U.S. DEPARTMENT OF ENERGY | Office of Science

# *Biomass 2010*

## *The Office of Basic Energy Sciences (BES)*

*Richard Greene, Lead*
*Photo- and Bio-Chemistry Team*
*Chemical Sciences, Geosciences, and Biosciences*
*Division of BES*

- *DOE and BES*
- *BES Program Planning*
- *Funding Modalities*
- *Fuels from Sunlight Hub*

# DEPARTMENT OF ENERGY

Federal Energy Regulatory Commission

**Office of the Secretary**
Dr. Steven Chu, Secretary

Daniel B. Poneman,
Deputy Secretary*

Chief of Staff

*Departmental Staff and Support Offices*

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- General Counsel
- Chief Financial Officer
- Chief Information Officer
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- Assistant Secretary for Policy & International Affairs
- Health, Safety & Security
- Inspector General
- Economic Impact & Diversity
- Hearings & Appeals
- Intelligence and Counterintelligence

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- Deputy Administrator for Defense Nuclear Nonproliferation
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Under Secretary for Science

Office of Science
Dr. William Brinkman

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- Biological & Environmental Research
- Fusion Energy Science
- High Energy Physics
- Nuclear Physics
- Workforce Development for Teachers & Scientists

- Energy Information Administration
- Southeastern Power Administration
- Bonneville Power Administration
- Western Area Power Administration
- Southwestern Power Administration

* The Deputy Secretary also serves as the Chief Operating Officer

26 May 09

# Office of Basic Energy Sciences

## Harriet Kung, Director

Wanda Smith, Administrative Specialist

### BES Budget and Planning

Bob Astheimer, Senior Technical Advisor
Margie Davis, Financial Management
Vacant, Program Support Specialist

### BES Operations

Rich Burrow, DOE Technical Office Coordination
Robin Hayes, AAAS Fellow
Katie Perine, Program Analyst / BESAC
Ken Rivera, Laboratory Infrastructure / ES&H
Vacant, DOE and Stakeholder Interactions

## Materials Sciences and Engineering Division

**Linda Horton, Director**

Christie Ashton, Program Analyst
☆ Charnice Waters, Secretary

### Materials Discovery, Design, and Synthesis

**Arvind Kini**
Kerry Gorey, P.A.

- Materials Chemistry — Mary Galvin, Dick Kelley, ● Darryl Sasaki, SNL
- Biomolecular Materials — Mike Markowitz
- Synthesis and Processing — Bonnie Gersten
- Tech. Coordination Program Management — John Vetrano; Vacant

### Condensed Matter and Materials Physics

**Jim Horwitz**
Marsophia Agnant, P.A.

- Exp. Cond. Mat. Phys. — Andy Schwartz, ●Doug Finnemore, Ames, Vacant
- Theo. Cond. Mat. Phys. — Vacant, △ Arun Bansil, NEU, ■ Jim Davenport, BNL, ● Kim Ferris, PNNL
- Physical Behavior of Materials — Refik Kortan
- Mechanical Behavior and Radiation Effects — John Vetrano

### Scattering and Instrumentation Sciences

**Helen Kerch**
Cheryl Howard, P.A.

- X-ray Scattering — Lane Wilson
- Neutron Scattering — Thiyaga P. Thiyagarajan
- Electron and Scanning Probe Microscopies — Jane Zhu
- DOE EPSCoR* — ◆ Tim Fitzsimmons, Jane Zhu, ● Helen Farrell, INL

* Experimental Program to Stimulate Competitive Research

**LEGEND**

- ◆ Detailee (from DOE laboratories)
- ■ On detail from SC-28
- ■ Detailee, ½ time, not at HQ
- ● Detailee, ¼ time, not at HQ
- ◆ On detail to EERE/SETP, 30%
- △ IPA (Interagency Personnel Act)
- ☆ On active military duty
- P.A. Program Assistant

## Scientific User Facilities Division

**Pedro Montano, Director**

Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant

### Operations

- X-ray and Neutron Scattering Facilities — Roger Klaffky, Vacant
- NSRCs & EBMCs** — Tof Carim, Carlos Sa de Melo, ◆ Joe Horton, ORNL
- Accelerator and Detector R&D — Eliane Lessner
- Facility Coordination; Metrics; Assessment — Van Nguyen

** Nanoscale Science Research Centers & Electron Beam Microcharacterization Centers

### Construction

- Linac Coherent Light Source — Tom Brown
- National Synchrotron Light Source II — Tom Brown
- Spallation Neutron Source Upgrades — Tom Brown
- Instrument MIEs*** — ■ Stephen Tkaczyk, ◆ John Tapia, LANL
- Advanced Light Source User Support Building — Tom Brown

*** Major Item of Equipment projects

## Chemical Sciences, Geosciences, and Biosciences Division

**Eric Rohlfing, Director**

~~Diane Marceau, Program Analyst~~
Michaelene Kyler-King, Program Assistant

### Fundamental Interactions

**Michael Casassa**
Robin Felder, P.A.

- Atomic, Molecular, and Optical Sciences — Jeff Krause
- Gas-Phase Chemical Physics — Wade Sisk, △ Larry Rahn, SNL
- Condensed-Phase and Interfacial Mol. Science — Greg Fiechtner
- Computational and Theoretical Chemistry — Mark Pederson

### Photo- and Bio-Chemistry

**Rich Greene**
Sharron Watson, P.A.

- Solar Photochemistry — Mark Spitler, ● Arthur Frank, NREL
- Photosynthetic Systems — Gail McLean
- Physical Biosciences — Robert Stack

### Chemical Transformations

**John Miller**
Teresa Crockett, P.A.

- Catalysis Science — Paul Maupin, Raul Miranda, ◆ Jan Hrbek, BNL
- Heavy Element Chemistry — Lester Morss, ● Norm Edelstein, LBNL
- Separations and Analysis — Bill Millman, △ Larry Rahn, SNL
- Geosciences — Nick Woodward, ● Jennifer Blank, LBNL
- Technology Office Coordination — Marvin Singer, Vacant

**January 2010**

Posted 21JAN10

# BES Council on Chemical and Biochemical Sciences Workshop on the Efficiency of Photosynthesis vs Photovoltaics

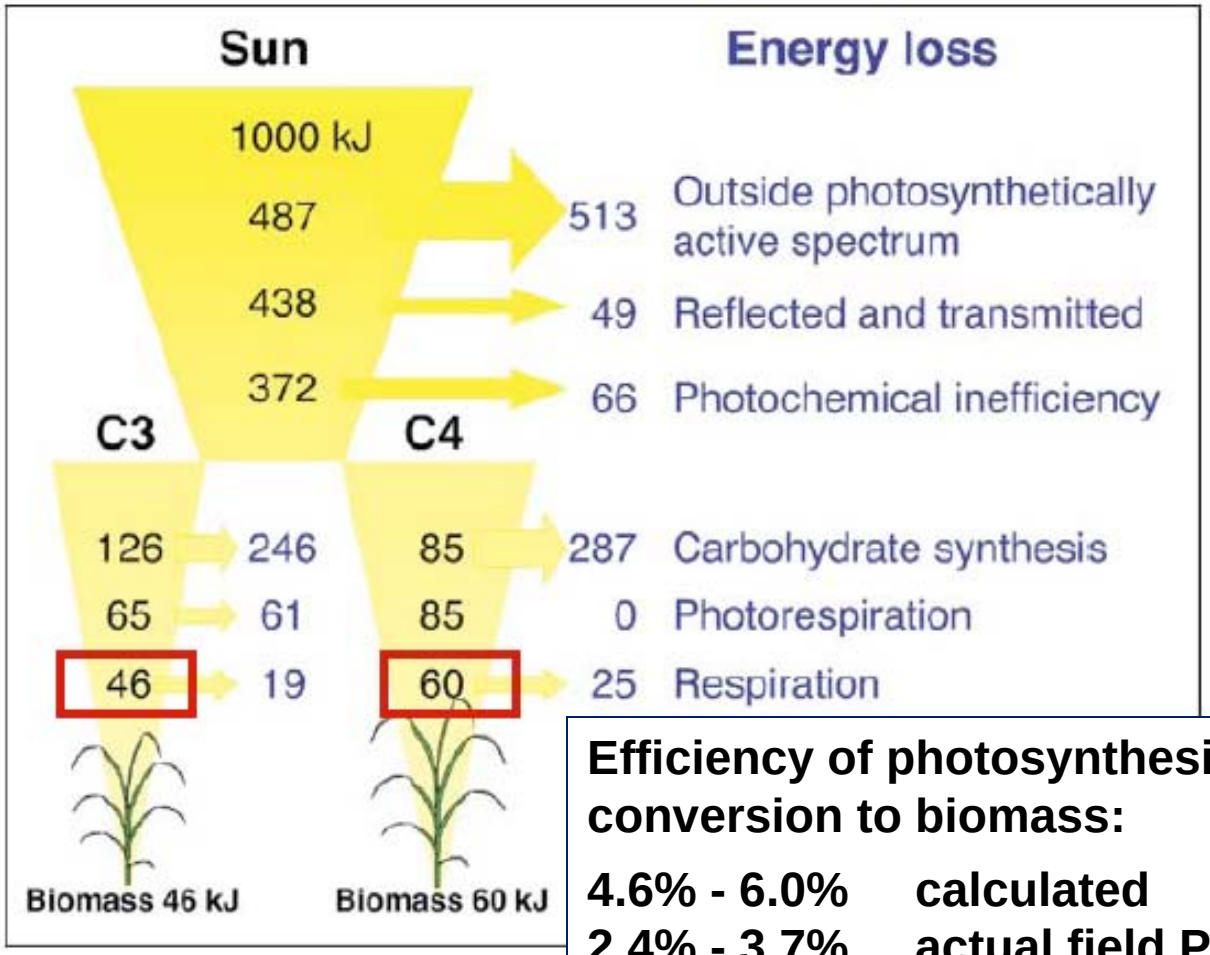
Robert Blankenship, Washington University (Co Chair)

David Tiede, Argonne National Laboratory (Co-Chair)

May 23, 24, - 2009
Albuquerque, NM

Jim Barber, Imperial College, UK
Gary Brudvig, Yale Univ.
Chris Moser, Univ. of Pennsylvania
Graham Fleming, UC Berkeley/LBNL
Maria Ghirardi, NREL
Marilyn Gunner, City College of NY
Wolfgang Junge, Univ. Osnabruck, Germany
David Kramer, Washington State Univ.
Tasio Meilis, UC Berkeley
Tom Moore, Arizona St. Univ.
Dan Nocera, MIT
Art Nozik, NREL
Don Ort, USDA-ARS
William Parson, Univ. of Washington
Roger Prince, Exxon
Richard Sayre, Danforth Plant Science Center

# What is the solar energy conversion efficiency of natural photosynthesis?*




**Efficiency of photosynthesis conversion to biomass:**

**4.6% - 6.0%** **calculated**
**2.4% - 3.7%** **actual field PS**

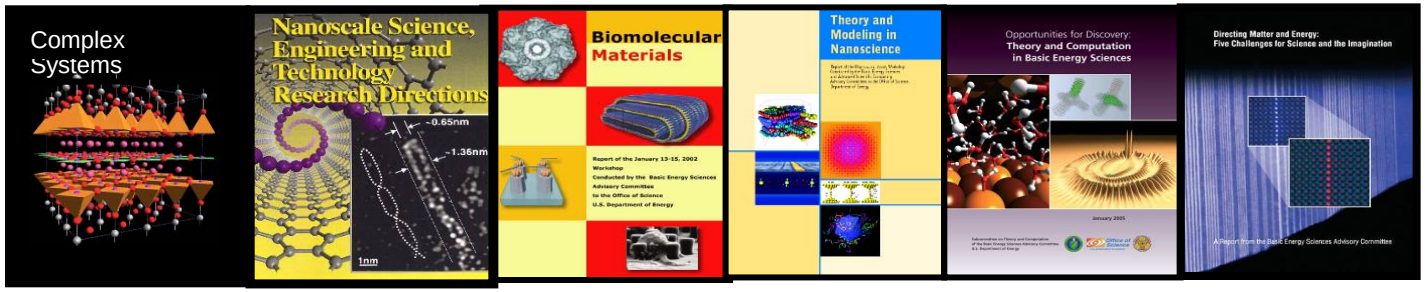
Don Ort, USDA-ARS



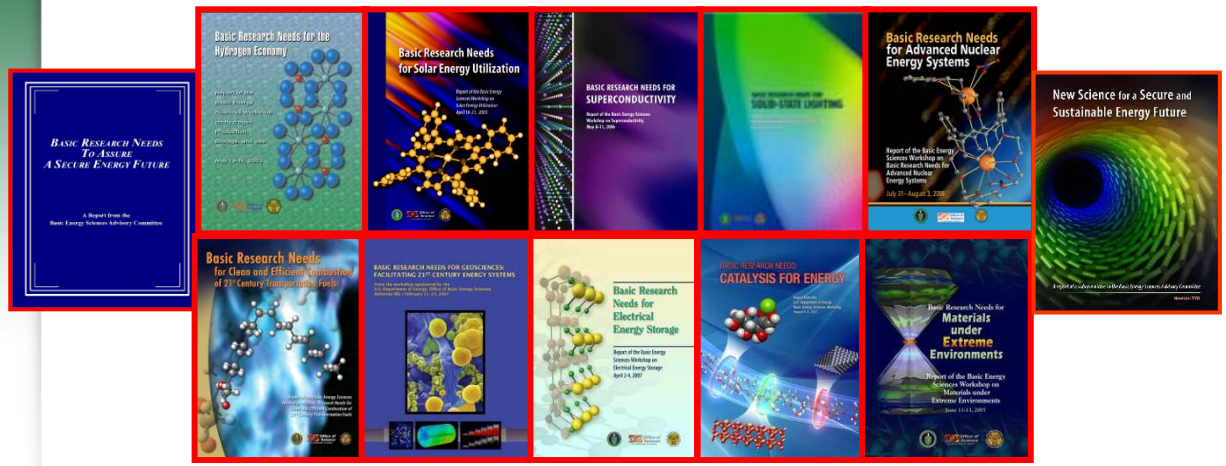
*Blankenship, Tiede, et. al., *Science*, submitted.

# BESAC & BES Strategic Planning Activities

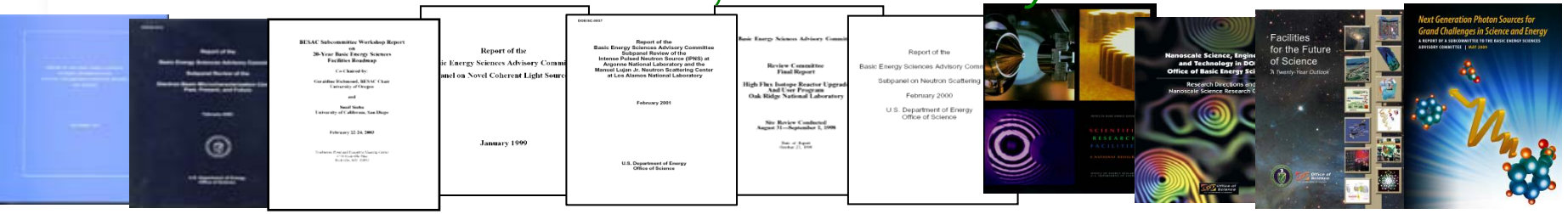
- *Science for Discovery*




- *Science for National Needs*




- *National Scientific User Facilities, the 21st century tools of science*

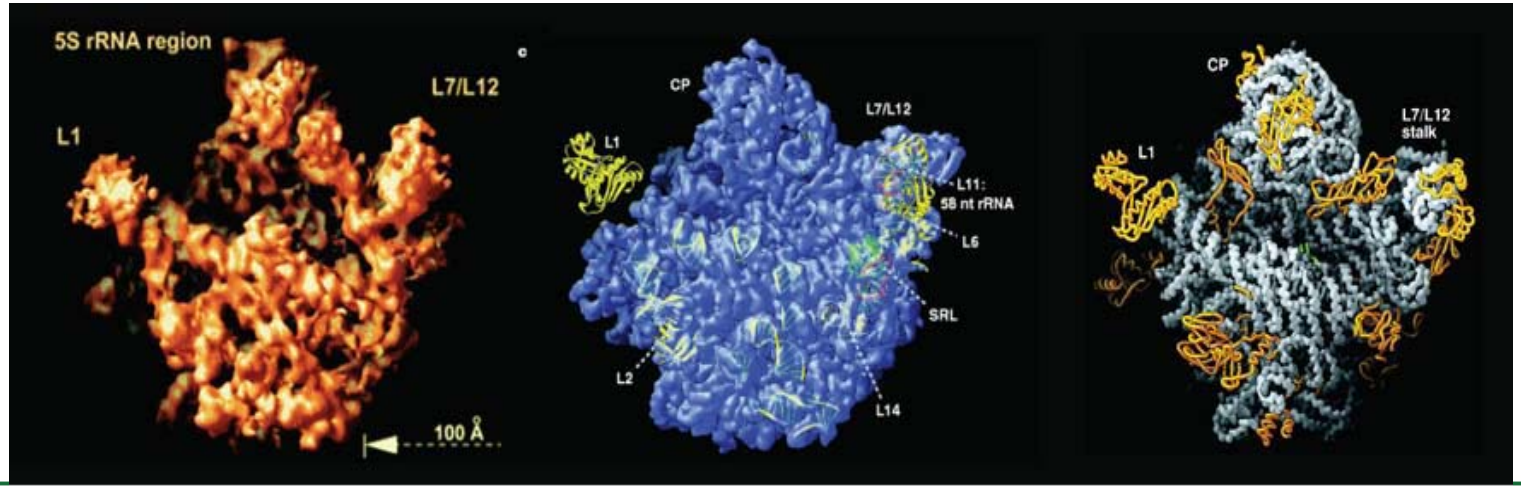



http://www.sc.doe.gov/bes/reports/list.html

# The 2009 Nobel Prize in Chemistry Work Used all Four BES Light Sources

*PIs were supported by DOE/SC and NIH National Center for Research Resources*

- Ribosome translates the genetic instructions encoded by DNA into chains of amino acids that make up proteins. The ribosome is composed of two subunits: 30S, which reads the code; and 50S, which links up the amino acids.
- The structures of 30S and 50S have been crucial to understanding everything from how the ribosome achieves its amazing precision to how different antibiotics bind to the ribosome.
  - **Ramakrishnan** and **Steitz** used x-ray crystallography at the **NSLS** to gather structures of these two ribosome subunits: Ramakrishnan on 30S and Steitz on 50S.
  - **Steitz, Ramakrishnan,** and **Yonath** also performed studies at the **APS**. Most work was performed at the DOE beamline; Steitz and Yonath also used two other beamlines – GMCA-CAT and BIOCARS.
  - **Steitz** also performed work at the **ALS**.
  - **Yonath** also did early work at **SSRL** related to developing the cryo-cooling of ribosome particles.

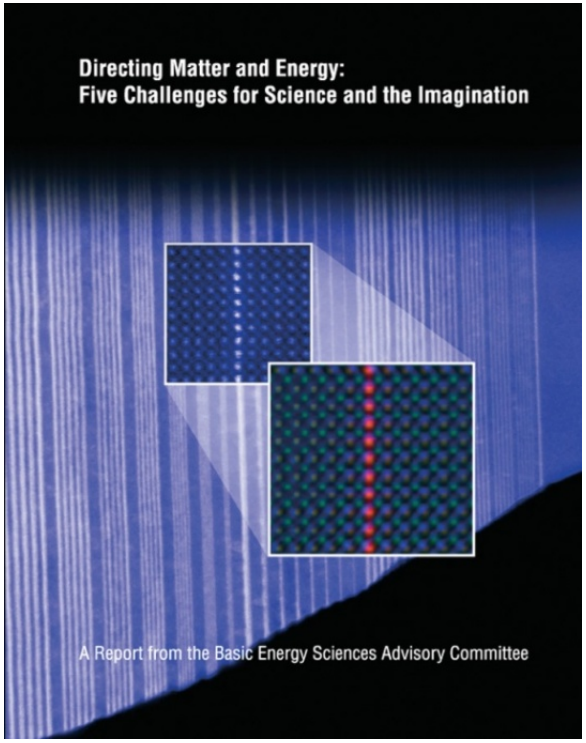



The 50S subunit structure at 9Å resolution (left, 1998), 5Å resolution (middle, 1999), and 2.4Å resolution (right, 2000) (From Ban et al., 1998; 1999; 2000).

# Directing Matter and Energy: 2007 BESAC Report

## Five Grand Challenges

- How do we control materials properties at the level of electrons?
- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from complex correlations of the atomic and electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?
- How do we characterize and control matter--especially very far away--from equilibrium?

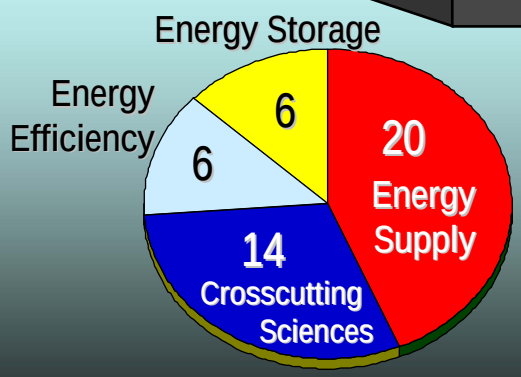


# The Status of the SC/BES Energy Frontier Research Centers

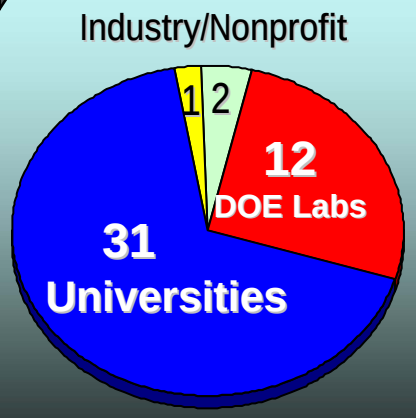
*46 EFRCs were launched in late FY 2009 using FY 2009 Appropriations and Recovery Act Funds*

46 centers awarded, representing 103 participating institutions in 36 states plus D.C

Energy Frontier Research Center Locations (★ Leads; • Participants)




By Topical Category

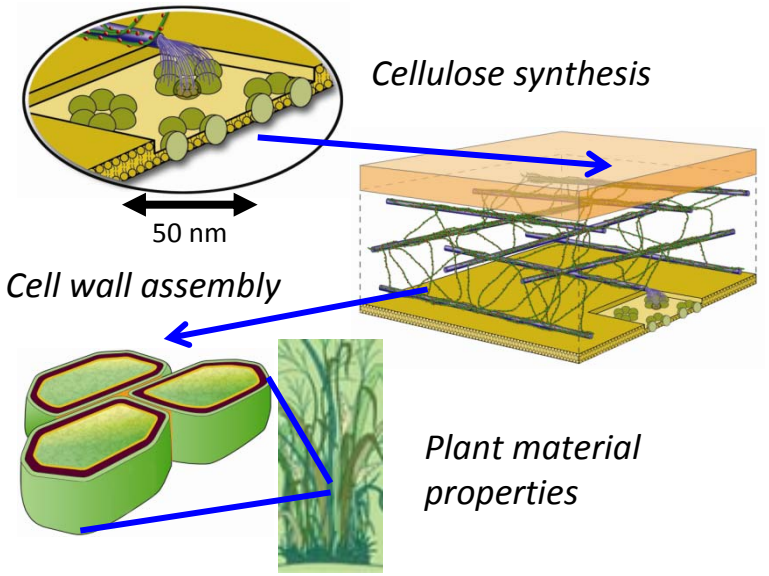



By Lead Institution

# Center for Lignocellulose Structure and Formation

Daniel Cosgrove (Penn State University)

Lignocellulose is the major structural material in plants and a vast source of renewable biomaterials and bioenergy. CLSF studies the physical structure of lignocellulose at the nano scale and the physicochemical rules by which plants create this most versatile of materials.



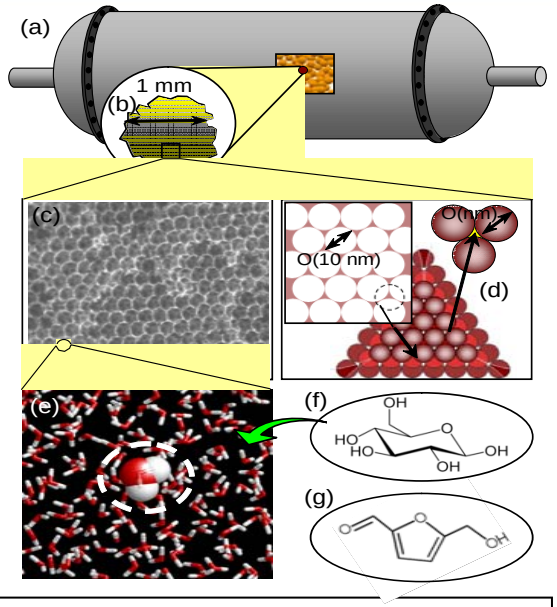

## RESEARCH PLAN AND DIRECTIONS

With a unique mix of molecular biologists, chemists, physicists, engineers and modelers, CLSF will tackle key questions of lignocellulose structure and formation. This is a key step towards unlocking the energy-rich biomaterial for the next generation of sustainable biofuels and for creating new cellulosic biomaterials with diverse economic applications.

U.S. DEPARTMENT OF ENERGY | Office of Science
PENNSTATE 1855
NORTH CAROLINA STATE UNIVERSITY
Virginia Tech VT

# Catalysis Center for Energy Innovation (CCEI)
# Dion Vlachos (Univ. of Delaware)

Summary statement: The central aim of the CCEI is to develop innovative heterogeneous catalytic technologies for future biorefineries and to educate the workforce needed to lead to further, sustainable economic growth of the US.




## RESEARCH PLAN AND DIRECTIONS

Biomass feedstocks vary considerably with source, and their transformation entails complex, multiscale reactions and processes. The CCEI members develop novel catalytic materials and processes, based on a fundamental understanding of the underlying chemistry, to set the foundations for the operation of modern biorefineries for carbon free production of chemicals and fuels.

# BER Bioenergy Research Centers

*Model for the Department's Energy Innovation Hubs*

## $75 million will support the fourth year of operations of the three BRCs

**Joint BioEnergy Institute (JBEI)**—research on model crops (*Arabidopsis* and rice) that can be transferred to bioenergy crops; lignin modification; synthetic biology approaches to fuels

- *Advanced biomass pretreatment using room temperature ionic liquids to remove lignin from plant cell walls improved biomass breakdown 5x.*
- *New cellulase enzyme more stable and active in ionic liquids at elevated temperatures and low pH.*

**Great Lakes Bioenergy Research Center (GLBRC)**—research on model plants and potential bioenergy plants; microbial biorefineries; sustainability of biofuel production

- *Improved screening of hydrolytic enzymes using gene expression approach coupled with enzyme screening and computational approaches – 100x more efficient than conventional methods*

**BioEnergy Science Center (BESC)**—research to overcome "recalcitrance" (resistance of plant fiber, or lignocellulose, to break down into sugars); gene discovery for recalcitrance; consolidated bioprocessing

- *New high throughput screening of chemical, structural, and genetic features of biomass – >100x faster than conventional methods.*
- *New imaging technologies to view cell wall at multiple scales to analyze recalcitrance*

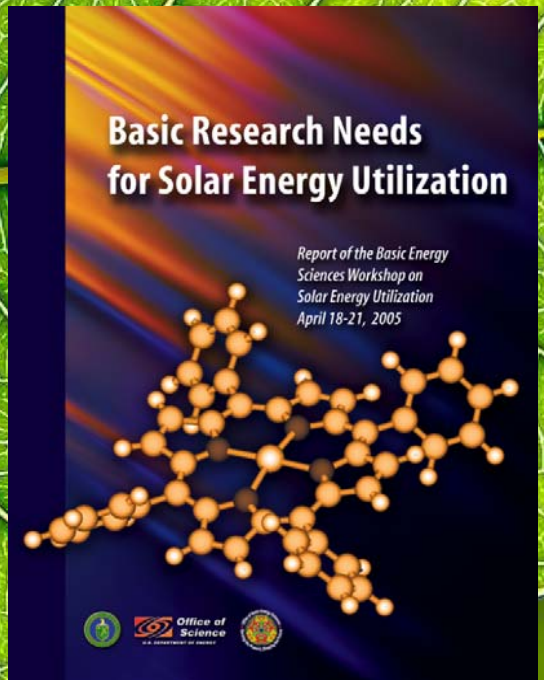
# Modalities of BES Research

| | Investigators and their Institutions | Diversity of Disciplines Per Award | Period of Award and Management | Annual Average Award Amount |
|---|---|---|---|---|
| **CORE** | Single or small-groups. Led by Universities or National Laboratories. | Few | Three–year renewable awards. Managed at the Division level. | ~$150-300 k |
| **EFRC** | Self-assembled group of ~6-12. Led by Universities, National Laboratories , Non-profits Organizations or Industry. | Several | Five years with 5-year renewal possible. Managed at the BES level. | ~$3-4M |
| **HUB** | Large set of investigators. May be led by Universities, National Laboratories , Non-profits Organizations or Industry. | Many; possibly, including areas such as energy policy, economics, and market analysis. | Five years with 5-year renewal possible; the "bar" is significantly higher for further renewals. Managed by DOE SC with broad DOE participation. A Board of Advisors consisting of senior leadership will coordinate across DOE. | ~$25 million per year for R&D |

# Fuels from Sunlight: A Hub Approach

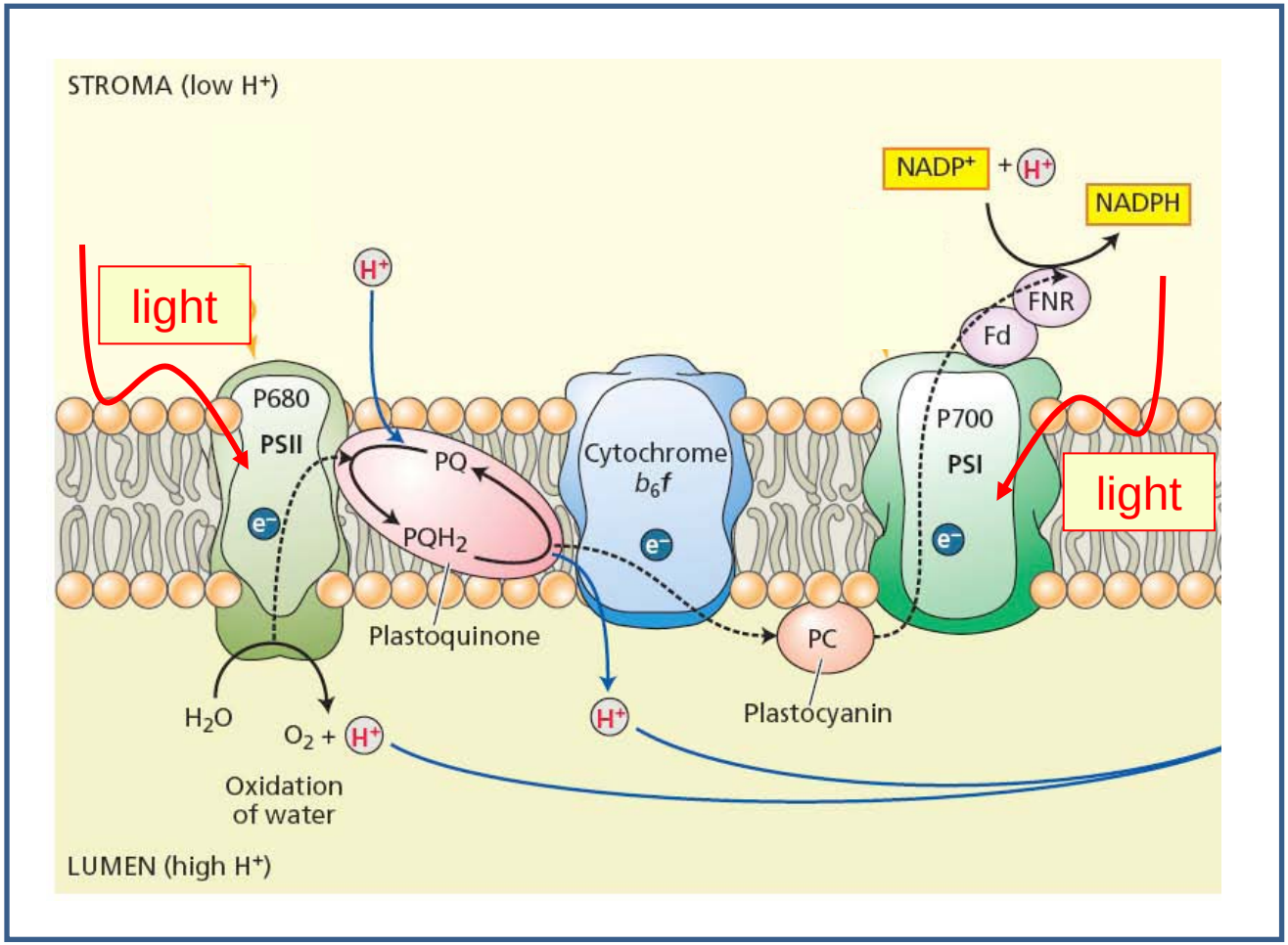
*Fuels from Sunlight: Nature's Way*

*We've wanted to copy Nature for a long time!*



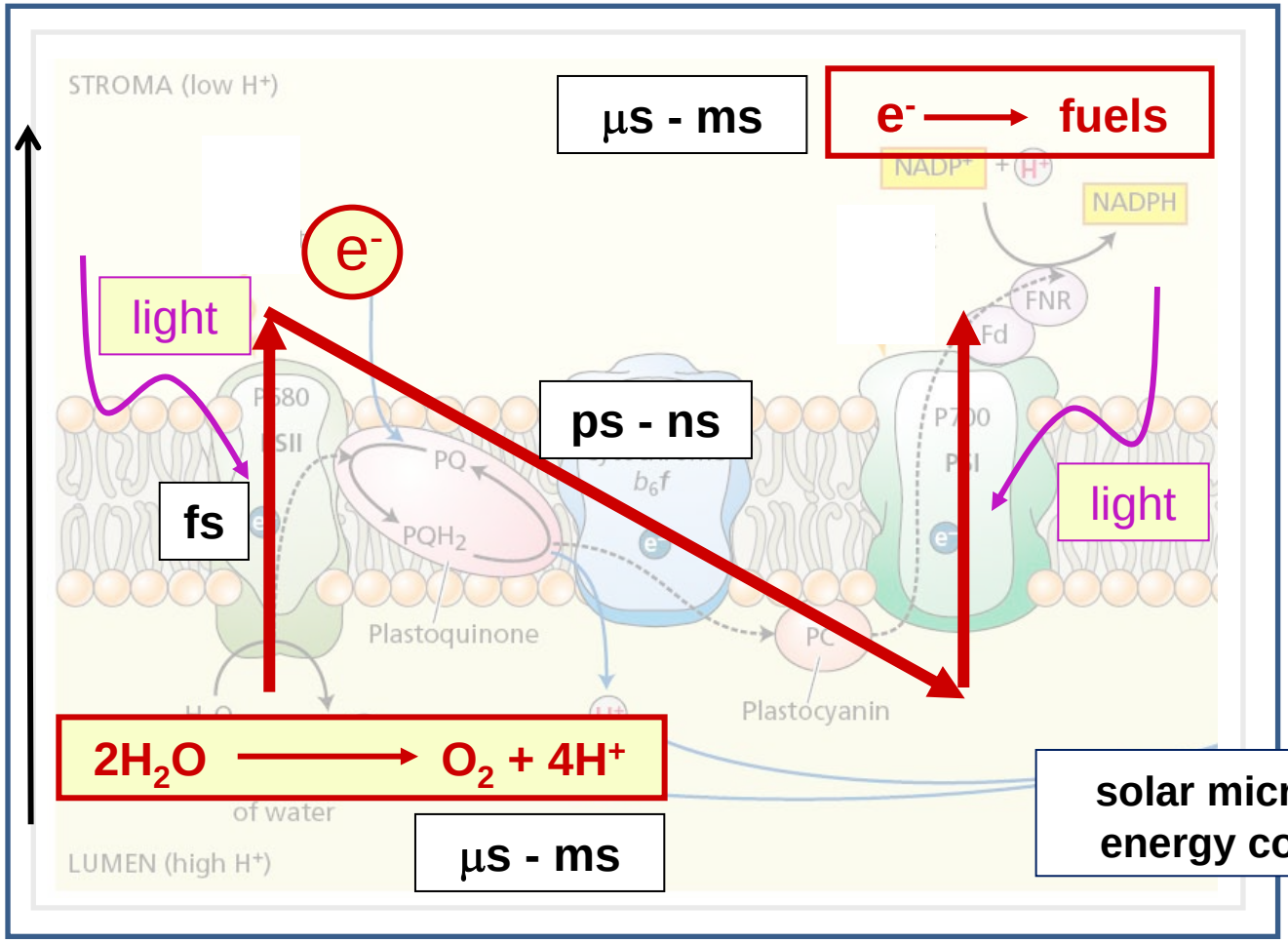
# Natural Photosynthesis: Focus on the Thylakoid Membrane

Matrix for reaction centers I & II, the electron transfer chain, and catalytic redox sites



# Artificial Photosynthesis: Working Definition

The “Z” scheme of photosynthesis is depicted in overlay on the structure




- Photon capture and energy transfer - fs
- Charge separation and electron transport – ps-ns
- Catalysis and fuel formation – μs-ms

# Fuels from Sunlight: Critical Issues in Research

## fs

**Photon absorption and harvesting**

*How do we control light harvesting to utilize all of the photons?*

-Need to know how to design and control exciton transfer in molecular systems

-Need red absorbers to harvest the bulk of the solar spectrum

## ps-ns

**Charge separation and transport**

*How do we avoid recombination of photo-generated charge carriers?*

-Need to overcome geminate recombination in organic systems

-Need to design transport to reduce non-geminate recombination in all systems

## μs-ms

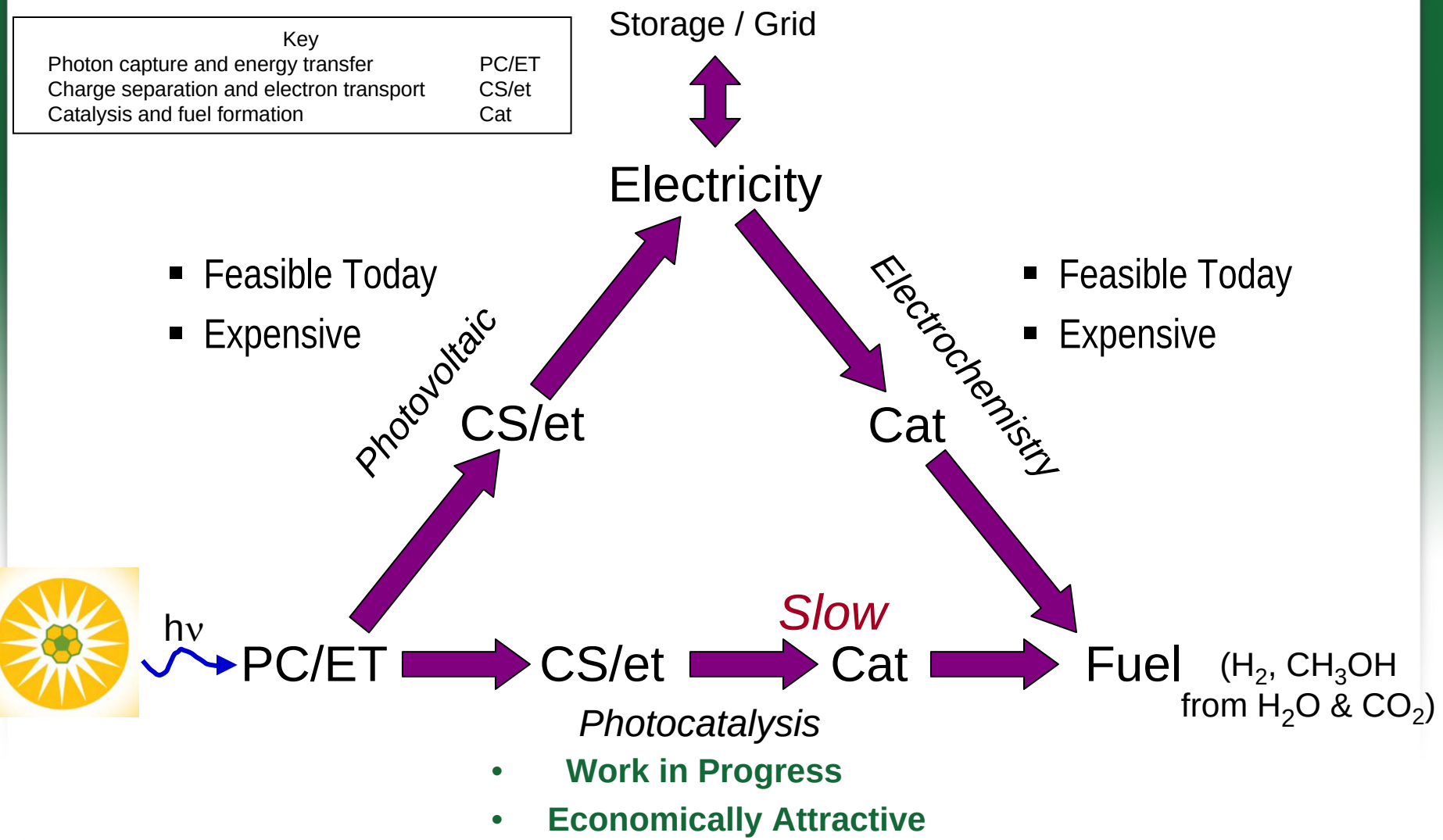
**Photocatalysis**

*How do we produce fuels with the energy provided by visible light absorption?*

-Need hetero/homo - geneous catalytic systems for water splitting

-Need to couple light absorption to catalytic processes for C-C bond formation

# Artificial Photosynthesis




- **Work in Progress**
- **Economically Attractive**

# Prospects for Solar Fuels Production

## Two Limits

### What we can do today:

$12/kg $H_2$ @ $3/pW PV
(BRN on SEU 2005)

PV cell
balance of system

current

electrolyzer

gas

fuel storage

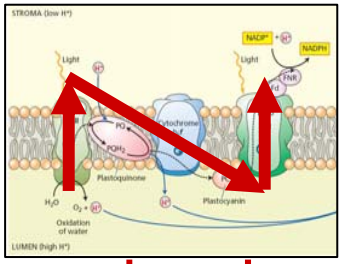
$H_2$ compression

High capital costs

We do not know how to produce fuels in a cost effective manner.

### Ultimate goal:

**solar microcatalytic energy conversion**



liquid

fuel storage

Low capital costs

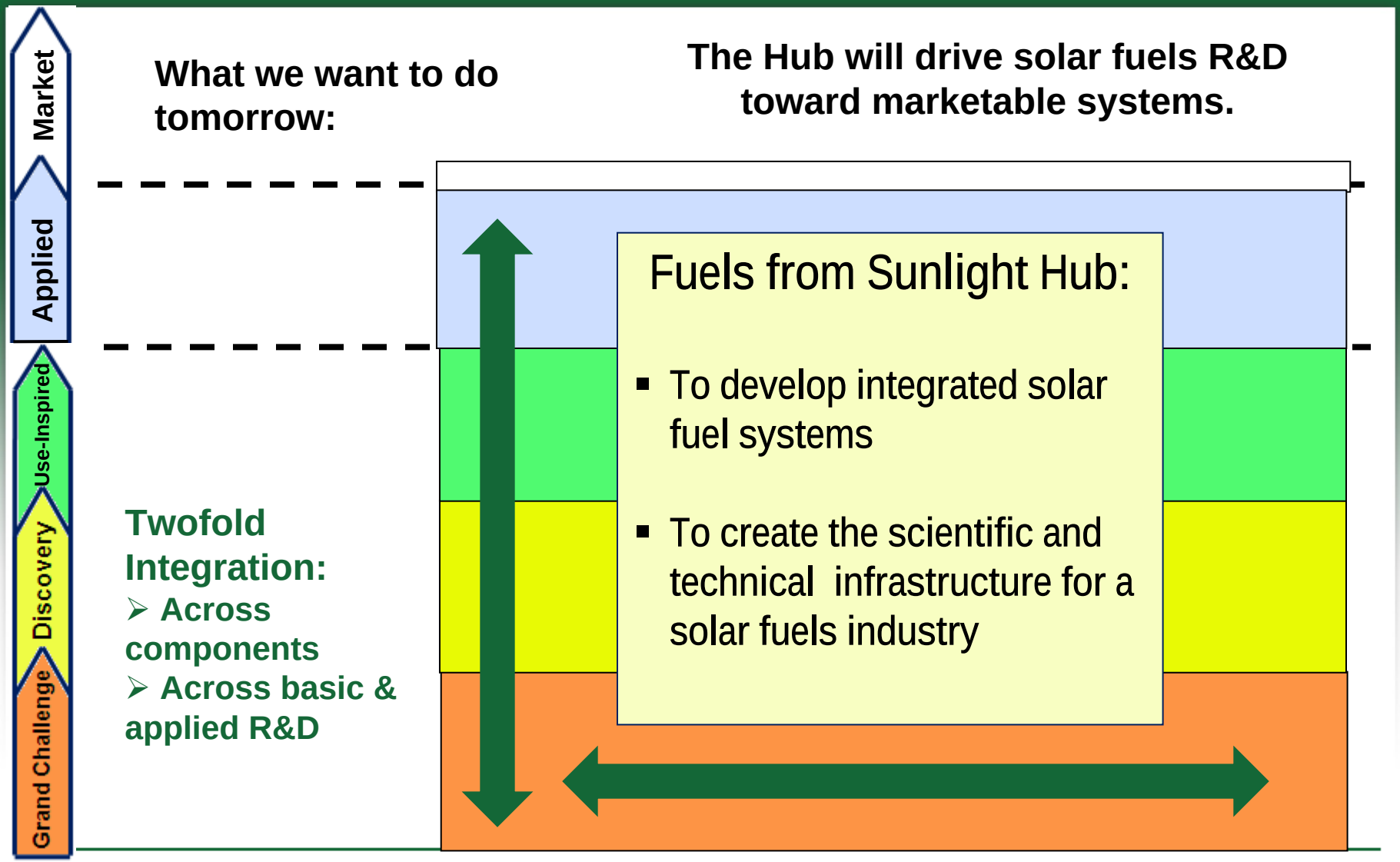
Chemists do not yet know how to photoproduce $O_2$, $H_2$, reduce $CO_2$, or oxidize $H_2O$ on the scale we need.

gas

fuel storage

compression

# Landscape for Solar Fuels Production: From Basic Research to Market



# Thank you!

## BES Website

## http://www.er.doe.gov/bes/BES.html