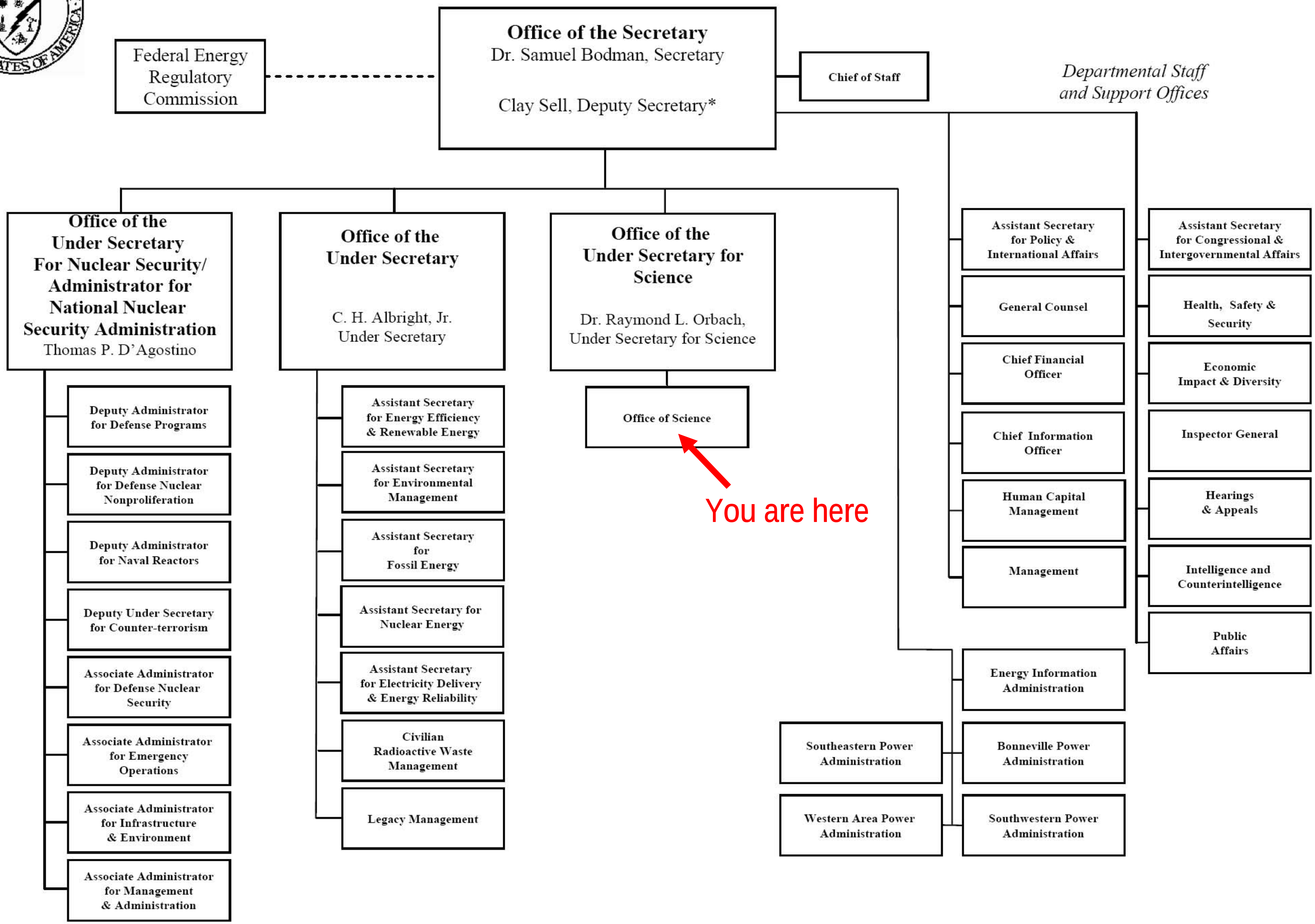
Biomass Research & Development Technical Advisory Committee Meeting – Dec 3, 2008

Basic Energy Sciences Overview

Richard V. Greene, Team Lead
Photo- and Bio-Chemistry

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

DEPARTMENT OF ENERGY

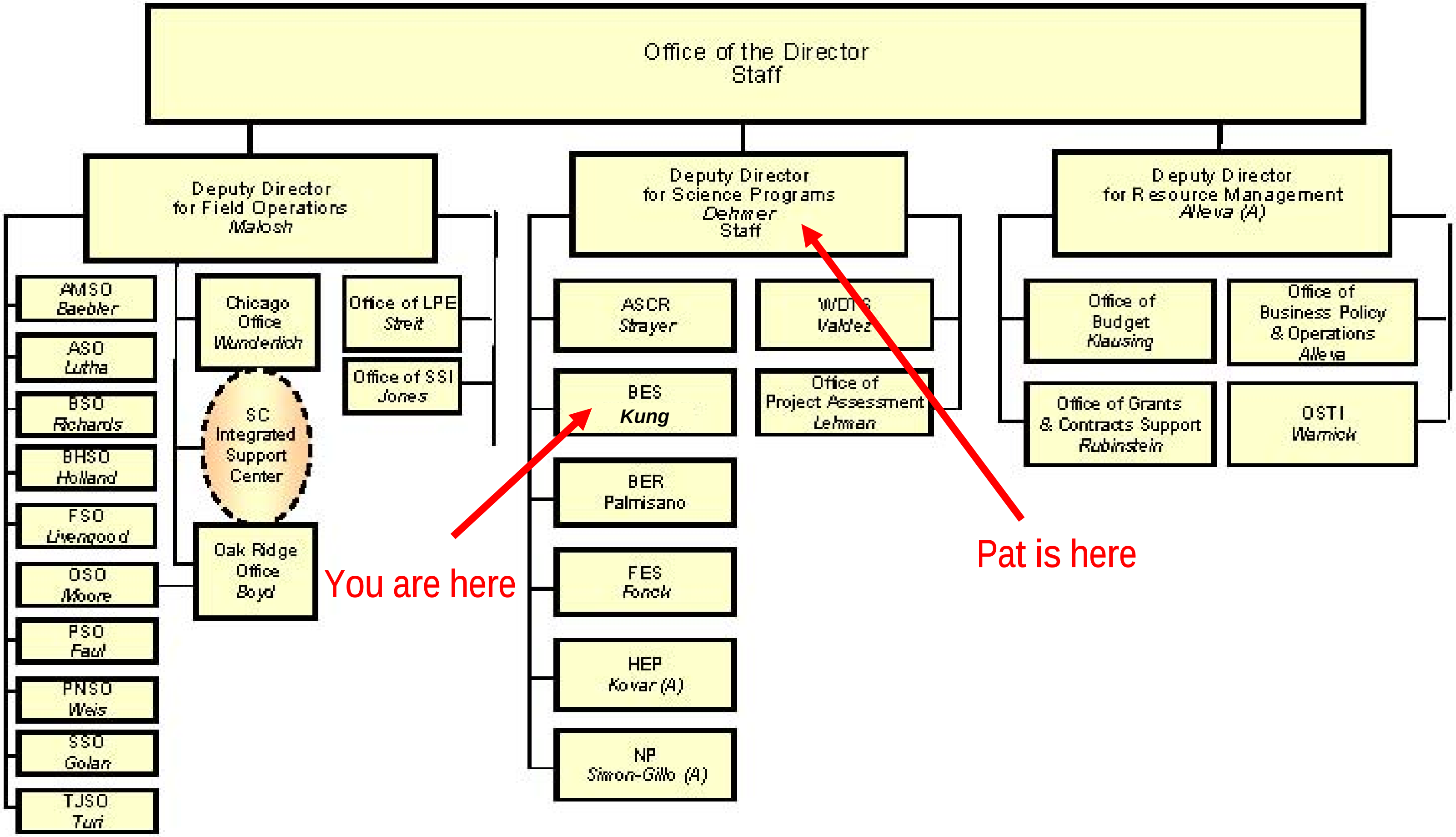


* The Deputy Secretary also serves as the Chief Operating Officer

06 Feb 08

U.S. Department of Energy's Office of Science

OFFICE OF SCIENCE



3/31/08

Relationships Between the Science and the Technology Offices in DOE

Discovery Research → **Applied Research** → **Technology Maturation & Deployment**

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

DOE Applied Energy Offices
EE/RE, NE, FE, OE, ...

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

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

Relationships Between the Science and the Technology Offices in DOE

Discovery Research → Use-inspired Basic Research → Applied Research → Technology Maturation & Deployment

DOE Office of Science
BES

DOE Applied Energy Offices
EE/RE, NE, FE, OE, …

- Basic research for fundamental new understanding, with the goal of addressing short-term showstoppers on real-world applications in the energy technologies

Basic Research Needs To Assure A Secure Energy Future

BESAC Basic Research Needs to Assure A Secure Energy Future Report February 2003

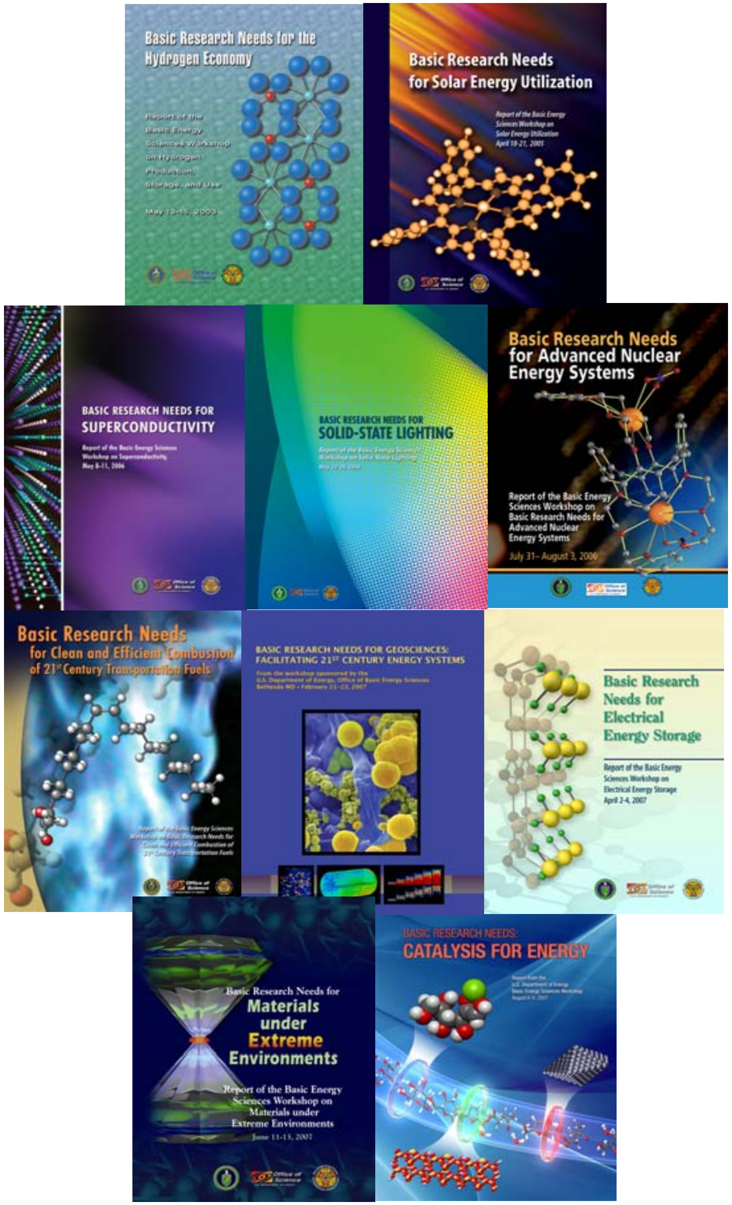
Current projections estimate that the energy needs of the world will more than double by the year 2050. This is coupled with increasing demands for "clean" energy—sources of energy that do not add to the already high levels of carbon dioxide and other pollutants in the environment. These enormous challenges cannot be fully met by existing technologies, and scientific breakthroughs will be required to provide reliable, economic solutions for our future energy security

This seminal workshop report indentified the broad basic research directions that will help provide the major scientific discoveries necessary for major technological changes in the largest industries in the world—those responsible for energy production and use.

The findings of this 2003 report gave birth to a series of ten follow-on *Basic Research Needs* workshops over the next five years, which together attracted more than 1,500 participants from universities, industry, and Department of Energy laboratories. These reports provide in-depth analyses on how the work of the scientific community can further our Nation's most challenging energy missions.

Basic Research Needs Workshops:

Help Define Research Directions and Provide the Links to Societal Needs



- Basic Research Needs for a Secure Energy Future (BESAC)
- Basic Research Needs for the Hydrogen Economy
- Basic Research Needs for Solar Energy Utilization
- Basic Research Needs for Superconductivity
- Basic Research Needs for Solid State Lighting
- Basic Research Needs for Advanced Nuclear Energy Systems
- Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels
- Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems
- Basic Research Needs for Electrical Energy Storage
- Basic Research Needs for Materials under Extreme Environments
- Basic Research Needs for Catalysis for Energy Applications

Energy Frontier Research Centers

Tackling our energy challenges in a new era of science

Energy Frontier Research Centers will bring together the skills and talents of multiple investigators to enable research of a scope and complexity that would not be possible with the standard individual-investigator or small-group award.

The DOE Office of Science, Office of Basic Energy Sciences, announced the Energy Frontier Research Centers (EFRCs) program. Pending appropriations, up to $100M will be available in FY2009 for EFRC awards that are $2–5 million/year for an initial 5-year period. Universities, labs, nonprofits, and for-profit entities are eligible to apply.

Energy Frontier Research Centers will pursue fundamental research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Catalysis for Energy
- Electrical Energy Storage
- Solid State Lighting
- Superconductivity
- Bioenergy and biofuels
- Geosciences for Nuclear Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Combustion of 21st Century Transportation Fuels
- Hydrogen Production, Storage, and Use
- Materials Under Extreme Environments

EFRC Funding Opportunity Announcement was published on April 4, 2008. See: http://www.sc.doe.gov/bes/EFRC.html

Single-Investigator and Small-Group Research
Tackling our energy challenges in a new era of science

- Pending appropriations, up to $60M will be available for single-investigator and small-group awards in FY2009.
- BES seeks applications in two areas: grand challenge science and energy challenges identified in one of the Basic Research Needs workshop reports.
- Awards are planned for three years, with funding in the range of $150-300k/yr for single-investigator awards and $500-1500k/yr for small-group awards (except as noted below)
- Areas of interest include:

  Grand challenge science: ultrafast science; chemical imaging, complex & emergent behavior

  Tools for grand challenge science: midscale instrumentation; accelerator and detector research (awards capped at $5M over 3-year project duration)

  Use inspired discovery science: basic research for electrical energy storage; advanced nuclear energy systems; solar energy utilization; hydrogen production, storage, and use; geological CO2 sequestration; other basic research areas identified in BESAC and BES workshop reports with an emphasis on nanoscale phenomena
- For full details see: http://www.sc.doe.gov/bes/SISGR.html

Office of Basic Energy Sciences

Harriet Kung, Acting Director
Vacant, Administrative Specialist

BES Budget and Planning
- Robert Astheimer, Technical Advisor
- Margie Davis, Budget Analyst

BES Operations
- Linda Blevins, International/Intergovernmental ☺
- Richard Burrow, DOE Technical Office Coordination
- Don Freeburn, DOE and Stakeholder Interactions
- Ken Rivera, Laboratory Infrastructure/ES&H
- Karen Talamini, Program Analyst/BESAC

Materials Sciences and Engineering Division

Helen Kerch, Acting Director
Christie Ashton, Program Analyst
Charnice Waters, Secretary

Materials Discovery, Design, and Synthesis
Arvind Kini
Vacant, Prog. Asst.

- Materials Chemistry — Richard Kelley; ■ James McBreen, BNL
- Biomolecular Materials — Arvind Kini
- Synthesis and Processing — Tim Fitzsimmons; Bonnie Gersten; ◆ Daniel Friedman, NREL
- Tech. Coordination Program Management — John Vetrano

Condensed Matter and Materials Physics
Jim Horwitz
M. Agnant, Prog. Asst.

- Exp. Cond. Mat. Phys. — James Horwitz; ● D. Finnemore, Ames; Daniel Friedman, NREL
- Theo. Cond. Mat. Phys. — Vacant; ■ James Davenport, BNL; ● Kim Ferris, PNNL
- Physical Behavior of Materials — Refik Kortan
- Mechanical Behavior and Radiation Effects — John Vetrano

Scattering & Instrumentation Sciences
Helen Kerch
C. Howard, Prog. Asst.

- X-ray Scattering — Lane Wilson
- Neutron Scattering — Lane Wilson
- Electron and Scanning Probe Microscopies — Jane Zhu
- Ultrafast Science and Instrumentation — Jim Glownia
- Exp. Program to Stimulate Competitive Research — Kristin Bennett; ● Helen Farrell, INL

Scientific User Facilities Division

Pedro Montano, Director
Linda Cerrone, Program Analyst
Secretary (Vacant)

Operations
- X-ray and Neutron Scattering Facilities — Roger Klaffky
- Nanoscience Centers & E-beam Centers — Altaf (Tof) Carim
- Accelerator and Detector R&D
- Facility Coordination, Metrics, Assessment

Construction
- Linac Coherent Light Source — Tom Brown
- NSLS II — Tom Brown
- Spallation Neutron Source Upgrades — Tom Brown
- TEAM — Altaf (Tof) Carim
- Instrument MIEs (SING, LUSI, etc.) — Tom Kiess
- ALS User Support Bldg — Tom Brown

Chemical Sciences, Geosciences, and Biosciences Division

Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant

Fundamental Interactions
Michael Casassa
R. Felder, Prog. Asst.

- Atomic, Molecular, and Optical Sciences — Jeffrey Krause
- Ultrafast Chemical Sciences — Michael Casassa
- Gas-Phase Chemical Physics — Richard Hilderbrandt; ◆ Larry Rahn, SNL
- Condensed-phase and Interfacial Mol. Sci. — Gregory Fiechtner
- Computational and Theoretical Chemistry — Richard Hilderbrandt

Photo- and Bio-Chemistry
Richard Greene
Vacant, Prog. Asst.

- Solar Photochemistry — Mark Spitler
- Photosynthetic Systems — Richard Greene
- Physical Biosciences — Richard Greene; ◆ Robert Stack, PNNL

Chemical Transformations
John Miller
T. Russ, Prog. Asst.

- Catalysis Science — Raul Miranda; Paul Maupin; ◆ Michael Chen, ANL
- Heavy Element Chemistry — Lester Morss; ● Norman Edelstein, LBNL
- Separations and Analysis — William Millman; ◆ Larry Rahn, SNL
- Geosciences — Nicholas Woodward; ◆ Patrick Dobson, LBNL
- Technology Office Coordination — Marvin Singer

☺ On Detail to SC-2
◆ Detailee
■ Detailee, 1/2 time, not at HQ
● Detailee, 1/4 time, not at HQ

December 2007

Construction is Complete and Initial Operations are Underway at all NSRCs

Center for Functional Nanomaterials
(Brookhaven National Laboratory)

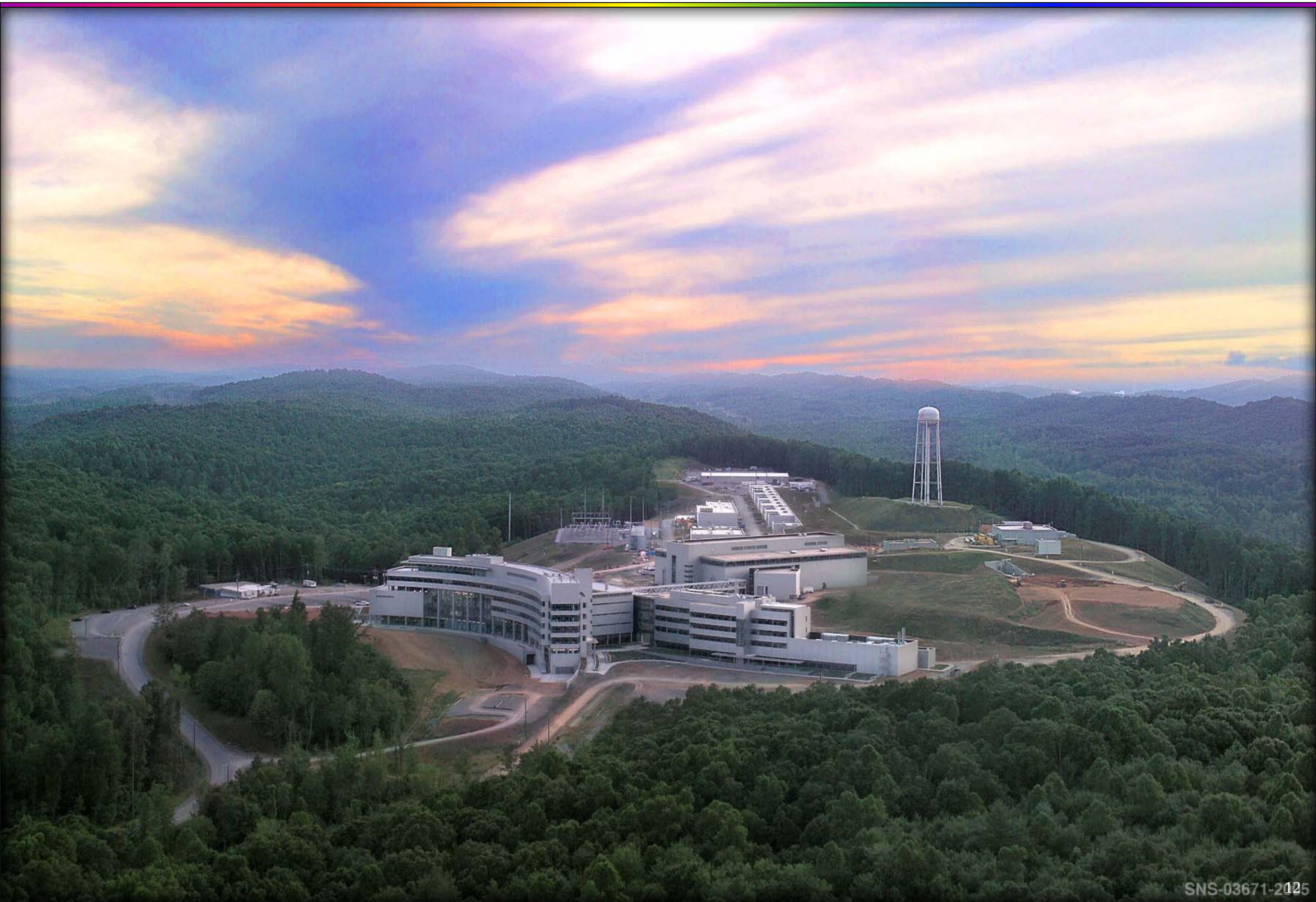
Molecular Foundry
(Lawrence Berkeley National Laboratory)

Center for Nanoscale Materials
(Argonne National Laboratory)

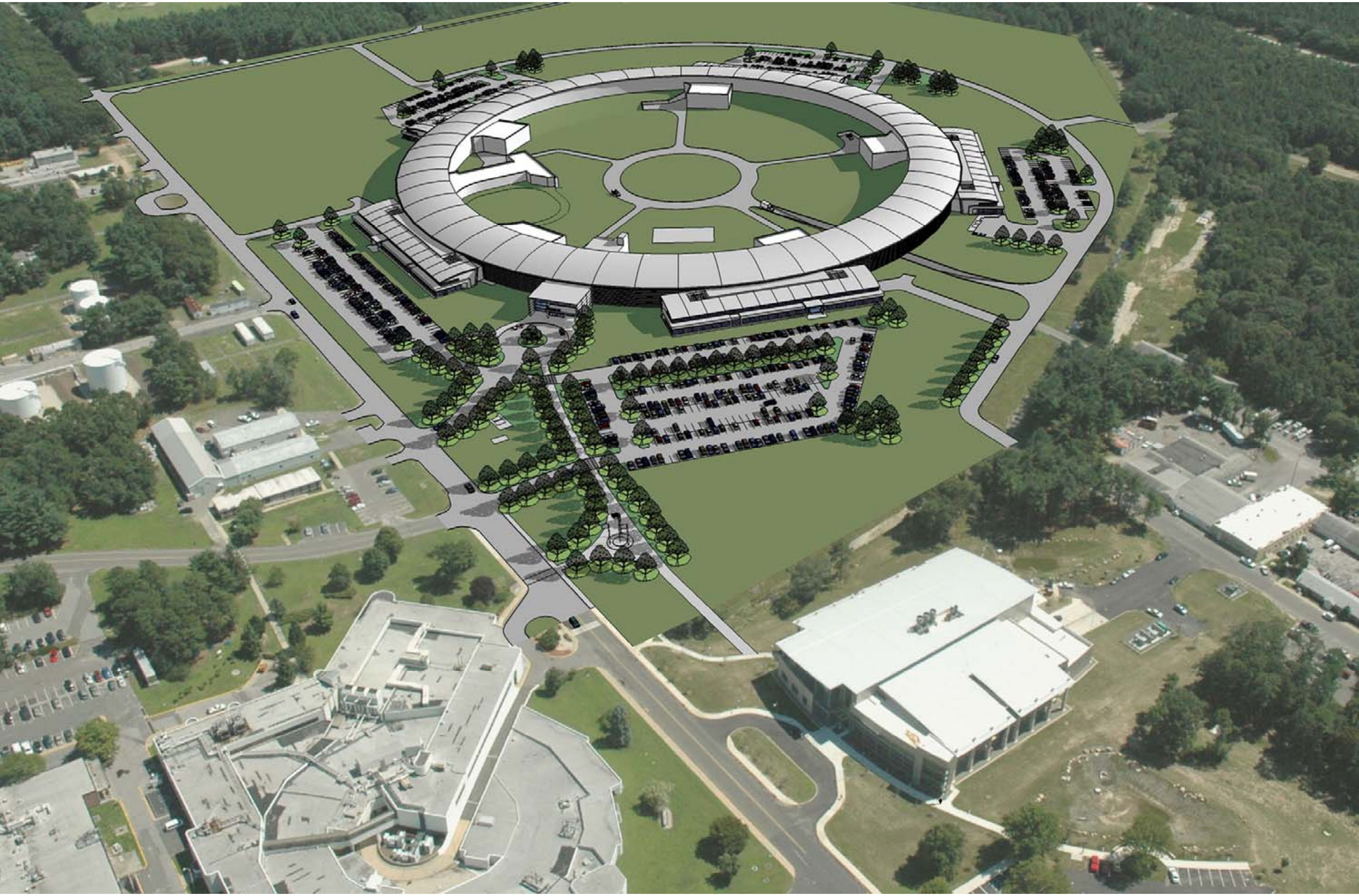
Center for Nanophase Materials Sciences
(Oak Ridge National Laboratory)

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

The Spallation Neutron Source Project is Complete!



Rendering of NSLS - II



April, 2008

Chemical Sciences, Geosciences, and Biosciences Division

Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant

- ● IPA
- ◆ Detailee
- ■ Detailee, 1/4 time, not at HQ

Fundamental Interactions

Michael Casassa
R. Felder, Prog. Asst.

- **Atomic, Molecular, and Optical Sciences** — Jeffrey Krause
- **Gas-Phase Chem Physics** — Vacant and Posted; ◆ Larry Rahn, SNL; ◆ Wade Sisk , BNL
- **Cond. Phase & Interfacial Molecular Science** — Gregory Fiechtner
- **Computational & Theoretical Chemistry** — Vacant; in process

Photo- and Bio-Chemistry

Richard Greene
S. Watson, Prog. Asst.

- **Solar Photochemistry** — Mark Spitler
- **Photosynthetic Systems** — Vacant
- **Physical Biosciences** — Vacant; ◆ Bob Stack, PNNL

Chemical Transformations

John Miller
T. Russ, Prog. Asst.

- **Catalysis Science** — Raul Miranda; Paul Maupin; ◆ Michael Chen, ANL
- **Heavy Element Chemistry** — Lester Morss; ■ Noman Edelstein, LBNL
- **Separations & Analyses** — William Millman; ◆ Larry Rahn, SNL
- **Geosciences** — Nicholas Woodward; ◆ Patrick Dobson, LBNL

Hiring 5 program managers in FY2008-9!

Major Historical Impacts of BES Biosciences

- **Predecessor programs established the effects of radiation on plants, leading to radiation-induced mutations used extensively in plant breeding.**
- **Established the AEC Plant Research Laboratory at Michigan State University in 1965 ("*The PRL*"). Strong basic science approach; trained over 500 post-docs and 250 graduate students in biomass-relevant areas.**
- **Program leads in developing *Arabidopsis* as a model laboratory plant for molecular genetic analysis (2007 Balzan Prize – Somerville & Meyerowitz)**
- **Identified multiple enzymes for the biological synthesis/consumption of molecular hydrogen**
- **Elucidated the metabolic pathway for the synthesis of methane. This novel biochemistry contributed to the recognition of the Archaea as a new kingdom.**
- **Initiated a focus on the structure and function of complex carbohydrates by establishing the Complex Carbohydrate Research Center at the University of Georgia ("*The CCRC*").**
- **Elucidated the biosynthetic pathway for plant lipid production.**
- **Platform information for cellulosic biofuel; e.g., determined structure of the cellulosome, the large multi-component complex that is involved in bacterial cellulose degradation.**
- **ATP Synthase; "Life's Energy Currency" (1997 Chemistry Nobel Prize – Boyer**, Walker, & Skou)

Biofuels – From Discovery Research to Technology

Discovery Research

- Fundamental molecular understanding (i.e., science grand challenges) of mechanisms that govern plant and microbial metabolism and growth that may be only peripherally connected to today's problems in energy technologies
- New tools and techniques for advanced modeling, imaging and structural analyses of plant and microbial energy transduction systems.

Use-inspired Basic Research

- Basic research for fundamental new understanding that address short-term showstoppers of plant cell wall recalcitrance and inability of biological systems to ferment sugars other than glucose to EtOH
- Fundamental projects on:

Lignocellulose biosynthesis

Cellulase structure-function

Carbohydrate metabolism

Thermodynamics and genetics of ethanolic fermentative pathways

Applied Research

- Proof of technology concepts
  - Development of cellulases and other enzymes with enhanced performance (high activity, thermotolerance, etc.) and reduced cost
  - Creation of microbes that ferment five and six carbon sugars to EtOH
  - Metabolic engineering to produce biofuels other than EtOH in microbes and plants

Technology Maturation & Deployment

- Scale-up research
- Cost reduction
- Manufacturing R&D (startup companies from BES PIs)
  - Mascoma – Lynd (Dartmouth), Cellulase Complex
  - Celunol (BES/EERE) – Ingram (U. Florida), Multiple Substrate Fermentation
  - Newco LS9 – Somerville (Carnegie), Alternative Biofuel

BER Bioenergy Centers

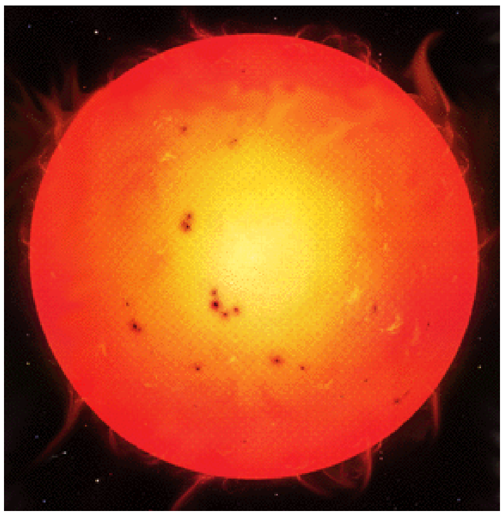
BES Energy Biosciences Program

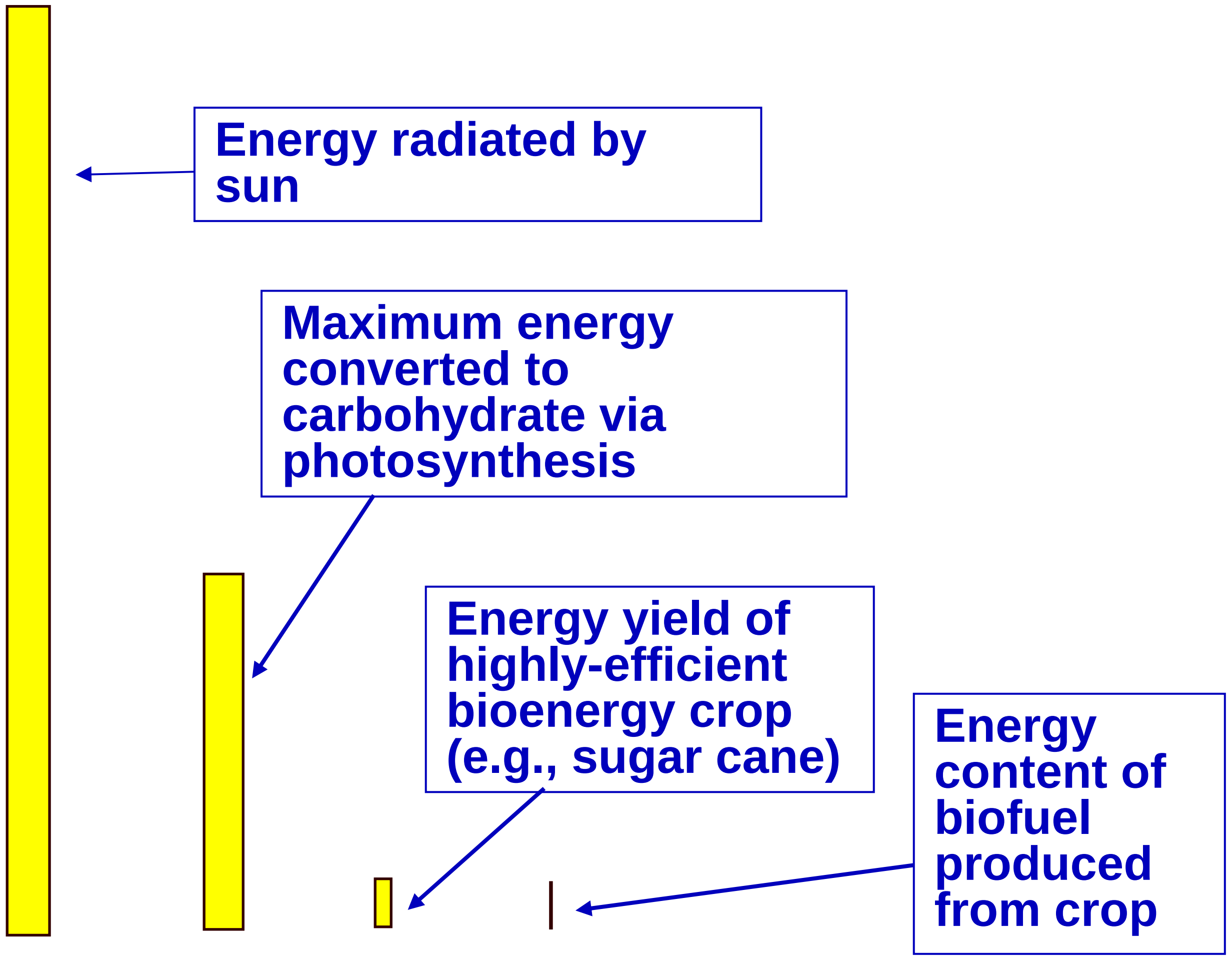
Goal: new knowledge / understanding
Mandate: open-ended
Focus: phenomena
Metric: knowledge generation

EERE Cellulosic Biorefineries

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

Seeking Greater Efficiencies by Moving "Upstream" to Photosynthesis



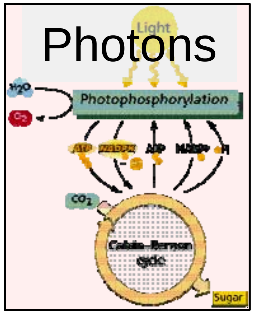


Photosynthetic Systems & Physical Biosciences Focus

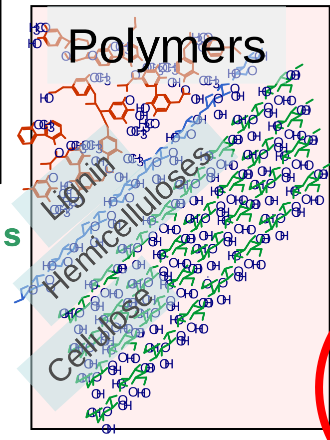
pathway for bioenergy

Photons CO_2 → Sugars → Polymers → Microfibrils → Cell Walls → Sugars → Biofuels

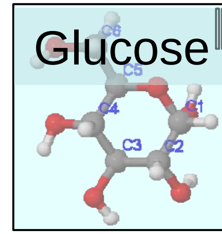
Photosynthesis | Bioassembly | Deconstruction | Fermentation

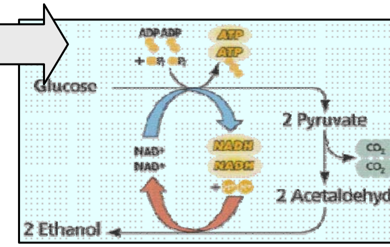


Photosynthesis



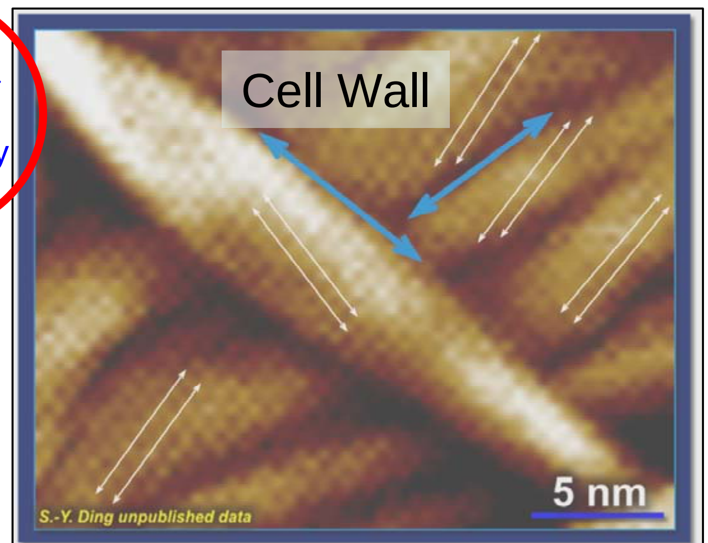
Bioassembly





Fermentation

Deconstruction



Atomic force micrograph of primary cell wall nanostructures (25 x 25 nm) (*Ding, S.-Y., NREL*)

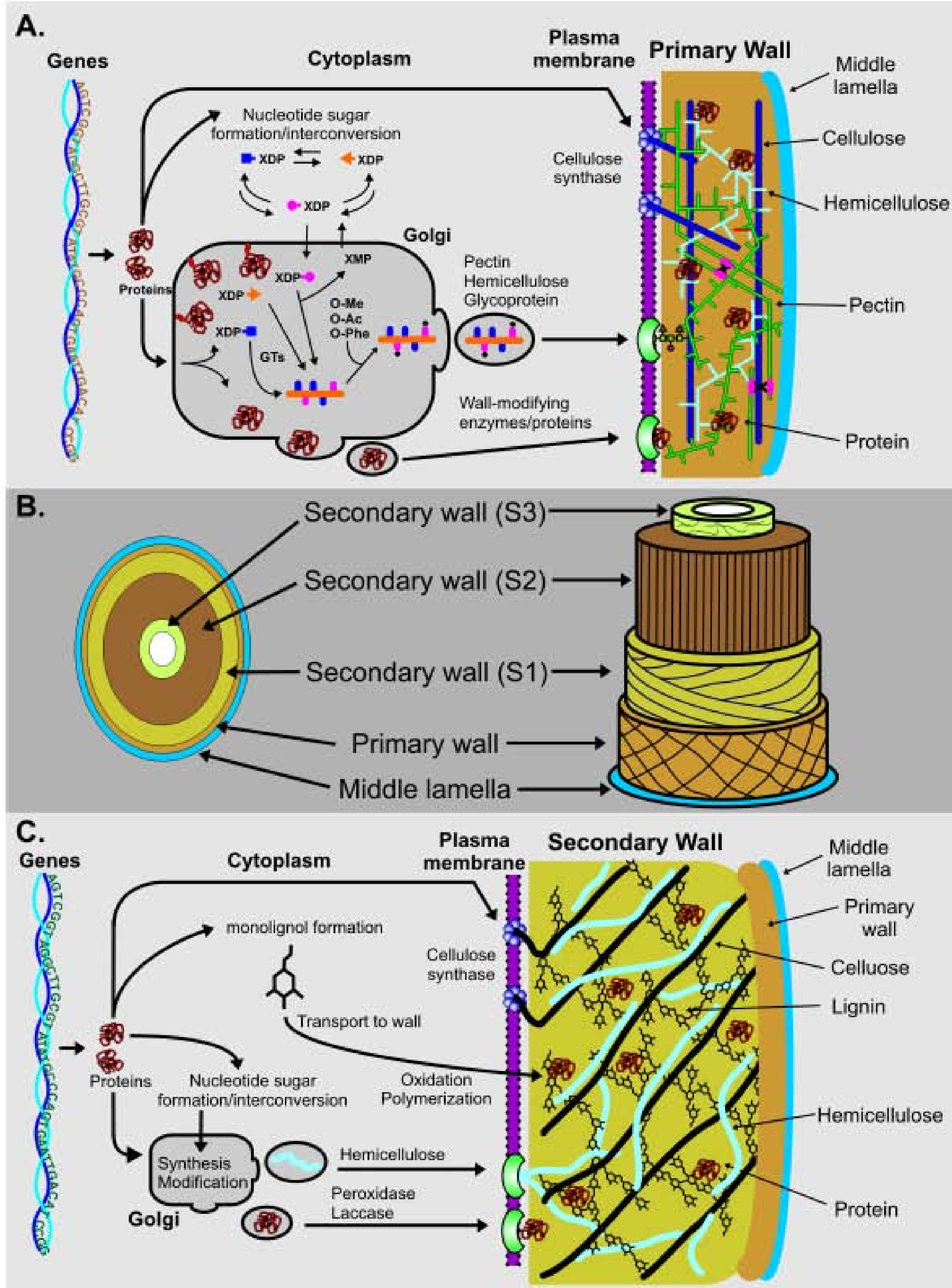
The microfibril is only 3-5 nm!

- 140,000 sq ft. facility; state-of-the-art MS, computing and NMR instrumentation
- Research on carbohydrates in biomedicine, plants and microbes

Synthesis of plant walls polysaccharides requires:
a coordinated expression of multiple types of biosynthetic and processing enzymes.

These enzymes require specific activated-sugar and acceptor substrates.

Malcolm O'Neill, CCRC
Mohnen et al. (2008)



Primary Wall

Dividing and growing cells

Pectin
Hemicellulose
Cellulose
(proteins)

Secondary Walls

Some cells with structural roles

↓ Pectin
Hemicellulose
Cellulose
Lignin
(proteins)

There is increasing research emphasis on identifying and understanding cell wall biosynthetic genes and enzymes.

$$\text{Substrate} + \text{acceptor}_{(n)} \xrightarrow{\textit{enzyme}} \text{acceptor } (n+1) + \text{xxx}$$

$$\text{UDP-sugar} + \text{acceptor}_{(n)} \xrightarrow{\textit{Glycosyltransferase / polysaccharide synthase}} \text{acceptor}_{(n+1)} + \text{UDP}$$

Current state: ≥ 2000 wall biosynthetic enzymes (*Arabidopsis*)

Current state: ≥ 200 wall polysaccharide transferases (*Arabidopsis*)
of these, only ~20 genes identified

Current state: ~20-30 lignin biosynthetic genes
of these ~40-60 % identified

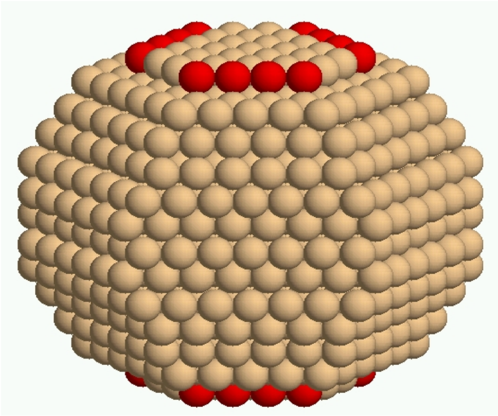
The goals of CarboSource Services continue to be:

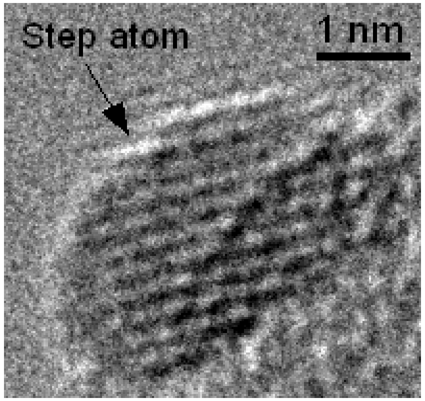
* synthesis of rare substrates for acquisition by researchers
* development of methods to produce rare substrates

"CarboSource Services", was established in 2001 at the CCRC at the University of Georgia under the direction of the Co-PI Debra Mohnen.

CarboSource Services was partially-funded by NSF from 2001-2007; beginning in FY2009 funding provided by DOE-BES.

Catalysis Science: The Acceleration and Control of Chemistry





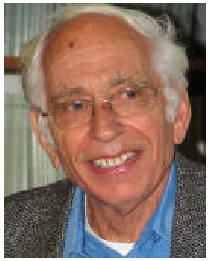
Model (top) and TEM image of a ruthenium nanoparticle active in ammonia synthesis. (Courtesy of J. Norskov)

- Catalysis rests on two foundations:
  - The acceleration of chemical reactions.
  - The control of competing reactions to selectively produce desired products and minimize undesirable ones.
- Catalytic processes now enable:
  - The production of chemicals with optimal utilization of energy and minimal production of environmentally damaging side products.
  - The development and use of renewable energy sources.
  - The creation of materials with tailored properties on the nano to macroscopic scale.
  - Precise synthesis of highly value-added molecules with stereo-isomeric specificity.
- Revolutions in experimental and theoretical techniques in the past 20 years make it feasible to study catalysis in many complex environments (solutions, interfaces, living systems, etc.) at the molecular level.
- The goal is to understand and harness the wide variety of catalytic phenomena – e.g., heterogeneous catalysis, homogeneous catalysis, and biocatalysis.
- BES is the largest supporter of fundamental catalytic science.

Nobel Prize in Chemistry 2005 Awarded to Two BES Investigators

Robert Grubbs,
Caltech

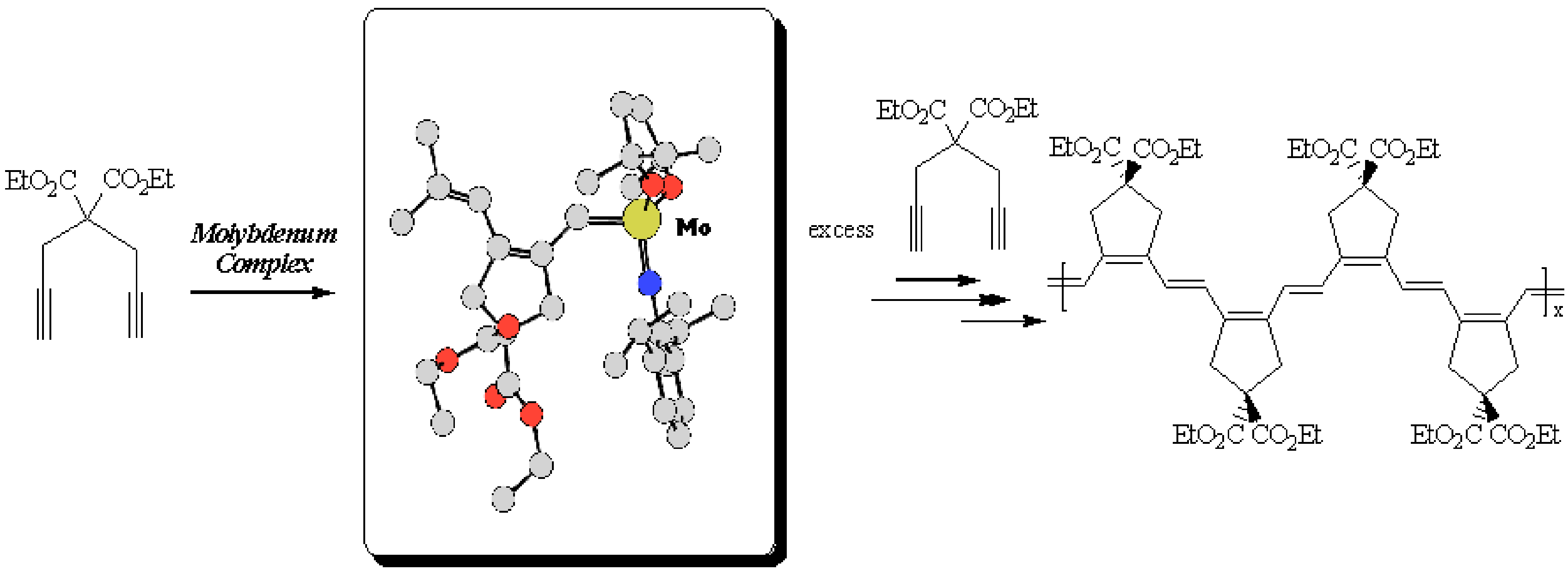
Richard Schrock,
MIT



Yves Chauvin,
Inst Francais du Petrole

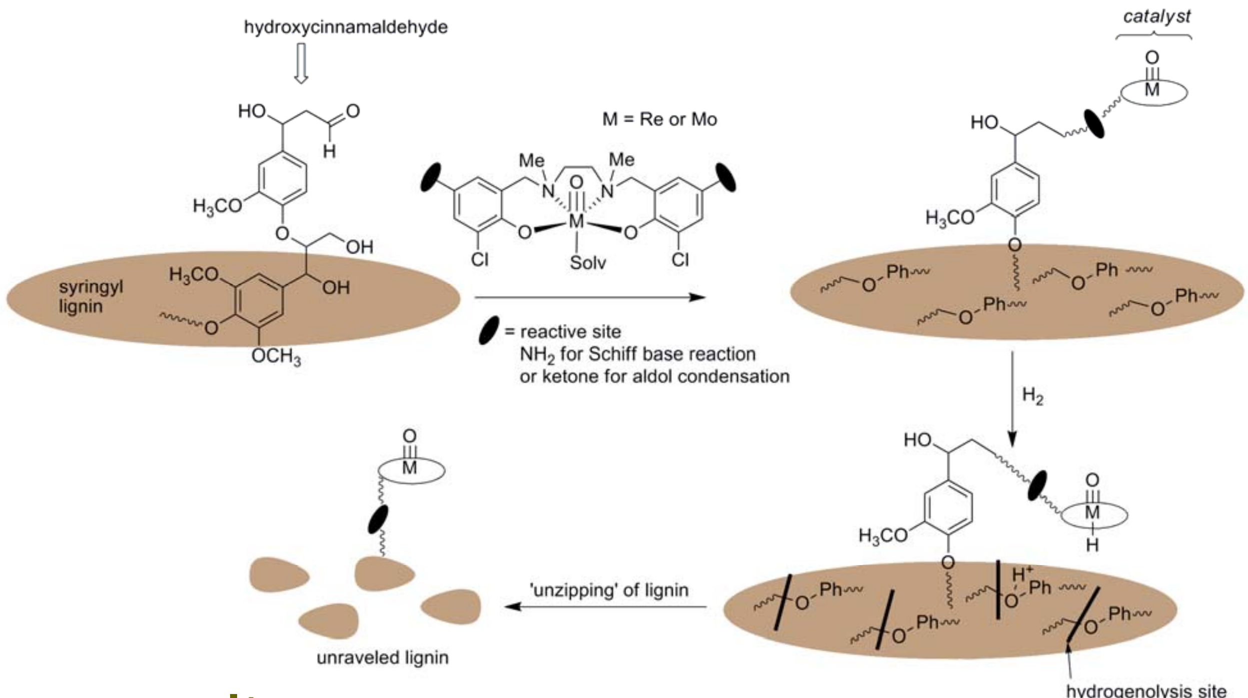
R. Schrock, DOE-BES grantee, 1979-present
R. Grubbs, DOE-BES grantee, 1979-1988, 2005

Their work led to understanding of the mechanistic steps of olefin metathesis and the development of successfully working catalysts for such chemistry. Olefin metathesis is a chemical process that is largely responsible for the production of fuels, pharmaceuticals, polymeric materials, detergents, and many other petrochemical products. Through exquisite control, catalysts direct organic molecules that might not react under mild conditions, to link together in specific ways and with minimum production of waste.

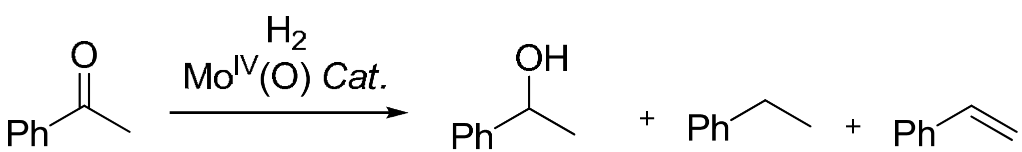


Schrock's polymerization of alkynes

Unzipping of lignin via *Trojan Horse* tandem catalysts



Preliminary result:



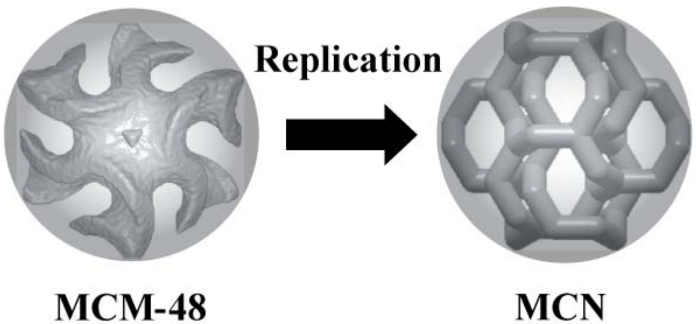
100% conversion

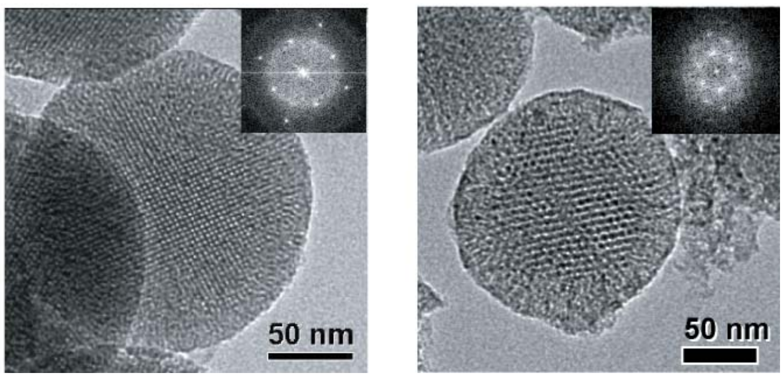
Becoming possible: biochemically engineered lignin that allows the introduction of a '*Trojan horse*' catalyst for deconstructing the lignin biopolymer…

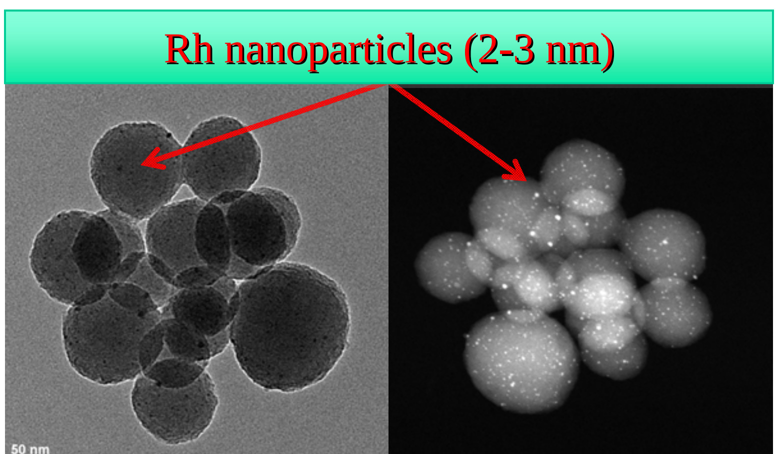
Abu-Omar, Purdue University

Mesoporous Carbon Nanosphere-supported Metal Catalysts for Selective Conversion of Biomass-generated Synthetic Gas to Ethanol

AMES LABORATORY







Victor Lin, Ames Lab and Iowa State University

$$x\,CO + y\,H_2 \xrightarrow[\text{Rh-MCN Catalyst}]{\text{Oxygenation}} CH_3CH_2OH$$

Catalyst	Product Selectivity (%)		
	CH_4	MeOH	EtOH
Impregnated Rh on Silica	87.4	2.9	8.7
Rh-MCN	< 2.0	26.7	71.3

- ✓ We have successfully synthesized a Mesoporous Carbon Nanosphere (MCN) material with graphene and tetragonal *I*4$_1$/*a* porous structure via the carbon replication process of a cubic *Ia*-3d (MCM-48 type) mesoporous silica template.
- ✓ The mesoporous surface of MCN was functionalized with MnO_2 and Rh nanoparticles (avg. diameter 2-3 nm) to yield a series of novel Rh-MCN catalysts.
- ✓ In contrast to the low product selectivity for alcohols of the conventional C2-oxygenation catalysts, our Rh-MCN catalysts show an unprecedented high selectivity for ethanol. (*"Turning Waste Material Into Ethanol"*, ***ScienceDaily***, August 14, 2008. *"Nanoscale catalyst converts syngas to ethanol"*, ***Ethanol Producer Magazine***, August 15, 2008. *"Nanoscale catalysts could tap syngas as cheap source of ethanol"*, ***Small Times***, August 18, 2008.)