

APPENDIX E
SUMMARY PRESENTATIONS

Topical Team Summary

Fossil Energy

Fossil Energy Topical Team

Marvin Singer (Chair)

Tim Armstrong, ORNL

Tof Carim, BES

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Eric Suuberg, Brown U

Anbo Wang, VPI

John Wimer, NETL

Mike Bockelie, Reaction Eng.

Bob Carling, SNL

Brian Gleeson, Ames/U of Iowa

Larry Myer, LBNL

Doug Ray, PNNL

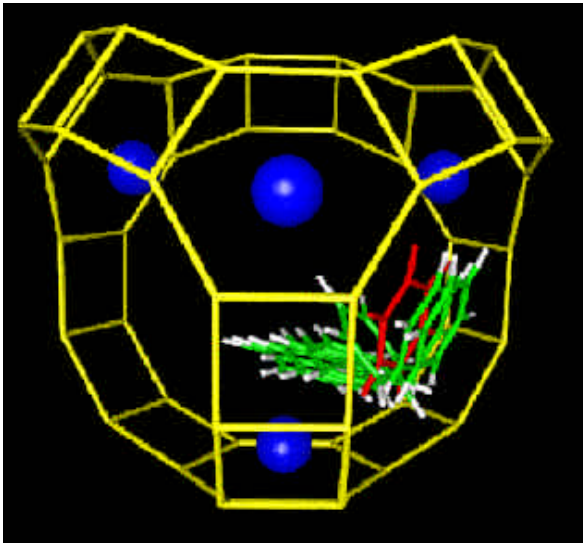
Roger Turpening, BES

Nick Woodward, BES

Proposed Research Directions

1. Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability
2. Advanced Subsurface Imaging and Manipulation of Fluid-Rock Interactions
3. Development of an Atomistic Understanding of High Temperature Hydrogen Conductors
4. Development of Predictive Fuel Conversion Models

Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability



Exploit the synergy between experimentation (inelastic neutron scattering) & theoretical simulations (QM and Monte Carlo methods) in heterogeneous catalysis.

Benefits: inorganic solid materials with predicted properties

Status: “Edisonian” Approach

Obstacles: reaction pathways (kinetics, binding energies, thermodynamics) are not well understood

Challenges: governing rules for behavior of inorganic solids

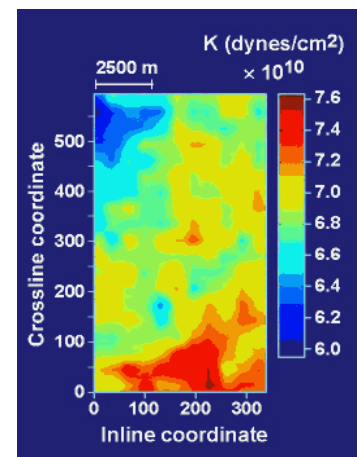
Advanced Subsurface Imaging and Manipulation of Fluid-Rock Interactions

Benefits: Increased production of domestic oil and gas resources along with the ability to tap unconventional gas reservoirs

Status: Production in continuous decline

Obstacles: Poor images of the subsurface, poor in information content, poor in resolution, and poor in registration. Most of the hydrocarbons remain trapped in the pore space.

Challenges: Imaging challenge--deployment of sensors, of all techniques, in the subsurface. Modify interfacial surface energies.



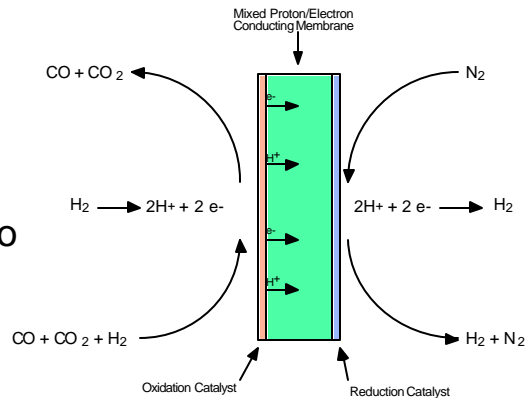
Development of an Atomistic Understanding of High-Temperature Hydrogen Conductors

Benefits: high flux, stable proton conductors

Status: Current proton conductors suffer from low conductivity and poor chemical stability - current approaches “Edisonian”

Obstacles: Need new materials, models to guide development and characterization methods to determine conduction mechanisms

Challenges: Development of models to predict H_2 conduction in materials



Development of Predictive Fuel Conversion Models

Combustion operates at the intersection of chemistry, hydrodynamics, and transport with approximations made along each axis

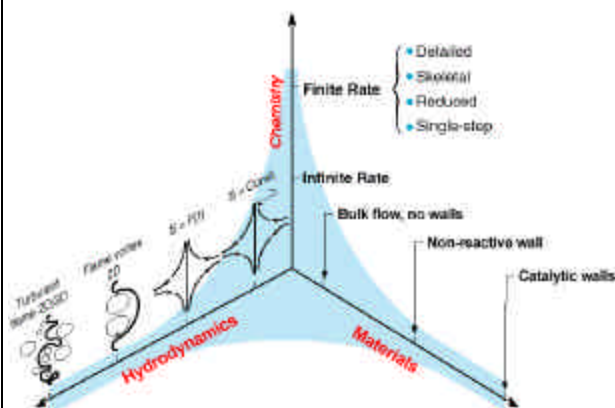
Benefits: Improved combustion devices

Status: Current models don't adequately describe today's experimental results

Obstacles: New codes to capture time-dependent events

Computer resources

Challenges: Development of the science base for simulation and validation



Topical Team Summary

Nuclear Fission Energy

Nuclear Fission Energy Topical Team

John Ahearne, Sigma Xi (chair)*	Jim Beitz, ANL
Allen Croff, ORNL (acting chair)	Bill Millman, DOE/SC-BES
Ralph Bennett, INEEL*	Jack Richards, Cal Tech
Bob Gottschall, DOE/SC-BES	Rob Versluis, DOE/NE
Andy Klein, Oregon State	Brian Wirth, LLNL
Frank Goldner, DOE/NE	Bill Weber, PNNL
John Taylor, EPRI*	Mike Kassner, Oregon State
Neil Todreas, MIT*	
Todd Allen, ANL-W	*Did not attend workshop

Background

- Nuclear fission currently provides 20% of U.S. electricity safely and reliably
- In light of expected population growth and energy demand and the expected need for large quantities of hydrogen produced without contributing to adverse climate change, nuclear fission is expected to be a critical component of the future energy mix

Background

- Current light water reactors are the first generation of commercial nuclear fission based technology. Technological improvements are desired in the areas of:
 - Sustainability-waste impact and fuel utilization
 - Safety and reliability
 - Economics
 - Proliferation resistance and physical protection

Background

- Generation IV initiative has identified six technologies that have the potential to meet the four goals
- Successful deployment of these technologies relies on significant advancements in
 - Materials-high temperature, unique coolants
 - Actinide chemistry-support recycle
 - Fuels-high temperature, support recycle
 - Heat transfer

Key Issue-1

Issue: Decade-long under-investment in science relevant to nuclear fission resulting from lack of interest in nuclear fission

Response: Need to invest in nuclear-related physical science topics, further incorporating available and emerging state-of-the-art tools and approaches: neutron scattering, light sources, advanced computing

Key Issue-2

Issue: Commonality of science investments across nuclear fission and other energy sources

Response: One size does not fit all

- Some areas have much commonality, e.g., fluid flow, hydrogen production cycles
- Other apparently similar areas are very different, e.g., materials degradation because of the effects of radiation and unique hostile environments

Approach to identifying PRDs-1

Review technology issues stemming from the “big four” nuclear fission issues: proliferation, cost, waste disposal, safety and environment

Round-table definition of potential PRDs based on previous topical group input and participant views

Discuss potential PRDs; refine and combine where appropriate

Approach to identifying PRDs-2

Select “top several” based on vote excluding DOE/SC staff

Sanity check: Any major problem with what is below the cut line

Documentation

- PRD write-up
- Coordination disposition of potential cross-cuts

First Priority PRD

Materials degradation: mechanical and chemical degradation of cladding, reactors, and waste package components. Examples

- Multiscale modeling of the complex microstructural development of alloys and ceramics and the relationship of these highly non-equilibrium changes to mechanical, dimensional stability, and corrosion properties
- Fundamental understanding of intergranular cracking in irradiated components
- These challenges amplified by the extreme environments envisioned by Generation IV
- Multiple year stability of nuclear waste packages.

Second Priority PRD

Actinide and fission product chemistry: to support a sustainable recycle system. Examples:

- Designer molecules for selected proliferation resistant group extractions
- Green chemistry to minimize waste impact
- Development of deliberately designed ligands (ion channels of biological membranes or carbon nanotubes) for improvements in mining and extraction techniques

Third Priority PRD

Fuel behavior: for advanced high temperature fuels

- Behavior of novel fuel forms to harsh environments (high temperature, radiation, stress). These include nitride fuels, metallic fuels, dispersion fuels, and non-fertile (inert matrix) fuels.
- Influence of recycle products on fuel behavior including radiation response
- Multiscale modeling of fuel behavior (similar to materials issues in PRD 1)

Fourth Priority PRD

Heat transfer: Examples

- Eliminate use of engineering correlation by developing a first principles understanding of multi-phase heat transfer and fluid flow mechanisms (including supercritical water, lead-alloy coolants, molten salts)
- Understanding of fluids with dispersed particles (i.e. nanofluid suspensions)

Other Cross-Cutting Candidates

Hydrogen generation chemical cycles

- Chemical cycles that work at lower temperatures

Welding and joining

- For high-temperature, high-strength materials

Multifunction materials

- Self-monitoring or self-healing

Direct energy conversion

- Processes and materials

Potential PRDs Considered

- 11 Actinide and fission product processing chemistry
- 11 Materials degradation: mechanical
- 11 Materials degradation: chemical
- 7 Heat transfer
- 5 Fuel behavior
- 5 Hydrogen generation
- 3 Welding and joining
- 2 Fundamental effects of radiation on biological organisms
- 2 Processes/materials for direct energy conversion to electricity
- 2 Evaluation and condition monitoring in harsh environments
- 1 Educating the public
- 0 Remote, non-invasive sensing
- 0 Sub-critical transmutation systems
- 0 Beneficial uses of depleted uranium
- 0 Multifunctional materials
- 0 Human factors and advanced instrumentation
- 0 Small reactors
- 0 Integrated power supplies
- 0 Extraction of energy from waste repositories
- 0 Synergistic energy sources
- 0 Infrastructure support

Topical Team Summary

Renewable and Solar Energy

Renewable and Solar Energy Topical Team

George Crabtree, ANL (Chair)	<u>Extra Attendees</u>
Sam Baldwin, EE	Tom Baker, LANL
John Cooke, ORNL	Dan Ginosar, INEEL
Jerry Hunt, ANL	Mack Kennedy, LBNL
Lonnie Ingram, Univ. of Florida	Joe Paladino, NETL
Lary Kazmerski, NREL	Sharlene Weatherwax, DOE-BES
Nate Lewis, Cal Tech.	Jane Zhu, DOE-BES
Jeff Mazer, EE	
Arthur Nozik, NREL	
Jay Spivack, GE	

Key Issues

Total energy/yr in 2000: 13 TW

Carbon free energy/yr required in 2050: 10-30 TW

Grand Challenges in basic research

> enable renewable use at this level

Proposed Research Directions

- Develop functional genomics and biochemistry for the tailoring of plants and microorganisms to increase the production of fuels and chemicals by 100-fold.
- Develop methods for solar energy conversion that result in a 10-50 fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity.
- Develop the knowledge base to enable the widespread creation of geothermal reservoirs.
- Effectively convert solar, wind and geothermal energy into stored chemical fuels.
- **Cross cutting:** Design and synthesize new classes of complex materials, including hybrids that integrate organic, inorganic and biological to revolutionize the development of renewable technologies.

Develop functional genomics and biochemistry for the tailoring of plants and microorganisms to increase the production of fuels and chemicals by 100-fold.

Genetic tailoring for materials, fuels, and chemicals

- understand limitations of plant efficiency
- improve energy efficiency - less water, nutrients, and land
- greater range of cultivation- salt tolerance and stress resistance
- rational design of enzymes for depolymerization of plant constituents
- simplify bioconversion process
- engineering of plants and microbes to produce renewable biomaterials and chemicals

Develop methods for solar energy conversion that result in a 10-50 fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity.

Robust for 20 -30 years

Cost of installed photoconversion : \$0.20/peak watt of solar radiation

- raise mobility of inexpensive photoconversion materials- polycrystalline, organic semiconductors
- interpenetrating networks- nanoscale charge separation and collector elements
- multiple junctions match solar spectrum, prevent carrier thermalization: efficiency 32% -> 65%
- quantum dots, quantum wells, and organic dyes

Develop the knowledge base to enable the widespread creation of geothermal reservoirs.

Entire western U.S. has high thermal gradient and untapped potential

Developed geothermal reservoirs limited to sites with surface hot water

Challenge: create geothermal reservoir where no fracture network exists

- create fracture network remotely
- map fracture network remotely
- understand interaction of injected fluid with fractured rock matrix
- develop materials and coatings for drilling above 300°C and 500-1000°C

Effectively convert solar, wind and geothermal energy into stored chemical fuels.

Solar, wind, and geothermal sources produce electricity far from end use

- convert electricity to storable fuels H₂ and O₂ from water, reduce CO₂ to methanol, ethanol or other C-based fuels
- direct conversion of solar photons to fuels or chemicals from H₂O, CO₂, N₂
- photoactive organic, inorganic, or biological molecules
- absorb solar irradiation and drive chemical reactions

Design and synthesize new classes of complex materials, including hybrids that integrate organic, inorganic and biological to revolutionize the development of renewable technologies

Entirely new classes of materials must be developed to bring renewables on line.

- nanostructures: single wall nanotubes for simultaneous bandgap and charge collection media, hybrid nanotube/metal materials, etc.
- semiconductor quantum dots as photovoltaic media
- organic semiconductors as inexpensive photovoltaics
- p -type transparent conducting oxides
- photocatalysts and photoelectrodes for water splitting
- engineered biosystems that carry out physical processes such as bugs that split water

Proposed Research Directions

- Develop functional genomics and biochemistry for the tailoring of plants and microorganisms to increase the production of fuels and chemicals by 100-fold.
- Develop methods for solar energy conversion that result in a 10-50 fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity.
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- **Cross cutting:** Design and synthesize new classes of complex materials, including hybrids that integrate organic, inorganic and biological to revolutionize the development of renewable technologies.

Topical Team Summary

Fusion Energy

Fusion Energy Topical Team

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J. Dahlburg, GA

P. Efthimion, PPPL

Fusion Energy Proposed Research Directions

- Multiscale modeling of microstructural stability of irradiated materials
- Deformation and Fracture Modeling
- BES Research Opportunity in Plasma-Surface Interaction
- Thermofluids and “Smart Liquids”
- BES Research Opportunity in Plasma Aerodynamics

Multiscale modeling of microstructural stability of irradiated materials

- **Brief statement of proposed research topic:** Fundamental research is needed to identify the key physical processes that will enable materials to maintain microstructural stability during prolonged fusion neutron irradiation.
- **New scientific opportunities:** By utilizing physically-rigorous bridging of the gaps between different spatial and temporal modeling regimes (nanoscale to continuum), a comprehensive predictive capability for modeling the stability of prospective advanced nanoscale materials can be attained.
- **Relevance & impact to Fusion Energy and other applied programs:** The successful development of fusion energy will require materials that are capable of withstanding exposure to intense radiation fields over a broad range of temperatures.
- **Estimated time scale:**
 - ~10 years: development of improved interatomic potentials
 - ~ 10 years: multiscale microstructural evolution and nanoscale solute segregation models
 - ~10 years: development of improved physics-based models of radiation-induced or – enhanced solute segregation to interfaces
- **Additional Information:**
 - Development of improved interatomic potentials, including directionality effects, magnetic effects (very important for ferritic steels)
 - Numerous recent molecular dynamics (MD) simulations (using interatomic potentials of dubious quantitative accuracy) have predicted the possibility of long range one-dimensional transport of matter via self-interstitial crowding bundles.
 - Development of physically rigorous multiscale microstructural evolution models based on Molecular Dynamics, kinetic Monte Carlo and kinetic rate theory techniques.
 - Phase stability under irradiation
 - Transport and clustering of He

Deformation and Fracture Modeling

- **Research direction:** New opportunities exist to understand and predict the effects of radiation on deformation and fracture. Multi-scale modeling involving atomistic simulations, mesoscopic simulations, and continuum simulations coupled with greatly expanded computational capabilities allow us to understand phenomena and predict behavior beyond that which has been possible with experimental approaches.
- **New Scientific Opportunities:** The current understanding of radiation effects on deformation and fracture of new materials is inadequate. New multi-scale modeling capability has the potential to make breakthroughs in understanding and designing these new materials.
- **Summary:** Some examples covering both new materials and a description of some well known problems are given below.
 - Nanoscale reinforced materials
 - Advanced radiation resistant ceramic composites
 - Flow localization
 - Atomistics of crack initiation and growth (radiation embrittlement)
 - Initiation and growth of subcritical sized flaws
 - High-temperature deformation mechanisms

BES Research Opportunity in Plasma-Surface Interactions

- **Research Direction:** To increase the basic understanding of critical issues related to plasma-surface interactions including photon radiation transport, “potential” sputtering, and material erosion under intense power loadings.
- **New Scientific Opportunities:** Development deeper understanding and models for key plasma -surface interactions involving intense particle and heat loads.
- **Relevance to DOE Mission:** One of the most important issues concerning the basic feasibility of fusion as an energy source, and a major issue for present-day high-temperature plasma confinement experiments, is the interaction of intense heat and particle fluxes with plasma-facing components. These interactions need to be understood in terms of the basic phenomena so they can be controlled. Potential impacts include contamination of the plasma and short lifetimes of the components.
- **Summary:**
 - One important area that determines many of the plasma -surface interaction effects is photon radiation transport in both optically thin and optically thick plasmas with intense line populations.
 - Another important topic is a recently new physical phenomenon that is not well understood is called "Potential Sputtering".
 - Understanding fundamental models of material erosion and destruction under intense power applications is another vital topic.

Thermofluids and “Smart Liquids”

- **Research Direction:** The proposed research is to develop a fundamental understanding of flowing, electrically conducting fluids in complex environments which include electromagnetic fields. Magnetohydrodynamic forces can affect liquid motion from the largest, integral scales down to the fine scales of turbulence. Ultimately, fluid properties can be tailored so that such “smart liquids” can be shaped and steered in a novel fashion using fields.
- **New Scientific Opportunity:** Computation methods for 3-D direct numerical solution and other methods of incompressible, turbulent, free-surface fluid flow in strong electromagnetic fields
- **Relevance and Impact:** Fusion energy seeks to contain star-like conditions within physical barriers. The environment includes elevated temperatures, radiation and kinetic debris. To solve the resulting materials problems, increasing attention is being given to liquid walls in both magnetic and inertial fusion. Liquids can be pumped through the harsh reactor environment and out to a benign area where liquid refurbishment can be performed. “Smart liquids” may enable unique solutions to directing flow, especially free-surface flow, in complex, fusion reactor geometries.
- **Summary -- Specific Suggestions that might be of interest to BES include the following:**
 - Numerical simulation of the effect of magnetohydrodynamic forces on turbulence in incompressible liquid conductor flows and their related transport of heat and mass, especially at solid and free interfaces.
 - Control of liquid metal flow motion and velocity profiles via applied magnetic and electric fields and currents.
 - Modification and control of fluid properties and behavior via complex chemical doping and micro-additives.

BES Research Opportunity in Plasma Aerodynamics

- **Research Direction:** To developed the basic understanding of the application of weakly ionized plasmas in aerodynamics for control of shock, turbulence, heat fluxes, drag, and related phenomena.
- **New Scientific Opportunity:** Develop new methods to control aerodynamic flows.
- **Relevance:** Weakly ionized air plasmas have a high potential for impact on advanced aerodynamics. Specifically, plasmas and MHD processes may be capable of mitigating peak thermal loads, extracting high levels of power, reducing drag, reducing observability, reducing sonic boom, and suppressing noise.
- **Summary:**
 - Because the plasmas are so expensive in power to establish and sustain, one of the critical areas to understand is the time scale of the phenomena.
 - In many of the plasma aerodynamic applications the presence of instabilities may become a serious limitation.
 - Mechanisms for the efficient creation of air plasmas also need to be understood.
 - Perhaps the most difficult issue is the establishment of scalability relations.

Topical Team Summary

Distributed Energy, Fuel Cells, and Hydrogen

Distributed Energy, Fuel Cells, and Hydrogen Topical Team

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Vitalij Pecharsky, Iowa State University

Philip N. Ross, Lawrence Berkeley National Laboratory

Subhash Singhal, Pacific Northwest National Laboratory

John Turner, National Renewable Energy Laboratory

Douglas Wheeler, UTC Fuel Cells

Mark Williams, National Energy Technology Laboratory

Key BES Topics

- Hydrogen synthesis
- High capacity hydrogen storage
- Novel Membranes
- Designed Interfaces

Hydrogen Synthesis

- Photocatalytic Synthesis of Hydrogen
Challenge: coupling of light harvesting systems with catalysis to produce hydrogen.
- Thermochemical Water Splitting Driven by Solar or Nuclear Heat
Challenge: feasible redox cycles
- Fossil Hydrogen Production
Challenge: advances in catalysis, membranes, gas separation

Photocatalytic Synthesis of Hydrogen

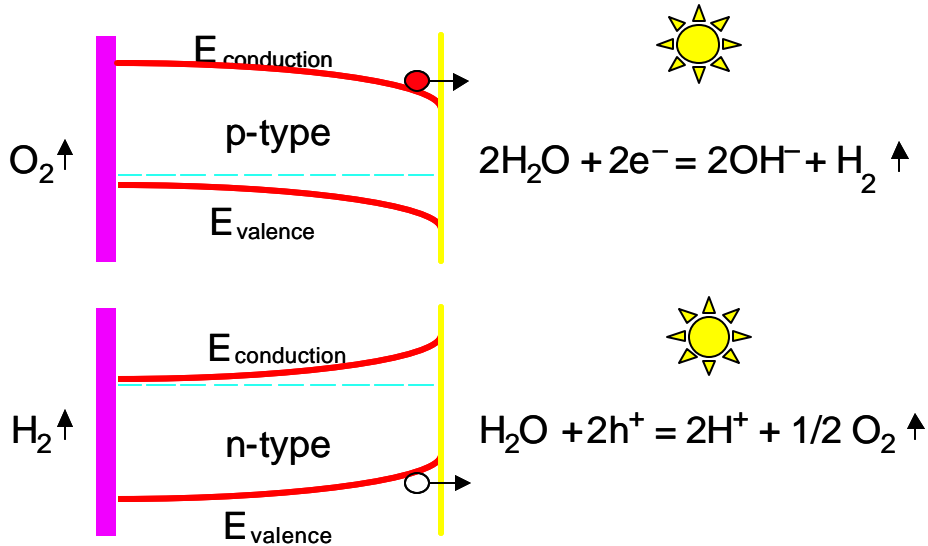
Approach:

- 1) semiconductor materials that have appropriate light absorption characteristics and are stable in aqueous solutions.
- 2) catalytic coatings on semiconductor surfaces.
- 3) Identification of environmental factors (e.g., pH, ionic strength, solution composition, etc.) that affect the energetics of the semiconductor, the properties of the catalysts, and the stability of the semiconductor.

Photocatalytic Synthesis of Hydrogen

Band Edges of p- and n-Type

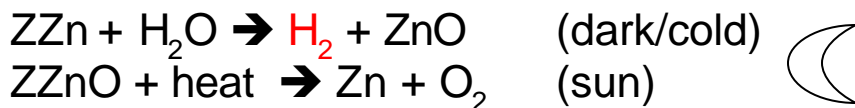
Semiconductors Immersed in Aqueous Electrolytes to Form Liquid Junctions



Thermochemical Water Splitting

Approach: Thermochemical cycles (typically at $\sim 700\text{-}900\text{ C}$) driving a set of hydrogen producing redox reactions.

Example:



Range of possibilities:

- Cycling between various oxidation states
- S-I cycles (corrosion issues!)

High Capacity Hydrogen Storage Materials

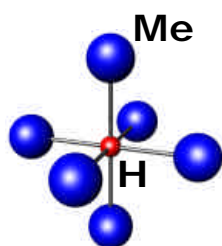
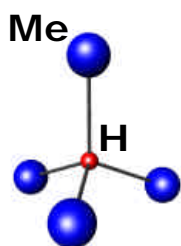
Challenge:

materials with 10+ percent mass and volume of hydrogen storage capacity

Approach:

replace C in CH_4 with light elements from which hydrogen can be more readily removed and reattached

High Capacity Hydrogen Storage

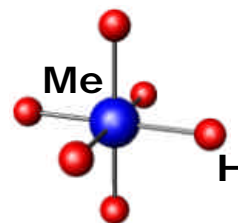
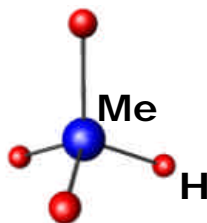


Metal hydrides

From encapsulating hydrogen

to encapsulating by hydrogen

Complex metal hydrides
Alanes, Borohydrides....



Novel Membranes

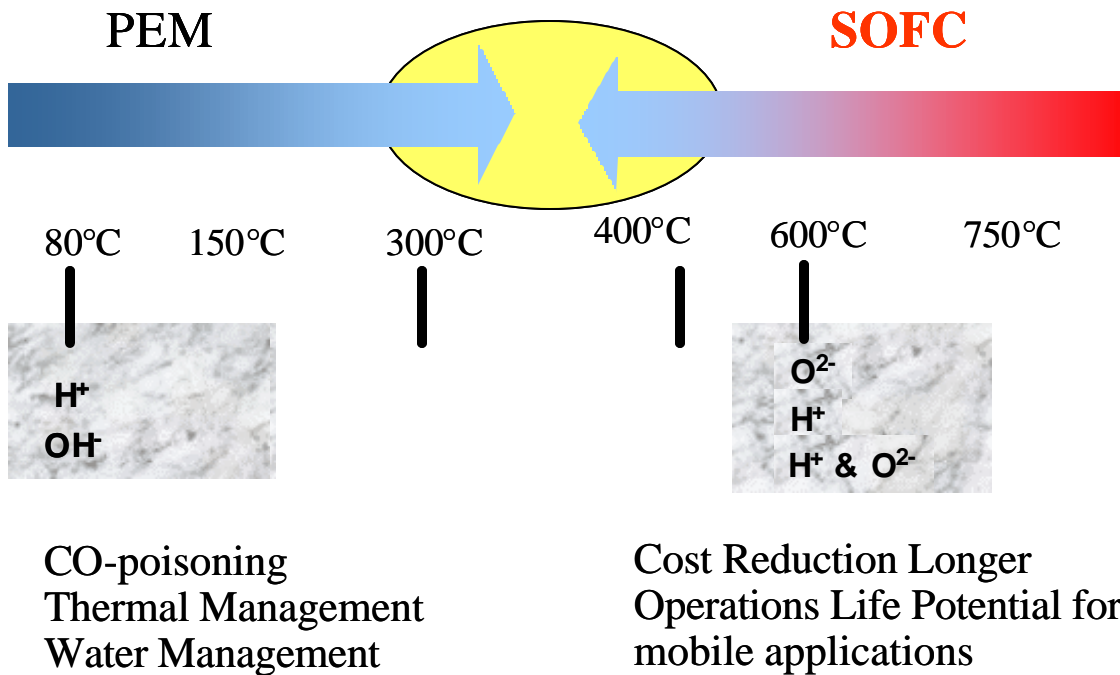
Challenge:

Design ionic and mixed-conducting membranes with high conductivity, stability, and selectivity over a broad temperature range.

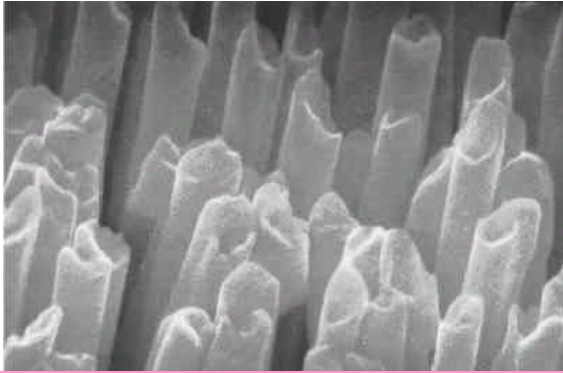
Impact:

Increased efficiency and reduced cost of fuel cells, batteries, hydrogen separation/purification, oxygen separation, reforming/partial oxidation of hydrocarbon fuels, contaminant removal, gas sensing, and other processes relevant to energy storage and conversion.

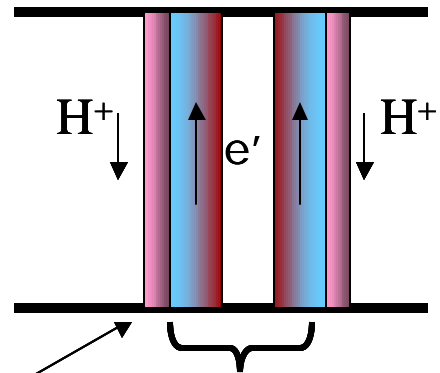
Ionic Membranes for Fuel Cells



Proton-Electronic Membranes



Proton transport along surfaces of nanotubes

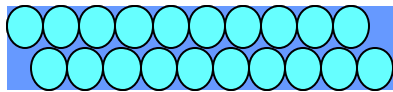


Nanotube for electron transport

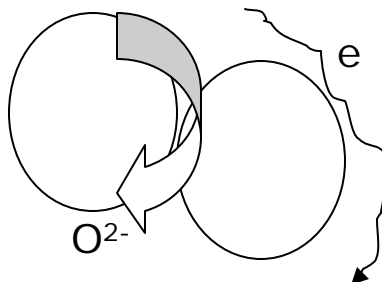
- Hydrogen separation/purification
- Electrodes for fuel cells based on proton conductors

Oxygen Ion-Electronic Membranes

Templated self-assembly of precursors to form functional membranes and interfaces



Ionic and electronic transport along interfaces



- Oxygen separation
- Reforming/partial oxidation of hydrocarbon fuels
- Cathodes/anodes for SOFCs
- Contaminants removal

Designed Interfaces

Challenge:

The generation and utilization of hydrogen or carbon-containing fuels depends critically on interfaces that need to fulfill specific and often conflicting functions. Among these functions are structural, dimensional and chemical stability, electron, ion, and mass transfer, catalysis, and electrocatalysis, under a wide range of temperature, temperature changes, and gas partial pressures variations. So far the approach has been largely Edisonian. Basic science must develop a reliable roadmap to designing solutions in this multidimensional space.

Proposed approach:

We propose the development of a computational equivalent of combinatorial synthesis, drawing on a multidisciplinary, theory-based approach.

The impact of the combinatorial science is broad. The approach can be of exceptional value in a wide range of energy conversion and generation, separation technology, hydrogen production, and energy storage.

Topical Team Summary

Transportation Energy Consumption

Transportation Energy Consumption

Topical Team

Jan Herbst, GM R&D (Chair)

Channing Ahn, California Inst. Tech.

Tarasankar DebRoy, Penn State Univ.

Jim Eberhardt, EE

Ed Grostic, ORNL

Oren Hadaller, The Boeing Company

Kenneth Hass, Ford Motor Company

Joseph Heremans, Delphi Research Labs

Chris Sloane, General Motors

Extra Attendees:

Iver Anderson, AMES

Suresh Baskaran, PNNL

Bill Kirchhoff, DOE-BES

Paul Lessing, INEEL

Paul Miles, SNL

Kevin Ott, LANL

Matesh Varma, DOE- BES

Integrated quantitative knowledge base for joining of lightweight structural materials for transportation applications

- Maximum benefits of lightweight transportation materials will not be achieved without an integrated knowledge base on joining.
- No integrated model exists of the various physical processes that constitute joining such as heat transfer, fluid flow, mass transport, gas sorption, vaporization, solidification, phase transformations, etc.
- Significant advances in computational hardware and models now permit integration of constituent models for the prediction of the response of new materials systems to a selected joining process.
- Integrated models will allow full incorporation of novel materials into future transportation systems with significant gains in fuel efficiency and, hence, enhanced energy security.

Vehicular energy storage

- Widespread use of hydrogen-powered and electric vehicles requires materials having greatly improved energy storage capability
- Current materials are limited in volumetric and/or gravimetric energy density relative to hydrocarbon fuels
 - H₂ @ 700 atm contains < 14% energy of equivalent volume of diesel fuel and the advanced Ni-M hydride battery only about 10% of that.
- Fundamental understanding of the phase stability, thermodynamics, and kinetics of both hydride and battery materials is needed to enable the discovery and development of new materials that satisfy system requirements.

Fundamental challenges in fuel cell stack materials

- Fuel cells have long been seen to offer the opportunity for high efficiency, pollution-free propulsion to meet the nation's transportation needs, but persistent technical barriers remain: membrane performance & durability, cathode kinetics, tolerance to contaminants, alternatives to noble metal catalysts,...
- Materials for fuel cells have been developed empirically.
- Achieving higher performance membranes and electrodes requires
 - Fundamental theoretical understanding and experimental validation of relationships among composition, structure and properties
 - Accelerated design, novel synthesis and characterization of improved materials
 - Integrated, predictive, computational chemical & materials models with adequate fidelity for subsequent system optimization

Integrated Heterogeneous Catalysis for Transportation

- Catalytic processes are central to transportation fuel production, storage, utilization, and emissions abatement today and => enhanced US energy security in the future
 - H₂ production (coal, petroleum, natural gas => electrolytic, photolytic, biomass)
 - Liquid fuels (coal, petroleum, nat. gas => biomass, biofuels, tailored high density naphthenic aviation fuels)
 - Fuel cell electrocatalysts (Pt => base metal catalysts, more rapid cathode kinetics, bioinspired O₂ manipulation)
 - Hydrogen storage materials (catalytic uptake and release at appropriate pressures, temperatures, rates in materials of high hydrogen content)
- U.S. energy security will require integrated experimental, theoretical thrusts to enable rational design of heterogeneous catalysts
 - Fundamental, detailed knowledge of active site structure and reactivity: need access to emerging and development of new local structure tools
 - Multiple experimental techniques, high throughput experimentation, modeling and simulation tools
 - Fusion of complementary experimental information to yield coherent description of catalyst active site(s)
 - => Accelerate heterogeneous catalyst design (similar to capabilities available to homogeneous catalysis researchers today)

Thermoelectric materials and energy conversion cycles for mobile applications

- Thermoelectric materials (TEs) offer dual use in transportation systems:
 - Waste heat recovery: potential for ~20% increase in fuel economy
 - Cooling/air conditioning: greenhouse gas free; potential to exceed efficiency of vapor compression
- Realization of high-efficiency TEs requires
 - Improved theoretical understanding of electrical & thermal transport in semiconductors, esp. nanostructures and low thermal conductivity systems
 - Discovery and synthesis of materials with high Seebeck coeff. and electrical conductivity, low thermal conductivity
- Opportunities for new TE module configurations

Complex Systems Science for Sustainable Transportation

- Sustainability of US transportation system
 - Challenging problem: petroleum dependence, complex interdependencies among system components
 - System = fuels + vehicles + infrastructure + policies + behaviors...
 - Technological advances alone may not be good enough
- Complex systems science
 - Building conscience among disparate fields (including physical, biological, computer, economic, behavioral sciences – e.g., genetic computer algorithms)
 - Emphasis on nonlinear, holistic, nonequilibrium behaviors
- Long-term basic research required to develop fundamental concepts, tools, and cross-disciplinary insights into non-traditional energy/transportation problems
 - An immediate example is the creation of a robust strategy for transporting nuclear waste from distributed sources to the Yucca mountain disposal site

Topical Team Summary

Residential, Commercial, and Industrial Energy Consumption

Residential, Commercial, and Industrial Energy Consumption Topical Team

Millie Dresselhaus (MIT, Chair)	Speakers:
Sam Baldwin (EE)	Dr. Anil Duggal (GE)
Hylan Lyon (Marlow Industries)	Dr. Jerry Simmons (SNL)
Gerald Mahan (Penn State Univ.)	Prof. Woods Haley (UMN)
Anne Mayes (MIT)	Dr. Ron Judkoff (NREL)
Steve Selkowitz (LBNL)	Dr. Ertugrul Berkcan (GE)
Jerry Simmons (SNL)	Dr. Dickson Ozokwelu (DOE/EE)
Harriet Kung (BES)	Prof. Vitalij Pecharsky (Ames/Iowa State)
Aravinda Kini (BES)	

Panel Members with Phase I Task:

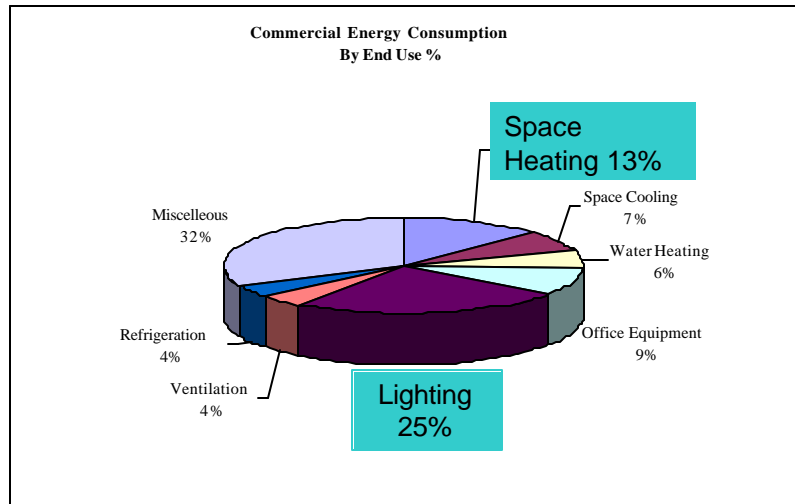
Paul Alivisatos (UC, Berkeley)
Sam Bader (ANL)
Terry Michalske (SNL)

Considerations for Selection of PRDs

- Importance of problem for energy security
- Potential of PRD to have impact on solving identified problem
- Potential of PRD to have impact on solving other problems of interest to DOE
- Potential for advancing science broadly
- PRD should lead to a new revolutionary technology

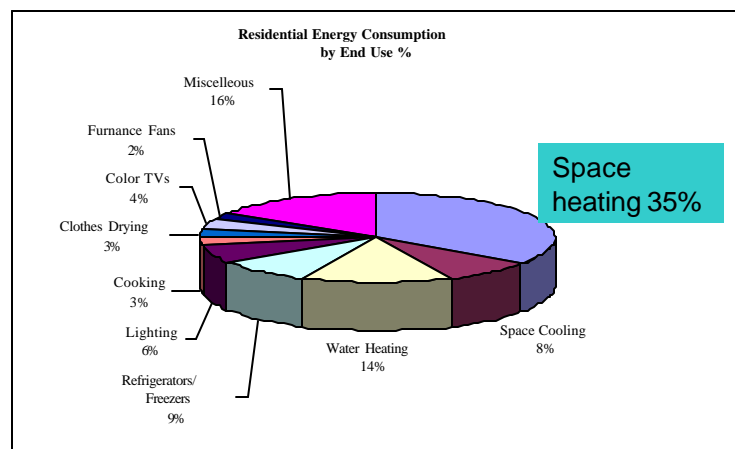
Commercial Energy Consumption

- Lighting is largest usage
- Second is space heating

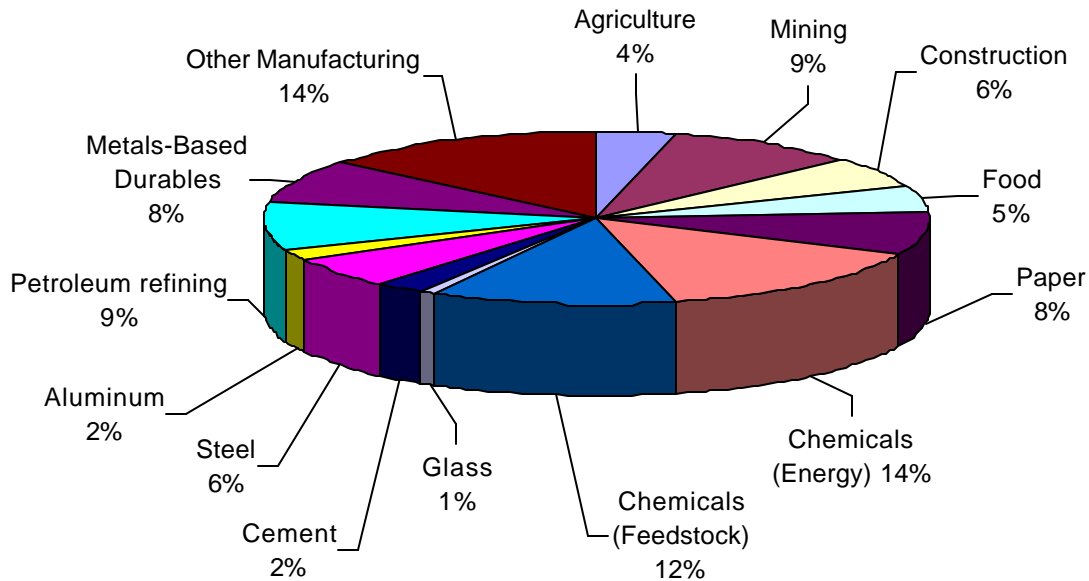


Residential Energy Consumption

- Space heating 35%
- Appliances 29%
- Lighting 6%



Industrial Sector Energy Use (%)



Key Proposed Research Directions

Four broad research themes were identified:

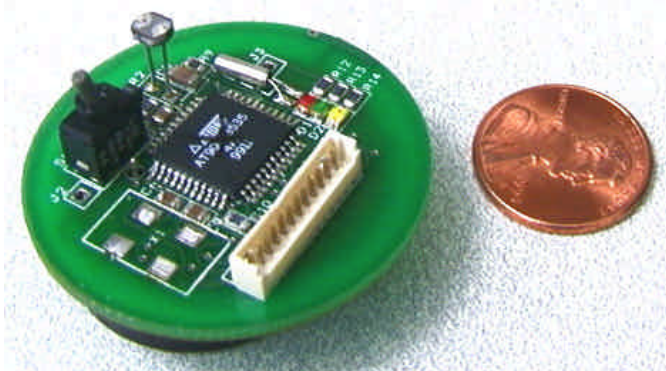
- Sensors
- Solid State Lighting
- Innovative Materials
- Multilayer Thin Film Materials and Deposition Processes

Sensors

- Ubiquitous, dense wireless sensor network, potential for large reduction in energy usage
- Sense and control energy flows, temperature, pollutants,...
- Equipment: e.g. smart dishwasher with turbidity sensor
- Buildings: Systems integration, diagnostics, comfort, safety.....

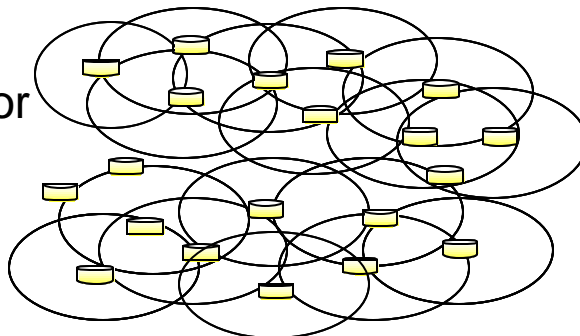
Smart Sensors

- Small self-powered sensors
- Robust, low cost
- Specific to each sensing function
- Sensors available for many different sensing functions
- Integrated signal processing for wireless transmission



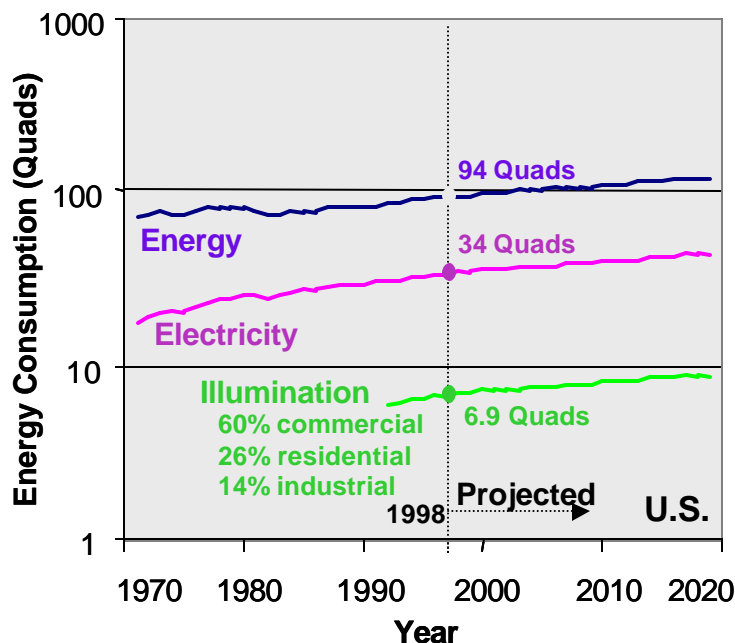
Smart Networks

- System integration of inputs from many sensors
- Information technology infrastructure for data collection
- On-chip signal processing linking sensors to actuators
- Wireless Communications protocols
- Self-organizing networks
- Adaptive logic, neural nets for real time control
- Optimization of linked sensors, actuators, controls



Solid-State Lighting

Lighting is large fraction of energy consumption, and very low efficiency

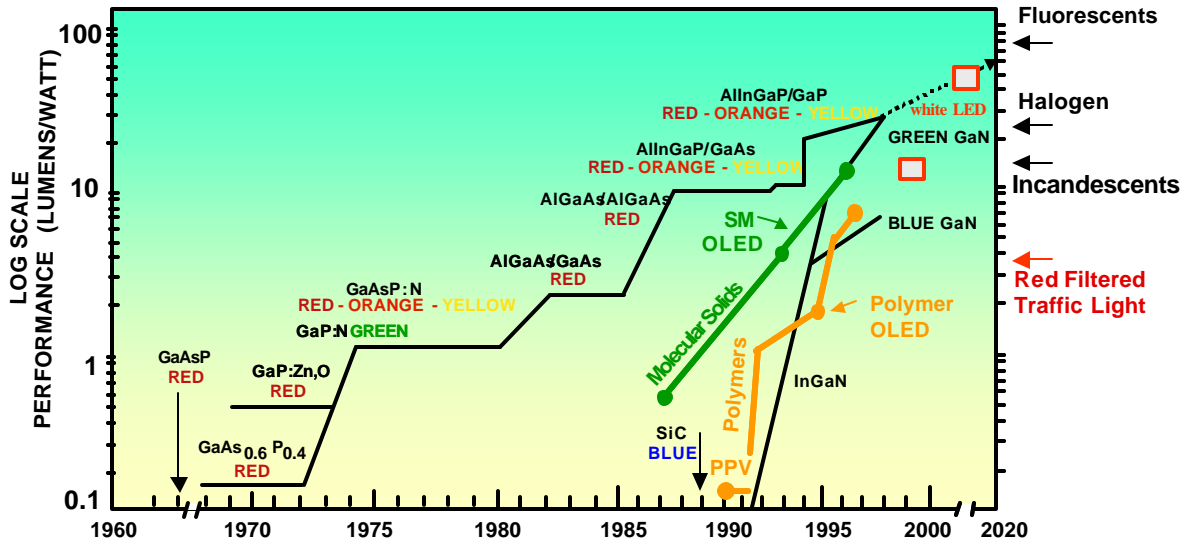


Efficiencies of energy technologies in buildings

Heating:	70 -80%
Electrical motors:	85-95%
Incandescent Lighting:	5-6%
Fluorescent Lighting:	20-25%

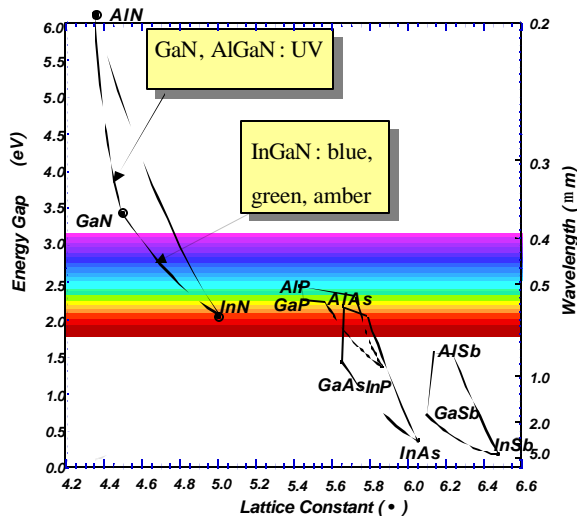
~20% of U.S electricity consumption is for general illumination

LEDs have been increasing in efficiency (and dropping in cost) at phenomenal rates



RED: lumens/Watt has improved at **30X/decade**, cost has decreased at **10X/decade**.
 BLUE: Recently blue Nitride-based LED materials have appeared.

AlGaN blue & UV LED materials are very new, considerably different from other III-Vs, and little understood



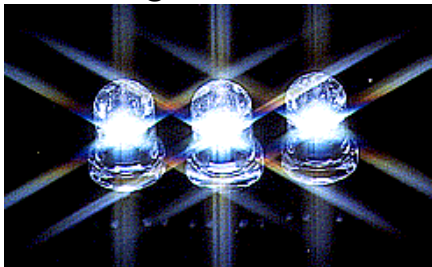
Nitride materials challenges:

- No lattice-matched substrate is known (dislocations therefore results)
- AlGaN not lattice-matched to GaN (dislocations and cracking)
- Mg p-type doping problematic (poor activation, high resistance)
- Growth process is poorly understood and difficult to control

Optical & electrical properties
dependent on defect concentrations

Organic LEDs are potentially low cost, large area light sources

Inorganic LEDs



- High brightness point sources
- Spot lighting applications:
 - Flashlights
 - Traffic lights
 - Projection lamps
- More like incandescent

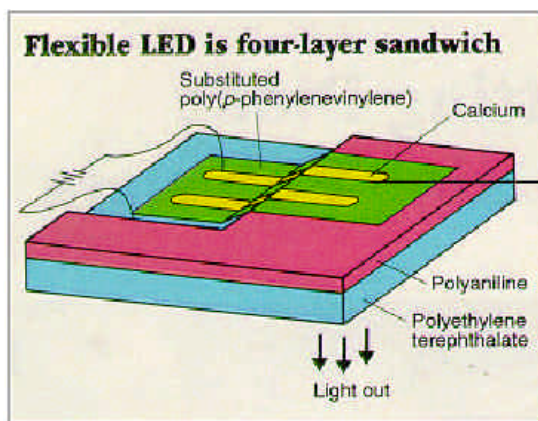
Organic LEDs



- Large area extended sources
- Diffuse lighting applications:
 - Backlights
 - Signs
 - General illumination
- More like fluorescent

Organic LEDs have several “simple” unanswered questions

- What is so special about the few “magic” materials? (Alq3, Polyfluorene)
- What is really going on at material interfaces?
- What controls the singlet-triplet exciton formation ratio in conjugated materials?
- Is it possible to make effective materials that are intrinsically stable to water?
- What are the mechanisms that lead to material degradation?
- Why is it so hard to make blue devices?

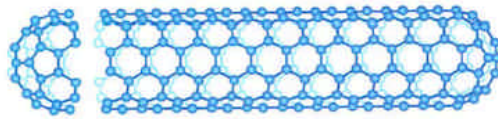


Innovative Materials- Independent Control of Multiple Materials Properties

- Available new nanoscale building blocks
- Large scale rapid synthesis methods
- Ability to control processing
- Utilize organic, inorganic, and biological elements

Nanoscale Patterning- some examples of new building blocks

■ Nanotubes

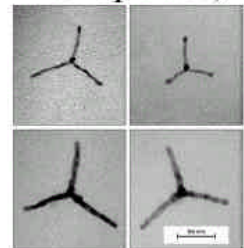


■ Nanocrystals

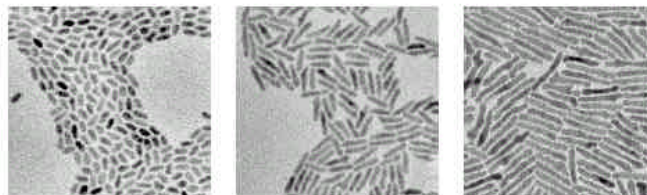


10 nm

(semiconductor
Tetrapods!)



■ Nanorods

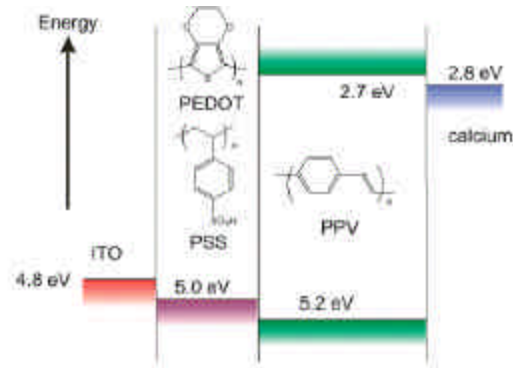


100 nm

Solar_Cell

More Building Blocks

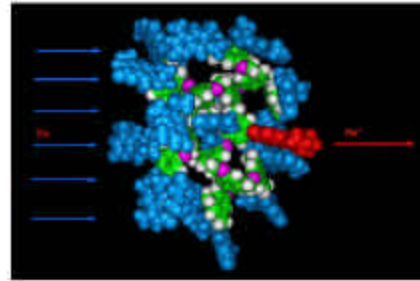
■ Electronic Polymers and Organics



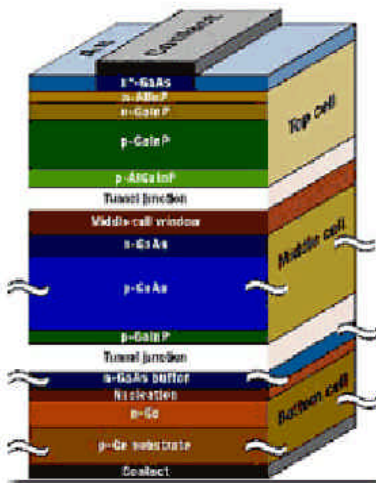
■ Block Polymers



■ Dendrimers



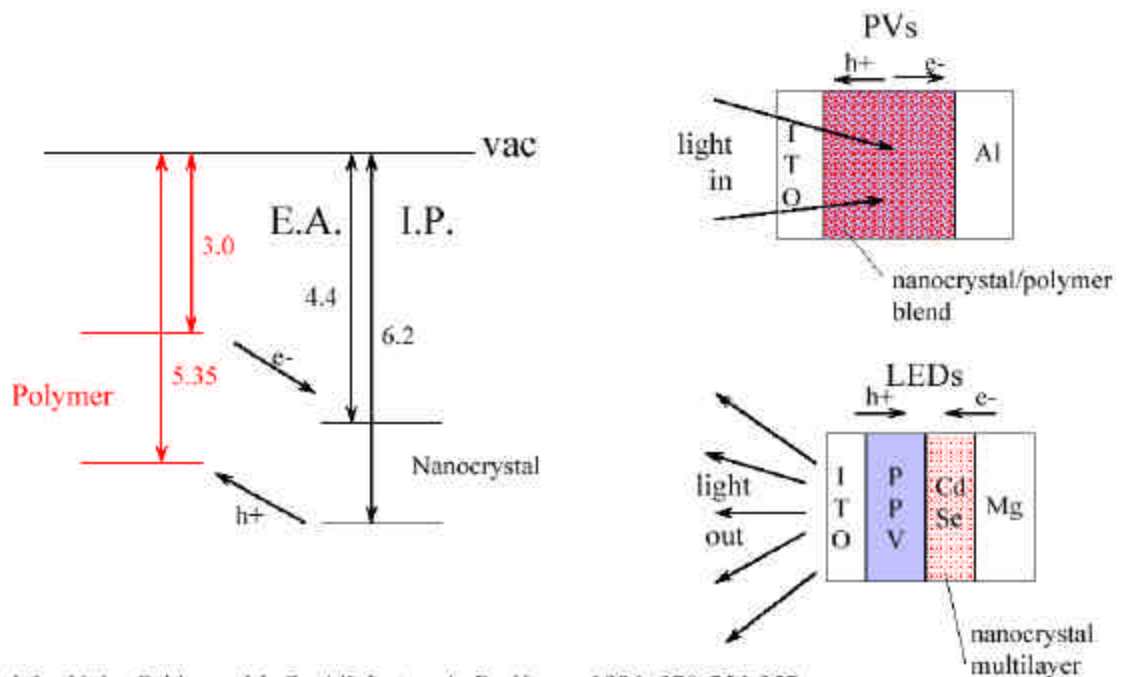
High end multi-gap tandem solar cells made by molecular beam epitaxy and used in satellites



This cell has achieved 34% conversion efficiency under a concentration of 600 suns.

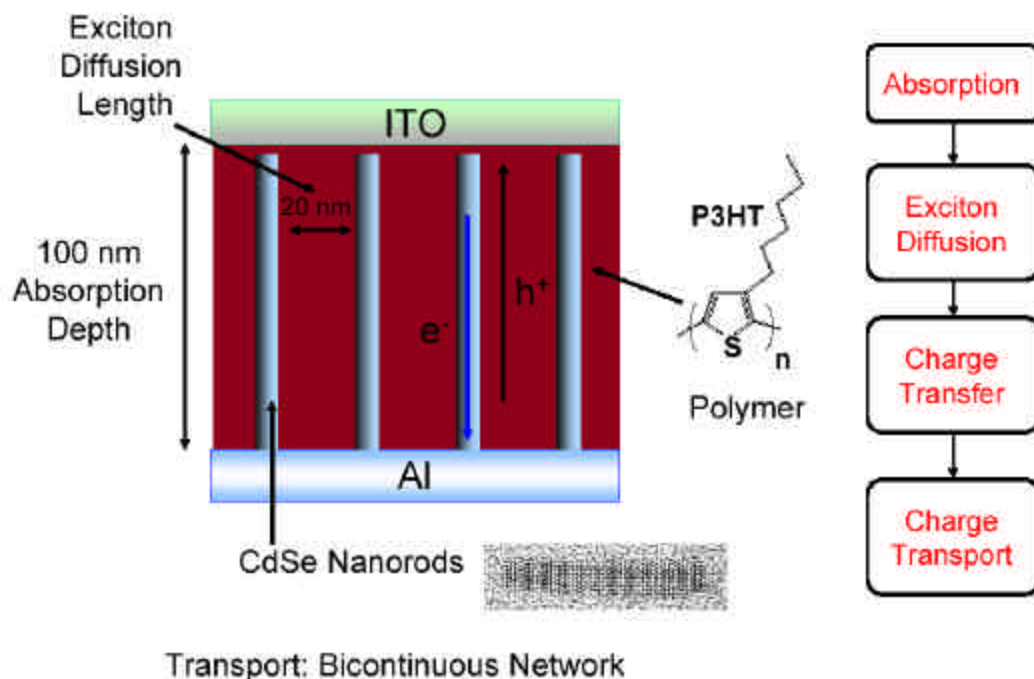
- Proof of concept 36% efficiency.
- Processing impractical for wide areas.
- Same materials can be assembled from inexpensive mass-produced colloidal nanorods.

Semiconductor Nanocrystals and Polymers Band Offsets and Electrical Devices



Colvin, V. L.; Schlamp, M. C.; Alivisatos, A. P., *Nature* **1994**, *370*, 354-357.
 Schlamp, M. C.; Peng, X.; Alivisatos, A. P., *J. Appl. Phys.* **1997**, *82*, 5837-5842.

Self-assembled Nanorod-Polymer Photovoltaics



Some Applications of Innovative Materials

- New LED for solid state lighting(50% efficiency)
- New low cost organic solar cells(30% efficiency)
- Thermoelectrics for self-powered sensors
- New sensor materials for selectivity
- New phase change materials for thermal storage

Multi-layer Thin Films

- First successful nano-dimensioned “products”, 5-50nm thick
- Ex: Low E coatings
 - 30% energy savings on 4% of U.S. total energy use
 - 40million sq.m/yr



- Broad potential applicability for new advanced coatings in buildings
- Needs - “New Materials technologies” and “Low-cost deposition technologies”

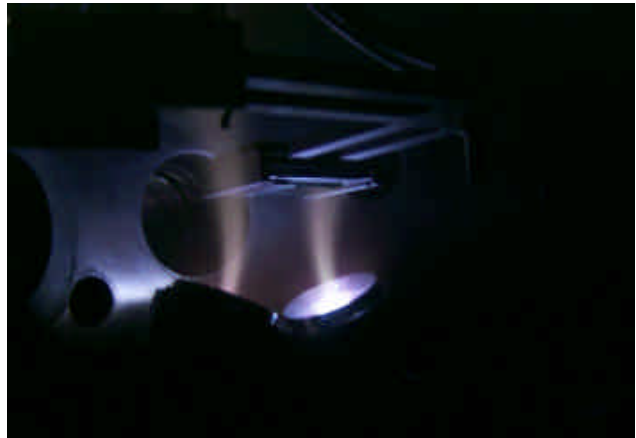
Opportunities for Novel Approaches to Materials

- Electrochromic window coatings - change in optical density with applied voltage
- Bendable, Transparent, conductive coatings
- Dynamic redirection of daylight

Opportunities for Novel Deposition Processes

- Modeling process parameters and film growth chemistry and kinetics
- Prediction of coating properties vs present “tweak and look” approach
- Energetic Deposition for improved rate and properties

e.g., plasma-assisted sputtering



Topical Team Summary

*Cross Cutting Research and
Education*

Cross-Cutting Research Topical Team

Rick Smalley, Rice Univ. (Chair)

Ivan Bekey, Bekey Designs

Kwan Kwok, DARPA

Gerry Lavin, DuPont

John Mankins, NASA

Yoram Shoham, Shell

Jeff Tester, MIT

Nathan Lewis, CalTech

Art Green, ExxonMobil

Agenda

Nate Lewis (Terrawatts)	1:10 – 1:30
Jeff Tester (HDR)	1:45 – 2:30
John Mankins (Solar Satellites)	2:45 – 3:15
Kwan Kwok (Darpa's approach)	3:30-3:40
New & Old Cross-Cutting Issues	
inputs and discussion	3:45-4:30
Workshop Summary & Closing	4:30-5:00 pm

Cross-Cutting PRDs

1. Education / Workforce
2. Nanomaterials –
 - Carbon nanotubes
 - etc.

Development of Proposed Research Directions

Education / Workforce

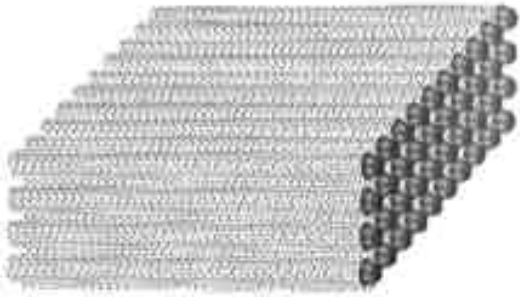
The 10-50 TW BY 2050 ENERGY CHALLENGE

Launch an Education Program within DOE to educate the public on the real problems in World energy supplies.

And how these can only be solved by Breakthrough research in the Garden of the Physical Sciences.

Single Crystal Fullerene Nanotube Arrays

A multifunctional supermaterial



- extreme strength / weight
- high temperature resistance
(600°C in air, 2000°C in space)
(for BN tubes ~900°C in air)
- unidirectional thermal conductor
- electromechanical structural component
- unidirectional electrical conductor
 - 0.7 to 1 eV direct band-gap semiconductor
 - or metallic conductor
 - or (for BN tubes) a 6 eV band-gap insulator

The Promise and the Challenge of Space Solar Power

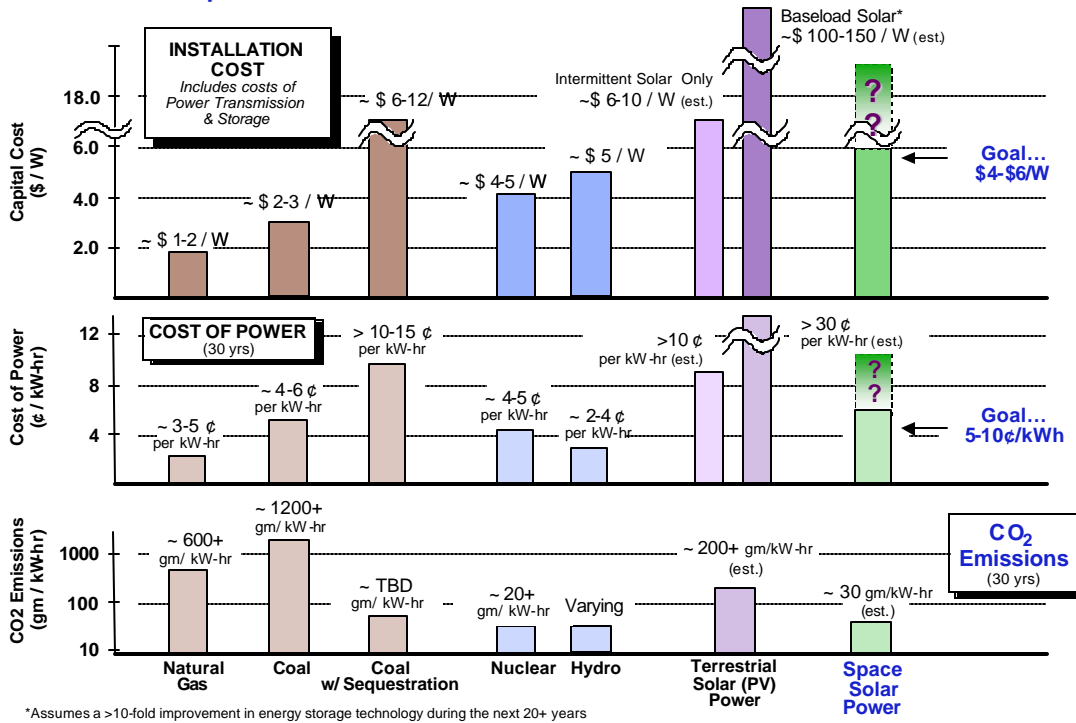
23 October 2002

John C. Mankins
Chief Technologist, Human Exploration & Development of Space
NASA Headquarters
Washington, DC, USA

Executive Summary

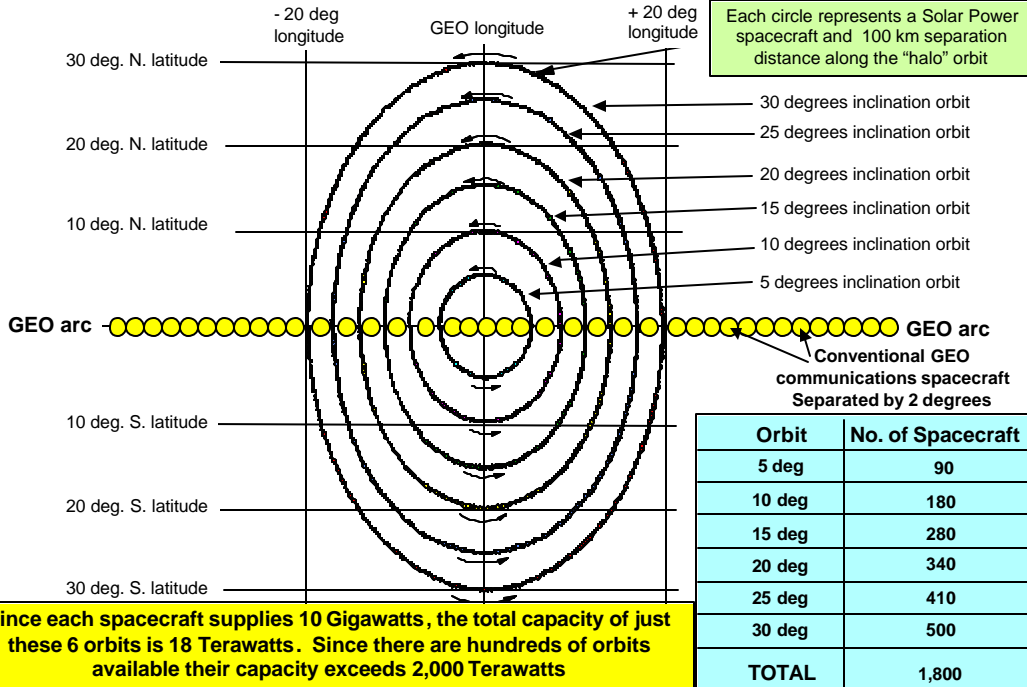
- **Global climate change caused by accumulating concentrations of greenhouse gases in the atmosphere is a growing concern**
 - Continuing improvements in efficiency are being more-than-offset by rapidly growing global demand for new power plants
- **Stabilizing the carbon dioxide-induced component of climate change is an energy problem**
- **By 2050-2100, ~ 15TW to 40TW of Carbon-neutral energy must be available if CO₂ levels are to be stabilized at 2- to 4- times pre-industrial levels**
- **Only a handful of baseload power options exist that can make a meaningful contribution to that level of generation capacity**
- **Space Solar Power (SSP) is one of those options**
- **A constellation of large Space Solar Power Satellites (SSPS) deployed in a family of geosynchronous Earth orbits has the potential to deliver 10s to 100s of Terawatts to markets worldwide**

What are the Options? Comparison of Some Baseload Power Alternatives

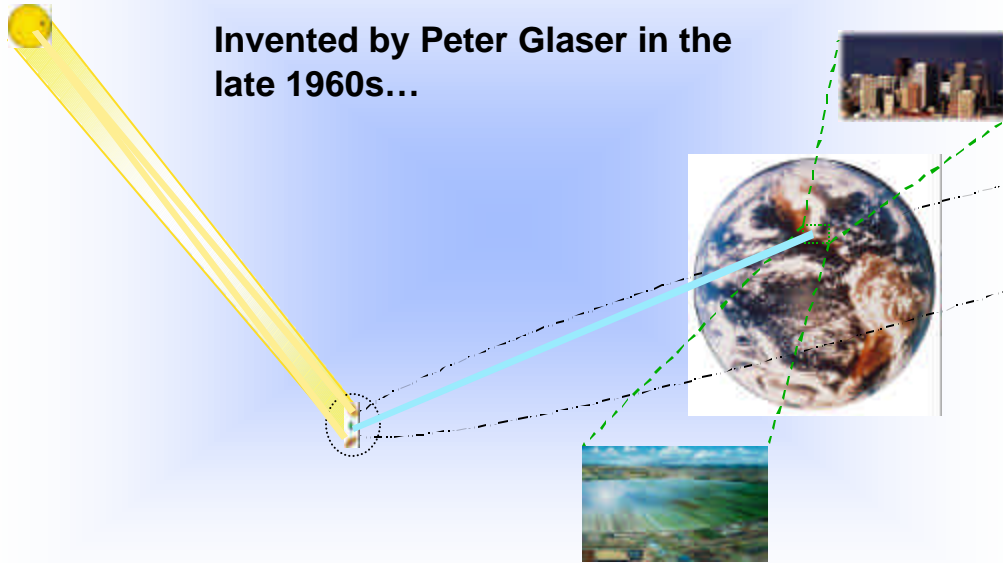


POWER CAPACITY OF GEOSYNCHRONOUS ORBITS

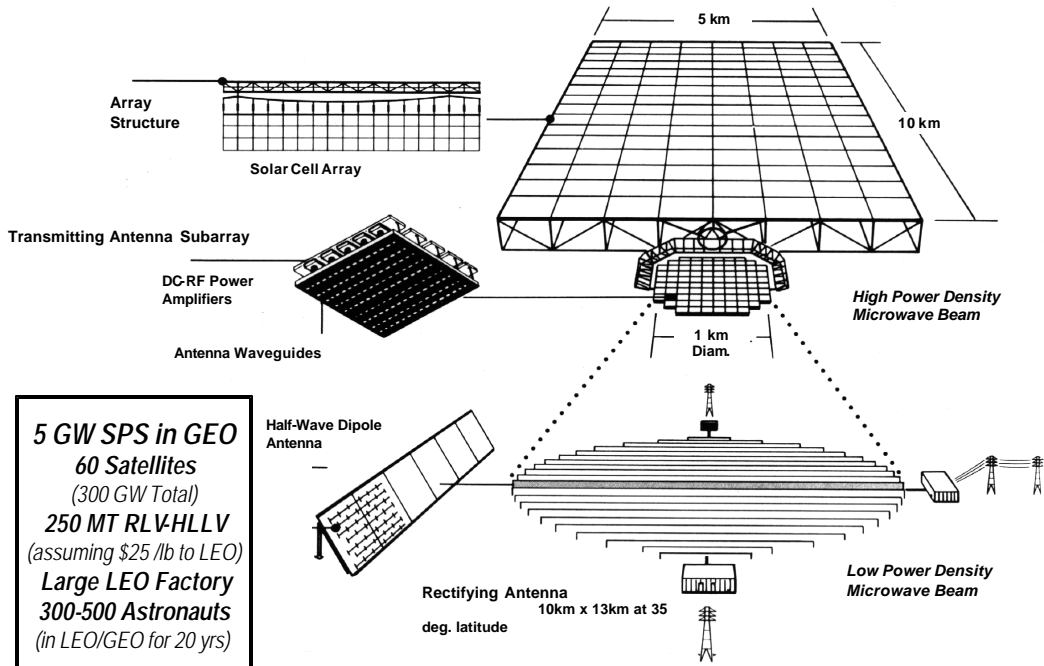
Space Solar Power Spacecraft placed into just 6 of hundreds of possible circulating "halo" orbits provide 18 Terawatts of power



Solar Power Satellites - Basic Concept

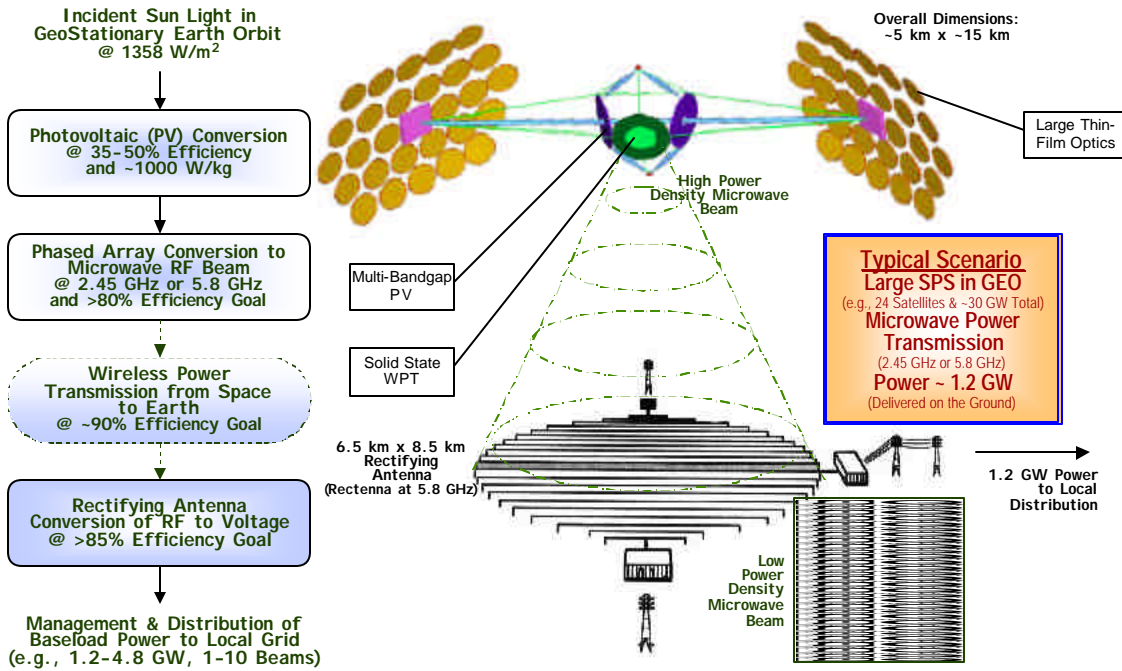


SOLAR POWER SATELLITES 1979 SPS Reference System Concept (GEO)

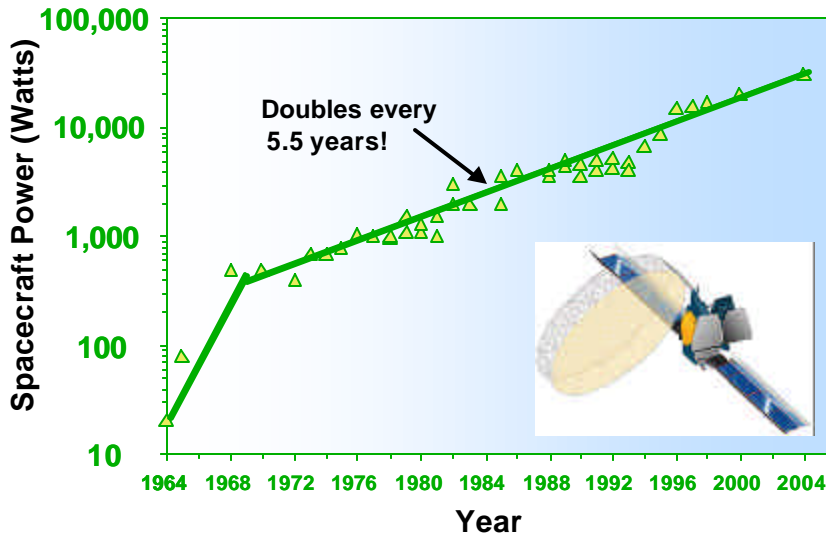


jmankins-6/97

SOLAR POWER SATELLITES 2000 Integrated Symmetrical Concentrator Concept



Space Solar Power Communications/National Security Satellite Power Trends



Courtesy of Boeing

Future National Security Needs

SBR: on critical roadmap for >25kW power needs

SBL: Increased power identified as a top enabler

NRO: > 100kW

SMC/XR (Don Gasner): >100-200kW

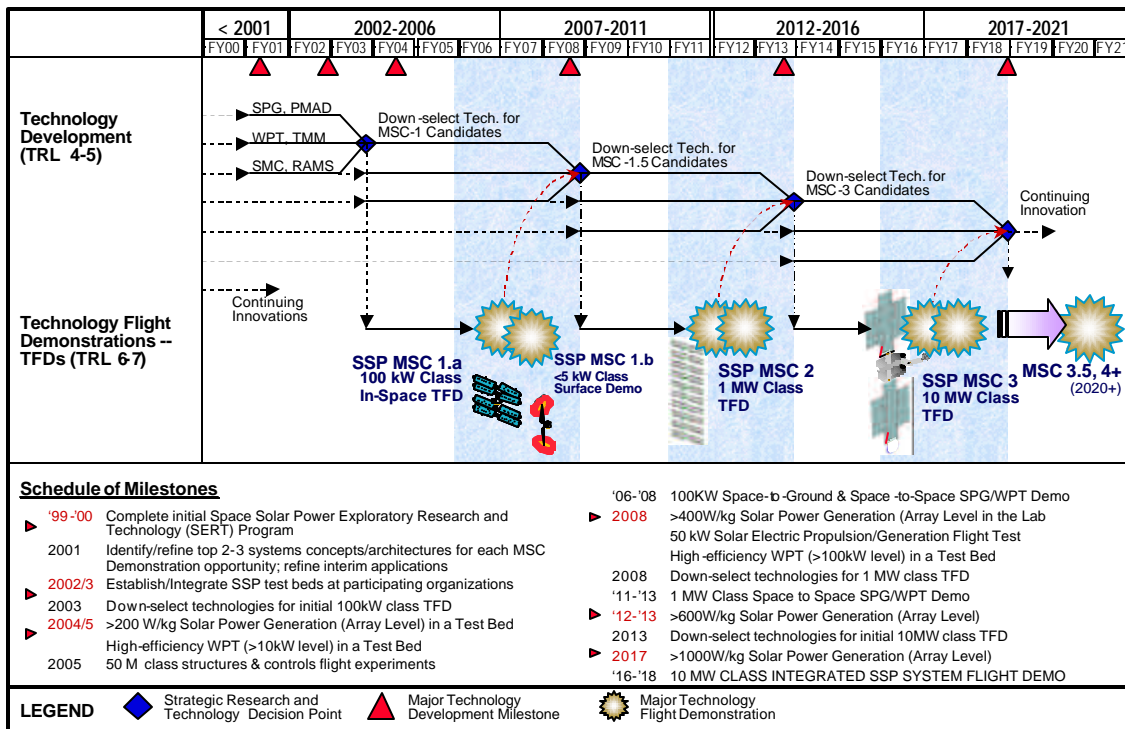
21st Century Space Mission Challenges and ... SSP Technology Areas

SPACE SOLAR POWER Technology Roadmap Areas

	Solar Power Gen.	Wireless Power Trans	Power Mgt & Dist	Structure, Matts & Controls	Thermal Mgt & Materials	Assy, Maint & Ops	Platform Systems	Ground Segment Systems	ETO Trans & Infr	In Space Trans & Infr	Environ & Safety Factors	Systems Integration
Human Health and Support											?	
Human-Machine Systems												
Information & Automation		?										
Instruments & Laboratories		?				?						
Space Transportation		?										
Space Power												
Space Platforms		?										
Surface Systems		?										
Systems Studies												

21st CENTURY SPACE MISSION
Technology Opportunities / Challenges

Space Solar Power Strategic Research & Technology Roadmap



Space Solar Power Background Results of the US NRC SSP Review (1 of 2)

- **During 2000-2001, the Aeronautics and Space Engineering Board (ASEB) of the NRC assessed the technology investment strategy of the “Space Solar Power” Program to determine its technical soundness and contributed the roadmap by...**

- Critiquing the overall technology investment strategy in terms of the plan’s likely effectiveness in meeting the program’s technical and economic objectives
- Identifying areas of highest technology investment necessary to create a competitive space-based electric power system
- Identifying opportunities for increased synergy with other research and technology efforts
- Providing an independent assessment of the adequacy of available resources for achieving the plan’s technology milestones, and
- Recommending changes in the technology investment strategy



- **Findings?**

- “SERT program has provided a credible plan for making progress toward the goal of providing space solar power for commercially competitive terrestrial electric power despite rather large technical and economic challenges
- “Current SSP technology is aimed at technical areas with important commercial, civil, and military application
- “Dedicated NASA team has defined a potentially valuable future program...
- “Current SSP program is operating on minimal budget and significantly higher funding and program stability will be necessary to attain aggressive goals of program
- “Funding plans during the first five years (leading to first flight test demonstration) are reasonable...”

Space Solar Power Background Results of the US NRC SSP Review (2 of 2)

- **Findings? (continued)**

- “Concern in committee that investment strategy is based on modeling efforts and individual mass, cost, and performance goals that may guide management toward poor investment decisions
- “Significant technical breakthroughs necessary to achieve final goal of cost-competitive terrestrial baseload power
- “Ultimate success of terrestrial power application critically depends on dramatic reductions in cost of transportation from Earth to GEO
- “Leveraging of technological advances made by organizations external to NASA must be done.”



- **The SSP R&T panel also made a series of recommendations for improving the management and focus of future program efforts, including**

- Need to prepare a formal technology plan
- Need for improvements in systems and cost modeling, including increased use of expert critique and review
- Continued use of technology flight demonstrations
- Early emphasis on environmental, health and safety issues
- Key technologies:
 - Solar Power Generation
 - Wireless Power Transmission
 - Space Power Management and Distribution
 - Assembly, Maintenance and Servicing
 - In-Space Transportation

But...

- **Despite our best efforts, we are NOT there yet...**
 - We have a better understanding of the issues and the challenges
 - We have an extensive database of options and alternatives
 - We have an strong, peer-reviewed Strategic R&T road map
 - We have made progress on many key technologies
 - Except the key area of very low cost access to space...
- **We have NOT yet gotten to clear economic viability**
 - Don't buy stock in an "SPS Start-Up Company" just yet...
- **What will a viable concept be like? -- "Concept-X"**

A Visionary Idea: "Concept-X" What Might It Be Like?

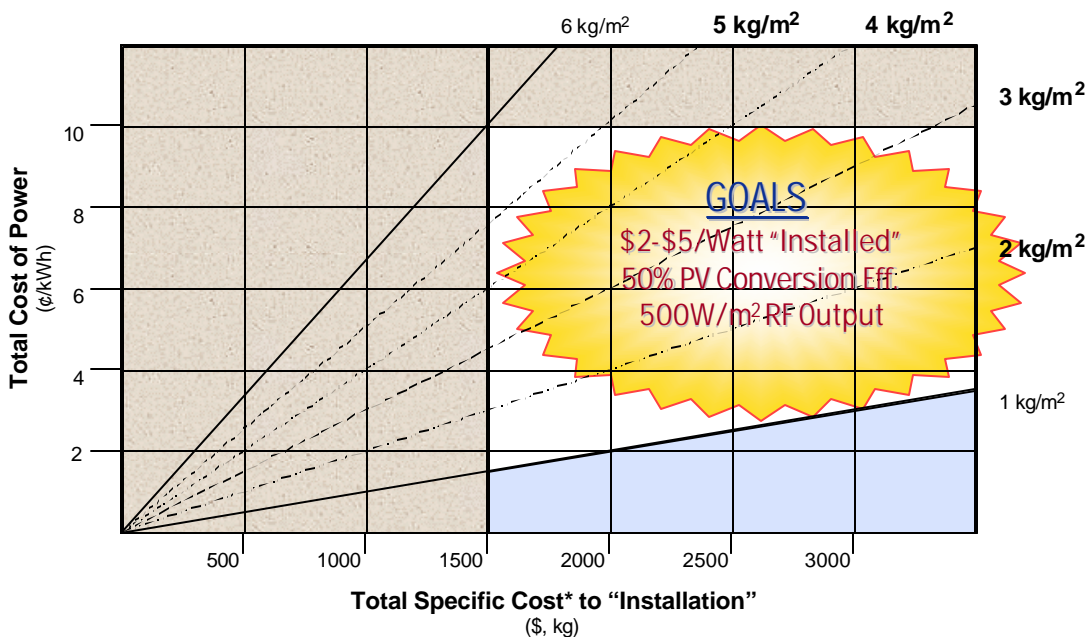
- **Most probably some version of the ISC/Sandwich approach**
 - Use of solar flux redirecting optics (e.g., large thin-film mirrors)
- **In the RF Case...***
 - Phased array must be very low mass per square meter...
 - All thermal should be local...
 - All PMAD should be local...with no converters...
 - Diameter of transmitter should be large, but send beam to multiple ground sites...
 - Reducing size of ground station
 - Find some way to avoid using a full 10:1 Gaussian distribution

* *Solar-pumped laser based concepts may also prove promising, but are not yet sufficiently mature to allow the definition of a "Concept-Y"*

A Visionary Idea: "Concept-X" What Might It Be Like?

- **Ambitious Goals must be achieved...**
 - Sandwich or ISC -like Optics (< 10% of total system mass)
 - PV Energy Conversion
 - Efficiency: > 50%
 - RF transmitter:
 - ~ 5 km diameter at 2.45 GHz (or another frequency...choice is not critical)
 - Efficiency: > 80%
 - RF Power Output per square-meter: ~ 500 W
 - Total Power Output: >10 GW
 - Ground Rectenna:
 - 10-20 stations at < 2 km diameter each (and @ < 500 MW output)
 - Cost per Receiving Station: < \$2/W

A Visionary Idea: "Concept-X" What Should We Seek to Achieve?



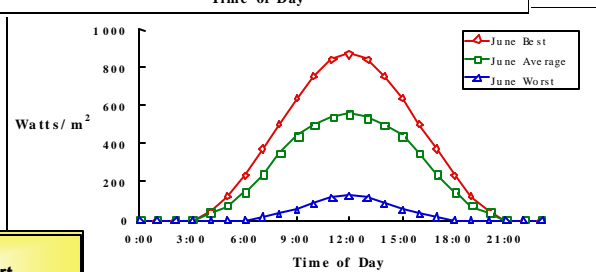
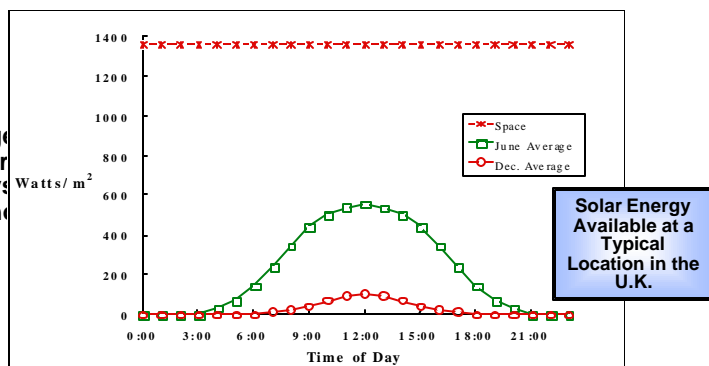
*Including cost of Money, H/W, Launch, etc....

SSP Research and Technology Some Key Directions

- **Continuing advances in / applications of intelligent systems and robotics -- pursuing the goals of self-assembly, large and self-sufficient “communities” of systems, etc.**
 - Including modular/distributed avionics -- e.g., wireless network avionics (massively redundant)
- **Higher strength-to-weight materials and structural concepts applicable in the space environment**
 - Both thin film / deployable and rigid structure / assembled
- **Higher temperature solid state devices of various types, including PV cells, FET amplifiers, phase shifters, etc.**
- **MEMS / μ -device thermal management, etc.**
- **Various Options, including**
 - Laser wireless power transmission (electric and solar-pumped)
 - High-voltage and/or HTc power management and distribution
 - Others...
- **PLUS...**
 - Very low cost space transportation

...Terrestrial Solar Power?

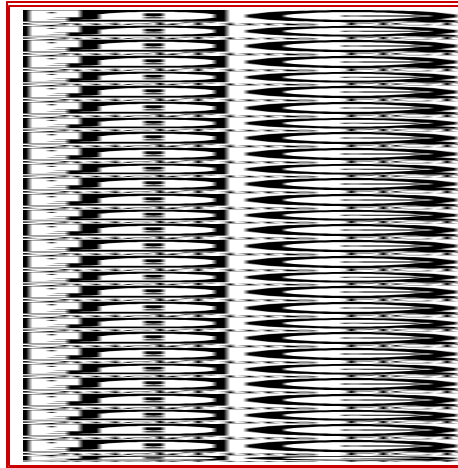
- There must be terrestrial solar...
- For baseload power, however, the challenges facing ground solar are in many ways harder than those for space-based systems
- The total solar energy available at a typical site on the Earth's surface is much less than in space
- Moreover, the energy available varies widely — seasonally and daily
- “Baseload” using ground solar requires substantial over-capacity and costly large-scale energy storage or global distribution networks...



BASIC TRADE:
WPT + Space Transport
Versus
Ground Solar + Energy Storage

...the Safety of Power Beaming?

- **There is a continuing concern regarding the health & safety issues associated electromagnetic radiation**
 - These must be treated seriously
 - At microwave frequencies, the only known physical effect on living tissue is thermal heating
- **The US Standard Limit for microwave exposure is = 100 W/m², for = 6 minutes**
- **For SSP, power densities would vary greatly across an incoming beam; a 2.45 GHz, 5 GW beam would have densities of**
 - Beam Center ~ 230 W/m²
 - Rectenna edge ~10 W/m²
 - Fence edge ~ 1 W/m²
- **Studies conducted in the late 1970s found that for exposure levels up to 500 W/m² for 30 min., there was no discernable effect on honey bee test subjects (3000 subjects, over 2 trials)**
- **Further research in 2001-2002 indicates no effect on plants “outside the fence”**
- **Further research required to ensure that any possible health factors associated to SSP/WPT (people and animals) were within acceptable limits**



Summary

- **Space solar power appears to be a technically-viable option capable of delivering large (>100's GW) essentially carbon-free electrical power globally**
 - No issues with any areas of fundamental physics
- **Significant advances have been made since the 1970s**
 - Concepts
 - Technology
 - Infrastructure
- **Technology developments needed in a number of areas...**
 - Materials, structures, devices, autonomy, robotics, others
- **Strategic R&T road maps for SSP have been developed and reviewed by the National Research Council**
 - “SSP technology ... aimed at technical areas with important commercial, civil, and military application
 - “... a potentially valuable future program...”
 - “... significantly higher funding and program stability ... necessary
 - “Funding plans during the first five years (leading to first flight test demonstration) are reasonable...”

Topical Team Summary

Energy Biosciences Research

Energy Biosciences Research

Topical Team

Mark Alper, LBNL
Heinz Frei, LBNL
Evan Hughes, EPRI
Laurie Mets, Univ. Chicago
John Shanklin, BNL
Chris Somerville, Stanford Univ.
Walt Stevens, BES
Lut De Jonghe, UCB

Other Attendees:

John Stringer, EPRI
Linda Horton, ORNL

October Workshop Suggested Need for Additional Discussion of Opportunities related to Biological Energy Research

- Team workshop held on January 13-14, 2003 in Palo Alto
- Presentations included:
 - World energy situation (Stringer)
 - Results from the October Workshop (Horton)
 - Current BES Biosciences research program (Stevens)
- Proposed Research Directions from the October workshop were included in the discussions
 - Renewable Energy; Transportation; Industrial Residential, Commercial; Distributed Energy

Proposed Research Directions

- Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Fuels and Chemicals
- Genomic Tools for the Development of Designer Energy and Chemical Crops
- Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Fuels and Chemicals

- Increase the efficiency of biomass production by plants by metabolic engineering
 - Control plant architecture and composition (lignin, cellulose, hemicellulose, starch and oils)
 - Enzyme design, metabolic modeling, and rational pathway engineering
- Increase the efficiency of microbial conversion of biomass to fuels and chemicals
 - Improved microbial biocatalysts
 - Understanding of the fundamental chemical and physical processes of fractionation and solubilization

100-Fold Increase in Contribution of Renewable Biomass

Genomic Tools for the Development of Designer Energy and Chemical Crops

- High yields of 3 to 5 times current energy crops are needed for economic viability and a major role for biomass energy
- High energy density and properties compatible for manufacturing the final product are critical
- Emerging genomic tools will enable high yields and other desirable properties within 10-20 years
 - Identify key genes that determine yields and important plant properties
 - Use genomic tools to breed plants that can be directly integrated into the energy conversion process (improve efficiency, cost effectiveness, etc.)
- Example genomic tools to be developed include single DNA molecule sequencing and mapping, improved bioinformatics for marker assisted breeding

Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

- Nanoporous inorganic, organic, and biochemical hybrid structures
 - Efficient synthesis of fuels (hydrogen, methanol) from renewable sources (water, CO₂) using sunlight energy
 - Efficient photochemical energy storage
- Self assembly using the principles of molecular recognition
- Strategies for organizing nanoscale assemblies relative to one another to achieve concerted, macro-scale effects
- Dynamic analysis for time-resolved spectroscopy, diffractometry, computational approaches and molecular genetics