Basic Energy Sciences Solar Energy

Challenges and Opportunities

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for
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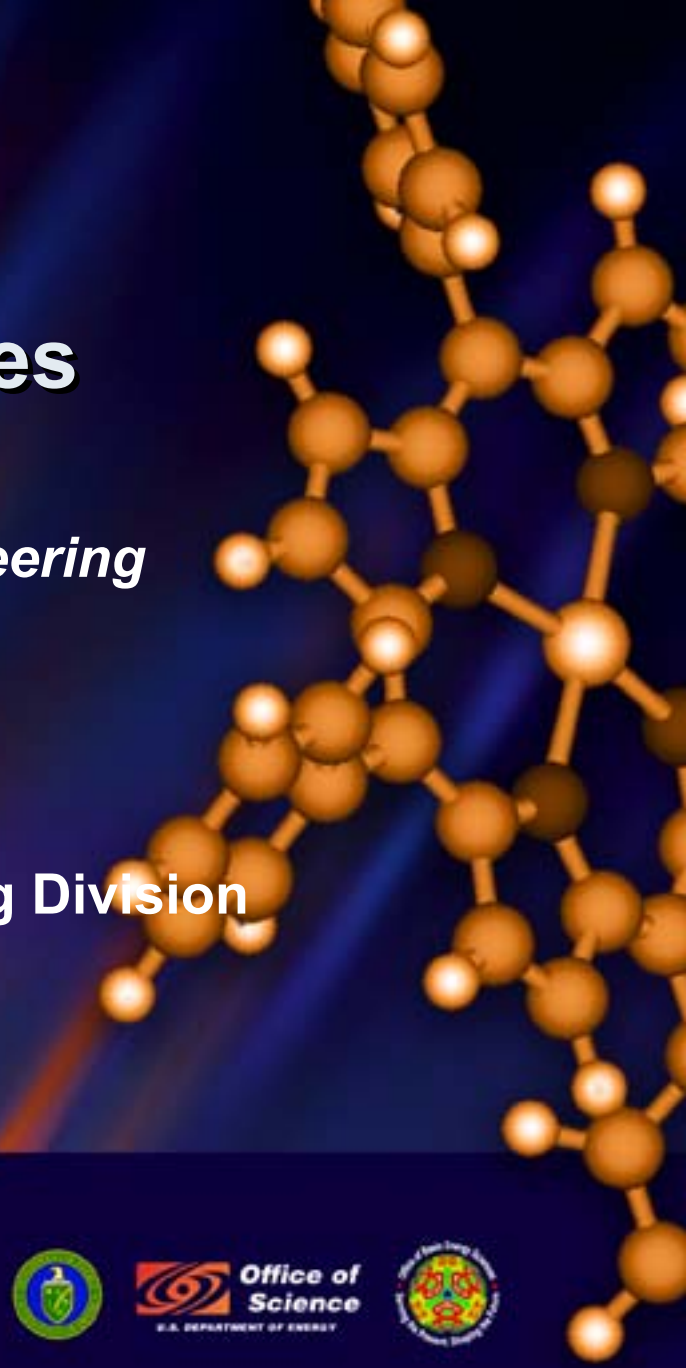
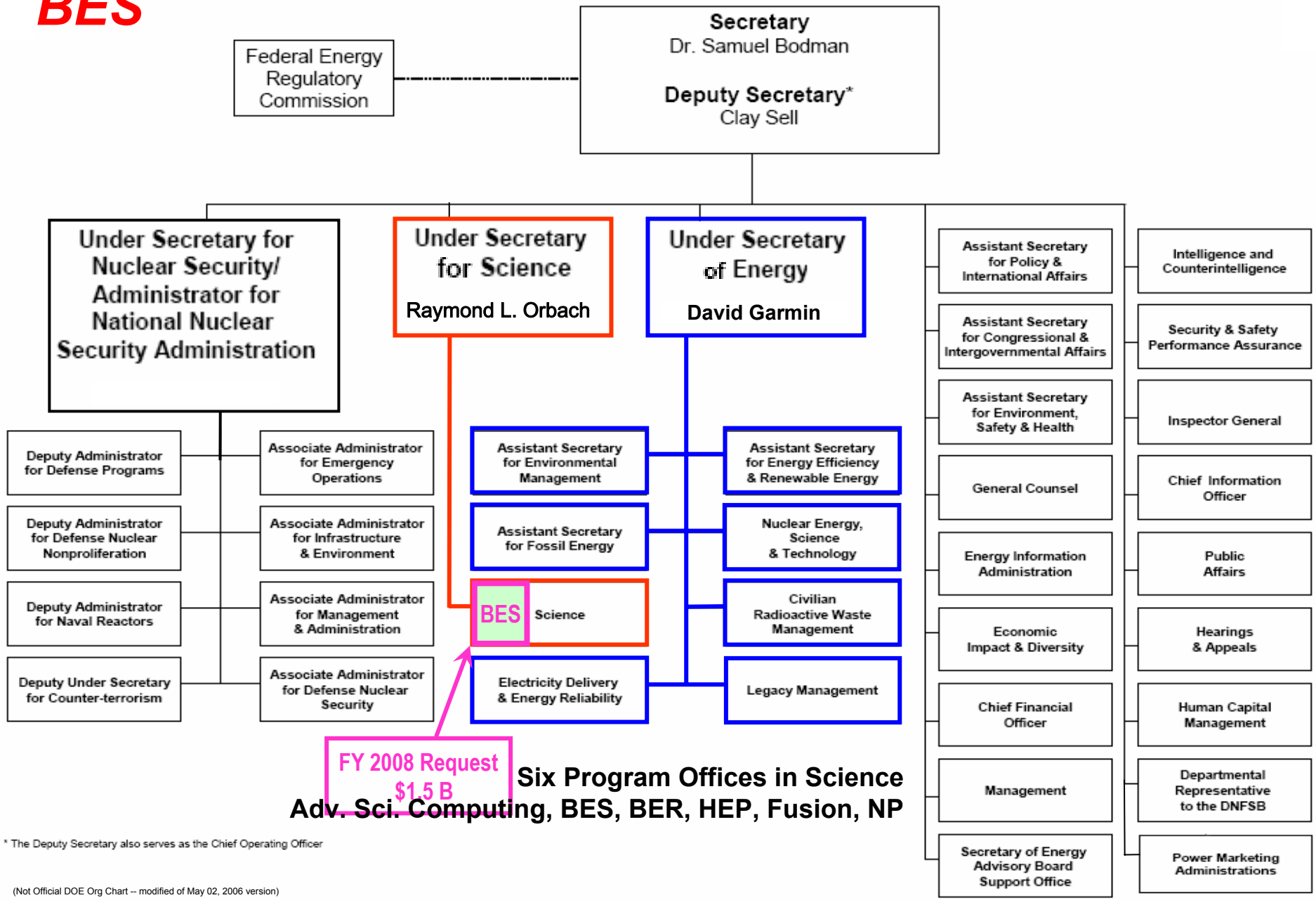


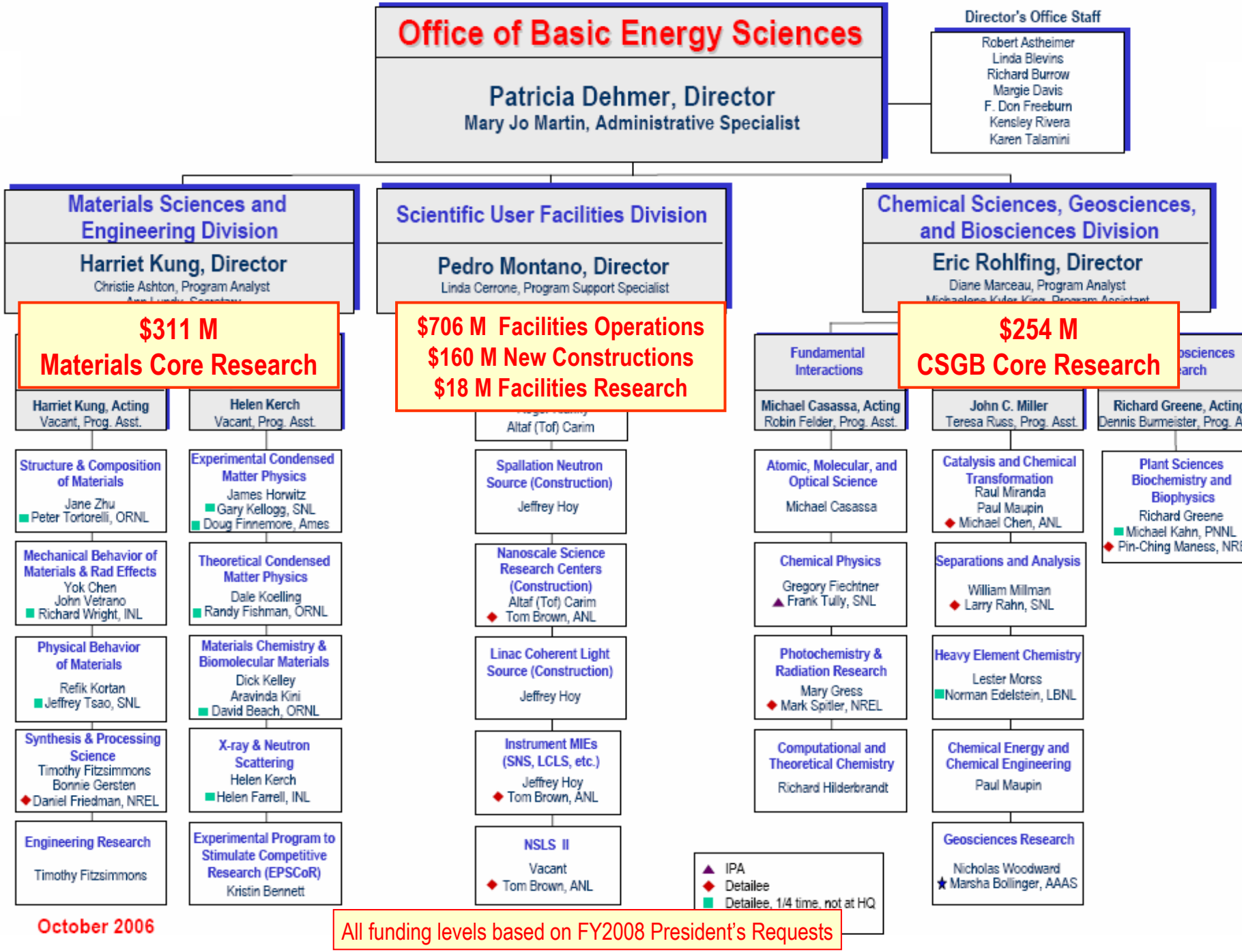
Office of Science
U.S. DEPARTMENT OF ENERGY

The Department of Energy: Office of Science and BES



* The Deputy Secretary also serves as the Chief Operating Officer

(Not Official DOE Org Chart -- modified of May 02, 2006 version)


Office of Basic Energy Sciences
Patricia Dehmer, Director
Mary Jo Martin, Administrative Specialist
Director's Office Staff
Robert Astheimer
Linda Blevins
Richard Burrow
Margie Davis
F. Don Freeburn
Kensley Rivera
Karen Talamini
Materials Sciences and Engineering Division
Harriet Kung, Director
Christie Ashton, Program Analyst
$311 M
Materials Core Research
Scientific User Facilities Division
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Linda Cerrone, Program Support Specialist
$706 M Facilities Operations
$160 M New Constructions
$18 M Facilities Research
Chemical Sciences, Geosciences, and Biosciences Division
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Diane Marceau, Program Analyst
$254 M
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Helen Kerch
Vacant, Prog. Asst.
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Peter Tortorelli, ORNL
Mechanical Behavior of Materials & Rad Effects
Yok Chen
John Vetrano
Richard Wright, INL
Physical Behavior of Materials
Refik Kortan
Jeffrey Tsao, SNL
Synthesis & Processing Science
Timothy Fitzsimmons
Bonnie Gersten
Daniel Friedman, NREL
Engineering Research
Timothy Fitzsimmons
Experimental Condensed Matter Physics
James Horwitz
Gary Kellogg, SNL
Doug Finnemore, Ames
Theoretical Condensed Matter Physics
Dale Koelling
Randy Fishman, ORNL
Materials Chemistry & Biomolecular Materials
Dick Kelley
Aravinda Kini
David Beach, ORNL
X-ray & Neutron Scattering
Helen Kerch
Helen Farrell, INL
Experimental Program to Stimulate Competitive Research (EPSCoR)
Kristin Bennett
Altaf (Tof) Carim
Spallation Neutron Source (Construction)
Jeffrey Hoy
Nanoscale Science Research Centers (Construction)
Altaf (Tof) Carim
Tom Brown, ANL
Linac Coherent Light Source (Construction)
Jeffrey Hoy
Instrument MIEs (SNS, LCLS, etc.)
Jeffrey Hoy
Tom Brown, ANL
NSLS II
Vacant
Tom Brown, ANL
Fundamental Interactions
Michael Casassa, Acting
Robin Felder, Prog. Asst.
John C. Miller
Teresa Russ, Prog. Asst.
Richard Greene, Acting
Dennis Burmeister, Prog. Asst
Atomic, Molecular, and Optical Science
Michael Casassa
Chemical Physics
Gregory Fiechtner
Frank Tully, SNL
Photochemistry & Radiation Research
Mary Gress
Mark Spitler, NREL
Computational and Theoretical Chemistry
Richard Hilderbrandt
Catalysis and Chemical Transformation
Raul Miranda
Paul Maupin
Michael Chen, ANL
Separations and Analysis
William Millman
Larry Rahn, SNL
Heavy Element Chemistry
Lester Morss
Norman Edelstein, LBNL
Chemical Energy and Chemical Engineering
Paul Maupin
Geosciences Research
Nicholas Woodward
Marsha Bollinger, AAAS
Plant Sciences Biochemistry and Biophysics
Richard Greene
Michael Kahn, PNNL
Pin-Ching Maness, NREL
IPA
Detailee
Detailee, 1/4 time, not at HQ
October 2006
All funding levels based on FY2008 President's Requests

Basic Energy Sciences

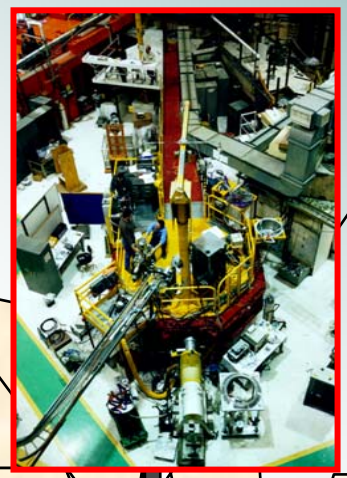
- The Basic Energy Sciences (BES) program supports fundamental research in focused areas of the natural sciences in order to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use.

- BES also supports work that creates knowledge and develops tools to strengthen national security. The BES program plans, constructs, and operates major scientific user facilities to serve researchers from universities, national laboratories, and private institutions.

BES Neutron and X-ray Scattering User Facilities Characterizing Nanoscale Materials for Energy Applications

Advanced Photon Source

Intense Pulsed Neutron Source



National Synchrotron Light Source

Advanced Light Source

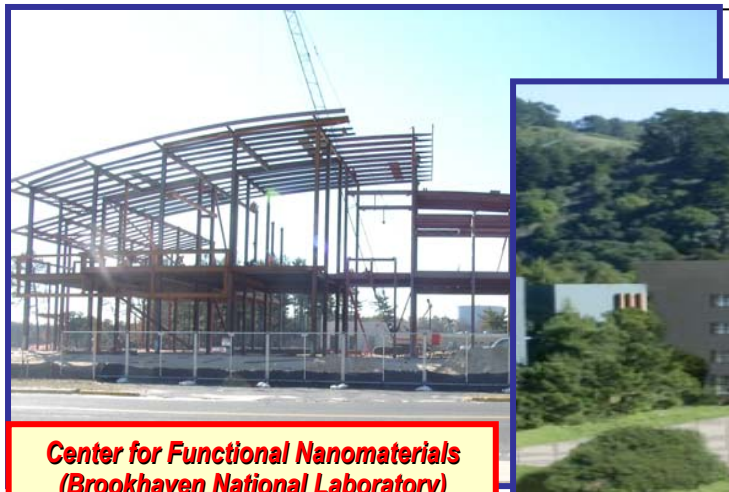
Stanford Synchrotron Radiation Laboratory

Manuel Lujan Jr. Neutron Scattering Center

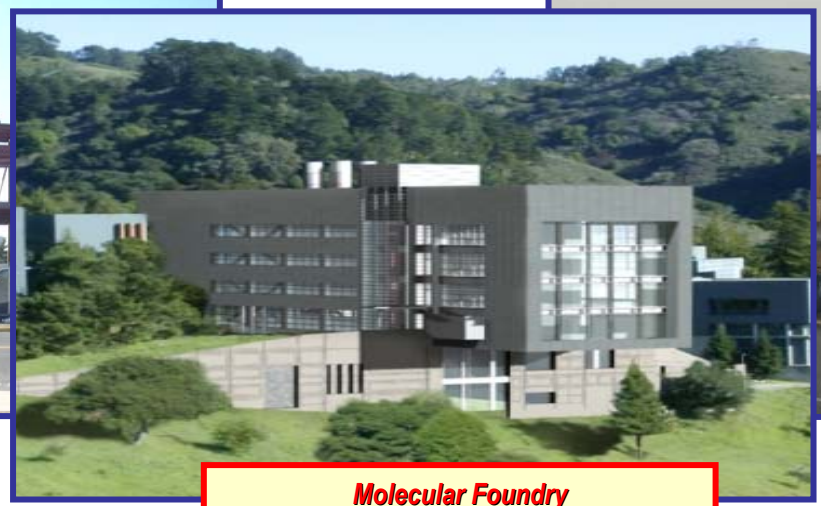
High-Flux Isotope Reactor

Spallation Neutron Source

DOE Nanoscale Science Research Centers



Center for Functional Nanomaterials
(Brookhaven National Laboratory)



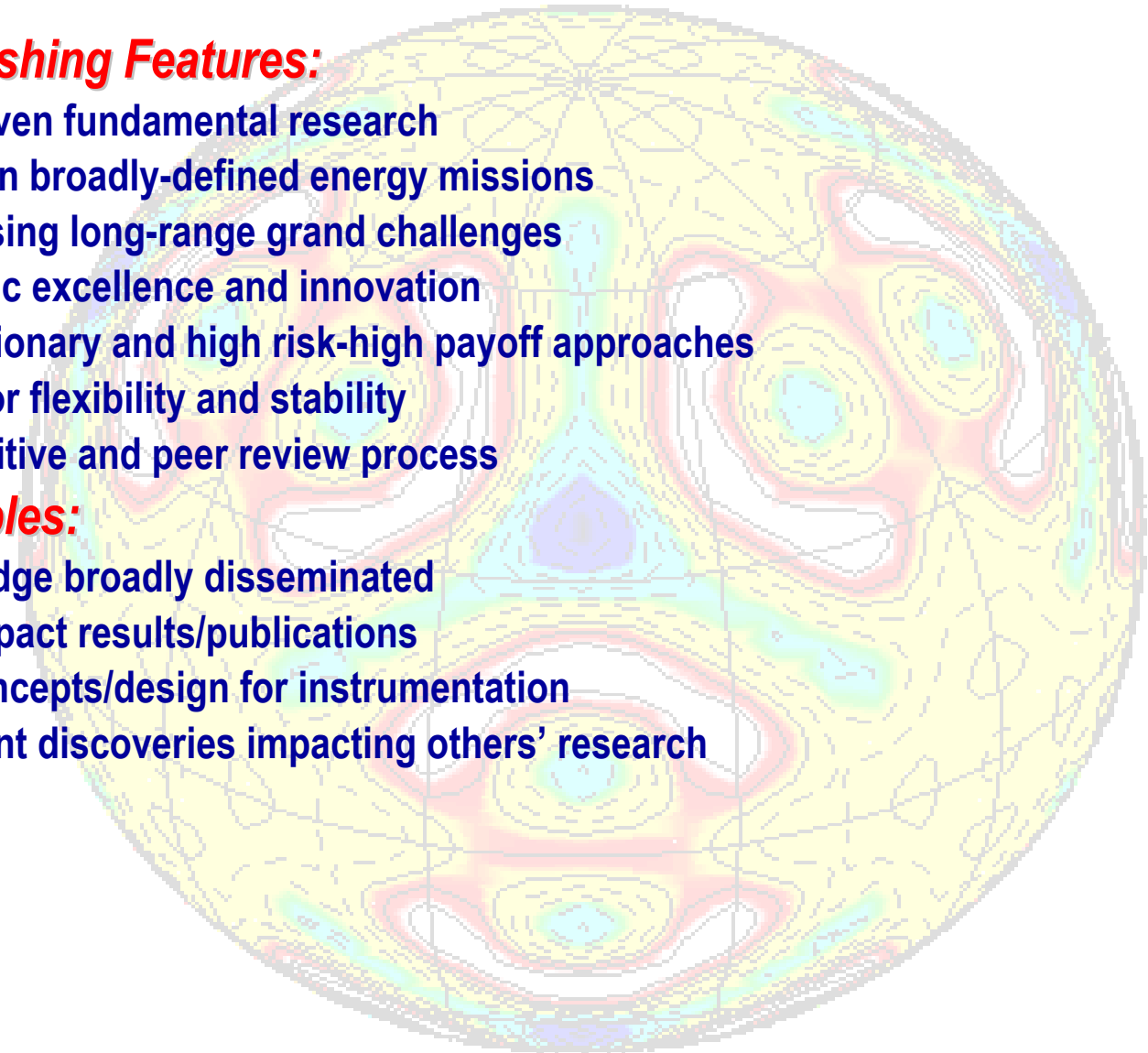
Molecular Foundry
(Lawrence Berkeley National Laboratory)

Center for Nanoscale Materials
(Argonne National Laboratory)

Center for Nanophase Materials Sciences
(Oak Ridge National Laboratory)

Center for Integrated Nanotechnologies (Sandia & Los Alamos National Labs)

BES Research Portfolio



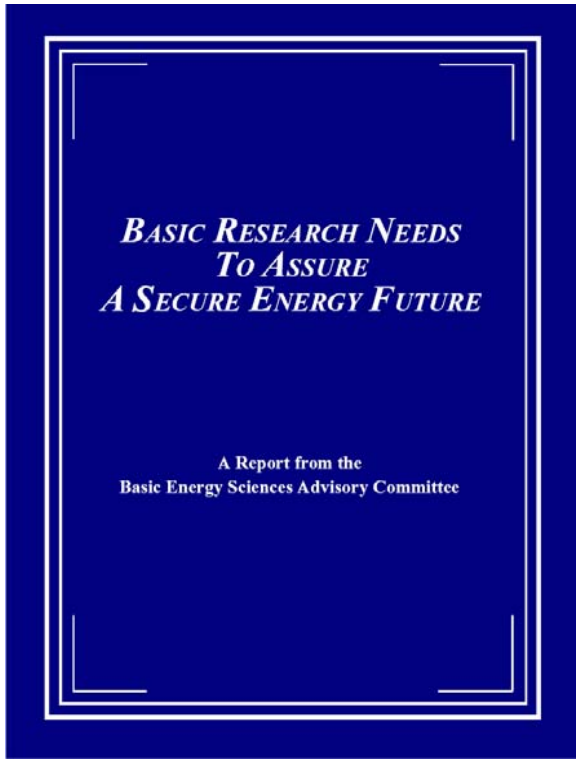
Distinguishing Features:

- Idea-driven fundamental research
- Underpin broadly-defined energy missions
- Addressing long-range grand challenges
- Scientific excellence and innovation
- Revolutionary and high risk-high payoff approaches
- Strive for flexibility and stability
- Competitive and peer review process

Deliverables:

- Knowledge broadly disseminated
- High impact results/publications
- New concepts/design for instrumentation
- Important discoveries impacting others' research

BESAC Energy Security Plan

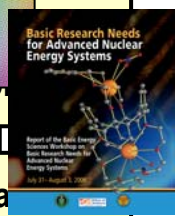


"Considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved."

A Comprehensive Decades-to-Century Energy Security Plan





Research for a Secure Energy Future

Supply, Distribution, Consumption, and Carbon Management

Decision Science and Complex Systems Science

nergy

Carbon Management

No-net-carbon Energy Sources

Distribution/ Storage

Energy Consumption

Energy Conservation, Energy Efficiency, and Environmental Stewardship

Natura

CO_2 Sequestration

- Geologic
- Terrestrial
- Oceanic

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Nuclear Fission

Nuclear Fusion

Renewables

- Hydropower
- Biomass
- Geothermal
- Wind
- Solar
- Ocean

Electric Grid

Electric Storage

Hydrogen

Alternate Fuels

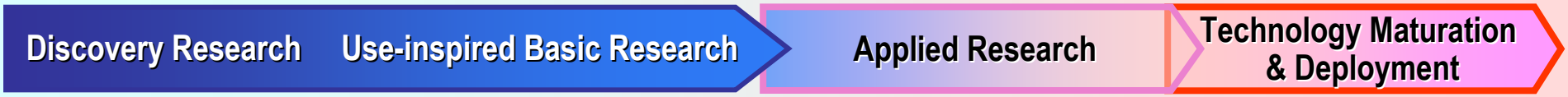
Transportation

Buildings

Industry

- Combustion Alternate Fuels (Oct 30 - Nov. 1 2006)
- Electric Storage (April 2-4, 2007)
- Materials under Extreme Environments June 2007
- Geosciences (FY 2007)
- Catalysis (FY 2007)

Relationships Between the Science and the Technology Offices in DOE



DOE Office of Science BES

- Basic research for fundamental new understanding (i.e., science grand challenges) on materials or systems that may be only peripherally connected or even unconnected to today's problems in energy technologies
- Development of new tools, techniques, and facilities, including those for advanced modeling and computation
- Basic research for fundamental new understanding, with the goal of addressing short-term showstoppers on real-world applications in the energy technologies

Goal:	new knowledge / understanding
Mandate:	open-ended
Focus:	phenomena
Metric:	knowledge generation

DOE Applied Energy Offices EERE, NE, FE, OE, EM, RW, …

- Research with the goal of meeting ***technical milestones***, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Proof of technology concepts
- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

Goal:	practical targets
Mandate:	restricted to target
Focus:	performance
Metric:	milestone achievement

BES Workshop on Basic Research Needs for Solar Energy Utilization

April 21-24, 2005

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

Panel Chairs

Arthur Nozik, NREL: Solar Electric
Mike Wasielewski, NU: Solar Fuel
Paul Alivisatos, UC-Berkeley: Solar Thermal

Topics

Photovoltaics
Photoelectrochemistry
Bio-inspired Photochemistry
Natural Photosynthetic Systems
Photocatalytic Reactions
Bio Fuels
Heat Conversion & Utilization
Elementary Processes
Materials Synthesis
New Tools

Plenary Speakers

Pat Dehmer, DOE/BES
Nathan Lewis, Caltech
Jeff Mazer, DOE/EERE
Marty Hoffert, NYU
Tom Feist, GE

200 participants

universities, national labs, industry
US, Europe, Asia
EERE, SC, BES

Charge

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

Solar Energy Challenges

Solar electric

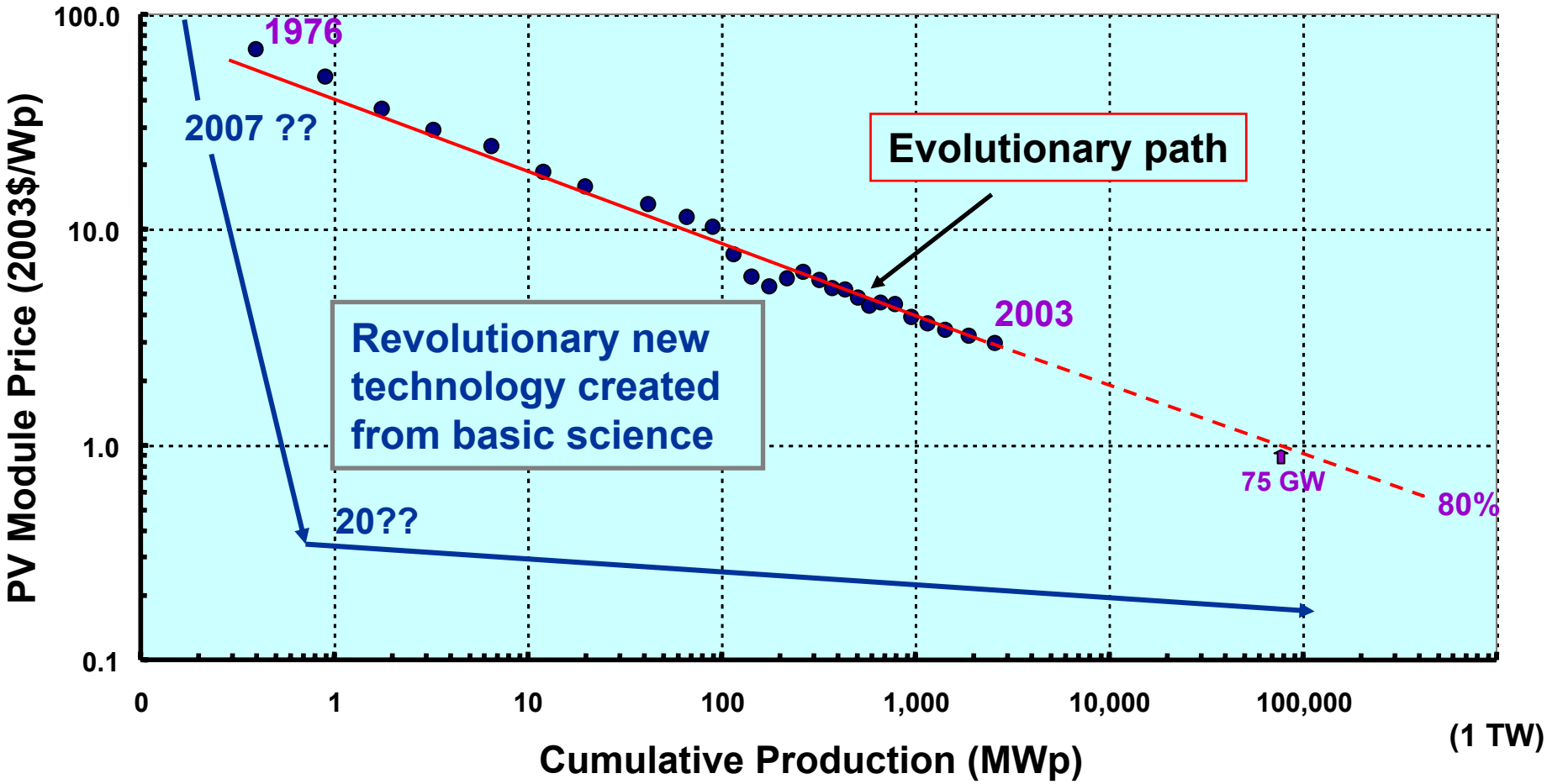
Solar fuels

Solar thermal

Cross-cutting research

Basic Scientific Challenges

Basic science to produce ***new unknown technologies***



13 Proposed Research Directions from BES Solar Energy Utilization Workshop

1. ***Revolutionary evolutionary photovoltaic devices ; 50% efficient solar cells***
2. ***Maximum energy from solar photons at low cost: Designed plastic photovoltaic structures***
3. ***Nanostructures for solar energy conversion: Low cost and high efficiencies***
4. Fuels from water and sunlight: New Photo-electrodes for efficient photo-electrolysis
5. Leveraging photosynthesis for sustainable solar production of biofuels
6. Using bio-inspired smart matrix to optimize energy landscapes for solar fuels production
7. Solar-powered catalysts for energy-rich fuels formation
8. Bio-inspired molecular assemblies for integrating photon to fuels pathways
9. ***Achieving defect tolerant and self repairing solar conversion systems***
10. Solar thermochemical fuel production
11. ***New experimental and theoretical tools to enable transformational research***
12. ***Solar energy conversion materials by design***
13. ***Materials architectures for solar energy: assembling complex structures***

Solar-to-Electric Conversion

Discovery Research

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

Use-inspired Basic Research

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

BES

Applied Research

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

Technology Maturation & Deployment

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

EERE

Solar-to-Fuels Conversion

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

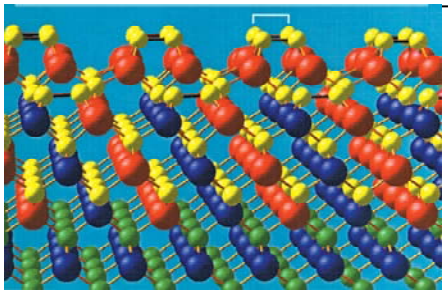
- Novel photoelectrode materials and molecular configurations for efficient photoelectrolysis
- Biomimetic multi-electron catalysts and proton-coupled electron transfer for solar water splitting
- Photocatalytic cycles for CO_2 reduction to alcohol fuels
- Multi-scale control of reactivity in hybrid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

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

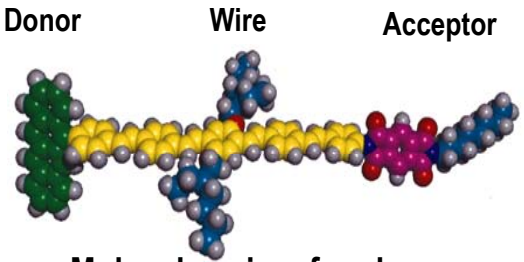
- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

BES | **EERE**

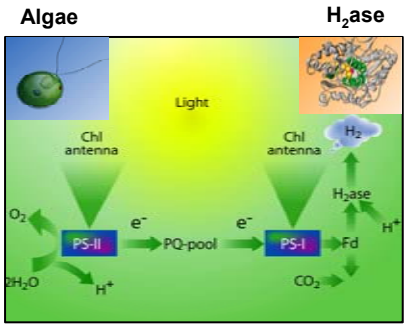
BES-Supported Research Related to Solar Energy Conversion



Ordering in GaInP modified band structure



Molecular wires for charge separation



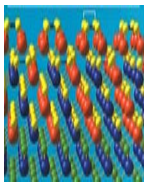
Enzymes in green algae convert water and light to hydrogen

Goal: To Obtain a fundamental understanding of atomic/molecular level interactions and reactions associated with solar energy conversion to electricity and fuels.

Major areas of current research:

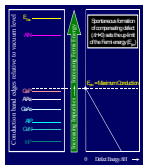
- **First-principles design of photoconversion materials**
- **Semiconductor physics and defects in III-V compounds**
- **Organic and inorganic photochemistry**
- **Electron and energy transfer in the condensed phase**
- **Molecular mechanisms in plants that convert solar energy into biomass and other chemical fuels**
- **Biomimetic synthetic assemblies for artificial photosynthesis**

BES/DMSE research support impacting solar technologies at NREL

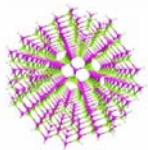


- **Properties of novel ordered semiconductor alloys:** Understanding the origin and effects of spontaneous long-range ordering in semiconductor alloys leads to world record → 40% efficient solar cells

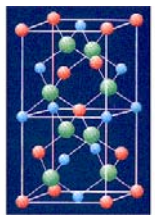
- **Isoelectronic alloys:** For 4-junction solar cells, how does one obtain a 1eV absorber lattice matched to GaAs? Dilute isoelectronic alloys offer the possibility of achieving this but these alloys are abnormal. Need to decipher the science underlying this abnormality



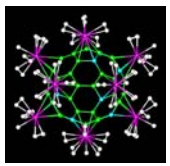
- **Overcoming the doping limits in semiconductors:** Develop microscopic models to understand the physics of doping bottlenecks in photovoltaic materials



- **Theory of energy-related nano materials:** Predict optical and electrical properties of nanocrystals (dots, wires, wells) suitable for energy-related applications



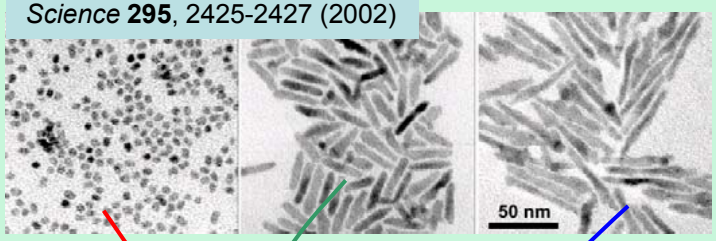
- **Polycrystalline PV materials:** Calculate effects of defects and grain boundaries on material properties which are difficult to measure: impacts thin-film PV materials.

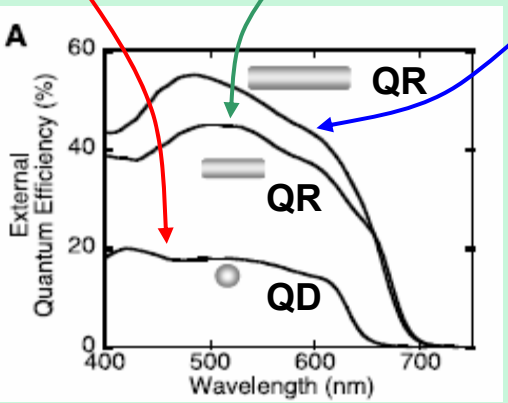


- **Theoretical study of carbon nanotubes:** for energy related applications in areas such as transparent conducting oxides and solar cells

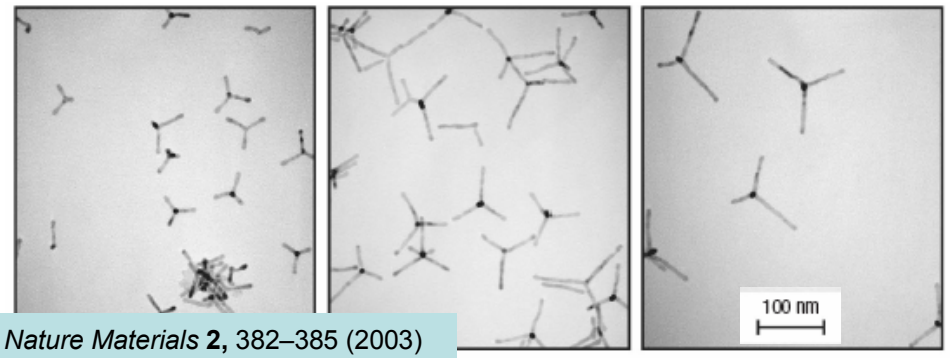
Nanocrystal Shape Control Boosts Efficiency of New Solar Cells

Science **295**, 2425-2427 (2002)



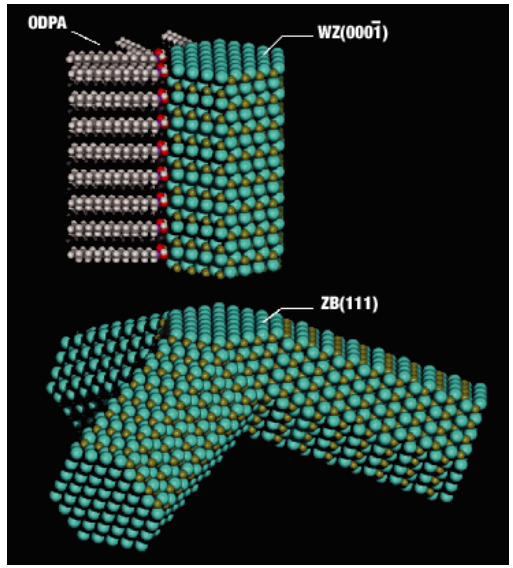


CdSe

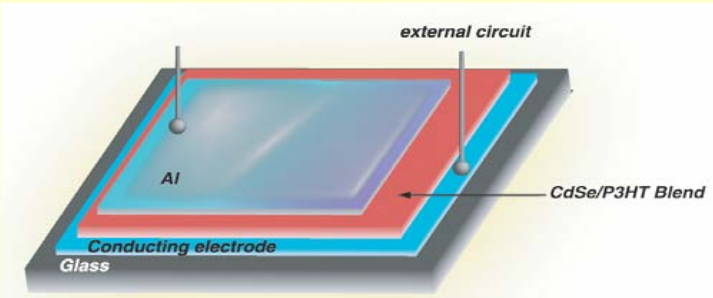


Nature Materials **2,** 382–385 (2003)

CdTe tetrapods

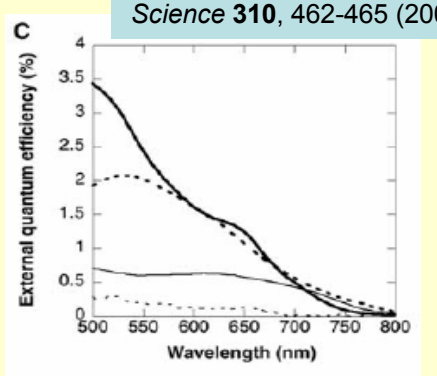


*Growth rates of two crystalline phases of CdTe are balanced to grow tetrapods. The zinc blend (ZB) phase nucleates initially, but the faster growing wurtzite phase continues the growth, resulting in a **tetrapod shape**.*



Organic/Inorganic Blended Cell

Science **310**, 462-465 (2005)

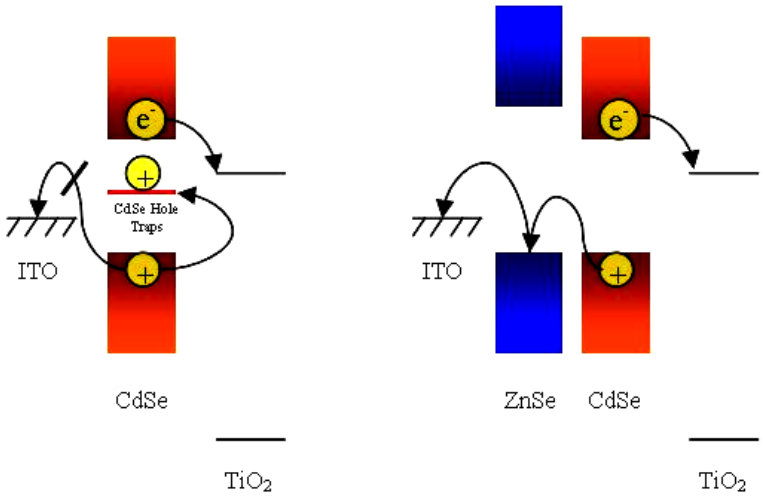


All-Inorganic Cell

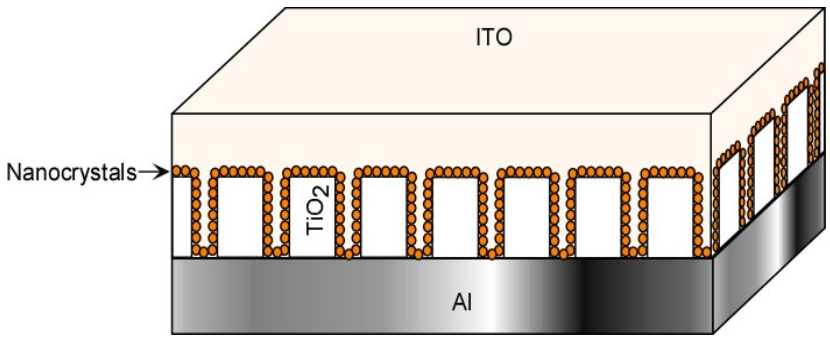
A. P. Alivisatos *et al.* (LBNL)

Nanostructured Photovoltaics or Quantum Dots That Produce White Light

Designing Materials with Minimal Carrier Loss for Use in Nanocrystal Photovoltaics



Rosenthal, Vanderbilt University



J. Am. Chem. Soc., **ASAP Article** 10.1021/ja055470d
S0002-7863(05)05470-3
Web Release Date: October 18, 2005

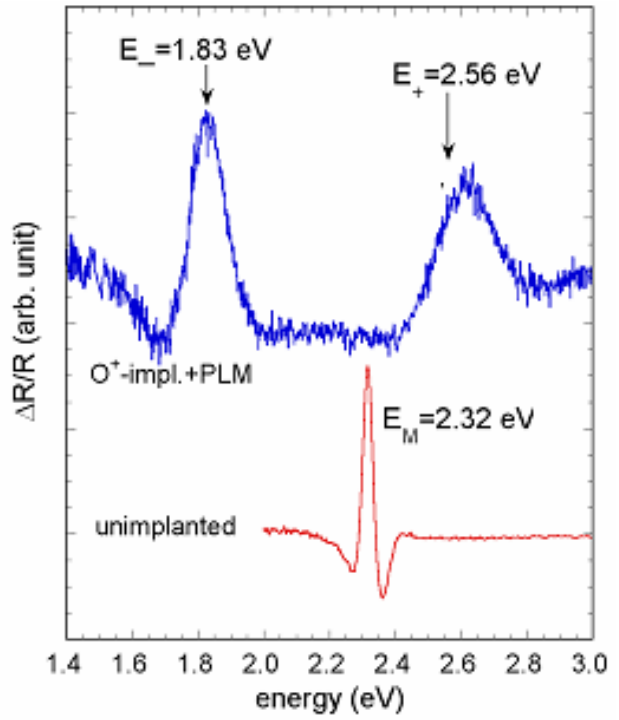
White-Light Emission from Magic-Sized Cadmium Selenide Nanocrystals

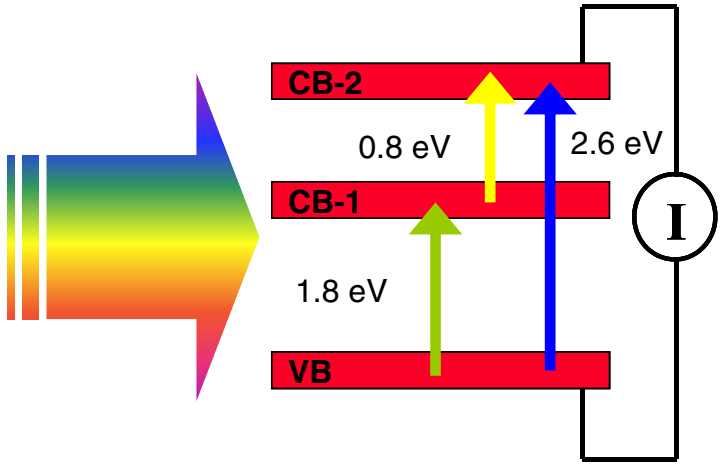
Michael J. Bowers II, James R. McBride, and Sandra J. Rosenthal*
Department of Chemistry, Vanderbilt University, Nashville, Tennessee 37235
sandra.j.rosenthal@vanderbilt.edu
Received August 22, 2005

Abstract:
Magic-sized cadmium selenide (CdSe) nanocrystals have been pyrolytically synthesized. These ultra-small nanocrystals exhibit broadband emission (420-710 nm) that covers most of the visible spectrum while not suffering from self absorption. This behavior is a direct result of the extremely narrow size distribution and unusually large Stokes shift (40-50 nm). The intrinsic properties of these ultra-small nanocrystals make them an ideal material for applications in solid state lighting and also the perfect platform to study the molecule-to-nanocrystal transition.

Multi-Band Semiconductor Synthesis for High Efficiency Solar Cells

Phys. Rev. Lett. **91**, 246403 (2003)

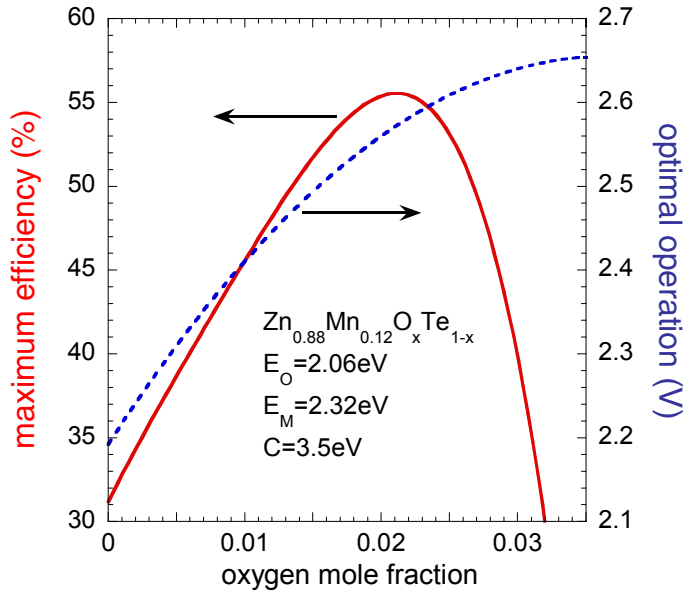




Band diagram of multiband semiconductor. Solar radiation can induce transitions between VB and CB-2 or CB-2. Absorption at 0.8 eV excites electron from CB-1 to CB-2.

Optical reflectance data demonstrates synthesis of a multiband semiconductor.

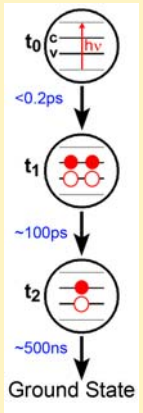
$Zn_{0.88}Mn_{0.12}Te$ has a band gap of 2.32 eV (red trace). Replacement of a small fraction of the Te atoms by O splits that band into two (blue trace).



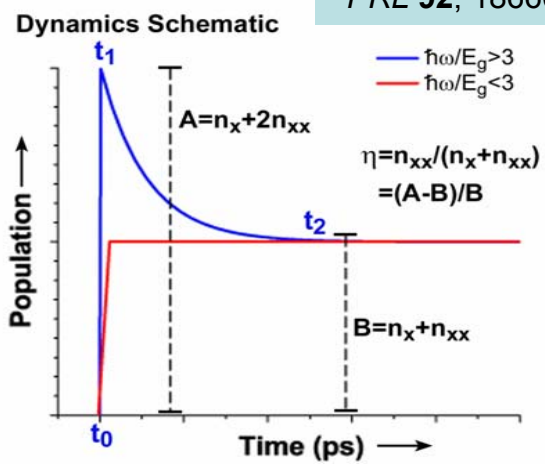
Optimization calculations predict an ultimate efficiency for this 3-band design of over 50%. The operating voltage can be controlled, as well, by adjusting the positions of the three bands by appropriate alloying.

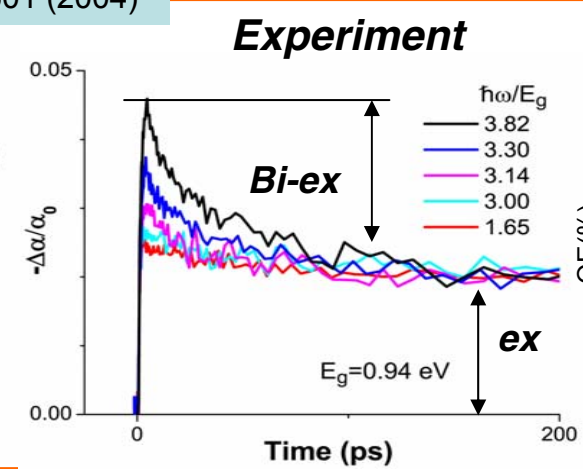
K. M. Yu, W . Walukiewicz *et al.* (LBNL)

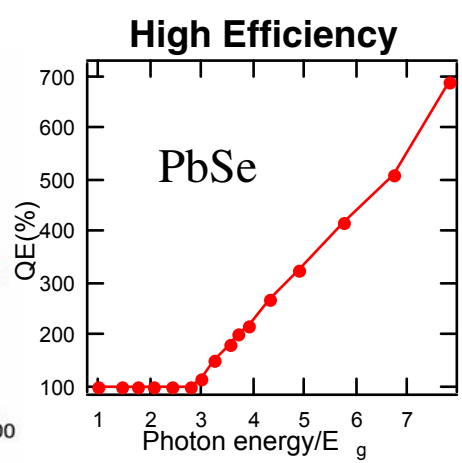
Exciton Multiplication in Semiconductor Nanocrystals



PRL **92**, 186601 (2004)





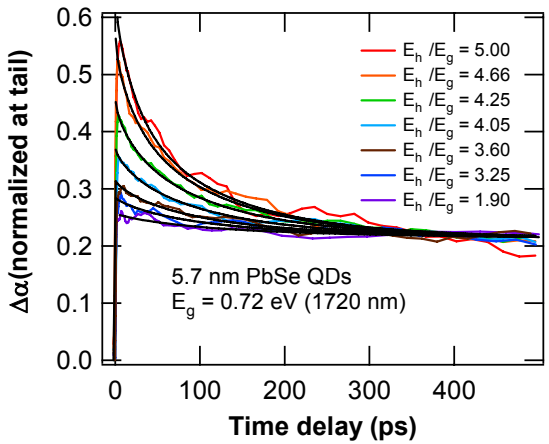


- Generality: PbSe and CdSe nanocrystals (*Appl. Phys. Lett.* **In Press**)
- 700% Efficiency in PbSe, 160% in CdSe
- Mechanism: instantaneous generation of multiexcitons via *virtual* single exciton states (*Nature Physics* **In Press**)

V. I. Klimov *et al.* (LANL)

- PbSe and PbS nanocrystals, QY of 300% at 4 E_g
- Proposed new model based on coherent superposition of quantum states

Nano Lett. 5, 865 (2004)



Solar H_2 Production

Strategy based on both **multiple exciton generation** and **singlet fission** (molecular analog of multiple exciton generation).

Proposed efficient carrier multiplication in QDs, to be utilized in QD-polymer blend or QD-sensitized TiO_2 solar cells

Ann. Rev. Phys. Chem. **52**, 193 (2001)

A. J. Nozik *et al.* (NREL)

Notice 06-15: Basic Research for Solar Energy Utilization

- Solar to electric conversion
  - Category 1: New concepts in solar electric conversion
  - Category 2: Organic and hybrid organic/inorganic conversion systems
  - Category 3: Photoelectrochemical solar cells
- Solar fuels production
  - Category 4: Natural photosynthetic systems
  - Category 5: Bioinspired molecular assemblies
  - Category 6: Defect tolerant and self-repairing conversion
  - Category 7: Solar hydrogen production
  - Category 8: Photocatalytic fuels formation
- Category 9: Solar thermal energy utilization
- Category 10: Novel nanoscale and self-assembled materials
- Category 11: Theory, modeling, and simulation
- FY2007 Funding (request) for Solar Energy Utilization is $34.1 M/yr

BES Proposals Full Proposals

BES received 656 pre-proposals (268 solar to electric)

Encouraged 346 for full proposal review

All full proposals were peer reviewed

Scientific and/or technical merit of the project;
Appropriateness of the proposed method or approach;
Competency of personnel and adequacy of proposed resources;
Reasonableness and appropriateness of the proposed budget.
Basic research that is relevant to improved utilization of solar energy (i.e., application is responsive to the solicitation).

Four large-scale or "center" proposals were encouraged and received.

Center proposals will receive two-stage review:

1) Technical review of each subtask (four per proposal)
2) Management review of each center proposal by a second panel in a reverse site visit format.

FY2007 BES Solar Energy Utilization Solicitation (Full proposals)

Panel	BES Program Manager	# of Proposals*
Nano Photovoltaics (PV)	Refik Kortan	32
Inorganic Tranport PV	John Miller/Jim Horwitz	20
Organic PV	Arvind Kini/ Bonnie Gersten	43
Hybrid PV	Greg Fiechtner/ Jim Horwitz	27
Photoelectrochemistry	Mark Spitler	27
Bioinspired Molecular Assemblies	Arvind Kini/ Bonnie Gersten	17
Natural Photosynthesis	Rich Greene	19
Hydrogen Production	Dick Kelley	28
Photocatalytic Fuel Formation	Mary Gress	35
Solar Thermal	Tim Fitzsimmons	34
Theory, Modeling, and Simulation	Dick Hilderbrandt	23
Solar Centers	Eric Rohlfing	4
	Total	**309**

309 full proposals received (23 lab; 286 university)

Rebinned from submission categories into 11 review panels for purpose of review only (not budget distribution)

150 reviewers from 14 countries

AUSTRIA	NETHERLANDS
IRELAND	SWITZERLAND
JAPAN	ITALY
AUSTRALIA	GERMANY
ISRAEL	SWEDEN
MEXICO	CANADA
FRANCE	UNITED KINGDOM

Total (annualized) budget request ~$146M/yr

With funding of $34.1 M/yr, Projected success rate = 23%

Budget range is enormous: $58 k/yr - $18.9 M/yr

FY2007 BES Solar Energy Utilization Solicitation

http://www.sc.doe.gov/bes/solar.html

- The joint Congressional resolution (H.J.R. 20) funding BES in FY2007 provides approximately $8M in funding for Notice 06-15, Basic Research for Solar Energy Utilization (SEU). FY2007 awards for SEU will be announced in mid-May, 2007.

- The proposed FY2008 budget contains full funding for the original SEU initiative ($34.1 M) plus additional funding for SEU ($5.9 M), for a total of $40.0 M.

- All full applications submitted in response to Notice 06-15 that are not funded in FY2007 will be held in consideration for funding in FY2008. Awards will be made only after the FY 2008 funds that are requested for this activity are appropriated by Congress.