research

NEDO – AIST – LANL Workshop

August 28, 2006
Santa Fe, NM

Fuel Cell Durability

Hydrogen Storage

Scientific Aspects of Polymer Electrolyte Fuel Cell Durability and Degradation

Rod L. Borup, Jeremy Meyers, Bryan Pivovar, Yu Seung Kim, Nancy Garland, Deborah Meyers, Rangachary Mukundan, Mahlon Wilson, Fernando Garzon, David Wood, Piotr Zelenay, Karren More, Tom Zawodzinski, James Boncella, James E. McGrath, Minoru Inaba, Kenji Miyatake, Michio Hori, Kenichiro Ota, Zempachi Ogumi, Seizo Miyata, Atsushi Nishikata, Zyun Siroma, Yoshiharu Uchimoto, Kazuaki Yasuda

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The Institute for Hydrogen and Fuel Cell Research

Chemical Hydrogen Storage Center of Excellence

A coordinated approach to identify, research, develop and validate advanced on-board chemical hydrogen storage systems to overcome technical barriers and meet 2010 DOE system goals with the potential to meet to 2015 goals

- Develop materials, catalysts and new concepts to control thermochemistry and reaction pathways
- Assess concepts and systems using engineering analysis and studies
- Develop life cycle inventory and demonstrate a 1 kg storage system

- More efficient borate-to-borohydride (B-OH to B-H) regeneration
- Alternative boron chemistry to avoid thermodynamic sinks using polyhedral boranes (B_xH_y) or amine-boranes
- Concepts using coupled endo/exothermic reactions, nanomaterials, heteroatom substitution for thermodynamic control

Chemical Hydrogen Storage System

- **Hydrogen stored in chemical bonds and released by chemical reaction**
- **Material undergoes an on-board reaction to release hydrogen and generate spent storage material**
  - Energy density (capacity)
  - Hydrogen release rates
  - Heat management
- **Regeneration of spent storage material**
  - Likely will need to be off-board vehicle
  - Energy efficiency of regeneration is key
- **Liquid or solid fuel infrastructure possible**
  - Potential for no H_2 handling by consumer
  - Potential for no need for hydrogen delivery or fueling station

Hydrogen could only appear transiently at a fuel cell anode when needed

Ammonia Borane for Hydrogen Storage

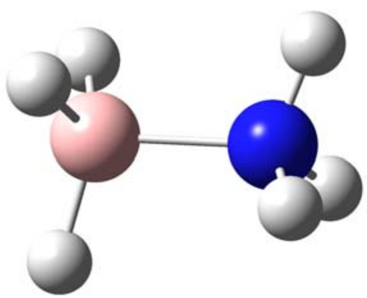
$$NH_4BH_4 \longrightarrow BN + 4\ H_2 \qquad (24.5\%\ H_2)$$

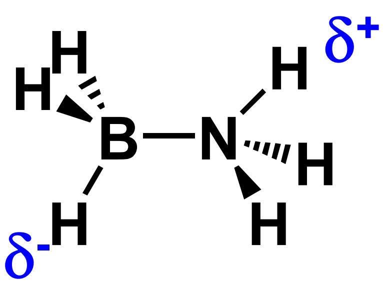
$$NH_3BH_3 \longrightarrow BN + 3\ H_2 \qquad (19.6\%\ H_2)$$

$$B_3N_3H_{12} \longrightarrow 3\ BN + 6\ H_2 \qquad (14\%\ H_2)$$

$$B_3N_3H_6 \longrightarrow 3\ BN + 3\ H_2 \qquad (7.5\%\ H_2)$$

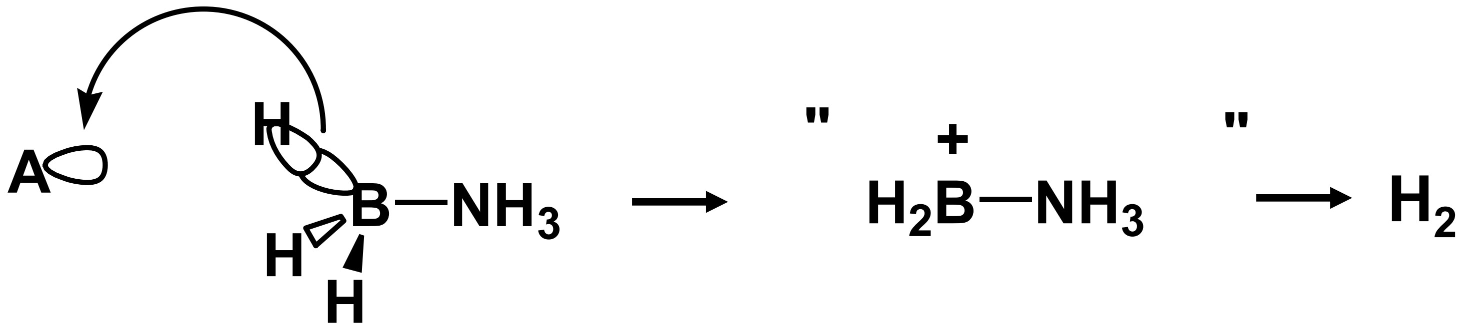
$$NH_3B_3H_7 \longrightarrow B_3N + 5\ H_2 \qquad (17.8\%\ H_2)$$

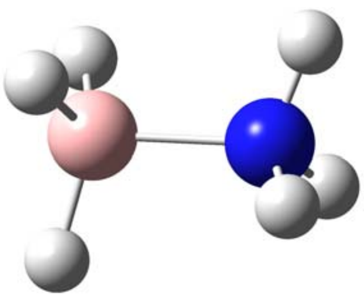




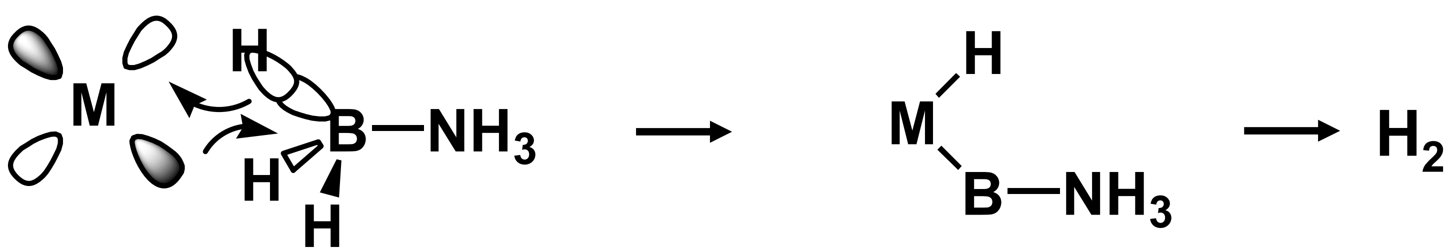
Catalytic Activation of Ammonia Borane

- Acid Catalysis (Lewis or Bronsted Acid)



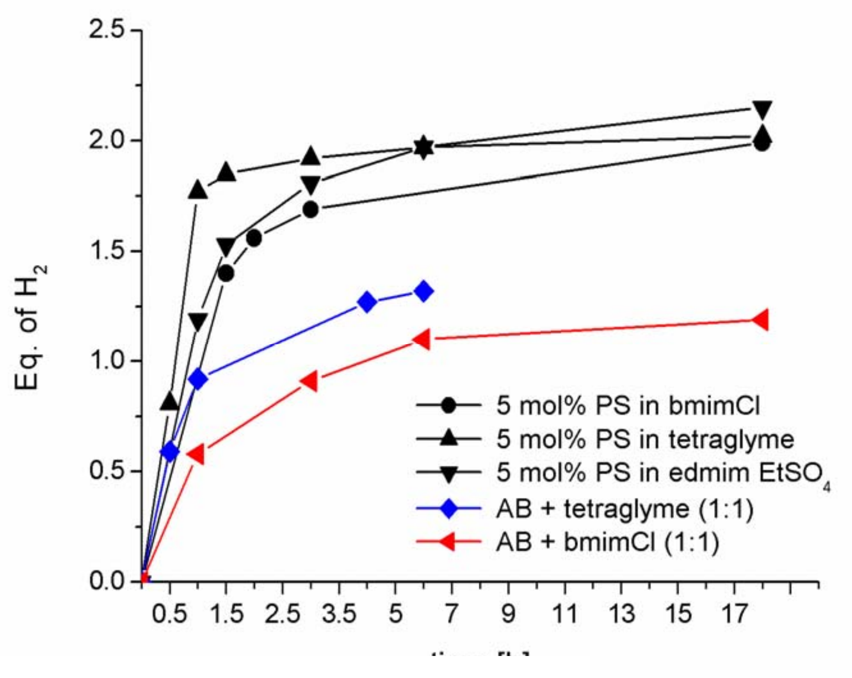


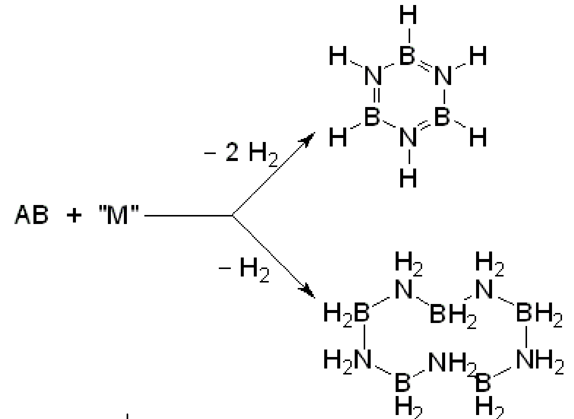
- Metal Catalysis

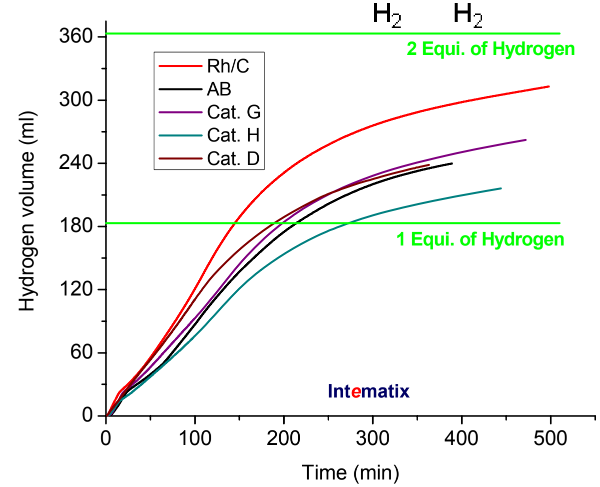


Mechanistic Understanding has led to Higher Rates

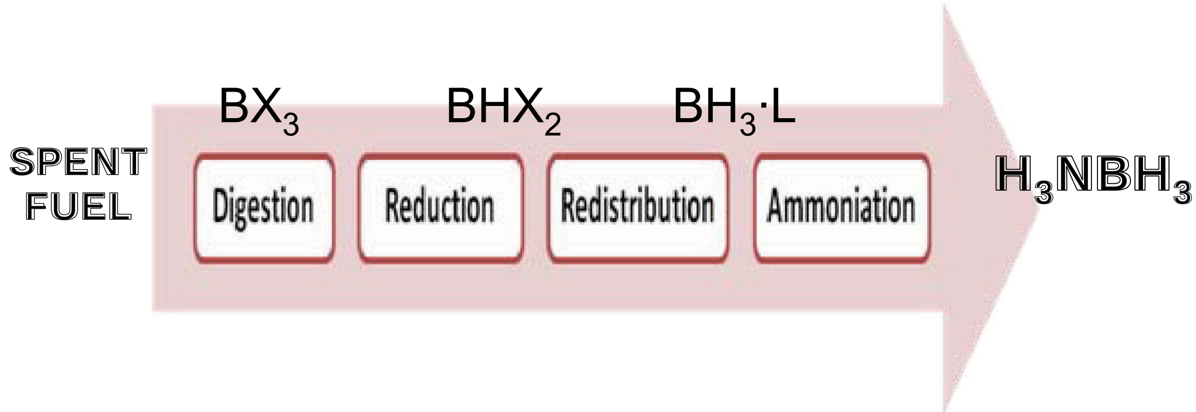
- Penn: Anionic mechanism in ionic liquids
- LANL: Metal catalyzed mechanisms explain selectivity/capacities, and guide catalyst design







Ammonia Borane Regeneration



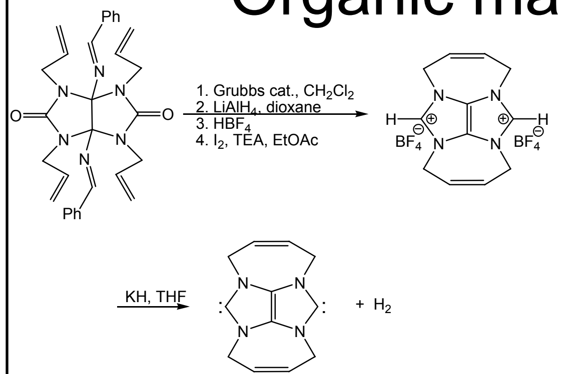
- **Regeneration of spent fuel demonstrated by two pathways**
  - **Spent fuel → BBr_3 → AB**
  - **Spent fuel → $B\text{-}(SR)_n$ → AB**

- **Capture of residual B-H with other ligands**
- **Energy efficiencies at DOE targets (60%) possible**
- **“One-pot” reduction/ammoniation demonstrated**

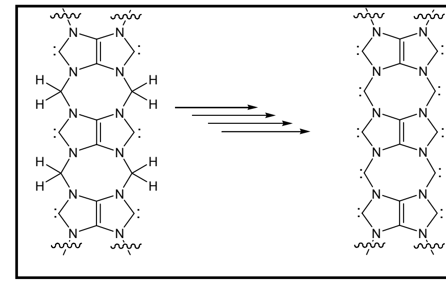
Additional Concepts for Hydrogen Storage under Investigation

- Coupled reactions
  - –Developed concepts with > 1 H/carbon atom
  - –Implemented 25 well reactor for catalyst screening and quantification (Center capability)
- Organic materials
  - –Demonstrated 1,1-elimination of hydrogen to make carbene
  - –Currently 2 wt% of possible 9-11 wt%
  - –Demonstrated hydrolysis of carbenes via 1,5-elimination to diimidazolium rings
- Nanomaterials
  - –Demonstrated hydrogen release from Si nanoparticles (TG/MS)
  - –Not reversible
- IPHE - new derivatives of AB w/ potential reversibility

Organic materials



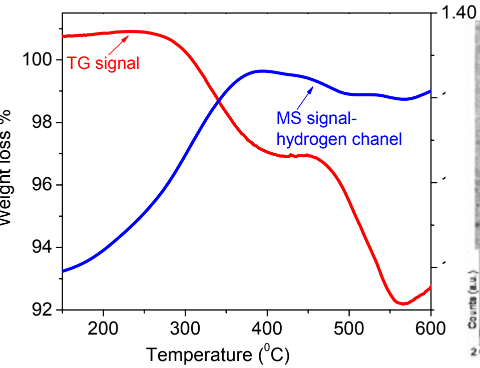
ST 27



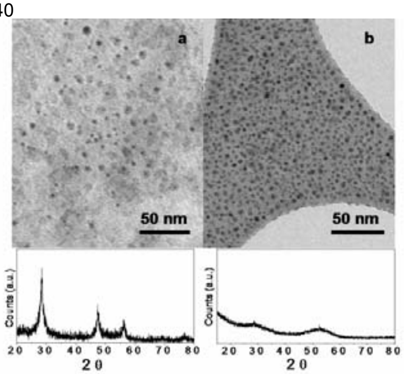
Prepared precursor to 11% polymer

THE UNIVERSITY OF ALABAMA

Nanomaterials



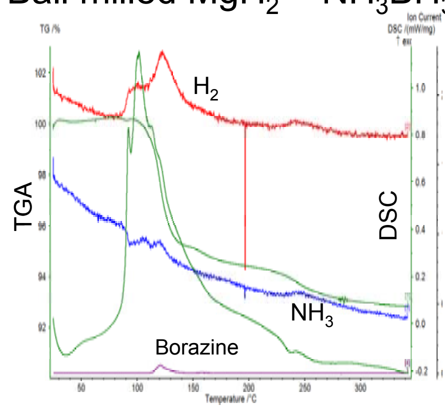
TG/MS showing ~3 wt % H_2 between 200-350°C.



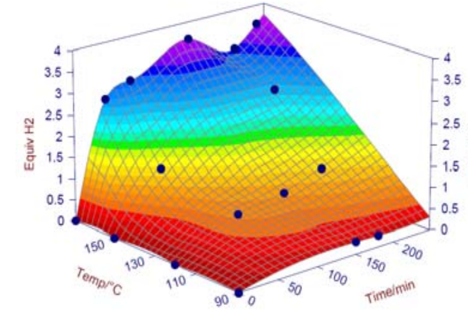
~5 nm diameter Si nanoparticles

IPHE materials

Ball milled MgH_2 + NH_3BH_3



New LANL compound



7.2 % H_2 quantified by GC

Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

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International Partnership for the Hydrogen Economy

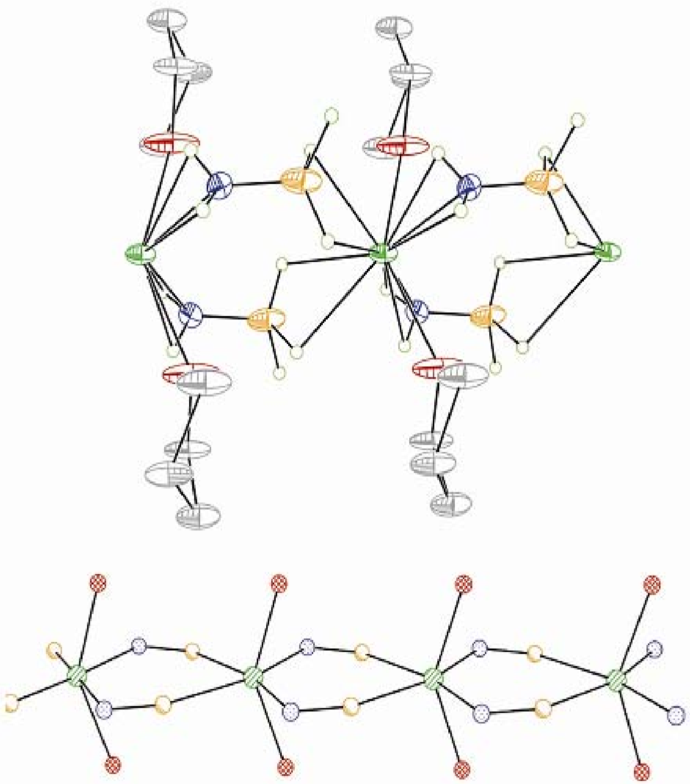
New Derivatives of Ammonia Borane (AB)

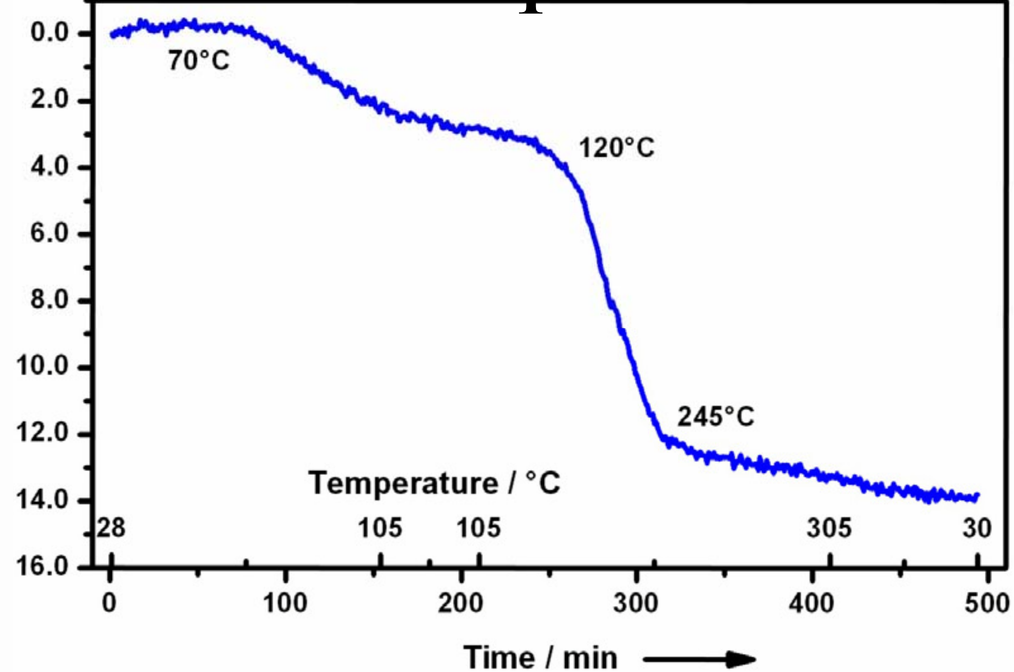
$$CaH_2 + 2\ NH_3BH_3 \longrightarrow Ca(THF)_2(NH_2BH_3)_2 + 2H_2$$

2

$$Ca(THF)_2(NH_2BH_3)_2 \longrightarrow Ca(NH_2BH_3)_2 + 2THF$$

1





H.V. K. Diyabalanage, R.PShrestha, T.A Semelsberger, B.L. Scott, M.E. Bowden, B. L. Davis and A K. Burrell
Angewandte Chemie in press

Los Alamos Neutron Scattering Center (LANSCE) Application to Hydrogen Storage Materials

- **Neutron scattering measurements are useful for determining both crystal structure and local structure.**
- **Local structure can be determined through analysis of the total scattering profile, even of amorphous, glassy, or liquid materials.**
- **Because neutrons are scattered strongly by H, neutron scattering experiments on hydrogen storage materials must be highly deuterated (>99% D) to avoid large background scattering from H.**
- **Using various pair distribution function analysis methods, location of deuterium atoms may be determined as a function of temperature and/or pressure.**

NPDF at LANSCE

Neutron Powder DifFractometer

- high resolution powder diffractometer
- located 32m from the spallation neutron target.
- large detector coverage in backscattering and is mainly used for PDF studies of disordered materials, liquids, and high resolution neutron crystallography.
- Sample environments: ranging from 10 to 1000K with a capability for controlling atmosphere and pressure.

AIST/LANL Collaboration

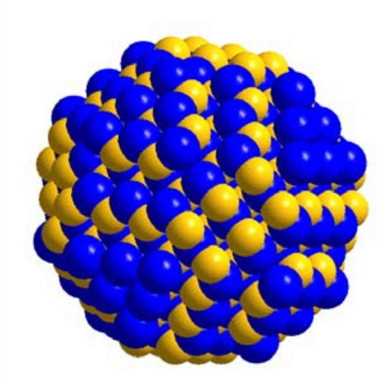
Center for Integrated Nanotechnologies

Sandia National Laboratories • Los Alamos National Laboratory

- Highly collaborative U.S. Dept. of Energy User Facility
- Focused on nanoscience integration
- Access to tools and expertise
- Pre-competitive and proprietary research options

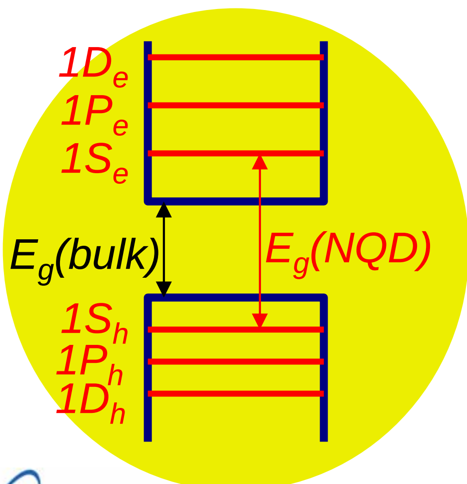
"One scientific community focused on nanoscience integration"

Nanocrystalline Quantum Dots

Molecules →  d = 2-10 nm → Bulk Material

NQD

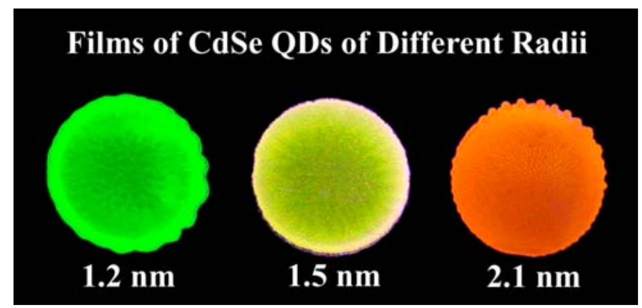
Discrete atomic-like states



$$E_g(NQD) = E_g(bulk) + \frac{\hbar^2 \pi^2}{2 m_{eh} R^2}$$

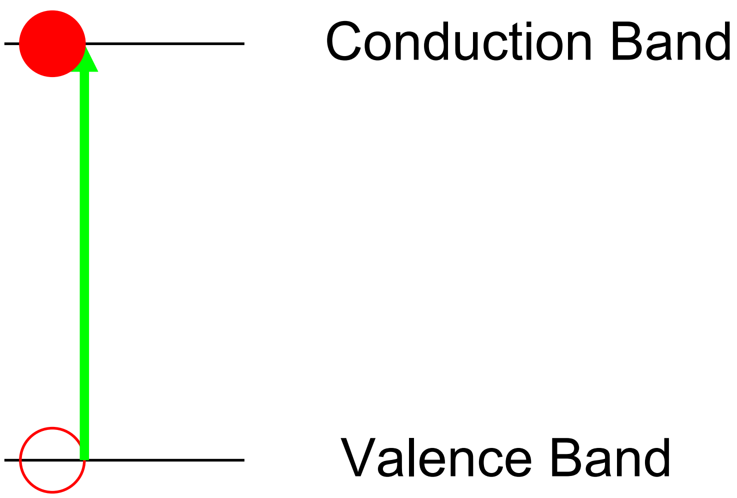
↑ *quantum confinement term*

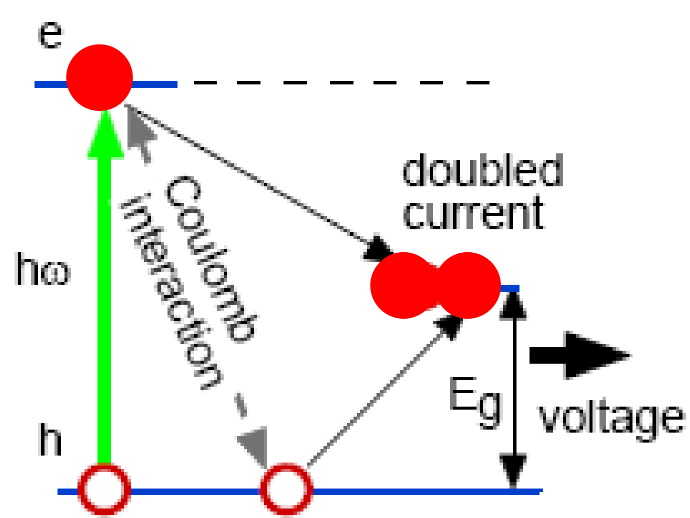
Tunable emission color



Carrier Multiplication in Quantum Dots

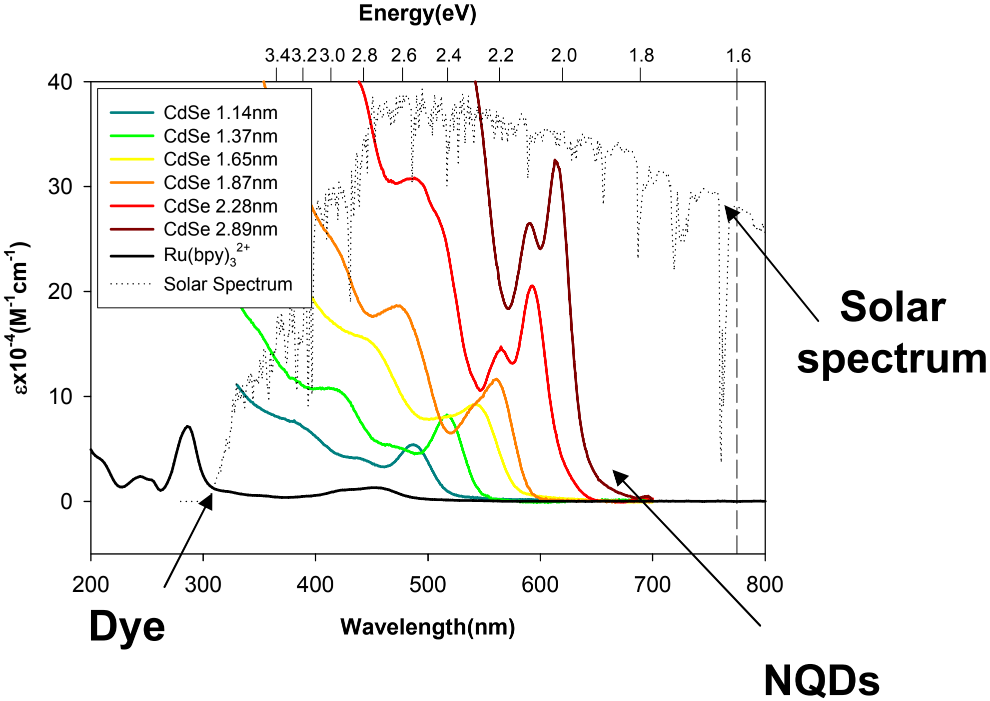
- **Nanoscale particles (quantum dots) exhibit different physics that the bulk materials**
- **LANL discovery that quantum dots can give multiple electrons for one photon**
- **Could significantly increase the efficiency of photovoltaic devices**





Schaller, Klimov *Phys. Rev. Lett.* **92,** 186601 (2004)

Generation of Multiple e-h Pairs by Single Photons

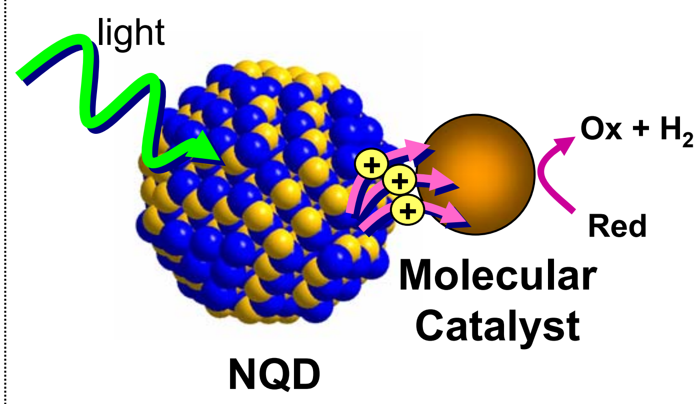


- *High absorptivities*
- *Easily tunable*
- *Increased efficiency from carrier multiplication*
- *Up to 7 electrons/photon for PbSe*

R. D. Schaller, M. Sykora, J. M. Pietryga, V. I. Klimov, *Nano Lett.* **6**, 123118 (2006)

Multifunctional Materials
Photocatalysis: Generating Solar Fuels

- Quantum Dots can convert solar light into chemical energy
- When coupled with a molecular catalyst this energy can be used to drive chemical reactions
- As a result of carrier multiplication effect improvement in efficiency of chemical reactions could be achieved



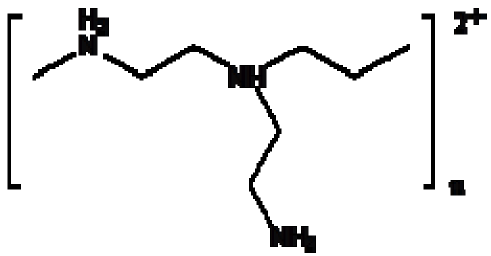
Hydrogen Production by Solar Water Splitting:

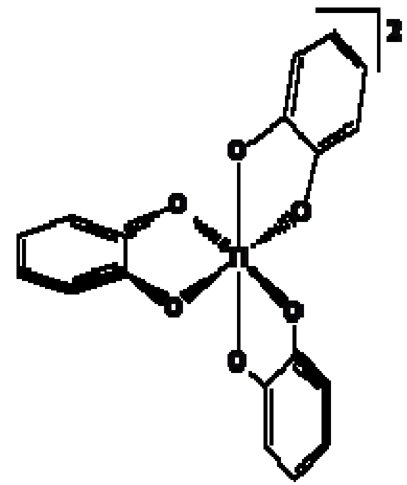
$$\text{Photoanode:}\quad 2H_2O \xrightarrow{h\nu} O_2 + 4H^+ + 4e^-$$
$$\text{Cathode:}\quad 4H^+ + 4e^- \rightarrow 2H_2$$
$$\text{Net:}\quad 2H_2O \rightarrow O_2 + 2H_2$$

4-electron process could be accomplished by absorption of a single, high energy photon through carrier multiplication

Thin Film Synthesis: Polymer-Assisted Deposition (PAD)

- Aqueous solution of metal precursor and polymer are deposited on a surface on then thermally treated
- Enhanced processability
- Polymer binding of metal precursor
  - control stoichiometry
  - control stability
  - control dopants

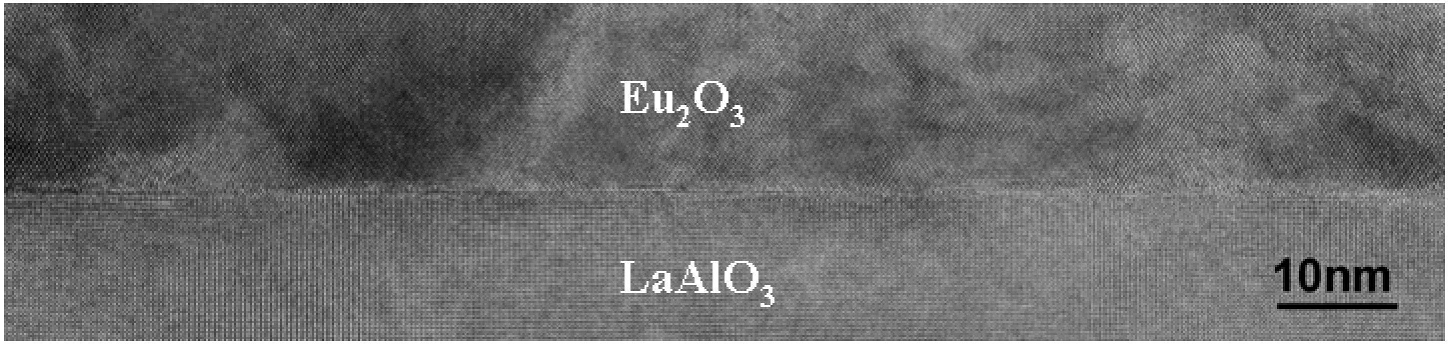


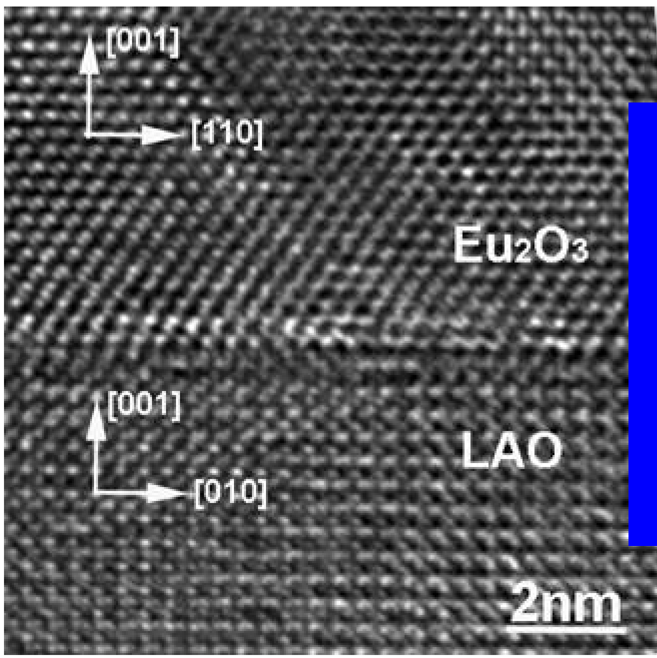


Final film (microstructure and physical properties) can be manipulated.
Access to metal systems previously to difficult to consider

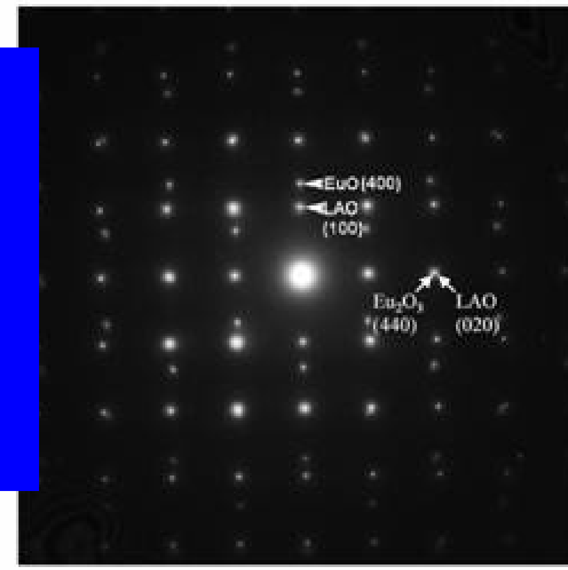
Burrell, McCleskey, Jia et al.

Example: Epitaxial Metal-Oxide Films





- High crystallinity Eu_2O_3 film on $LaAlO_3$ by PAD.
- Sharp interface between the substrate and the film.
- No voids and 2nd phases detectable



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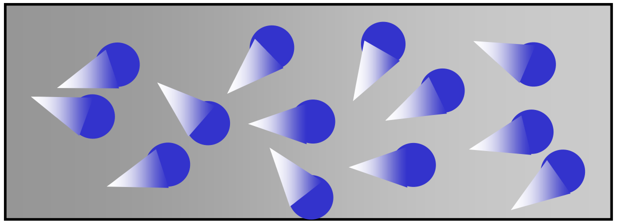
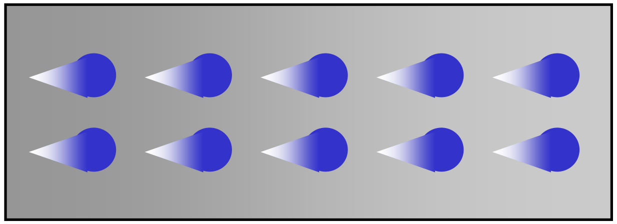
Operated by Los Alamos National Security, LLC for DOE/NNSA

Metal oxides, sulfides and nitrides

Superconductors for Electricity Transmission: Electricity Flow without Loss of Energy



Ordinary conductor: electrons moving at random lose energy in collisions, generating heat.



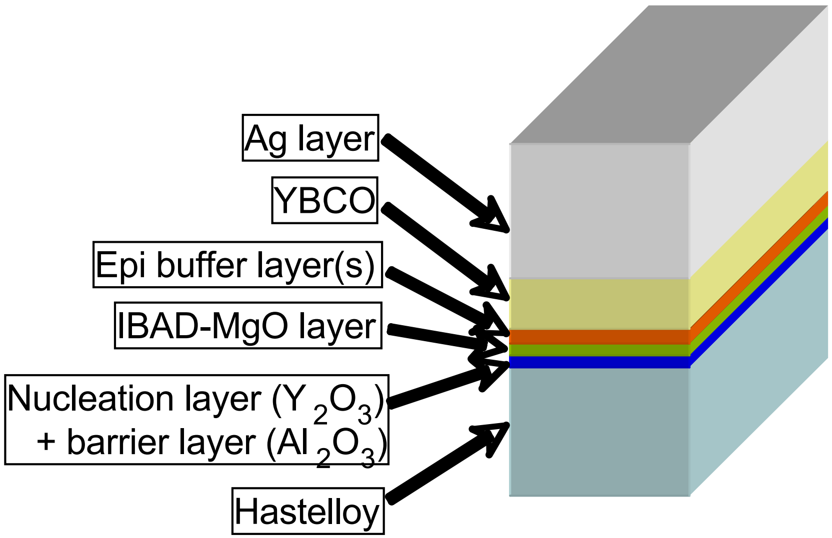
Superconductor: electrons moving in pairs don't collide, generating no heat and losing no energy!

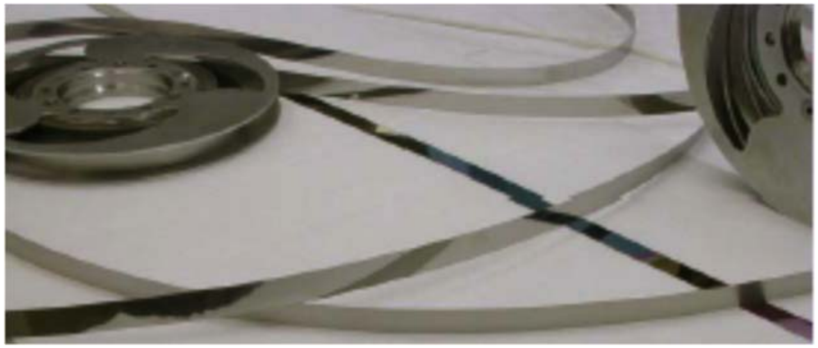
- **High Temperature Superconducting (HTS) Wires**
  - **No electrical resistance (cooled with liquid nitrogen)**
  - **More powerful, efficient, smaller, lighter**
  - **Increased energy infrastructure security**
  - **Congestion corridors**

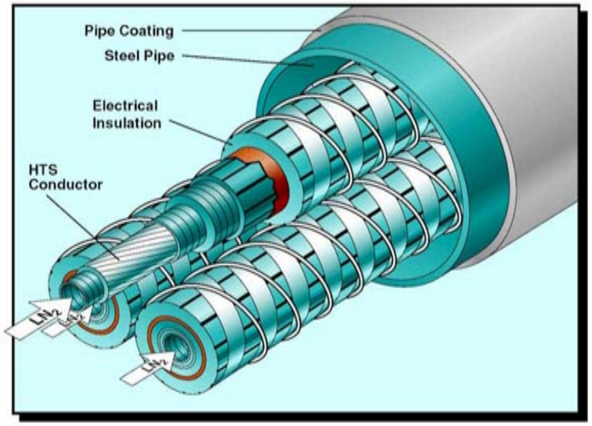
Compliments of ASC

Superconductivity Technology Center (STC)

- ***Energy efficient superconductor technologies in collaboration with industry and universities***





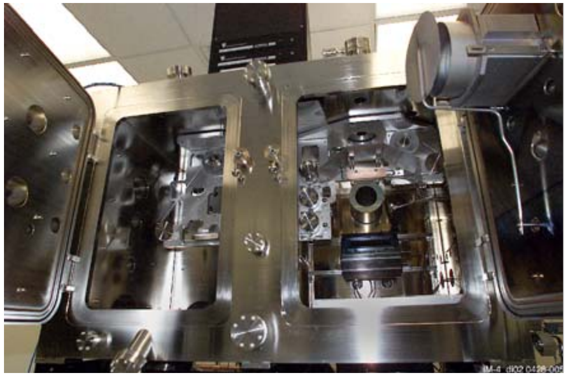


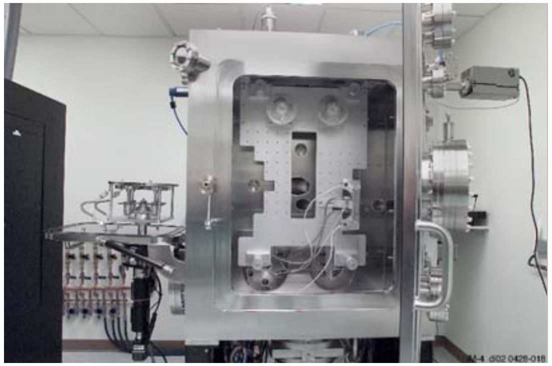
Capabilities: Los Alamos Research Park

Research Park

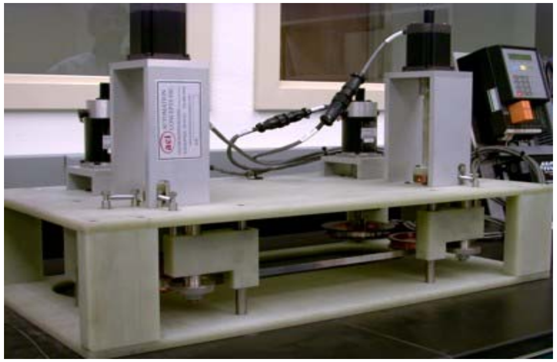
Tape Polish

IBAD Film





HTS Film

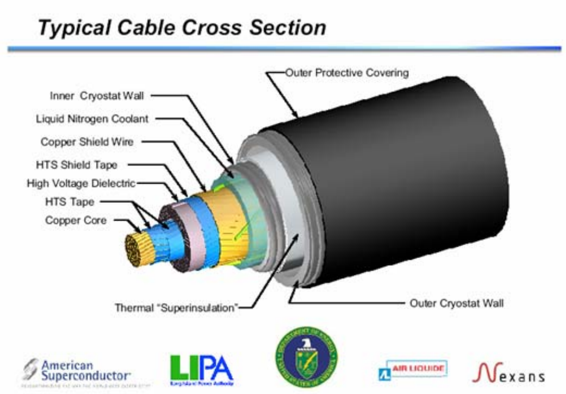


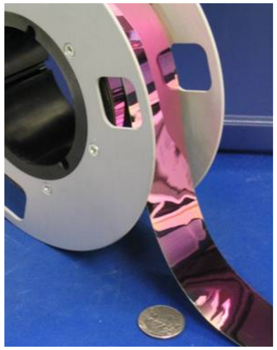
Tape Characterization

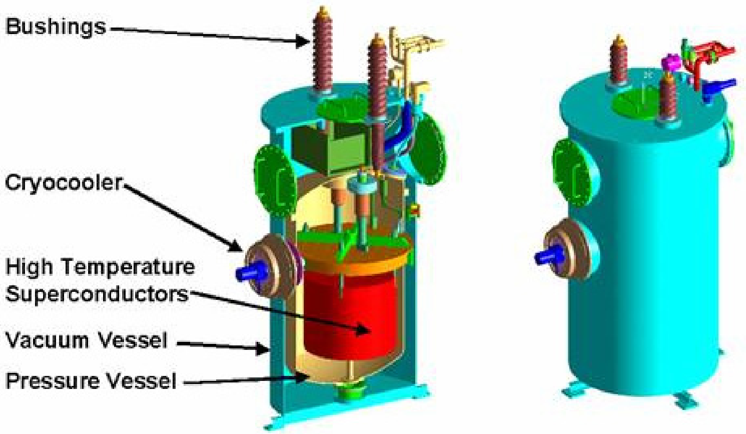
Power Applications (HTS Motors, Cables, etc.)

HTS Power Applications

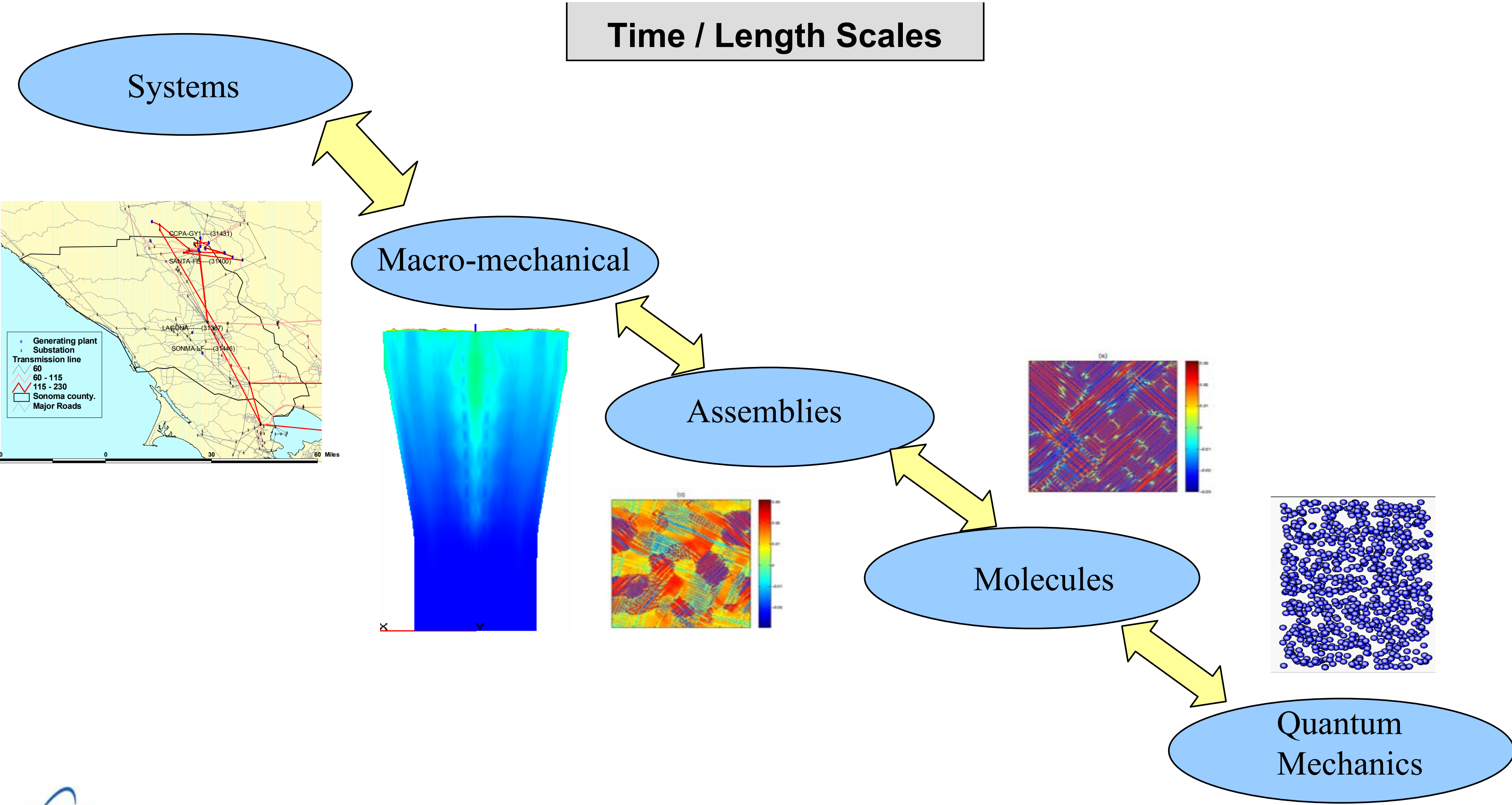
- **Underground Power Transmission Cables**
  - Can carry 3-5 times the current of a copper cable in the same duct
  - Environmentally safer – no oil to leak, magnetic field contained
- **Transformers**
  - Much smaller (X2) and lighter (X4) making transportation and siting in urban environments (close to load) easier
  - Environmentally safer (no oil, fire hazard much reduced)
- **Fault Current Limiters**
  - Limits current to protect grid components during a fault (short circuit)







Multiscale Theory, Modeling and Simulation



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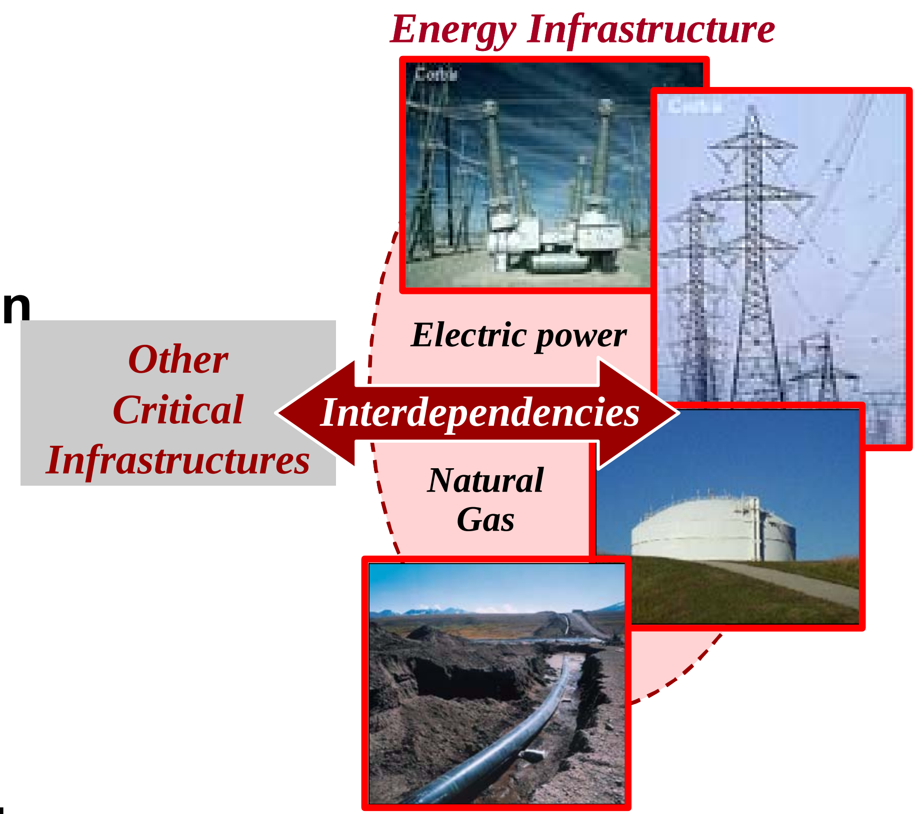
Energy Infrastructure Modeling and Simulation

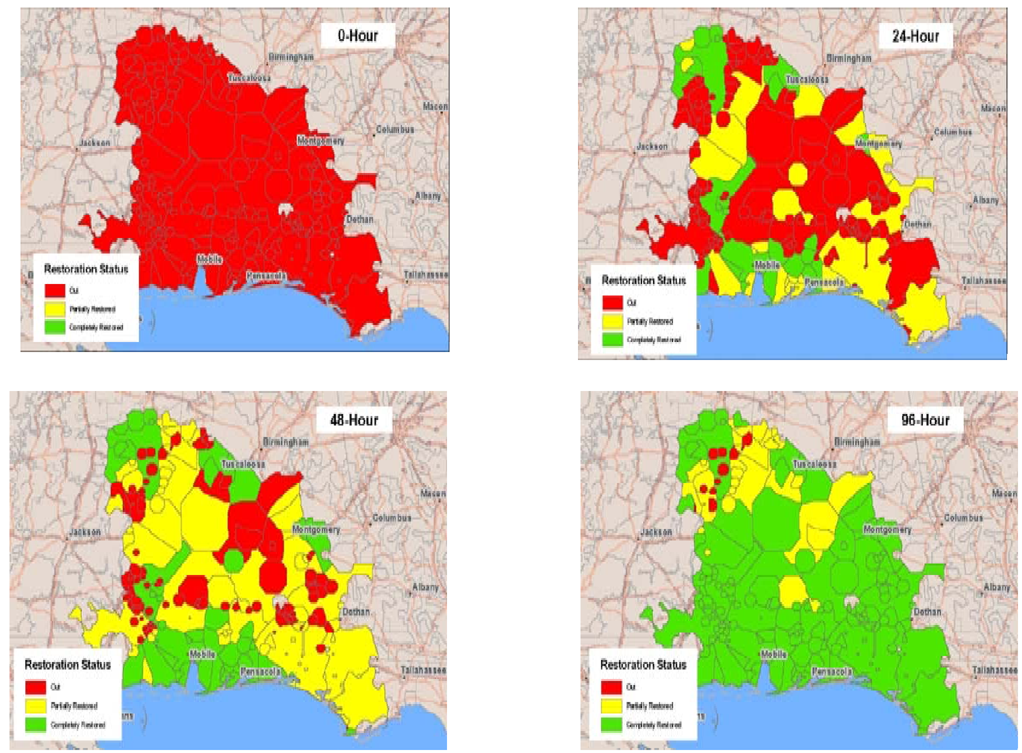
- **National Infrastructure Simulation and Analysis Center (NISAC)**
- **LANL/Sandia partnership**
- **Advanced modeling and simulation capabilities for the analysis of critical infrastructures, interdependencies, and complexities**
- **Address the nation's potential vulnerabilities and the consequence of disruption among our critical infrastructures.**



Electric Power Grid Modeling

- ***Impacts of Deregulation and Mergers***
- ***A National Electric Power Model***
- ***Earthquake Impact on Electric Power***
- ***Restoration of Electric Power after Hurricanes***
- ***Long-Term Climate Change Impact on Energy Security***

Restoration of electrical service after Hurricane Dennis



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Summary

- **Work in alternative energy is synergistic with other national security work**
  - **capabilities, facilities and scientific challenges**
- **Significant developments have been made, but innovation is required to lower costs and (in some cases) increase durability for widespread application**
- **Los Alamos historical strengths and accomplishments align well with needed advances**
  - **An integrated, multidisciplinary approach**
  - **A complete look at the problem**
    - **From fundamental science to applied techniques**
    - **Theory, modeling, simulation, experiment**
- **Collaboration and alliances are needed**
  - **No one institution or country can do it alone**

August 14, 2006
Los Alamos National Laboratory

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- **Fuel Cells**
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  - Ben Davis, John Gordon
  - Chemical Hydrogen Storage Center of Excellence Partners
    - L. Sneddon (Penn)
    - D. Dixon (Alabama)
  - **IPHE Partners**
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- **Solar Energy Conversion**
  - V. Klimov, R. Schalller, M. Sykora
  - D. Dattelbaum, B. Dyer
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  - Ken Marken
  - Jeff Willis
- **Solid-State Lighting**
  - Brian Crone
  - Darryl Smith
  - Tony Burrell
- **Infrastructure Modeling**
  - Jim Doyle, Sam Flaim
- **Tech Transfer**
  - Duncan McBranch

Department of Energy

Hydrogen for Transportation

Petroleum-based transportation will be difficult to replace

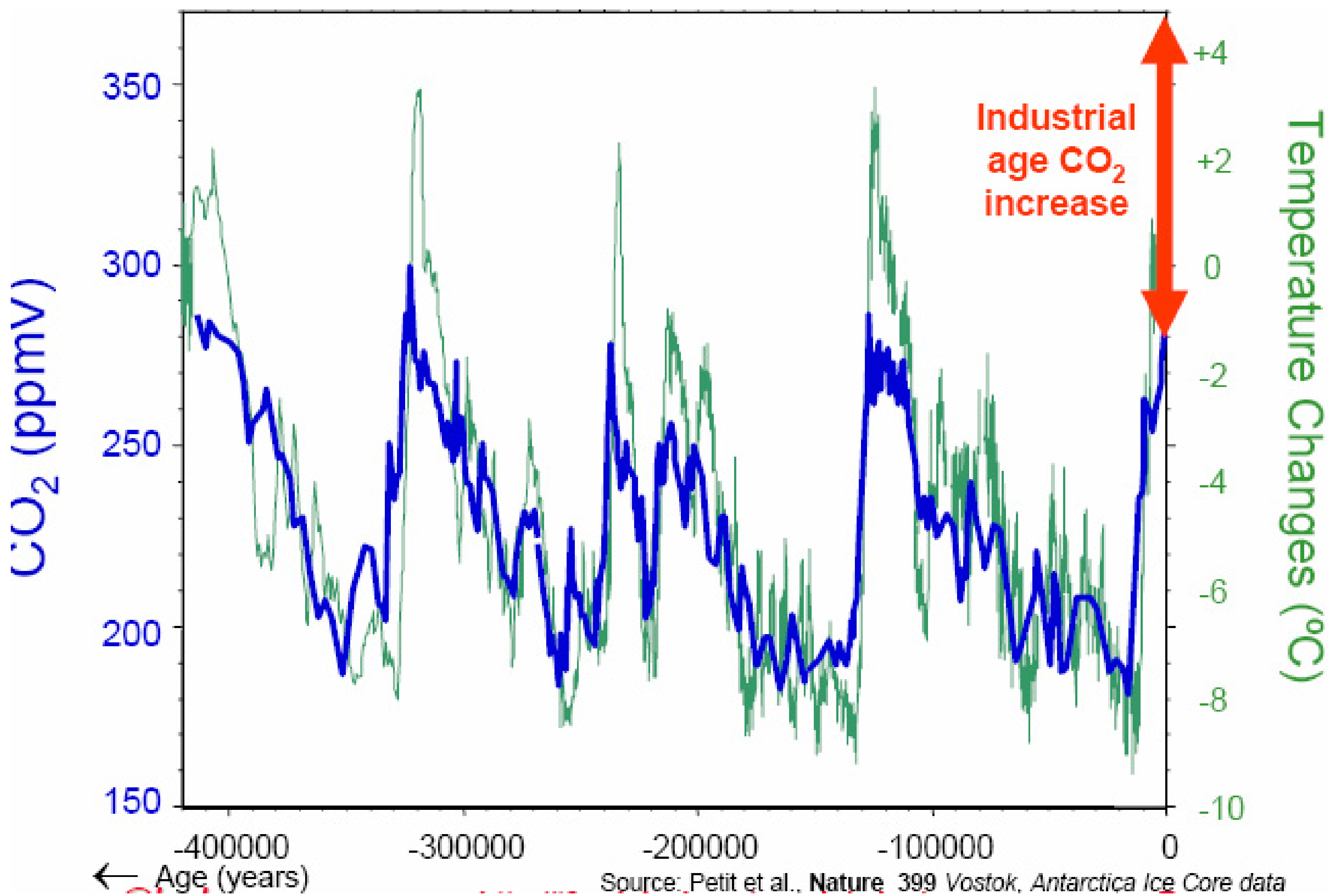
- Gasoline is both an energy source and an energy storage medium
- High energy density
- Easy to handle and cheap (for now)
- 100 years of optimization and infrastructure

U.S. Department of Energy 2015 Targets for Hydrogen:

- Hydrogen delivered at cost equivalent to cost of gasoline
- On-board hydrogen storage to allow > 300 mile range
- Fuel cell system cost of $30/kW
- Fuel cell durability of > 5000 hours
- Cold start to -20 °C and survivability to -40 °C
- Safe operation

Scientific Advances are Needed

Carbon Dioxide



Source: Petit et al., **Nature** 399 *Vostok, Antarctica Ice Core data*