Five-Year Goals and 2012 Progress Summaries

Following the 2012 midterm science reviews of the Energy Frontier Research Centers (EFRCs), one-page summaries of the progress each EFRC had made towards reaching their five-year scientific research goals were developed; these also include the five-year award total; the staffing headcount by type of staff; the number of peer-reviewed journal publications; the number of invention disclosures, patents/ patent applications, and associated licenses; and the number of companies using the results from the research. This information was collected in May 2012.

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Five-Year Goals and 2012 Progress

Argonne-Northwestern Solar Energy Research Center
Director: Michael R. Wasielewski
Lead Institution: Northwestern University

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To revolutionize our understanding of molecules, materials and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production.

Partner Institutions: Argonne National Laboratory; Yale University; University of Illinois, Urbana-Champaign; University of Chicago

Award: $19.0 M

Senior Investigators: 25 **Postdoctoral Staff:** 28 **Graduate Students:** 32 **Technical Staff:** 12
Publications: 109 **Invention Disclosures:** 2 **Patents/Applications:** 4 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Develop a fundamental understanding of the interaction of light and charge with molecules and materials necessary to convert solar energy into fuels and electricity.	▪ Developed light-driven hydrogen generation catalysts that mimic the behavior of the active site within hydrogenase enzymes, and use ultrafast multi-step electron transfer to extend charge separation lifetimes. ▪ Prepared the most active water oxidation catalyst known to date and have integrated it with a light-harvesting molecule to power it with solar energy.
Develop a fundamental understanding of how the electronic energy levels in molecules and materials impact solar energy conversion.	▪ Developed an integrated, predictive theoretical model of organic photovoltaics (OPVs) that takes into account all critical interfacial charge transport processes. ▪ Experiments and theoretical modeling demonstrated that surface plasmon resonance effects can boost light absorption in light-harvesting molecules by 15-fold.
Develop a fundamental understanding of the dynamics of photoinduced charge generation, separation, and transport across various interfaces with unparalleled temporal and spatial resolution.	▪ Prepared and characterized a new thin layer, highly-active, water oxidation catalyst using a combination of x-ray absorption and high energy scattering as well as computational modeling to determine its structure. ▪ Demonstrated a quantitative correlation between active layer nanostructure and power efficiency in OPVs using grazing incidence x-ray scattering.
Develop a fundamental understanding of the materials interfaces at which charge generation, separation, transport, and selective chemical reactions occur.	▪ Fabricated organic photovoltaics on graphene oxide interfacial layers, which provide a 20-fold increase in the lifetime compared to conventional organic interfacial layers. ▪ Iron oxide, Fe_2O_3 "rust", is a stable solar absorber and water oxidation catalyst, but has poor electronic properties that limit its efficiency. Demonstrated a new route to "folded" Fe_2O_3 electrodes that overcome these deficiencies.
Develop a fundamental understanding of the properties of unique materials, from self-assembling, bio-inspired materials for hydrogen fuel production from water, to transparent conductors and nanostructured hard and soft materials for solar electricity generation.	▪ Found that the molecular self-assembly of novel light absorbers with polymer electrolytes and new nickel catalysts produce artificial membranes that photo-generate hydrogen. ▪ Discovered that porous chalcogenide materials (chalcogels) mimic the composition and architecture of water-splitting proteins by providing a 3D platform to assemble nanostructured catalysts that carry out solar hydrogen production.

Website: http://www.ansercenter.org

Five-Year Goals and 2012 Progress

Catalysis Center for Energy Innovation
Director: Dionisios (Dion) G. Vlachos
Lead Institution: University of Delaware

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To design and characterize novel catalysts for the efficient conversion of the complex molecules comprising biomass into chemicals and fuels.

Partner Institutions: University of Pennsylvania; University of Massachusetts; University of Minnesota; Lehigh University; Brookhaven National Laboratory; California Institute of Technology; Princeton University

Award: $17.5 M, ARRA

Senior Investigators: 28 **Postdoctoral Staff:** 15 **Graduate Students:** 30 **Technical Staff:** 2
Publications: 55 **Invention Disclosures:** 0 **Patents/Applications:** 4 **Patents Licensed:** 3
Companies using EFRC research: Anellotech, Argilex Technologies

5 Year Research Goals	Progress
Develop heterogeneous catalysts for the conversion of sugars to intermediates for the production of fuels and chemicals – Intensify conversion processes for improved economics – Develop methods for mechanistic understanding of the underlying chemistry	▪ Introduced a new tin-zeolite catalyst for the conversion of a broad range of sugars to useful intermediates, such as glucose isomerization to fructose and xylose isomerization to xylulose. ▪ Developed "single-pot" technology for the production of various platforms with reduced cost. ▪ Revealed the mechanisms for several key reactions and demonstrated for the first time Lewis acid catalysis in water that exhibits an enzyme-like mechanism.
Develop a computational engine for the *a priori* discovery of novel (metal and transition-metal carbide) catalysts – Predict catalysts for reforming and hydrodeoxygenation of bio-oil to produce fuels and chemicals – Understand the reaction mechanisms and reveal the effect of functional groups of various bio-oil components	▪ Developed computational engine for catalyst discovery for biomass derivatives and demonstrated theory-guided experiments for reforming and hydrodeoxygenation. ▪ Identified surface bimetallics (Ni-Pt and Ni-WC) as highly active and selective reforming catalysts and transition-metal carbides (Mo_2C) as highly selective deoxygenation catalysts. ▪ Revealed (reaction) pathways of thermal cracking and steam reforming of small bio-oil components.
Develop catalysts and processes for the selective production of aromatics (monomers for green plastics) – Optimize para-xylene production to enable production of green plastics – Optimize yield of aromatics in catalytic fast pyrolysis as drop-ins to gasoline	▪ Developed Brønsted and Lewis acid catalysts in a multiphase reactor for the production of para-xylene. ▪ Achieved >75% yield to para-xylene from dimethylfuran and ethylene, compared to 16% in the literature, and gained understanding of the role of the catalyst. ▪ Achieved 40% increase in aromatics in catalytic fast pyrolysis as drop-ins to gasoline using a zeolite catalyst (Ga/ZSM-5).
Develop direct carbon fuel cells using molten metal electrolytes that convert solid biomass to electricity for power generation	▪ Demonstrated feasibility of direct carbon fuel cells, identified materials, characterized electrodes, developed a fundamental understanding, and optimized the technology.

Website: http://www.efrc.udel.edu

Five-Year Goals and 2012 Progress

Center for Advanced Biofuel Systems	Energy Frontier Research Centers
Director: Jan Jaworski	Basic Energy Sciences
Lead Institution: Donald Danforth Plant Science Center	DOE Office of Science

Mission: To generate the fundamental knowledge required to increase the efficiency of photosynthesis and production of energy-rich molecules in plants.

Partner Institutions: Michigan State University; New Mexico Consortium; University of Missouri-St. Louis; University of Nebraska-Lincoln; Washington State University

Award: $15.0 M

Senior Investigators: 10	**Postdoctoral Staff:** 17	**Graduate Students:** 2	**Technical Staff:** 9
Publications: 16	**Invention Disclosures:** 0	**Patents/Applications:** 4	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Enhance photosynthetic efficiency and carbon uptake in plants and algae	▪ Used molecular biology approaches to increase the pool size of plastoquinone in *C. reinhardtii*. ▪ Transformed constructs to overexpress cyanobacterial *ftpI* and *ftpII* into the chloroplast genome of *C. reinhardtii*. ▪ Transformed plasmids to overexpress *C. reinhardtii* bicarbonate transporter (HLA3), human carbonic anhydrase (HCA II) and bacterial carbonic anhydrase into Arabidopsis and camelina.
Understand regulatory networks controlling lipid metabolism in plants and algae	▪ Identified transcriptional factors that interact with lipid metabolites and characterized some of the interactions. ▪ Demonstrated that phospholipase-mediated phospholipid turnover plays a key role in mediating lipid accumulation.
Produce novel molecules that are components of jet fuel	▪ Produced camelina plants that accumulate oil (mono-and sesquiterpene) in seed. Patent application has been filed. ▪ Generated over 40 different seed-specific gene expression constructs with different combinations of candidate short- and medium-chain specific fatty acid biosynthetic genes and added to the camelina transgenic pipeline. Tested the resulting oil for jet-fuel-like functions. ▪ Engineered lipid and phenylpropanoid biosynthesis in yeast, Arabidopsis, and camelina. Analyzed fatty acid synthase complex in Arabidopsis and, based on protein interaction assays, identified two novel regulators of fatty acid synthesis.
Develop robust platforms for analysis of transcripts, proteins and metabolites in plants and algae	▪ Developed and utilized two liquid chromatography-based quantitative proteomics methods (iTRAQ and label-free). Several methods in place for extracting and quantifying a wide variety of metabolites, from primary metabolites to volatiles and non-volatiles, including many lipid classes. Used transcriptional profiling with state of the art next-generation sequencing technologies (e.g., RNA-sequencing).
Develop flux analysis platforms for wild type and transgenic camelina and Chlamydomonas	Developed platforms for flux analysis, including: ▪ Cell and embryo culturing methods mimicking *in planta* conditions. ▪ Steady-state/kinetic labeling protocols. ▪ Analysis of labeling in metabolic intermediates and products. ▪ Computer-aided metabolic flux models. ▪ Validated flux maps for wild type strains. Flux analysis of transgenic strains is underway.

Website: http://www.danforthcenter.org/CABS

Center for Advanced Solar Photophysics Energy Frontier Research Centers
Director: Victor I. Klimov Basic Energy Sciences
Lead Institution: Los Alamos National Laboratory DOE Office of Science

Mission: To capitalize on recent advances in the science of how nanoparticles interact with light to design highly efficient materials for the conversion of sunlight into electricity.

Partner Institutions: National Renewable Energy Laboratory; University of California, Irvine; Rice University; George Mason University; University of Minnesota; University of Colorado at Boulder; Colorado School of Mines

Award: $19.0 M

Senior Investigators: 16 **Postdoctoral Staff:** 14 **Graduate Students:** 14 **Technical Staff:** 3
Publications: 58 **Invention Disclosures:** 1 **Patents/Applications:** 3 **Patents Licensed:** 0
Companies using EFRC research: Sharp Corporation

5 Year Research Goals	Progress
Demonstrate efficient conversion of excess absorbed photon energy into extra charges in quantum-confined semiconductor nanocrystals (NCs) through predictive understanding of carrier multiplication (CM) and competing processes	▪ Demonstrated efficient CM in quantum dots (QDs) with the threshold approaching the fundamental two-energy-gap limit. ▪ Experimentally demonstrated that further enhancement in the CM efficiency can be obtained by using elongated NCs (quantum rods). ▪ Developed a generalized theory of CM, unifying coherent and incoherent models. ▪ Elucidated the physics of processes competing with CM such as phonon emission, coupling to surface species, and photoionization.
Establish the utility of semiconductor NCs as a new material platform for efficient, solution-processed solar cells through detailed understanding of interfacial phenomena, charge transport, recombination processes and environmental and photo-stability	▪ Produced photoconductive and robust QDs layers via new QD surface-treatment, electronic-coupling, and infilling methods. ▪ Developed new method for synthesis and solution-based film deposition of ligand-free silicon and germanium QDs. ▪ Explored p-n junction architectures for incorporation of photoactive QD-based layers into practical solar cells. ▪ Demonstrated 1000+ hours of air stability of QD-based solar cells. ▪ Created the first certified, record efficiency QD solar cell, included as a new photovoltaic (PV) platform in NREL's PV efficiency chart.
Demonstrate facile control of electronic and optical properties of NCs through size/shape control, doping, and heterostructuring, in order to optimize light harvesting, charge separation and recombination dynamics	▪ Developed new, highly efficient syntheses of QDs of solar relevant near-infrared materials (CuInS(Se), PbSSe and PbS(Se)Te). ▪ Demonstrated nanoscale charge-separating heterojunctions (specifically PbSe/CdSe/CdS QDs and tetrapods) with ultra-long carrier lifetimes. ▪ Developed core/shell QDs with suppressed Auger decay and NCs with optically-active p-type copper (Cu^{2+}) dopants. ▪ Combined semiconductor NCs and metal nanoparticles of arbitrary compositions and shapes into well-defined nanohybrids with widely tunable exciton-plasmon interactions.
Demonstrate prototype third-generation solar cells with enhanced performance due to novel nanoscale physics	▪ Developed the first p-n junction lead selenide QD-based solar cell with an external quantum efficiency greater than 100%. ▪ Demonstrated that the photovoltage of a QD-based solar cell can be enhanced by quantum-confinement. ▪ Theoretically showed that solar concentration can greatly increase the effect of CM on PV performance.

Website: http://casp.lanl.gov

Five-Year Goals and 2012 Progress

Center for Atomic Level Catalyst Design
Director: James J. Spivey
Lead Institution: Louisiana State University

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To build effective catalysts from first principles via computational catalysis and atomic-level synthesis.

Partner Institutions: Clemson University; University of Florida; Georgia Institute of Technology; Grambling State University; Ohio State University; Pennsylvania State University; Texas A&M University; Oak Ridge National Laboratories; Utrecht University; Tech University Vienna

Award: $12.5 M
Senior Investigators: 20 **Postdoctoral Staff:** 20 **Graduate Students:** 32 **Technical Staff:** 2
Publications: 41 **Invention Disclosures:** 1 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Develop computational methods to identify catalyst compositions for the production of clean fuels such as ethanol.	▪ Quantum-based computational studies identified promising bimetallic catalysts; initial experimental testing has proven the validity of the model predictions.
Develop new tools for quantitative analysis of the 3D structure of metal catalysts supported within mesopores.	▪ Developed a new calorimetric method to characterize pore entrance sizes in ordered mesoporous materials, yielding information not possible by conventional measurements.
Develop a fundamental understanding of carbon dioxide (CO_2) conversion using electrocatalysts that can be powered by solar energy.	▪ For the first time, intermediates in the electrocatalytic reduction of carbon dioxide to methanol have been predicted with simulation and then verified with experiment.
Develop tools to prepare atomically precise catalysts, and follow their formation in real time.	▪ Demonstrated a millifluidic reactor by synthesizing gold clusters as small as 1 nanometer and following their growth using synchrotron x-ray absorption spectroscopy.
Develop tools to correlate fundamental electronic properties of atomically precise catalysts, synthesized using wet-chemistry, with their catalytic activity.	▪ Demonstrated for the first time the presence of s–d hybridization in ligand stabilized clusters of gold atoms (Au_{38}).
Design and test adsorbents to remove sulfur in syngas produced from biomass.	▪ Successfully predicted with computational chemistry, for the first time, the relative order of desulfurization activity for mixed oxide adsorbents.
Develop a high-quality experimental database as input for modeling of atomically complex catalyst surfaces.	▪ Observed the active site for adsorption and irreversible splitting of water at room temperature.
Synthesize new graphene templates by tuning the graphene-substrate interactions.	▪ Synthesized graphene moiré structures on metal surfaces.

Website: http://www.efrc.lsu.edu

Five-Year Goals and 2012 Progress

Center for Bio-Inspired Solar Fuel Production Energy Frontier Research Centers
Director: Devens Gust Basic Energy Sciences
Lead Institution: Arizona State University DOE Office of Science

Mission: To construct a complete system for solar-powered production of hydrogen fuel via water splitting. Design principles are drawn from the fundamental concepts that underlie photosynthetic energy conversion.

Partner Institutions: None

Award: $14.0 M, ARRA
Senior Investigators: 11 **Postdoctoral Staff:** 13 **Graduate Students:** 18 **Technical Staff:** 3
Publications: 43 **Invention Disclosures:** 1 **Patents/Applications:** 6 **Patents Licensed:** 5
Companies using EFRC research: Mattium Corporation

5 Year Research Goals	Progress
Investigate fundamental science necessary to produce a complete system for solar hydrogen production by water splitting	▪ Bio-inspired organic materials, designed and synthesized at the Center, were employed in construction of an initial version of an artificial photosynthetic cell that uses sunlight to split water and generate hydrogen. This cell is being used to develop principles for preparation of useful solar fuel production systems. ▪ Created a design for a more efficient, tandem system.
Design and prepare artificial photosynthetic reaction centers for water splitting systems	▪ Developed dyes for reaction centers absorbing short-wavelength sunlight for water oxidation, and for those absorbing long-wavelength sunlight for hydrogen production. ▪ Incorporated a bio-inspired electron relay, reflective of pathways in natural photosystems, to transfer oxidation potential between reaction centers and water oxidation catalysts to improve water oxidation efficiency. ▪ Devised new methods for the synthesis of reaction center molecules.
Discover new catalysts for water oxidation	▪ Developed new functional catalysts based on iridium, an expensive but effective catalyst, and cobalt, an abundant, inexpensive element. ▪ Evaluating several approaches to synthesize catalysts based on earth abundant elements including manganese. ▪ Initial demonstration (with others) of femtosecond x-ray crystallography, a revolutionary new method for molecular structural analysis.
Discover new catalysts for hydrogen production	▪ Developed two new bio-inspired catalysts that produce hydrogen gas. ▪ Initiated the design of catalysts with higher efficiency and stability.
Discover new transparent electrode materials for use in solar fuel production systems	▪ Discovered a new, mesoporous, transparent, high surface area, conductive metal oxide material for use as electrodes. A startup company is developing other uses for this material. ▪ Other mesoporous transparent metal oxide materials are under development.

Website: http://solarfuel.clas.asu.edu/

Five-Year Goals and 2012 Progress

Center for Catalytic Hydrocarbon Functionalization — Energy Frontier Research Centers
Director: T. Brent Gunnoe — Basic Energy Sciences
Lead Institution: University of Virginia — DOE Office of Science

Mission: To develop, validate, and optimize new methods to rearrange the bonds of hydrocarbons, implement enzymatic strategies into synthetic systems, and design optimal environments for catalysts that can be used to reversibly functionalize hydrocarbons, especially for more efficient use of natural gas including low temperature conversion to liquid fuels.

Partner Institutions: Brigham Young University; California Institute of Technology; Iowa State University; Princeton University; The Scripps Research Institute; University of Maryland; University of North Carolina, Chapel Hill; University of North Texas; Yale University

Award: $11.0 M

Senior Investigators: 10	**Postdoctoral Staff:** 16	**Graduate Students:** 20	**Technical Staff:** 2
Publications: 54	**Invention Disclosures:** 0	**Patents/Applications:** 2	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Design and study new catalysts for selective and low temperature conversion of natural gas (methane) to liquid fuel based on electrophilic catalysts.	▪ Developed new palladium [Pd(II)] catalysts for carbon-hydrogen (CH) functionalization using oxygen (O). ▪ Demonstrated the use of new single-site catalysts supported on mesoporous silica nanoparticles. ▪ Demonstrated functionalization of platinum-methyl (Pt-Me) bonds to make methanol on mesoporous silica nanoparticles. ▪ Identified new metal (rhodium and iridium) catalysts for methane functionalization.
Design and study new catalysts for selective and low temperature conversion of natural gas (methane) to liquid fuel based on nucleophilic catalysts.	▪ Identified new mechanisms for oxygen atom insertion into metal-hydrocarbyl bonds, which are central to new strategies for catalytic cycles for gas-to-liquid conversion. ▪ New organo-catalysts for oxygen insertion into metal-methyl bonds. ▪ Demonstrated that basic media can be used to accelerate metal-mediated CH activation.
Design and study new catalysts for selective and low temperature conversion of natural gas (methane) to liquid fuel based on the formation of oxo complexes.	▪ Developed new manganese-based catalysts for halogenation of CH bonds including those with strong bonds (sp^3 CH). ▪ Demonstrated that vanadium-oxygen complexes should be capable of breaking strong C–H bonds, including methane. ▪ Developed new approach to catalytic CH functionalization using water oxidation catalysts. ▪ Developed new iridium catalysts that oxidize hydrocarbons. ▪ Developed procedures to bind ruthenium catalysts on transparent conducting oxide (ITO, FTO, TiO_2 and nanoITO) surfaces and demonstrated electrocatalytic oxidations of hydrocarbons.
Design and study new molecular electrocatalysts for anodic oxidation of methane at low temperatures, high current and low over potentials (for ultimate application in methane fuel cells).	▪ Developed strategies to covalently attach catalysts for CH activation to electrode surfaces. ▪ Demonstrated that the modified complexes show similar CH activation reactivity to the original system. ▪ Synthesized and studied anodic oxidation of low valent transition metal alkyl complexes that provide insight into the anodic oxidation of methane.

Website: http://artsandsciences.virginia.edu/cchf/

Center for Defect Physics in Structural Materials Energy Frontier Research Centers
Director: G. Malcolm Stocks Basic Energy Sciences
Lead Institution: Oak Ridge National Laboratory DOE Office of Science

Mission: To enhance our fundamental understanding of the defects, defect interactions, and defect dynamics that determine the performance of structural materials in extreme environments.

Partner Institutions: Ames Laboratory; Brown University; University of California, Berkeley; Carnegie Mellon University; University of Illinois at Urbana-Champaign; Lawrence Livermore National Laboratory; Ohio State University; University of Tennessee

Award: $19.0 M

Senior Investigators: 23 **Postdoctoral Staff:** 6 **Graduate Students:** 9 **Technical Staff:** 4
Publications: 27 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Understand the formation and time-evolution of displacement cascades in determining radiation damage production on the sub-picosecond time scale and their influence on damage accumulation at much longer times (seconds to years).	▪ Simulations of x-ray scattering of atomic configurations obtained at discrete times from molecular dynamics (MD) cascade simulations: (1) showed cascade-induced shock waves contain sub-picosecond information on cascade dynamics that may provide direct insight into energy partitioning between the electronic and ionic systems, and (2) identified a statistically-based technique for sub-picosecond resolution x-ray measurements of cascade dynamics at the Linac Coherent Light Source. ▪ Developed a new self-evolving atomistic kinetic Monte Carlo method that extends the time scale for highly accurate atomistic simulations by 10 orders of magnitude.
Understand quantitatively the interactions of dislocations with defects and microstructure in materials at the unit event level of single dislocations and the local stresses that drive fundamental deformation processes.	▪ Demonstrated the ability to detect single dislocations and micro-rotations surrounding dislocation arrays by sub-micron resolution x-ray microscopy at the Advanced Photon Source. ▪ Identified crystal orientations favorable for the controlled injection of dislocations in metal alloys (Ti-7Al and Mg) with combined nanoindentation and cross-sectional transmission electron microscopy (TEM) studies. ▪ Produced full 3D maps of the dislocation structures in deformed molybdenum nanofibers using electron tomography; conditions under which fibers undergo hardening were established using *in situ* TEM deformation. ▪ Designed and assembled an *in situ* nanoindenter-based system for combined 3D x-ray microscopy and small-scale instrumented mechanical testing at the Advanced Photon Source.
Treat unit events involving dislocations and radiation damage cascades within an *ab initio* framework and thereby relate defect properties to the underlying atomic, electronic and magnetic structure	▪ Essentially exact Quantum Monte Carlo methods, producing the most accurate electronic structures to date for aluminum (Al), have remedied the failure of existing density functional theory (DFT) to accurately predict the density and unequivocally resolved a discrepancy between theory and experiment regarding the sign of the di-vacancy binding energy in Al. ▪ Developed a coarse-grained DFT methodology that can treat the multi-million atom configurations used in classical molecular dynamics. The new method, which retains DFT accuracy, was used to understand and model magnetic effects on displacement cascade evolution in iron.

Website: http://cdp.ornl.gov

Five-Year Goals and 2012 Progress

Center for Direct Catalytic Conversion of Biomass to Biofuels Energy Frontier Research Centers
Director: Maureen McCann Basic Energy Sciences
Lead Institution: Purdue University DOE Office of Science

Mission: To integrate fundamental knowledge and enable technologies for catalytic conversion of engineered biomass to advanced biofuels and value-added products.

Partner Institutions: National Renewable Energy Laboratory; University of Tennessee; Northeastern University; Argonne National Laboratory

Award: $20.0 M, ARRA

Senior Investigators: 24	**Postdoctoral Staff:** 12	**Graduate Students:** 28	**Technical Staff:** 10
Publications: 33	**Invention Disclosures:** 7	**Patents/Applications:** 3	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Add value to lignin by enabling its catalytic conversion. Lignin is an abundant by-product of biorefinery operations, and comprises 40% of energy content in biomass, but is not widely utilized to make fuels and products.	▪ Demonstrated control of lignin composition by modulating its biosynthesis—a control science approach generating unique and tailored materials. ▪ Developed a selective, robust catalyst system for the disassembly of lignin via molecular cleavage (β-O-4-glycerolaryl ether) and subsequent deoxygenation of the resulting fragments without hydrogenating the aromatic groups. ▪ Developed highly flexible oxidative catalyst systems for product composition and reaction control.
Control synthesis, assembly and deconstruction of cellulose microfibrils. The structure of the cellulose microfibril, its size, crystallinity and potential aggregation in macrofibrils in plant cell walls, is a second major factor in the recalcitrance of biomass to deconstruction.	▪ Achieved new understandings of cellulose synthesis by demonstrating that catalytic domains form dimers. ▪ Developed computational models of cellulose structure that enable predictive behaviors. ▪ Demonstrated that maleic acid is a dual-function catalyst that releases pentoses from biomass and catalyzes their conversion to furfural at high yields. ▪ Incorporated sulfonic acid or ionic liquid groups on the surfaces of silicate supports to utilize solid acid catalysts for release of glucose from cellulose.
Engineer tailored biomass for highly efficient, direct catalytic conversion to liquid fuels and value-added products. By engineering biomass variants to incorporate catalysts, co-catalysts, or functionalized catalytic sites into cell walls, reaction steps in subsequent processing may be simplified, and the biphasic barrier between the catalyst in solution and the solid polymeric biomass alleviated.	▪ Elucidated the effects of iron co-catalysts in pretreatment of biomass and demonstrated that in vitro impregnation of corn stover (leaves and stalk) with soybean ferritin plus ferric iron (Fe^{+3}) significantly increases glucose and xylose yields. ▪ Generated Arabidopsis and rice transformants that express iron-binding peptides targeted to the cell wall for testing in physical and chemical conversion processes.
Design fast-hydropyrolysis to maximize carbon efficiency. Fast-hydropyrolysis has the potential to generate intermediates for catalytic upgrading to fuels from highly recalcitrant biomass components.	▪ Demonstrated that the primary products of fast-pyrolysis of cellulose are much simpler mixtures than bio-oil, making the discovery and design of a catalyst, or catalysts series, more feasible as the number of compounds to deoxygenate is greatly reduced.

Website: http://www.C3Bio.org

Five-Year Goals and 2012 Progress

Center for Electrochemical Energy Storage: Tailored Interfaces Energy Frontier Research Centers
Director: Michael Thackeray Basic Energy Sciences
Lead Institution: Argonne National Laboratory DOE Office of Science

Mission: To acquire a fundamental understanding of interfacial phenomena controlling electrochemical processes that will enable dramatic improvements in the properties and performance of energy storage devices, notably lithium-ion batteries.

Partner Institutions: University of Illinois at Urbana-Champaign and Northwestern University

Award: $19.0 M
Senior Investigators: 17 **Postdoctoral Staff:** 11 **Graduate Students:** 17 **Technical Staff:** 12
Publications: 30 **Invention Disclosures:** 4 **Patents/Applications:** 9 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Create synthetic procedures for designing novel electrode/electrolyte materials and architectures and understand surface and interfacial phenomena that occur during electrochemical reactions.	▪ Used lithographic patterning to reveal the anisotropic expansion of silicon electrodes. ▪ Designed anode architectures with nano-silicon particles in graphene, yielding high-charge/discharge rates. ▪ Created novel architectures of carbon and carbon-coated electrodes using autogenic reactions.
Explore and exploit novel concepts of 'self-repair' and 'activated shutdown' in lithium-ion battery systems.	▪ Demonstrated the *in situ* thermal shutdown of a lithium cell using polyethylene-encapsulated microcapsules on a carbon anode surface. ▪ For the first time, demonstrated autonomic restoration of electrical conductance with an encapsulated gallium-indium (Ga-In) liquid alloy.
Develop, by *in situ* and *ex situ* techniques, a thorough understanding of the structural and electrochemical behavior of materials at the electrode/electrolyte interface by capitalizing on the comprehensive facilities at the EFRC partner institutions.	▪ Developed an *in situ* scanning electron microscopy technique to measure local lithium-ion currents and topography of electrodes. ▪ Designed inelastic x-ray scattering methods to probe the solid-electrolyte-interphase (SEI) layers which are formed on battery electrodes during operation.
Use first-principles calculations, based on density functional theory and atomistic simulations, to explore the structure, energetics and kinetic properties of electrode/electrolyte materials and their interfaces with the fidelity to understand accompanying processes at an atomic/electronic scale.	▪ Simulations of unique electrode material of carbon spheres revealed a mixture of graphene fragments with diamond-like linkages and no strong spatial correlation beyond 8 angstroms. ▪ Simulations and calculations provided evidence of a 'superoxide-like' species on the surface of the discharge product in a lithium-air cell that has a low overpotential for decomposition during charging.

Website: http://web.anl.gov/energy-storage-science/

Five-Year Goals and 2012 Progress

Center for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage
Director: Grigorii Soloveichik
Lead Institution: GE Global Research

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To develop the fundamental basis for an entirely new high-density energy storage system that combines the best properties of a fuel cell and a flow battery.

Partner Institutions: Lawrence Berkeley National Lab; Stanford University; Yale University

Award: $15.0 M
Senior Investigators: 17 **Postdoctoral Staff:** 4 **Graduate Students:** 9 **Technical Staff:** 2
Publications: 10 **Invention Disclosures:** 5 **Patents/Applications:** 1 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Determine the correlation between the structure of potential organic hydrogen carriers (fuels) and the thermodynamics and kinetics associated with their electrochemical oxidation pathways.	▪ Developed a method to predict the open circuit potential and fuel electrooxidation potential in fuel cells. ▪ Calorimetrically determined free energy of dehydrogenation of fuels to validate model; promising fuels identified. ▪ Discovered and quantified an enhancing effect of bases on fuel electrooxidation.
Understand the correlation between catalyst structure and selectivity of electro(de)hydrogenation of the organic hydrogen carriers.	▪ Developed methods to accurately calculate and tune the redox potentials of electrocatalysts. ▪ Demonstrated electrodehydrogenation of model fuels with organocatalysts; selected inner sphere electrocatalysts for further development. ▪ Observed and studied the reaction pathways for a metal hydride species as a model for a key intermediate in the targeted cycle for an inner-sphere, organometallic mechanism.
Develop methods to attach catalysts to electrodes for electrochemical dehydrogenation/hydrogenation.	▪ Developed a controlled, tunable and scalable process to attach metal complexes to various carbon surfaces without loss of electrocatalytic activity.
Understand transport phenomena in proton exchange membranes working at low humidity that are compatible with organic carriers.	▪ Developed a model based on solubility parameters of polymer, electrolyte and fuel that predicts membrane/fuel cross-over.
Understand the interactions among the components of an organic fuel cell/flow battery system.	▪ Identified compatible proton exchange membrane (PEM)/fuel couples that retain high proton conductivity. ▪ Developed polybenzimidiazole membrane with significantly improved oxidative stability for use in the integrated system.

Website: http://www.ge.com/efrc

Five-Year Goals and 2012 Progress

Center for Emergent Superconductivity
Director: J.C. Séamus Davis
Lead Institution: Brookhaven National Laboratory

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To discover new high-temperature superconductors and improve the performance of known superconductors by understanding the fundamental physics of superconductivity.

Partner Institutions: Argonne National Laboratory; University of Illinois, Urbana Champaign

Award: $22.5 M

Senior Investigators: 28 **Postdoctoral Staff:** 20 **Graduate Students:** 18 **Technical Staff:** 4
Publications: 76 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: Superpower Inc., AMSC (American Superconductor)

5 Year Research Goals	Progress
Understand and control the interaction among disparate pinning defects in composite pinning landscapes in commercial superconducting tapes and iron-based superconductors.	▪ Revealed that heavy-ion irradiation in the barium-122 (Ba-122) superconductor system induces short nanorod-like defects that enhance the field and temperature dependence of the critical current without any reduction in the superconducting critical temperature (Tc). ▪ Formulated a time-dependent Ginzburg-Landau simulation that accurately predicts the interaction among thousands of defects. ▪ Demonstrated that correlated arrays of nanorods and linear tracks due to heavy-ion irradiation interact destructively.
Develop a microscopic model of the superconducting mechanism in the iron-based pnictide superconductors and understand the role of electron matter in the normal state of these materials.	▪ Theoretically predicted direct phase sensitive experimental tests of pairing symmetry. ▪ Evidence for $s\pm$ symmetry seen in pressure dependent measurements of the penetration depth. ▪ Angle-resolved photoemission spectroscopy, scanning tunneling microscopy and point contact spectroscopy studies all provided evidence of nematic order.
Understand and exploit nearby electronic phase in the high-Tc cuprate superconductors.	▪ Identified Fermi pockets with an area scaling with the doping level as the system emerges from the Mott insulating state. ▪ Demonstrated electric field dependent tuning of Tc in high-temperature superconductor field effect transistor grown by molecular beam epitaxy.
Perfect growth of families of new superconductors and provide samples over a broad range of composition for experimental characterization.	▪ Established phase diagrams of several iron-based superconductors. ▪ Grew and characterized thin films of iron chalcogenides.
Develop new chemical phases in search of new families of superconductors, guided by rational design criteria informed by theory and phenomena.	▪ Demonstrated that strong correlations and multi-band dynamics lead to pairing interactions in iron-based superconductors; supports the conclusion that strong electronic correlations are common to all high Tc superconductors. ▪ Demonstrated superconductivity in a 3D half-Heusler compound.

Website: http://www.bnl.gov/energy/ces/

Five-Year Goals and 2012 Progress

Center for Energy Efficient Materials — Energy Frontier Research Centers
Director: John E. Bowers — Basic Energy Sciences
Lead Institution: University of California, Santa Barbara — DOE Office of Science

Mission: To discover and develop materials that control the interactions among light, electricity, and heat at the nanoscale for improved solar energy conversion, solid-state lighting, and conversion of heat into electricity.

Partner Institutions: National Renewable Energy Laboratory; Los Alamos National Laboratory; University of California, Santa Cruz

Award: $19.0 M, ARRA

Senior Investigators: 22 **Postdoctoral Staff:** 12 **Graduate Students:** 28 **Technical Staff:** 20
Publications: 76 **Invention Disclosures:** 2 **Patents/Applications:** 5 **Patents Licensed:** 1
Companies using EFRC research: LifeCel Technology LLC; Next Energy Technologies; Unite to Light (non-profit)

5 Year Research Goals	Progress
Develop new molecular semiconductors that optimize absorption and charge transport properties for solar cells that can be manufactured by printing and coating technology to enable low-cost solar energy conversion.	▪ Designed a new class of small molecule donor materials that circumvents the statistical nature of polymer structures and the typical variability of polymerization reactions. The materials achieved world-record power conversion efficiencies of 7%.
Develop novel materials for high efficiency solar cells suitable for concentrator applications such as multi-junction thin films of indium gallium nitride (InGaN) integrated with arsenide and phosphides to achieve a full-spectrum solar cell.	▪ Demonstrated record high internal efficiencies and coupling efficiencies in nitride solar cells ▪ Demonstrated a bonded three-junction cell with excellent mechanical and electrical coupling, comprising a two-junction tandem cell bonded to a single-junction cell using a new interconnection topology.
Develop novel materials having increased thermoelectric efficiency for conversion of waste heat to electricity and for solid-state refrigeration.	▪ Imbedded metallic nanoparticles in semiconductor alloys [(In,Ga)As] to substantially increase the thermoelectric properties at around 800K. ▪ Fabricated and evaluated the thermoelectric properties of highly ordered silicon nanowire arrays.
Develop bio-inspired, kinetically controlled, catalytic synthesis of novel high performance nanocomposites for high power and high stability batteries and fuel cells.	▪ Created very high power, high stability battery anodes and cathodes using catalysis to grow nanocrystals of tin and lithium manganese oxide ($LiMn_2O_4$) in matrices of graphite and carbon nanotubes. Synthesis of nanocrystalline platinum has yielded fuel cells with performance matching present commercial cells but with 33% less platinum.
Address the basic materials science and engineering required to achieve all semiconductor-based white-light sources with output greater than 300 lumens/watt, corresponding to greater than 80% wall-plug efficiency.	▪ Made the first fully quantum-mechanical calculations of indirect Auger recombination and free-carrier absorption in any semiconductor to understand intrinsic loss processes in nitride light emitters. ▪ Used photonic crystals to achieve light extraction efficiencies as high as 94% at the chip level (for p-side up geometries).

Website: http://ceem.ucsb.edu/

Five-Year Goals and 2012 Progress

Center for Energy Frontier Research in Extreme Environments	Energy Frontier Research Centers
Director: Ho-kwang Mao	Basic Energy Sciences
Lead Institution: Carnegie Institution of Washington	DOE Office of Science

Mission: To accelerate the discovery and creation of energy-relevant materials using extreme pressures and temperatures.

Partner Institutions: Argonne National Laboratory; Arizona State University; Brookhaven National Laboratory; Caltech; Cornell University; Florida International University; Jefferson National Laboratory; Lehigh University; Lawrence Livermore National Laboratory; Missouri State University; Oak Ridge National Laboratory; Pennsylvania State University; Stanford University; University of Texas-Austin

Award: $15.0 M

Senior Investigators: 35	**Postdoctoral Staff:** 16	**Graduate Students:** 8	**Technical Staff:** 1
Publications: 89	**Invention Disclosures:** 0	**Patents/Applications:** 0	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Develop methods for isolating potentially useful functional and structural materials with novel structural forms.	▪ Metastably quenched a new amorphous diamond material from high pressure. ▪ Discovered long-range topological order in a bulk metallic glass. ▪ Developed a nanocasting method for the synthesis of mesoporous silicas, which have potential use as fluid catalytic cracking catalysts.
Establish a fundamental understanding of the behavior of hydrogen in hydrogen-rich systems.	▪ Studied the stepwise addition of molecular hydrogen (H_2) to rhodium (Rh) metal at low pressures to produce stoichiometric RhH and RhH_2 at 4 and 8 GPa, respectively. ▪ Used deep-UV Raman spectroscopy to reveal structural features in poly-aromatic hydrocarbons that may be exploited in the physisorption of H_2.
Use the concept of chemical precompression to predict the stabilities of new energy materials in hydrogen-containing systems.	▪ Theoretically predicted that a hydrogen-rich compound ($BaReH_9$) should develop discrete H_2 units with very short H-H contacts at the onset of metallization at 51 GPa. ▪ Theoretically predicted that molecular benzene will convert to a fully saturated network hydrocarbon material at elevated pressures. ▪ Predicted that at high pressure, one of the three metallic, superconducting phases predicted for disilane (Si_2H_6) will have a transition temperature of 139K.
Establish a framework for understanding the interactions between magnetic, structural and electronic degrees of freedom in materials.	▪ Elucidated the relationship between structural distortions and metallic behavior in a colossal magnetoresistance material ($LaMnO_3$). ▪ Identified a strong coupling between 4f- and 3d-based electronic effects in a strongly electron-correlated material ($Yb_xFe_4Sb_{12}$). ▪ In both iron-based and cuprate superconductors, identified competing states of electronic order, which lead to maxima in the transition temperature in two separate pressure regimes.
Enhance capabilities for structural analysis of materials by neutron and x-ray methods.	▪ Optimized the Spallation Neutrons and Pressure (SNAP) beamline at Oak Ridge National Laboratory and manufactured pressure cells for neutron diffraction measurements to above 50 GPa. ▪ Contributed to the development of new diffraction and imaging techniques to study nanoscale materials at the Advanced Photon Source. ▪ Fabricated new types of diamond anvils designed to maximize signals from very small samples.

Website: https://efree.gl.ciw.edu/

Five-Year Goals and 2012 Progress

Center for Energy Nanoscience
Director: P. Daniel Dapkus
Lead Institution: University of Southern California

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To explore the light absorption and emission in organic and nanostructure materials and their hybrids for solar energy conversion and solid state lighting.

Partner Institutions: University of Illinois, Urbana-Champaign; University of Michigan; University of Virginia

Award: $12.5 M, ARRA
Senior Investigators: 16 **Postdoctoral Staff:** 12 **Graduate Students:** 46 **Technical Staff:** 0
Publications: 71 **Invention Disclosures:** 1 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: Universal Display Corporation, Global Photonics Energy Corporation

5 Year Research Goals	Progress
Synthesize, characterize and model the properties of semiconductor nanostructures on low cost substrates as a vehicle for efficient, cost-effective solar cells.	▪ Synthesized dense, uniform arrays of gallium arsenide (GaAs) nanowires on silicon substrates as a step towards efficient tandem solar cells. ▪ Achieved a 30-fold improvement in the recombination properties of nanowires whose surfaces are passivated with aluminum gallium arsenide (AlGaAs). ▪ Revealed through simulations of nanowire tandem solar cells that high efficiency solar cells can be fabricated using nanowire tandem designs while using 20 times less material.
Synthesize, characterize and model the properties of organic polymeric and nanocrystalline materials to enable the rational design of efficient, ultra-low cost organic and hybrid solar cells.	▪ Synthesized molecular and polymeric materials to move the absorption onset to ~800 nm to increase the fraction of the solar spectrum that can be absorbed by these materials. ▪ Used femtosecond pump-probe measurements to determine the pathway and the fraction of light-generated excitons that become long-lived triplet excitons to potentially increase the electrical power generation in a solar cell. ▪ Observed singlet exciton fission for the first time in a low cost amorphous material. ▪ Synthesized infrared absorbing nanocrystals from earth-abundant materials.
Develop an understanding of the limitations to high efficiency in organic and inorganic light emitting diodes (LEDs).	▪ Used femtosecond laser pump-probe measurements to show the existence of a transient absorption process in indium gallium nitride (InGaN) LED active regions that may contribute to high efficiency fall-off in InGaN/GaN LEDs. ▪ Synthesized core-shell nanowire and nanosheet InGaN/GaN structures to create emitting regions for LEDs that may avoid current droop issues. ▪ Resolved issue of efficiency loss in fluorescent organic light emitting diodes (OLEDs), caused by singlet-triplet annihilation, by doping the OLED emission layer with a third molecule having the lowest triplet energy.

Website: http://www.CEN-EFRC.org

Five-Year Goals and 2012 Progress

Center for Excitonics Energy Frontier Research Centers
Director: Marc Baldo Basic Energy Sciences
Lead Institution: Massachusetts Institute of Technology DOE Office of Science

Mission: To understand the transport of charge carriers in synthetic disordered systems, which hold promise as new materials for conversion of solar energy to electricity and electrical energy storage.

Partner Institutions: Harvard University; Brookhaven National Laboratory

Award: $19.0 M, ARRA
Senior Investigators: 21 **Postdoctoral Staff:** 16 **Graduate Students:** 42 **Technical Staff:** 2
Publications: 58 **Invention Disclosures:** 5 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: Ubiquitous Energy

5 Year Research Goals	Progress
Understand and exploit effects of coherence and disorder in locally-ordered excitonic materials	▪ Found interplay of disorder and coherence improves efficiency of energy transport in photosynthetic excitonic antennas. ▪ Developed theory of quantum state and process tomography for excitonic systems and applied it to double-walled, J-aggregate nanotubes.
Understand the physics of semiconductor nanocrystals and develop their applications	▪ Revealed blinking phenomena in quantum dots with single dot spectroscopy in the infrared using superconducting nanowire single-photon detectors. ▪ Demonstrated and characterized bright, quantum dot-based light emitting devices (LEDs) which has led to new understanding of high brightness losses in quantum dot based LEDs and the effect of electric field on quantum dot photoluminescence quenching and shifting. ▪ Developed a nanofabrication process to enable studies of excitonic antennae with the placement of single semiconductor quantum dots with 5 nm lithography.
Develop new light collecting antennas for solar cells	▪ Built solar laser for concentration and wavelength conversion of sunlight. ▪ Observed and quantified singlet exciton fission in a tetracene-based device demonstrating that exciton fission can efficiently compete with exciton dissociation on the nanoscale and increase overall device efficiency. ▪ Observed a key intermediate in singlet exciton fission and improved the understanding of a major potential loss mechanism which can be avoided by device design.
Understand and develop hybrid excitonic systems consisting of strongly coupled excitons and photons	▪ Characterized significant exciton-exciton annihilation in thin films of J-aggregates suggesting a loss process which can significantly increase the lasing threshold in polariton microcavities. ▪ Demonstrated room temperature lasing from an exciton-polariton in a generalized device structure. ▪ Used strong coupling to generate first quad polaritons.

Website: http://www.rle.mit.edu/excitonics/

Center for Frontiers of Subsurface Energy Security Energy Frontier Research Centers
Director: Gary A. Pope Basic Energy Sciences
Lead Institution: The University of Texas at Austin DOE Office of Science

Mission: To pursue the scientific understanding of multiscale, multiphysics processes and to ensure safe and economically feasible storage of carbon dioxide and other byproducts of energy production without harming the environment.

Partner Institutions: Sandia National Laboratories

Award: $15.5 M

Senior Investigators: 25 **Postdoctoral Staff:** 11 **Graduate Students:** 20 **Technical Staff:** 6
Publications: 22 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Coupled Physical and Biogeochemical Complexity at the Subpore Scale – Determine solubility of carbon dioxide (CO_2) in brine and its effect on density and viscosity for brines with calcium and magnesium. – Determine the effect of CO_2 injection on subsurface microbial communities.	▪ Performed the first measurements of CO_2 dissolution kinetics and solubility using hard brines commonly found in aquifers. ▪ Characterized the contact angle of CO_2 on minerals by unique micro x-ray-tomography experiments and molecular dynamics simulations. ▪ Measured the influence of water chemistry and mineralogy on microbial viability after CO_2 injection.
Multiphase Reactive Flow and Mechanics at Pore to Continuum Scales – Understand the coupling of physical and chemical phenomena from the pore to the continuum scale. – Investigate the emergence of unexpected phenomena.	▪ Discovered that suitably treated nanoparticles qualitatively change the nature of multiphase flow in sedimentary rocks with the potential for more secure CO_2 storage in the subsurface. ▪ Developed a game changing approach for how to scale up CO_2 behavior from the pore scale to the field scale. ▪ Measured deformation/fracturing in geologic materials.
Coupled Mechanics, Reactions, Flow, and Transport at the Continuum to Field Scales – Apply core and outcrop structural and diagenetic observations at the field scale using models that mimic the physical processes. – Use advanced parameter estimation techniques to better characterize basin scale heterogeneity.	▪ Developed methods for scale up of static and dynamic attributes accounting for the underlying spatial structure of subsurface geology. ▪ Derived a model and explanation for variation in shear and compressional velocity as a function of frequency in chemically altered rocks. ▪ Created a new seismic inversion method. ▪ Developed new insights into emergent phenomena associated with the Crystal Geyser field (Utah).
Simulation of Multiscale, Multiphysics, Heterogeneous Systems – Develop cutting-edge numerical and computational techniques across spatial and time scales. – Test and verify models of CO_2 sequestration using field data.	Improved numerical and computational methods and model physics greatly extend the capability to accurately simulate complex field observations in diverse locations such as: ▪ Crystal Geyser natural CO_2 driven geyser (Utah) ▪ Cranfield CO_2 injection demonstration (Mississippi) ▪ Bravo Dome natural CO_2 field (New Mexico)
Broad impact of basic research on wider scientific community.	▪ Advanced numerical and computational methods apply widely to other problems such as CO_2 utilization for enhanced oil recovery.

Website: http://www.utefrc.org

Five-Year Goals and 2012 Progress

Center for Gas Separations Relevant to Clean Energy Technologies Energy Frontier Research Centers
Director: Berend Smit Basic Energy Sciences
Lead Institution: University of California, Berkeley DOE Office of Science

Mission: To develop new strategies and materials that allow for energy efficient gas separations based on molecule-specific chemical interactions, with a focus on carbon capture.

Partner Institutions: University of California, Davis; Lawrence Berkeley National Laboratory; University of Minnesota; National Energy Technology Laboratory; Texas A&M University

Award: $10.0 M
Senior Investigators: 16 **Postdoctoral Staff:** 21 **Graduate Students:** 24 **Technical Staff:** 1
Publications: 65 **Invention Disclosures:** 0 **Patents/Applications:** 6 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Synthesis of novel solid adsorbents for gas separations	Novel metal organic frameworks (MOFs) have been synthesized for the following separations: ▪ Separations of oxygen and nitrogen (O_2/N_2) at high temperature. ▪ Separations of hydrocarbons using iron-based MOFs with an open metal site. Results published in *Science* showed that they operate at higher temperatures and pressures than current commercial materials that require low pressure and cryogenic conditions, potentially saving the oil and chemical industries large energy costs. ▪ Carbon capture using amine functionalized MOFs.
Synthesis of novel membranes for gas separations	Synthesized novel classes of membranes: ▪ Self-assembly of polymer tethered cyclic peptides in block copolymers into nanotubes with controlled radius to separate specific gases from mixtures. ▪ Polymer membrane based on amine grafted polyaniline, which exhibits facilitated transport for carbon dioxide (CO_2) from natural gas.
Novel characterization tools to better understand the molecular properties of these novel materials	▪ A soft x-ray technique has been developed that uses the polarization of the beam to investigate orientational order of polymer films at the molecular level.
Novel computational tools	Developed computational techniques: ▪ To predict the performance of a material for carbon capture. ▪ To screen large databases of porous materials for CO_2 separation for optimal performance. By integrating this method with other DOE programs, results published in *Nature Materials* identified many different materials with a potential to reduce the parasitic energy of carbon capture and separation by 30–40% compared to near-term technologies. ▪ To obtain accurate force fields from high-level quantum chemical calculations.

Website: http://www.cchem.berkeley.edu/co2efrc/

Five-Year Goals and 2012 Progress

Center for Interface Science: Solar Electric Materials | Energy Frontier Research Centers
Director: Neal R. Armstrong | Basic Energy Sciences
Lead Institution: University of Arizona | DOE Office of Science

Mission: To advance the understanding of interface science underlying solar energy conversion technologies based on organic and organic-inorganic hybrid materials; and to inspire, recruit and train future scientists and leaders in the basic science of solar electric energy conversion.

Partner Institutions: Georgia Institute of Technology; National Renewable Energy Laboratory; Princeton University; University of Washington

Award: $15.0 M, ARRA
Senior Investigators: 16 **Postdoctoral Staff:** 13 **Graduate Students:** 36 **Technical Staff:** 13
Publications: 60 **Invention Disclosures:** 1 **Patents/Applications:** 6 **Patents Licensed:** 0
Companies using EFRC research: 2

5 Year Research Goals	Progress
Develop new theories to better understand charge transfer between organic semiconductors, oxides, metals, and emerging nontraditional conductors.	▪ Used density functional theory for the first time to study the effects of lattice defects, hydroxylation, adsorbed water, and dipolar molecules on the electronic properties of important transparent conducting oxides.
Develop new methodologies for the characterization of the atomic and molecular composition of interfaces, and new approaches for the nanoscale characterization of electrical and electrochemical properties of these interfaces.	▪ Integrated surface vibrational spectroscopies, attenuated total reflectance spectroscopies, and synchrotron-based near-edge x-ray absorption fine structure spectroscopy to understand orientation and structure of molecular interface modifiers, and their influence on energetics in organic photovoltaics (OPVs). ▪ Developed novel waveguide spectroscopies/ spectroelectrochemistries to correlate molecular orientation of interface modifiers with rates of electron transfer relevant to OPVs. Made foundational observations correlating electron transfer rates, orientation, and aggregation for redox-active modifiers. ▪ Created new scanning probe microscopies to characterize electronic properties at sub-micron length-scales/nanosecond time-scales in organic semiconductor, OPV-relevant materials.
Develop new nanostructured hybrid materials that will lead to the formation of chemically and physically robust interfaces, with full control of their composition, their molecular architecture, and their physical (electrical, optical, and thermo-mechanical) properties.	▪ Developed new metal oxide nanolaminates (Al_2O_3:ZnO) and unique low-work function polymer electron-selective interlayers that may simplify the manufacturing of low-cost and large-area OPVs. The polymer interlayers work was recently published in *Science*.
Apply our understanding of nanoscale organic/oxide, organic/metal and organic/organic interfaces to existing and future solar energy conversion photovoltaic platforms.	▪ Characterized the interfacial chemistry and energetics of new metal oxide (NiO_x [hole-selective] and MoO_x [hole-transport]) interlayers, and have, for the first time, determined the relationship between interfacial composition and energetics with diode electrical properties and OPV efficiencies.

Website: http://solarinterface.org/

Five-Year Goals and 2012 Progress

Center for Inverse Design Energy Frontier Research Centers
Director: William Tumas Basic Energy Sciences
Lead Institution: National Renewable Energy Laboratory DOE Office of Science

Mission: To revolutionize the discovery of new materials by design with tailored properties through the development and application of a novel inverse design approach powered by theory guiding experiment with an initial focus on solar energy conversion.

Partner Institutions: University of Colorado, Boulder; Colorado School of Mines; Northwestern University; Oregon State University; SLAC National Accelerator Laboratory

Award: $20.0 M
Senior Investigators: 18 **Postdoctoral Staff:** 12 **Graduate Students:** 10 **Technical Staff:** 2
Publications: 27 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Develop the necessary theoretical and experimental tools to enable inverse design including high-throughput computation, rapid and detailed synthesis and characterization techniques	▪ Dramatically improved theory, and integrated this theory with algorithms into a platform for high-throughput calculations of advanced materials and properties. ▪ Implemented two methods for rapid synthesis/measurement of optoelectronic materials, upgraded thin film synthesis tools, and developed methods for structural characterization.
Design nanostructures with specific properties by search of large numbers of atomic configurations	▪ Applied inverse band structure calculations to predict novel silicon-germanium nanostructures with very strong direct bandgap absorption of light, an ideal property for solar cells.
Develop and use design principles to search large numbers of known materials and structures for targeted, yet unknown, functionalities	▪ Integrated theory and experiment to understand limitations of binary earth abundant materials, such as iron sulfide, as solar absorbers and developed improved alternatives by incorporating silicon and germanium into iron sulfides. ▪ Developed a new design principle for predicting performance of solar materials based on fundamental properties (spectroscopic limited maximum efficiency), applied it to 260 ternary materials, and identified 20 high-performance materials. ▪ Used inverse design to understand the origins of electrical conductivity in oxides and accelerated the development of transparent contacts crucial for efficiency of solar cells. ▪ Developed cobalt based oxides as a p-type transparent conductors and increased conductivity by a factor of 10,000.
Discover, synthesize and characterize heretofore-unknown materials (“missing materials”) with predicted targeted sets of properties or functionalities	▪ Used high-throughput theory (over 80,000 total calculations) to theoretically predict and characterize “missing materials”, including 235 new ternary materials (ABX) and 100 new ternary metal chalcogenides (A_2BX_4). ▪ Successfully applied inverse design to develop phase diagrams to predict the processing conditions for enabling synthesis of new materials. ▪ Demonstrated viability of inverse design through prediction and synthesis of new tantalum, cobalt and tin materials.

Website: http://www.centerforinversedesign.org/

Five-Year Goals and 2012 Progress

Center for Lignocellulose Structure and Formation Energy Frontier Research Centers
Director: Daniel J. Cosgrove Basic Energy Sciences
Lead Institution: Pennsylvania State University DOE Office of Science

Mission: To dramatically increase our fundamental knowledge of the formation and physical interactions of bio-polymer networks in plant cell walls to provide a basis for improved methods for converting biomass into fuels.

Partner Institutions: North Carolina State; Virginia Tech

Award: $21.0 M, ARRA

Senior Investigators: 21 **Postdoctoral Staff:** 17 **Graduate Students:** 34 **Technical Staff:** 10
Publications: 17 **Invention Disclosures:** 1 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Solve the structure of cellulose synthase (CESA), including its plasma membrane (PM) interactions, and determine the mechanisms involved in synthesis of the cellulose polymer.	▪ Developed a 3D structure of the CESA catalytic domain, using advanced computational methods. ▪ Tested its fidelity by identifying locations of known structural and catalytic features, e.g., point mutations and uridine diphosphate(UDP)-glucose substrate binding sites. ▪ Cloned and expressed CESA protein fragments in heterologous systems; started crystallization trials. ▪ Used spectroscopic and computational methods to analyze packing of transmembrane segments of CESA.
Identify proteins in the cellulose synthesis complex (CSC); elucidate how it is assembled, how it is controlled, and how it produces cellulose microfibrils.	▪ With advanced electron microscopy methods, showed that most of the CESA protein is below the exterior surface of the plasma membrane. ▪ Developed a set of anti-CESA antibodies; used them to identify CESA isoforms found in isolated CSCs in membrane extracts. ▪ Isolated CSCs, showed their activity, and identified associated proteins. ▪ Sequenced the *Gluconoacetobacter* genome and deposited in Genbank. ▪ Identified a protein linker ('CSI1') between CSCs and microtubules that likely participates in CSC movement control.
Develop a molecular-level understanding of the structure of the cellulose microfibril and its larger scale properties.	▪ Developed sum frequency generation (SFG) for analysis of cellulose crystallinity without interference from other cell wall components. ▪ Used SFG to detect developmental gradients in cellulose structure. ▪ Used simulations (quantum mechanical, molecular dynamics and coarse-grain) to interpret SFG spectra of cellulose, to predict microfibril twisting, and to predict periodic breakdown of its order.
Test the current model of cell wall architecture with cellulose-matrix interactions and refine/update the model to account for their nm- to mm-scale properties.	▪ Showed that only a minor fraction of xyloglucan connects cellulose microfibrils, and in its absence other wall components take on a larger biomechanical role; this calls for a revision of the current model. ▪ Analyzed wall structure with small angle neutron scattering, showing a mesh of 3-nm microfibrils set in a matrix of random-coil shaped polymers. ▪ With atomic force microscopy, imaged the arrangement of microfibrils and matrix on the inner surface of never-dried cell walls, and showed complicated microfibril movements when the walls were extended.
Develop multiscale models of cell walls to account for their physical properties.	▪ Developed computational models of cellulose-matrix interactions with molecular dynamic simulations and finite element methods to test the strength and stability of different network configurations and guide future tests of cellulose-matrix interactions.

Website: http://www.lignocellulose.org

Five-Year Goals and 2012 Progress

Center for Materials at Irradiation and Mechanical Extremes Energy Frontier Research Centers
Director: Amit Misra Basic Energy Sciences
Lead Institution: Los Alamos National Laboratory DOE Office of Science

Mission: To understand, at the atomic scale, the interactions of defects at interfaces in materials subjected to extreme radiation doses and mechanical stress in order to synthesize new interface-dominated materials that can tolerate such conditions.

Partner Institutions: Massachusetts Institute of Technology; University of Illinois at Urbana-Champaign; Carnegie Mellon University; University of Nebraska-Lincoln

Award: $19.0 M
Senior Investigators: 17 **Postdoctoral Staff:** 15 **Graduate Students:** 8 **Technical Staff:** 3
Publications: 51 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Understand helium storage at interfaces.	▪ Developed an equation that correlates the concentration of stored helium (He) at interfaces with the interface structure. ▪ Developed an equation-of-state for He bubbles at interfaces. ▪ Demonstrated suppression of material hardening due to He bubbles at interfaces. ▪ Collectively, the new understanding gained and the predictive capability that results will provide design principles for structural materials in fusion energy.
Understand sink efficiency of interfaces for radiation-induced point defects.	▪ Identified the types of point defect interactions at interfaces in terms of interface atomic structure and defect energetics and kinetics. ▪ Developed a model that accounts for the balance between irradiation conditions and recovery processes in nanoporous and multilayer materials.
Understand response of structure-less interfaces to radiation-induced point defects.	▪ Elucidated how point defects redistribute at interfaces in terms of defect energetics and kinetics. These results are being integrated into a predictive model that will enable the design of materials for fission energy applications.
Understand evolution of stable interfaces under severe plastic deformation.	▪ Discovered stable interfaces under accumulative roll bonding and developed theory for crystallographic and chemical stability of interfaces. Predictive capabilities are being developed.
Understand dislocation or twin nucleation at interfaces.	▪ Discovered deformation twin nucleation from specific interfaces in bulk accumulative roll bonding nano-composites. ▪ Identified how the interface structure affects defect (glide dislocation or deformation twin) nucleation at the interface. ▪ Initiated a predictive model, based on these results, which will provide the design principles for processing bulk nanocomposites for structural and nuclear energy applications.
Understand shock response of interfaces.	▪ Discovered varying shock response (e.g., stable or migrating boundaries, transgranular or intergranular spall) as a function of boundary structure. These results are being integrated into a predictive model that will enable the design of materials with a tailored response in high strain rate applications.

Website: http://cmime.lanl.gov/

Center for Materials Science of Nuclear Fuels Energy Frontier Research Centers
Director: Todd R. Allen Basic Energy Sciences
Lead Institution: Idaho National Laboratory DOE Office of Science

Mission: To develop an experimentally validated multi-scale computational capability for the predictive understanding of the impact of microstructure on thermal transport in nuclear fuel under irradiation, with ultimate application to UO_2 as a model system.

Partner Institutions: Colorado School of Mines; Oak Ridge National Laboratory; Purdue University; University of Florida; University of Wisconsin

Award: $10.0 M

Senior Investigators: 12 **Postdoctoral Staff:** 5 **Graduate Students:** 10 **Technical Staff:** 1
Publications: 11 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Understand how anharmonicity, fission product impurities, and chemical stoichiometry impact phonon lifetimes and thermal transport as a function of temperature in pure single crystal uranium dioxide (UO_2).	▪ First ever measurements of phonon lifetimes in UO_2 as a function of temperature showed that: – Phonon lifetimes accurately predict thermal conductivity. – Optical phonons are major heat carriers. – Anharmonicity has a very strong impact on thermal conductivity. – Fission product impurities have a small impact on phonon lifetimes. ▪ First ever prediction of thermal conductivity of UO_2 based on first principles calculations of phonon dynamics.
Understand how microstructural features such as grain boundaries, dislocations, interfaces, voids and bubbles affect thermal transport in UO_2 before and after irradiation.	▪ Measured thermal transport across a single bi-crystal interface and found agreement with an atomistic model informed by characterization using high-resolution transmission electron microscopy and electron energy loss spectroscopy. Predicted the same using molecular dynamics simulations.
Determine the type of clusters produced by irradiation of UO_2, understand the energies and kinetic paths of formation of clusters in UO_2, and predict atomic scale mechanisms of nucleation in UO_2.	▪ Determined the formation energies and migration barriers of elementary defects in UO_2. ▪ Discovered a non-intuitive kinetic path for the formation of previously observed cuboctahedral clusters. ▪ Determined the composition, energies and kinetic barriers of small, irradiation-induced clusters in UO_2.
Understand the impact of temperature and local oxygen environment on the stoichiometry of homogeneous and heterogeneous UO_2.	▪ A first model of defect disorder in UO_2 based on quantum mechanical results of defect energies showed that defects self-organize near surfaces to screen the charge associated with interaction with oxygen and that voids in UO_2 must include oxygen gas. This has important implications for the analysis of UO_2 performance under irradiation, e.g., in reactors.
Understand how voids, dislocation loops and gas bubbles form and grow in irradiated UO_2.	Models and experiments performed on defects and microstructure dynamics in irradiated UO_2 have shown that: ▪ Void growth in irradiated materials is controlled by reactions of point defects with void surfaces, contrary to the traditional belief that void growth occurs by diffusion. ▪ Void and dislocation loop development in the ion irradiated UO_2 and cerium oxide (CeO_2) are consistent.

Website: http://www.inl.gov/efrc

Five-Year Goals and 2012 Progress

Center for Molecular Electrocatalysis Energy Frontier Research Centers
Director: R. Morris Bullock Basic Energy Sciences
Lead Institution: Pacific Northwest National Laboratory DOE Office of Science

Mission: To understand, design, and develop molecular electrocatalysts for solar fuel production and use.

Partner Institutions: University of Washington; Pennsylvania State University; University of Wyoming

Award: $22.5 M
Senior Investigators: 15 **Postdoctoral Staff:** 15 **Graduate Students:** 4 **Technical Staff:** 0
Publications: 33 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Develop a fundamental knowledge of the design of molecular electrocatalysts that incorporate proton relays for fast, efficient catalysis of important reactions for solar fuel production and use. These proton relays are based on similar functionalities in naturally occurring enzyme catalysts.	Demonstrated that proton relays play important roles in synthetic molecular catalysts for hydrogen (H_2) oxidation, H_2 production, and oxygen (O_2) reduction. Proton relays can: ▪ Accelerate intra- and inter-molecular proton transfer reactions. ▪ Facilitate substrate (H_2 or O_2) binding. ▪ Enhance the rate of formation and cleavage of hydrogen-hydrogen, oxygen-hydrogen, and nitrogen-hydrogen bonds.
Develop quantitative and predictive knowledge of the structural and energetic factors that account for contributions from both first and second coordination sphere to multi-proton, multi-electron catalytic processes.	▪ Used high-level theory and experimental results to develop a simple model that accurately predicts the energies of all intermediates for nickel-based catalysts for H_2 oxidation and production. This approach enables the rational design of new molecular catalysts and the extension of these concepts to other energy storage/utilization reactions.
Apply this knowledge to the development of electrocatalysts of unprecedented efficiency for reactions of importance to a secure energy future: oxidation of hydrogen, production of hydrogen, reduction of oxygen, and reduction of nitrogen.	▪ Reported the fastest known molecular catalyst for production of hydrogen by proton reduction. ▪ Developed the fastest known molecular catalyst for oxidation of hydrogen, a key reaction in hydrogen fuel cells. Our catalyst uses nickel, an abundant, inexpensive metal, versus the currently used precious metal platinum. ▪ Reported an iron catalyst for reduction of oxygen to water, with remarkable selectivity. ▪ Synthesized novel metal complexes with nitrogen ligands, which are currently being studied for reduction of nitrogen to ammonia. ▪ Developed a molecular catalyst for *reversible* oxidation and production of hydrogen, similar to that in hydrogenase enzymes in nature.

Website: http://efrc.pnnl.gov/

Five-Year Goals and 2012 Progress

Center for Nanoscale Control of Geologic CO_2 — Energy Frontier Research Centers
Director: Donald J. DePaolo — Basic Energy Sciences
Lead Institution: Lawrence Berkeley National Laboratory — DOE Office of Science

Mission: To build a fundamental understanding of molecular-to-pore-scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow, transport, and mineralization in porous rock media as applied to the injection and storage of carbon dioxide (CO_2) in subsurface reservoirs.

Partner Institutions: Lawrence Livermore National Laboratory; Massachusetts Institute of Technology; Oak Ridge National Laboratory; Ohio State University; University of California, Davis; Washington University in St. Louis

Award: $20.0 M

Senior Investigators: 30	**Postdoctoral Staff:** 13	**Graduate Students:** 7	**Technical Staff:** 2
Publications: 23	**Invention Disclosures:** 2	**Patents/Applications:** 0	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Define molecular scale mechanisms and parameters governing carbonate dissolution and precipitation in reservoir conditions, with the goal to enable validated pore-to-reservoir scale modeling of these processes	▪ Measured calcium carbonate ($CaCO_3$) nucleation rates on mineral surfaces and in pores and developed validated methods for the simulations of $CaCO_3$ nucleation at relevant conditions. ▪ Quantified relative stabilities of $CaCO_3$ phases for input into precipitation models. ▪ Developed advanced instrumentation to measure impurity and isotope signatures and appropriate models to interpret results.
Develop the scientific basis for engineering approaches for controlled carbonate dissolution and precipitation	▪ By using newly synthesized designer biomimetic polymers demonstrated the ability to control as well as dramatically enhance the $CaCO_3$ nucleation and growth rate. ▪ Demonstrated nucleation rate enhancement by microbes.
Determine how the properties of confined fluids differ from those of bulk fluids	▪ Quantified the effect of confinement on the density of supercritical carbon dioxide ($scCO_2$) in nano- and meso-pores. ▪ Developed techniques (including synchrotron x-rays, neutron methods and high-performance supercomputing) to probe CO_2-water mixtures in nanopores with molecular-scale resolution in a broad range of temperature, pressure, and salinity conditions.
Determine how mineral wetting properties arise from molecular-scale properties of fluid-fluid and fluid-solid interfaces	▪ Carried out first-of-a-kind, nanometer-scale resolution observations of water films on mineral surfaces in the presence of CO_2 using synchrotron x-rays- based methods. ▪ Quantified CO_2 adsorption on the surface of liquid water and the impact of CO_2 on the hydrophilicity of mineral surfaces.
Understand and predict the mesoscale physical and chemical structures that emerge due to coupling of processes (flow, transport, reactions) at the pore scale	▪ Carried out the first mapping and quantification in 3D of the accessible reactive surface area in a $scCO_2$ reservoir rock from the Cranfield CO_2 injection demonstration site (Mississippi). ▪ Developed a lattice Boltzmann approach to modeling multiphase CO_2-brine flow at the pore scale. ▪ Developed a world-class high performance computing approach to modeling 3D pore scale reactive transport. ▪ Mapped the accumulation of carbonate due to precipitation at the micron scale at temperatures and pressures of a deep saline aquifer using synchrotron x-ray microtomography and upscaled this to the continuum scale.

Website: http://esd.lbl.gov/research/facilities/cncgc/

Center on Nanostructuring for Efficient Energy Conversion — Energy Frontier Research Centers
Director: Fritz Prinz and Stacey Bent — Basic Energy Sciences
Lead Institution: Stanford University — DOE Office of Science

Mission: To understand how nanostructuring can enhance efficiency for energy conversion and to solve fundamental cross-cutting problems in advanced energy conversion and storage systems.

Partner Institutions: Technical University of Denmark (DTU); Carnegie Institution; HRL Laboratories

Award: $20.0 M
Senior Investigators: 15 **Postdoctoral Staff:** 14 **Graduate Students:** 32 **Technical Staff:** 3
Publications: 56 **Invention Disclosures:** 1 **Patents/Applications:** 3 **Patents Licensed:** 3
Companies using EFRC research: QuantumScape

5 Year Research Goals	Progress
Use nanoscale confinement to develop new materials for use in energy conversion and storage.	▪ Examined effects of nano-confinement on thermodynamics, photon and electron harvesting, and catalysis of photoelectrochemical reactions. ▪ Demonstrated the effect of nanostructured size in hydrogen storage, batteries, and supercapacitors. ▪ Stabilized new phases of nanoscale materials by controlling size and composition in nanoparticles and thin films.
Utilize photonic concepts, including optical confinement, and quantum confinement for enhanced light absorption.	▪ Performed pioneering work on the use of plasmonic resonances in metallic nanostructures to enhance the rate of water splitting. ▪ Developed nanowire-based solar cells and nanocone-based light trapping layers. ▪ Using 3D modeling, showed how to select nanostructured designs that are optimal for photovoltaics.
Perform atomic scale engineering of catalysts/photocatalysts using theory-driven, bio-inspired design.	▪ Predicted, on the basis of theoretical analyses, doped surface structures of titania (TiO_2) that approach the electrocatalytic performance of the best noble metal catalysts for the oxygen evolution reaction. ▪ Developed bio-inspired, nanostructured manganese oxide catalysts with activity close to that of precious metals (platiunum, iridium, and ruthenium) in their bi-functional activity for the oxygen evolution and oxygen reduction reactions. ▪ Observed the dynamics of Photosystem II (a critical enzyme in the photosynthesis process) in real time using atomic-scale imaging methods. ▪ Synthesized manganese oxide catalysts mimicking the oxygen evolving center in Photosystem II.
Develop and/or modify techniques and strategies to fabricate and observe nanostructured materials .	▪ Developed a novel atomic layer deposition tool with an *in situ* scanning probe microscope to produce and analyze size- and position-controlled nanometer structures. ▪ Built nanostructured photovoltaic architectures via nature-inspired self-organization.

Website: http://cneec.stanford.edu/

Five-Year Goals and 2012 Progress

Center for Solar Fuels
Director: Thomas J. Meyer
Lead Institution: University of North Carolina at Chapel Hill

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To integrate academic and translational research to study light/matter interactions and chemical processes for the efficient production of solar fuels.

Partner Institutions: Duke University; North Carolina State University; North Carolina Central University; University of Florida; Research Triangle Institute; University of Maryland; Georgia Institute of Technology

Award: $17.5 M, ARRA

Senior Investigators: 30 **Postdoctoral Staff:** 25 **Graduate Students:** 31 **Technical Staff:** 12
Publications: 71 **Invention Disclosures:** 1 **Patents/Applications:** 4 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Catalyst Development Rapid, robust molecular and nanocatalysts for water oxidation and carbon dioxide (CO_2) reduction. Integration in assemblies for Dye Sensitized Photoelectrosynthesis Cells (DSPEC).	▪ Developed a new generation of water oxidation catalysts including first row transition metal complexes and assemblies. Integrated theory and experiment. ▪ Achieved large rate enhancements for water oxidation electrocatalysis on oxide surfaces. ▪ Synthesized electrocatalysts for CO_2 reduction to carbon monoxide (CO) and formate; synthesized single site catalysts for CO_2 splitting into CO and oxygen (O_2).
Materials Development High surface area metal oxide semi-conductors & electrodes for DSPEC and electrocatalysis. Surface modification & stabilization of oxide semiconductors.	▪ Synthesized metal oxide semiconductors (TiO_2, Nb_2O_5, $SrTiO_3$, and NiO) by sol-gel and pulsed laser deposition. ▪ Photoelectrochemically evaluated metal oxide photoanodes, and photocathodes, and high surface area optically transparent, conducting oxide electrodes.
Assemblies Interfacial chromophore-catalyst molecular assemblies for DSPEC applications; light harvesting and photocatalysis in polymers, peptides, and framework materials.	▪ Developed synthetic protocols for interfacial chromophore-catalyst assemblies in solution and on oxide surfaces by ligand bridging and oligoprolines. ▪ Demonstrated efficient light-harvesting with rapid electron and energy transfer in derivatized polymers and peptides and metal organic frameworks.
Integration Assembly/electrode integration and binding on oxide surfaces; surface characterization.	▪ Developed strategies for surface attachment and assembly synthesis based on phosphonate binding, surface coupling, and multi-layer synthesis on titania. ▪ Developed methods to study surface binding and characterization on oxide surfaces (Nb_2O_5, $SrTiO_3$, NiO).
Interface Structure and Dynamics Use surface spectroscopy and dynamics to explore structure, stability, binding, and interface dynamics.	▪ Characterized structure and binding of catalysts linked to metal oxide surfaces. ▪ Analyzed energy transfer and interfacial electron transfer of light harvesting and catalyst containing assemblies attached to metal oxide surfaces.
Device Prototypes and Characterization DSPEC, photoanode & photocathode characterization by electrochemical and photocurrent measurements. Applications to water splitting, CO_2 reduction, organic oxidations.	▪ Evaluated DSPECs for hydrogen (H_2) evolution; evaluated DSPEC dynamics by integrated transient absorption and photocurrent measurements. ▪ Utilized dye sensitized solar cell measurements to characterize assembly derivatized interfaces. ▪ Conducted systems analysis of DSPEC.

Website: http://www.efrc.unc.edu

Five-Year Goals and 2012 Progress

Center for Solar and Thermal Energy Conversion
Director: Peter Green
Lead Institution: University of Michigan

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To study complex material structures on the nanoscale to identify key features for their potential use as materials to convert solar energy and heat to electricity.

Partner Institutions: None

Award: $19.5 M, ARRA
Senior Investigators: 29 **Postdoctoral Staff:** 8 **Graduate Students:** 28 **Technical Staff:** 4
Publications: 85 **Invention Disclosures:** 2 **Patents/Applications:** 8 **Patents Licensed:** 7
Companies using EFRC research: Global Photonic Energy Corp.

5 Year Research Goals	Progress
Design and synthesize inorganic low dimensional materials that maximize the absorption of energy from sunlight and minimize energy losses associated with carrier transport to achieve high efficiency solar energy conversion.	▪ Developed novel methods for nanopatterning quantum dots at high densities to control the electronic states and photoresponse. ▪ Demonstrated that spatial separation of electrons and holes is promising for photovoltaic energy conversion. ▪ Engineered the electronic structure of highly mismatched alloys for both photovoltaic (PV) and thermoelectric (TE) applications. ▪ Developed experimental tools for real-time studies of photo-induced atomic-scale structure and electrical properties of nanoscale systems. ▪ Developed novel experimental tools to examine carrier dynamics in nanoscale structures, which enables tailoring of carrier excitation and relaxation mechanisms for optimum PV conversion efficiency.
Understand and exploit fundamental mechanisms and processes associated with electron and hole transport, with the goal of achieving high figures of merit in thermoelectric (inorganic, hybrid or molecular) materials.	▪ Developed scientific understanding for engineering the transmission characteristic of junctions to approach the limit of Carnot efficiency. ▪ Developed experimental ability to probe the basic mechanisms of charge and energy transport at the smallest molecular length scales. ▪ Developed novel beam-assisted nanostructuring techniques to fabricate thermoelectric and photovoltaic materials with improved charge and energy transport. ▪ Uncovered how molecular properties control thermopower in molecular systems. ▪ Uncovered the possibility of using non-equilibrium effects to increase the energy conversion efficiency of hybrid systems. ▪ Gained new fundamental insights into superior thermoelectric conversion characteristics in nanostructured materials.
Understand the molecular and structural origins of energy conversion phenomena in organic and hybrid material systems, with the goal of producing materials for efficient energy conversion.	▪ Developed theory to predict fundamental limits of excitonic PVs. ▪ Uncovered how molecular orientation affects organic PV performance. ▪ Developed organic solvent-free annealing method for polymer PV. ▪ Developed novel spectroscopies to probe nanoscale energy and charge transfer dynamics in low dimensional materials. ▪ Performed coordinated molecular design and synthesis of new compounds for high efficiency excitonic dye-sensitized solar cells. ▪ Developed theoretical and chemical synthesis approaches to understand the use of cage compounds for optical applications. ▪ Developed novel nano-structures for plasmonic enhancement of PV.

Website: http://cstec.engin.umich.edu

Five-Year Goals and 2012 Progress

Combustion Energy Frontier Research Center (CEFRC) Energy Frontier Research Centers
Director: Chung K. Law Basic Energy Sciences
Lead Institution: Princeton University DOE Office of Science

Mission: To develop a validated, predictive, multi-scale combustion modeling capability which can be used to optimize the design and operation of evolving fuels in advanced engines for transportation applications.

Partner Institutions: Argonne National Laboratory; Cornell University; Massachusetts Institute of Technology; Sandia National Laboratories; Stanford University; University of Connecticut; University of Minnesota; University of Southern California

Award: $20.0 M

Senior Investigators: 14 **Postdoctoral Staff:** 32 **Graduate Students:** 29 **Technical Staff:** 9
Publications: 79 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Advance fundamental understanding and practice of combustion and fuel science.	▪ Developed accurate *ab initio* quantum chemistry based methods for thermochemistry and kinetics at high pressures and for large fuel molecules. ▪ Discovered and exploited new phenomena involving the turbulent combustion of alternative, non-petroleum based fuels.
Create experimental validation platforms/databases for chemical kinetics, thermochemistry, transport processes, and flame structure through application of advanced diagnostic methods.	▪ Developed a comprehensive array of experimental tools and facilities with new and expanded experimental capabilities covering a wide range of thermodynamic conditions. ▪ Applied uncertainty quantification methods to better utilize the experimental data. ▪ Formed alliances with DOE Bioenergy Research Centers. Performed combustion tests and analysis of the biofuels synthesized by collaborators to provide feedback on fuel viability and design.
Implement validated, multi-scale, quantitative prediction methods for novel energy conversion design/control concepts tailored to the physical and chemical properties of alternative fuels.	▪ Predicted thermochemical and kinetic properties of key combustion species. ▪ Developed new methods to treat complex reactions. ▪ Developed advanced models for turbulent combustion including a detailed description of the chemistry.
Develop and implement methodologies for generating comprehensive, validated, detailed and reduced-order reaction mechanisms for alternative fuels, especially biofuels.	▪ Demonstrated a systematic approach towards developing reaction mechanisms of foundation fuels, butanols, and biodiesel. ▪ Developed systematic procedures for reducing the dimensionality of reaction mechanisms and for making them more amenable to numerical simulations. ▪ Tabulated reaction maps of detailed mechanisms for turbulent combustion modeling.

Website: http://www.princeton.edu/cefrc/

Five-Year Goals and 2012 Progress

Energy Frontier Research Center for Solid-State Lighting Science Energy Frontier Research Centers
Director: Michael E. Coltrin Basic Energy Sciences
Lead Institution: Sandia National Laboratories DOE Office of Science

Mission: To explore energy conversion in tailored photonic structures and materials to enable revolutionary breakthroughs in the efficiency and performance of light emitting diode (LED)-based lighting; to improve energy-efficiency in the way we light our homes and offices, which currently accounts for 20 percent of the Nation's electrical energy use. Solid-state lighting has the potential to cut that energy consumption in half, or even more.

Partner Institutions: Los Alamos National Laboratory; University of New Mexico; Northwestern University; Rensselaer Polytechnic Institute; University of California, Irvine; University of California, Merced; University of California, Santa Barbara; Philips Lumileds Lighting; Caltech

Award: $18.0 M
Senior Investigators: 32 **Postdoctoral Staff:** 5 **Graduate Students:** 9 **Technical Staff:** 8
Publications: 39 **Invention Disclosures:** 0 **Patents/Applications:** 4 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Explore gallium nitride/indium gallium nitride (GaN/InGaN) nanowires as a low-defect-density materials architecture for high-efficiency light-emission throughout the visible spectrum.	▪ Developed a novel "top-down" dry-plus-wet etching method for fabricating high-structural-and-optical-quality periodic GaN nanowire arrays with uniform heights and diameters, and with straight, faceted non-polar sidewalls. ▪ Demonstrated yellow-red electroluminescence from a vertically integrated radial-nanowire-based LED created by growth of InGaN/GaN multiple-quantum wells.
Discover new materials architectures for stable, efficient and narrow-linewidth wavelength down-conversion for improved efficacy and functionality of solid-state lighting.	▪ Demonstrated narrowband red emission at 609-614 nm from europium (Eu^{3+}) incorporated into non-centrosymmetric sites in tantalate and niobate host lattices. ▪ Initiated new approach to colloidal synthesis of cadium telluride (CdTe)-based multiple shell heterostructures with narrow linewidth red emission in the range 615-635 nm.
Develop a microscopic understanding of the radiative and non-radiative processes whose competition ultimately determines electroluminescence or photoluminescence efficiency.	▪ Developed a microscopic, physics-based model of InGaN recombination processes that goes far beyond the heuristic model usually used to explain LED efficiency droop. ▪ Found that large differences in electron and hole mobilities play an important role in InGaN efficiency droop. ▪ Showed that efficiency droop occurs not only in InGaN blue-emitting LEDs, but also in red-emitting LEDs (InGaP).
Develop in-depth understanding of InGaN defects, i.e., atomistic structure, carrier capture cross-sections, and how their spatial distribution depends on growth environment.	▪ Achieved first-ever measurement of defect depth profiles in multi-quantum-well regions of c-plane InGaN/GaN LEDs. ▪ Discovered conditions under which a multi-level defect can give rise to efficiency-droop behavior.
Investigate nanophotonic approaches to tailor the environments around light-emitters to enhance (or modify) spontaneous emission rates.	▪ Novel synthesis of a GaN photonic crystal that enables 3D mode confinement. ▪ Designed a new plasmonic core-shell nanoparticle geometry for enhancing luminescence quantum yield.
Explore solid state lighting architectures based on coherent light emission as a possible route to substantial improvements in efficiency.	▪ Showed that high color quality (comparable to conventional white light sources) is possible with a 4-color laser source. ▪ Demonstrated single-mode lasing from GaN nanowires.

Website: http://ssls.sandia.gov/

Five-Year Goals and 2012 Progress

Energy Materials Center at Cornell
Director: Héctor Abruña
Lead Institution: Cornell University

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To advance the science of energy conversion and storage by understanding and exploiting fundamental properties of active materials and their interfaces.

Partner Institutions: Lawrence Berkeley National Laboratory

Award: $17.5 M, ARRA
Senior Investigators: 18 **Postdoctoral Staff:** 22 **Graduate Students:** 23 **Technical Staff:** 0
Publications : 44 **Invention Disclosures:** 6 **Patents/Applications:** 17 **Patents Licensed:** 3
Companies using EFRC research: General Motors, NOHMs Tech., Inc., A123 Systems, American Aerogel

5 Year Research Goals	Progress
Design, characterize, evaluate, and understand the electrochemical behavior of new electrocatalysts and catalyst supports for fuel cell applications.	▪ Enhanced anode catalyst activity on a titanium-doped tungsten oxide ($Ti_{1-x}W_xO_2$) support. ▪ Developed novel catalyst supports with designed porosity. ▪ Developed and evaluated high performance, robust catalysts for the oxygen reduction reaction (ORR).
Employ high-throughput, combinatorial methods to elucidate trends in activity (electrical- , electro-catalytic, …) of multi-component materials correlated to key physical chemical parameters (composition, electronic structure, …).	▪ Developed and deployed high-throughput crystallography and phase analysis of combinatorial libraries. ▪ Used high-throughput methods to identify a highly active non-platinum containing catalyst for methanol oxidation. ▪ Identified promising new compositions for ORR electrocatalysis.
Develop polymer science and methodologies to produce enhanced electrolyte membranes, separators and structured, porous electrode materials for batteries and fuel cells.	▪ Developed and evaluated best-in-class hydroxide conducting membranes for alkaline fuel cells. ▪ Epitaxially deposited nanosized single-crystal domains for batteries and other applications. ▪ Developed vascular macro/mesoporous fuel cell materials.
Understand and control the chemical physics responsible for unique electro-chemical properties of inorganic and organic-inorganic hybrid materials and novel architectures for electrical energy storage.	▪ Developed sulfur-carbon composites for advanced lithium-sulfur battery cathodes. ▪ Developed nanostructured metal oxides composites for advanced anodes. ▪ Demonstrated scalable, high-volume production of silicon nanowire anodes.
Exploit complex oxides' chemical stability and electronic properties tunability for energy applications.	▪ Engineered the band gap of strontium titanate ($SrTiO_3$), a promising water splitting catalyst, by lowering it by 10%. ▪ Synthesized sodium cobalt oxide ($NaCoO_2$) nanosheets and demonstrated epitaxial film growth of pyrochlores.
Develop and implement new theories to support the science of energy conversion and storage.	▪ Predicted key electrochemical interfacial phenomena under realistic conditions with density functional theory. ▪ Calculated the "phase diagram" for polysulfides.
Develop and deploy *in situ* characterization methods and instrumentation to study fuel cells and battery systems *in operando*.	▪ Studied fuel cell electrode aging by *in situ* microscopy. ▪ Used synchrotron x-rays (at CHESS, APS, and NSLS) to understand "bottlenecks" of lithium sulfur system. ▪ Studied battery electrolyte degradation using differential electrochemical mass spectrometry.

Website: http://www.emc2.cornell.edu

Five-Year Goals and 2012 Progress

Fluid Interface Reactions, Structures and Transport Center Energy Frontier Research Centers
Director: David J. Wesolowski Basic Energy Sciences
Lead Institution: Oak Ridge National Laboratory DOE Office of Science

Mission: To develop fundamental understanding and validated, predictive models of the unique nanoscale environment at fluid-solid interfaces that will enable transformative advances in electrical energy storage and catalysis for energy.

Partner Institutions: Argonne National Laboratory; Drexel University; Georgia State University; Northwestern University; Pennsylvania State University; Suffolk University; Vanderbilt University; University of Virginia

Award: $19.0 M
Senior Investigators: 28 **Postdoctoral Staff:** 17 **Graduate Students:** 4 **Technical Staff:** 0
Publications: 56 **Invention Disclosures:** 1 **Patents/Applications:** 2 **Patents Licensed:** 1
Companies using EFRC research: Asylum Research; Y-Carbon, Inc.

5 Year Research Goals	Progress
Develop accurate, experimentally-guided multiscale computational models of fluid-solid interface structures, dynamics and reactivity.	▪ Published first *ab initio* molecular dynamics (MD) simulations of typical lithium-ion battery electrolytes ($LiPF_6$ in ethylene, propylene, dimethyl carbonates) to understand lithium ion diffusion rates. ▪ Performed highly integrated nuclear magnetic resonance, laser fluorescence, small angle x-ray, quasielastic and spin echo neutron scattering, and MD simulations of room-temperature ionic liquid (RTIL) structures and dynamics in bulk, at surfaces, and in confined spaces. ▪ Conducted highly integrated x-ray reflectivity, wetting angle studies, and classical MD (CMD) simulations of water structure at graphene surfaces. ▪ Discovered oscillatory capacitance in nanoporous carbon/RTIL interfaces using CMD simulation and classical density functional theory. ▪ Used CMD to predict unexpected curvature effect in carbon capacitors.
Achieve a fundamental understanding of fluid-solid interfaces when the interface exhibits nanoscale textures and tailored surface chemistry, including interactions and reactions with electrolyte ions and solvent molecules with distinct molecular sizes and shapes.	▪ Synthesized composite mesoporous carbon electrode materials with superior conductivity and hierarchical nanoscale pore distributions. ▪ Developed onion-like carbon (OLC) micro-supercapacitors with superior energy and power density and extremely high charge/discharge rates. ▪ Developed entirely new scanning probe methods for mapping lithium-ion mobility in electrode materials with tens of nm spatial resolution. ▪ Observed anomalous diffusion rates of water in sub-nm pores in carbide-derived carbon & RTILs in mesoporous carbons by neutron scattering. ▪ Evaluated dewetting, solvation-driven charge imbalance and ion-size-dependent diffusion in carbon nanopores as a function of pore size, temperature and solvent type with new CMD simulations.
Understand how the complex fluid-solid interface environment mediates the mechanisms and kinetic pathways for interfacial reactions that require transfer of protons and electrons between the catalytic surface sites, adsorbates and fluid.	▪ Demonstrated first application of laser sum frequency generation to probe molecular sorbate bonding orientation on carbon substrates. ▪ Developed *ab initio* MD models of water oxidation by polypyridyl ruthenium complexes at functionalized graphite surfaces. ▪ Demonstrated reversible proton-coupled electron transfer reactions that control quinone redox chemistry at the water/OLC interface. ▪ Applied quasielastic and inelastic neutron scattering and *in situ* UV Raman spectroscopy to characterize structures, diffusion dynamics and redox chemistry of quinones on OLC surfaces. ▪ Showed photoinduced cobalt redox chemistry at water/titania interface.

Website: http://www.ornl.gov/sci/first/

Five-Year Goals and 2012 Progress

Heterogeneous Functional Materials for Energy Systems Energy Frontier Research Centers
Director: Ken Reifsnider Basic Energy Sciences
Lead Institution: University of South Carolina DOE Office of Science

Mission: To create control science to build a bridge between synthesis and modeling by understanding, designing, and synthesizing heterogeneous functional materials from the atomistic to nano-scale to macro-scale for energy storage and conversion systems such as fuel cells, batteries, supercapacitors, electrolyzers, and solid membranes.

Partner Institutions: Georgia Institute of Technology; University of Utah; Princeton University; Rochester Institute of Technology; University of Connecticut; Savannah River National Laboratory; University of California, Santa Barbara

Award: $12.5 M
Senior Investigators: 15 **Postdoctoral Staff:** 11 **Graduate Students:** 30 **Technical Staff:** 2
Publications: 88 **Invention Disclosures:** 0 **Patents/Applications:** 7 **Patents Licensed:** 0
Companies using EFRC research: Topsoe Fuel Cell, Pall Corp., MSRI

5 Year Research Goals	Progress
Understand charge transport and storage in heterogeneous functional materials (HeteroFoaM)	▪ Used nano-porous HeteroFoaM architecture to achieve unprecedented super-capacitance (>2500 F/g) demonstrating new energy storage concept that is not solely dependent on redox reactions of cations. ▪ Established first-ever effect of crystalline content and morphology on hydrogen transport in ceramic membranes. ▪ Demonstrated model-based microstructure design of porous cathode resulting in 12-fold decrease in polarization losses in fuel conversion devices.
Establish science of functional surfaces and interfaces	▪ Created nano-island surface modification of a nickel-yttrium stabilized zirconia (Ni-YSZ) anode using barium oxide (BaO) to eliminate carbon formation from hydrocarbon fuels enabling direct utilization of legacy fuels. ▪ Addressed the “activity vs. stability” tradeoff by discontinuously coating a ceramic oxide cathode to demonstrate the advantage of a heterogeneous cathode surface layer with controlled morphology. ▪ Developed first ever closed-form model of surface charge development in non-dilute, heterogeneous mixtures of dielectric and conductive constituents.
Create synthesis methods to control morphology and functionality	▪ Created optimally reducible mixed conductor ceramic anode [$SrTi(Nb,Ga)O_3$] guided by first principles atomic level analysis. ▪ Developed unique direct write, freeze cast, and flash sintering methods of controlling nano- and micro-morphology in porous, heterogeneous materials. ▪ Achieved first-ever demonstration of regenerative *in-situ* formation of catalyst /ceramic, fuel-flexible anodes to enhance fuel flexibility during conversion.
Establish a multi-physics, multi-scale methodology for "HeteroFoaM by Design"	▪ Created 3D multiphysics model that resolves the microstructure of the anode to be used to follow functional changes during operation. ▪ Established new paradigm for design of mixed-electronic/ionic conducting electrodes using a new atomic modeling approach to structure-property predictions and validated the method for a perovskite anode material. ▪ Invented conformal design of anode for H_2 oxidation with heterogeneous methane reformation based on *ab initio* modeling of local sulfur poisoning. ▪ Established quantum mechanics-based design principles for solid oxide fuel cell cathode materials.

Website: http://www.HeteroFoaM.com

Institute for Atom-efficient Chemical Transformations
Director: Christopher L. Marshall
Lead Institution: Argonne National Laboratory

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To address key catalytic conversions that could improve the efficiency of producing fuels from biomass. The Institute for Atom-Efficient Chemical Transformations (IACT) is focusing on advancing the science of catalysis for the efficient conversion of energy resources into usable forms. IACT's goal is to find ways to achieve control and efficiency of chemical conversions comparable to those in nature.

Partner Institutions: Brookhaven National Laboratory; Northwestern University; Purdue University; University of Wisconsin, Madison

Award: $19.0 M
Senior Investigators: 21 **Postdoctoral Staff:** 20 **Graduate Students:** 15 **Technical Staff:** 3
Publications: 33 **Invention Disclosures:** 0 **Patents/Applications:** 1 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Synthesize nanobowls for the controlled catalysis and protection of small metal particles.	▪ Established the shape- and size-selectivity of nanobowl catalysts prepared by templated atomic layer deposition (ALD) for the photocatalytic oxidation of alcohols. ▪ Demonstrated enhanced thermal stability and selectivity of ALD over-coated noble metal nanoparticle catalysts.
Improve catalyst activity and selectivity for the reforming of small alcohols.	▪ Created a new highly active and stable bimetallic catalyst that produces hydrogen from biomass under aqueous reaction conditions. ▪ Discovered a highly active and selective new bimetallic catalyst that hydrogenates oxygen-rich biomolecules to gasoline-compatible fuels under aqueous reaction conditions.
Improve fundamental understanding in the catalytic conversion of furfural to levulinic acid.	▪ Found that one of the major reaction pathways for conversion of furfuryl alcohol to levulinic acid in water takes place via a geminal diol species formed by the addition of two water molecules. ▪ Identified multiple reaction pathways for the conversion of furfuryl alcohol in ethanol solvent to ethyl levulinate, one of which leads to the co-production of diethylether.
Selectively convert glucose and fructose to chemical intermediates.	▪ Studied the pathways and intermediates for the conversion of fructose to hydroxymethylfurfural (HMF) in dimethyl sulfoxide with theoretical and experimental techniques. HMF is a desirable compound for further processing into chemical feedstocks. ▪ High level calculations provided detailed data on the energetics and pathways for a variety of relevant reactions including lactic acid hydrogenation to propylene glycol and propanoic acid on Pt(111), and the mechanism for furfural hydrogenation and decarbonylation on transition metal surfaces.

Website: http://www.iact.anl.gov/

Light-Material Interactions in Energy Conversion
Director: Harry Atwater
Lead Institution: California Institute of Technology

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To tailor the morphology, complex dielectric structure, and electronic properties of matter to sculpt the flow of sunlight, enabling light conversion to electrical and chemical energy with unprecedented efficiency.

Partner Institutions: University of Illinois at Urbana-Champaign and Lawrence Berkeley National Laboratory

Award: $15.0 M

Senior Investigators: 11 **Postdoctoral Staff:** 11 **Graduate Students:** 28 **Technical Staff:** 1
Publications: 47 **Invention Disclosures:** 0 **Patents/Applications:** 4 **Patents Licensed:** 0
Companies using EFRC research: Semprius, Alta Devices, Caelux, MC10

5 Year Research Goals	Progress
Design an optical system for full spectrum photon conversion via optically independent multijunction solar converter architectures to greatly enhance the efficiency of photovoltaic energy conversion.	▪ Demonstrated flexible concentrator photovoltaics based on microscale crystalline silicon solar cells embedded in downshifting luminescent waveguides, increasing power output by over 300%. ▪ Completed initial designs for spectrum splitting optical structures used in optically-in-parallel multijunction solar cells.
Define the limits to absorption and spontaneous emission in optical materials, yielding principles for design of ultrathin photovoltaic cells with scaling of light absorbers to nanoscale dimensions, enabling advances in photovoltaic conversion efficiency and reduced material utilization.	▪ Achieved record solar cell efficiency: discovered that to maximize conversion efficiency, photon emission from the solar cell should be maximized. Theoretical results led to Alta Devices' 28.4% efficient flat plate single-junction gallium arsenide (GaAs) solar cell that exceeded the previous record by 2 percentage points. ▪ Demonstrated the first optoelectronically active photonic crystal light emitting diode (LED) in a single crystal GaAs photonic crystal with light-emitting heterostructures.
Establish fundamental transformation optics principles for light absorption and emission in complex metamaterial structures.	▪ Implementing wafer-scale transformation optics using photoelectrochemical etching of silicon to produce refractive indices ranging from 2.5 to 1.2 and optical properties that vary continuously across a device.
Develop light-driven material synthesis processes that enable energy conversion materials to develop their own complex architectures in response to illumination conditions and tailor light absorption in dielectric materials with complex architectures.	▪ Investigating light-mediated formation of nanoscale lamellar patterns during the electrodeposition of photoresponsive selenium-tellurium (Se-Te) alloys. ▪ Using varied illumination conditions during growth to control film morphology and build in structural complexity to create structures that may be able to naturally evolve into the optimal light trapping geometry.

Website: http://lmi.caltech.edu

Five-Year Goals and 2012 Progress

Materials Science of Actinides
Director: Peter C. Burns
Lead Institution: University of Notre Dame

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To understand and control, at the nanoscale, materials that contain actinides (radioactive heavy elements such as uranium and plutonium) to lay the scientific foundation for advanced nuclear energy systems.

Partner Institutions: University of Michigan; University of California, Davis; George Washington University; University of Minnesota; Rensselaer Polytechnic Institute; Oak Ridge National Laboratory; Savannah River National Laboratory; Sandia National Laboratories

Award: $18.5 M, ARRA

Senior Investigators: 18 **Postdoctoral Staff:** 18 **Graduate Students:** 24 **Technical Staff:** 13
Publications: 109 **Invention Disclosures:** 0 **Patents/Applications:** 2 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Understand ionic substitutions in fluorite-structure-related actinide oxides and nuclear fuels.	▪ Characterized the energetics of lanthanum and yttrium substitution in thoria, and studied size mismatch and defect clustering in the fluorite-structure series. ▪ Determined that water is bound strongly and partially dissociated on the surface of thoria.
Synthesize, characterize, and determine the energetics of revolutionary new actinide materials.	▪ Created and tested a promising thorium borate with ion exchange properties for technetium. ▪ Measured the energetics of uranyl peroxide cage clusters for the first time. ▪ Synthesized hybrid uranyl-organic solids and studied their thermochemistry.
Create, characterize, and understand a family of new actinide-based nano-materials.	▪ Synthesized and characterized 80 uranium-based clusters with diameters up to 3.5 nm. Computational studies showed that peroxide bridges between uranyl ions create the needed curvature, and that counter ions stabilize specific structural units.
Develop applications of nano-scale control of actinides.	▪ Demonstrated the assembly and stability of uranium cage clusters used for separation of uranium from complex solutions.
Understand actinide materials under the coupled extreme conditions of radiation, pressure, and temperature using experimental strategies.	▪ Performed systematic irradiations of cerium oxide at extreme pressures and temperatures that have provided insight into the influence of structure, composition and bonding on the radiation stability of actinide-bearing materials.
Investigate actinide materials under extreme conditions of irradiation, pressure and temperature using theoretical approaches.	▪ Calculated the energetics of incorporation of uranium, neptunium, and plutonium into garnet-type structures. ▪ Used simulations and thermal spike models to understand track formation, internal structural, and phase changes for radiation induced pyrochlore. ▪ Predicted computationally the electronic structures of uranium oxides (UO_2 and $UO_{2.03}$) under pressure.

Website: http://www.ndefrc.com

Molecularly Engineered Energy Materials
Director: Vidvuds Ozolins
Lead Institution: University of California, Los Angeles

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To acquire fundamental understanding and control of nanoscale materials for solar energy generation and electrical energy storage.

Partner Institutions: University of California, Berkeley; Eastern Washington University; University of Kansas; National Renewable Energy Laboratory; Lawrence Berkeley National Laboratory

Award: $11.5 M

Senior Investigators: 13	**Postdoctoral Staff:** 13	**Graduate Students:** 25	**Technical Staff:** 0
Publications: 40	**Invention Disclosures:** 0	**Patents/Applications:** 1	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Understand how the nanometer-scale structure of polymer blends controls separation, transport, recombination, and extraction of charge carriers in organic solar cells.	▪ Demonstrated that molecular self-assembly offers a practical route to controlling the structure of organic solar cells. ▪ Showed that the exciton diffusion length in highly crystalline polymers is at least twice as long as previously reported. ▪ Showed how molecular packing and the spatial extent of electronic states controls carrier mobility in self-assembled fullerenes. ▪ Obtained evidence that energy-transfer plays an important role in moving excitations within organic solar cells.
Control the structure of polymer blends through the synthesis of novel materials and self-assembly, with the goal of making optimal nanometer scale structures for organic solar cells.	▪ Used controlled crystallization and sequential processing to tune the fullerene distribution and orientation of crystalline polymer domains. ▪ Realized molecular co-assembly of photo-donors and electron acceptors in water to enable facile and stable charge separation. ▪ Synthesized a family of titania-binding fullerenes and showed that these facilitate electron transfer between polymers & titania nanorods.
Determine why capacitive storage from metal oxides is much less than theoretical predictions.	▪ Used novel mesoporous electrodes to show that electrolyte access to redox-active walls and short ion and electron diffusion paths are both crucial for enabling all of the active electrode material to contribute to charge storage. ▪ Proved the importance of fast ion transport in a new supercapacitor material, niobium oxide (Nb_2O_5), in which nearly 75% of theoretical capacitance is achieved within one minute.
Design hierarchical architectures as electrode structures, which integrate electronic and ionic conduction with charge storage.	▪ Made hierarchical electrode materials with enhanced charging rates using intertwined nanotubes and nanowires. ▪ Designed a novel hierarchical architecture based on a thin, conformal redox-active layer coated on a 3D porous, conductive scaffold. ▪ Developed conductive carbon nanotube scaffolds with controlled porosity and deposited redox-active materials onto these scaffolds.
Elucidate the relation between the structure of a zeolitic imidazolate framework (ZIF) and performance; develop strategies for optimizing performance of ZIFs for highly selective carbon separation.	Integrated computational and experimental studies, identified preferred adsorption sites for carbon dioxide (CO_2) and methane (CH_4) in ZIFs, and formulated the following design principles: ▪ To increase adsorption at low pressures, use smaller pores, highly polarizable functional groups, & asymmetrically functionalized linkers. ▪ For higher-pressure separations, use larger pore topologies. ▪ To increase CO_2 selectivity, optimize linker functionality.

Website: http://meem.ucla.edu

Five-Year Goals and 2012 Progress

Nanostructures for Electrical Energy Storage Energy Frontier Research Centers
Director: Gary Rubloff Basic Energy Sciences
Lead Institution: University of Maryland DOE Office of Science

Mission: To understand and build nano-structured electrode components as the foundation for new electrical energy storage technologies.

Partner Institutions: Sandia National Laboratories; University of California, Irvine; Los Alamos National Laboratory; University of Florida; Yale University

Award: $14.0 M
Senior Investigators: 18 **Postdoctoral Staff:** 12 **Graduate Students:** 25 **Technical Staff:** 1
Publications: 52 **Invention Disclosures:** 1 **Patents/Applications:** 3 **Patents Licensed:** 0
Companies using EFRC research: General Motors

5 Year Research Goals	Progress
Cathodic Nanostructures: Identify and optimize the specific factors controlling power and energy in heterogeneous nanostructures for use as cathodes in electrical energy storage systems.	▪ Fabricated manganese oxide (MnO_2) nanowires and characterized electrochemical properties to determine the limitations to reaching the theoretical capacity for charge storage. ▪ Deposited MnO_2 onto a single carbon nanotube and studied the electron transfer across the interface between the carbon electron conductor and the MnO_2 charge storage material. ▪ Fabricated nanowire cathodes with electrically conductive polymer and metal-oxide charge storage regions and determined how architecture affects charge storage capacity and cycle life. ▪ Developed layered cathode of decomposed sulfur on carbon nanotubes which improved cyclability and efficiency of the lithium sulfide cell by preventing cathode polysulfide dissolution.
Anodic Nanostructures: Develop mechanistic understanding and design principles to maintain electrochemical performance and stability during charge cycling of nanostructured anodes used in electrical energy storage systems.	▪ Developed *in situ* transmission electron microscopy (TEM) technique to observe in real time nanoscale structural changes in silicon (Si) or tin oxide nanowire anodes due to lithiation. ▪ Used tobacco mosaic virus as a self-assembled template for the preparation of uniform, high capacity Si nanowire anode arrays. ▪ Prevented metal-silicide formation and vastly improved Si nanowire cycle life by growing nanowires with the benefit of an anodic aluminum oxide template. ▪ Using *in situ* TEM, observed the interfacial failure mechanism for silicon layers and carbon nanotubes in composite anodes.
Enabling Science & Methods: Develop real-time *in-situ* characterization of nanoscale electrochemistry, methods for synthesizing heterogeneous nanostructures, and experimental and computational approaches to understand electrochemical interfaces and materials.	▪ Controlled growth of functional bands on carbon nanotubes, allowing for the control of both conductivity and solubility. ▪ Created an encapsulated electrochemical cell to monitor electrochemical processes in volatile, organic electrolytes at very high resolution using *in situ* TEM. ▪ Used density functional theory to model breakdown of an organic electrolyte and predicted the products that form solid electrolyte interphases and their resulting impact on electrode conductivity.
Nanowire Forests: Discover new phenomena to inform design of energy storage in constrained nanoscale environments.	▪ Controlled ion transport and water transport in nanopores by tuning hydrophobic islands on pore walls with chemical inhomogeneities. Hydrophobic gating through pores lays the foundation for controlling electrolyte flow.

Website: http://www.efrc.umd.edu

Five-Year Goals and 2012 Progress

Non-equilibrium Energy Research Center Energy Frontier Research Centers
Director: Bartosz A. Grzybowski Basic Energy Sciences
Lead Institution: Northwestern University DOE Office of Science

Mission: To understand self-organization in dissipative, far-from-equilibrium systems and to use this knowledge to synthesize adaptive, reconfigurable materials for energy storage and transduction.

Partner Institutions: Harvard University; University of Michigan; Pennsylvania State University

Award: $19.0 M, ARRA
Senior Investigators: 12 **Postdoctoral Staff:** 42 **Graduate Students:** 26 **Technical Staff:** 5
Publications: 130 **Invention Disclosures:** 1 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Develop general laws that describe how systems waste energy and how that energy can be harvested and channeled productively.	▪ Developed a theoretical description and statistical model of how energy that would otherwise be wasted can be harvested to do useful mechanical, chemical, or electrical work. ▪ Used theoretical understanding to guide experimental design and analysis of results for model dissipative, far-from-equilibrium systems.
Develop materials that produce chemical/electrostatic energy from energy sources that are otherwise wasted.	▪ Discovered that high-value products can be produced with high efficiency from polymer waste simply by squeezing them. The products include hydrogen peroxide and other materials relevant for nanotechnology. ▪ Provided fundamental insight into a 2000-year old question on how/why static electricity develops and how it can be utilized.
Develop materials that convert chemical, light, or electrical energy into mechanical energy using machines made from molecules.	▪ Discovered the principles by which molecules (e.g., molecular switches) can be assembled into machines (e.g., artificial muscles or nanorobots), which are programmed to do work by harvesting wasted thermal energy from the environment.
Harness the energy that is otherwise lost in nanoantennas, such as in arrays of plasmonic materials, to drive chemical reactions or generate electrical power.	▪ Fabricated and characterized the first ever solar cell based entirely on plasmonic materials, harvesting electrical energy from sunlight. ▪ Constructed a versatile platform for designing crystalline superlattice structures from DNA and plasmonic nanoparticles, which allows the channeling of energy in plasmonically-driven nanofabrication. ▪ Developed theoretical and computational approaches to the dynamic control of nanoparticle assemblies which are designed to perform functions (e.g., self-replication, nanocatalysis of chemical reactions, or swarming) under non-equilibrium conditions.
Revolutionize chemical synthesis by identifying new sequences of chemical reactions that can be performed in an energy efficient manner.	▪ Theoretically identified and experimentally verified how to execute multi-step reactions in a single reactor without purification of intermediates after each step. ▪ Demonstrated that this new synthetic paradigm of chemical networks saves energy and money by comparison to conventional methods used in the chemical industry.

Website: http://www.nercenergy.com/

Five-Year Goals and 2012 Progress

Northeastern Center for Chemical Energy Storage — Energy Frontier Research Centers
Director: M. Stanley Whittingham — Basic Energy Sciences
Lead Institution: Stony Brook University — DOE Office of Science

Mission: To understand how fundamental chemical reactions occur at electrodes and to use this knowledge to design new chemical energy storage systems.

Partner Institutions: Argonne National Laboratory; Binghamton University; Brookhaven National Laboratory; Lawrence Berkeley National Laboratory; Massachusetts Institute of Technology; Rutgers University; University of California, San Diego; University of Michigan

Award: $17.0 M

Senior Investigators: 16	**Postdoctoral Staff:** 22	**Graduate Students:** 25	**Technical Staff:** 8
Publications: 32	**Invention Disclosures:** 1	**Patents/Applications:** 1	**Patents Licensed:** 0

Companies using EFRC research: none

5 Year Research Goals	Progress
Understand the transformations that occur in an electrode composite structure, from the atomistic level to the macroscopic level, throughout the lifetime of the functioning battery.	▪ Produced flux-grown olivine (lithium iron phosphate, $LiFePO_4$) crystals with antisite defects below the detection limit as a pure model compound for *in-situ* studies of intercalation reactions. ▪ Characterized the phase progression and reversibility of structural changes for iron oxyfluorides (FeF_y, and FeOF), establishing these cathode materials as model compounds for conversion reactions. ▪ Probed the structural, phase, and compositional changes of the model compound in functioning batteries using newly developed *in situ* metrologies: *in situ* total scattering experiments to assess local structure (PDF), magnetic resonance imaging, x-ray Raman scattering, and x-ray absorption near-edge structure/transmission x-ray microscope.
Identify the key parameters that are required to optimize intercalation reactions in electrodes. (What are the ultimate limits to intercalation reactions, the core of today's batteries?)	▪ Developed theoretical model that explains high rate for nanosized olivine particles, using single phase reaction – Identified overpotential as controlling reaction path. – Identifying suitable experimental tests of models. ▪ Showed that doping of olivine enhances reaction kinetics. ▪ Identified tin cobalt carbon (SnCoC) and FeOF as crossover materials that exhibit both intercalation and conversion reactions. Demonstrated that hybrid reactions of the crossover material FeOF perform better than pure conversion of isostructural FeF_2.
Determine how to achieve total control over a conversion reaction, over the entire lifetime of the working battery, by deriving an understanding of the relevant chemistries that occur at the molecular (atomic) level and that involve control of the morphology and microstructures of the composite.	▪ Showed that a low diffusion metal (M) in MF_2 is needed to maintain the nanostructure, and therefore the reversibility. Thus FeF_2 is reversible whereas copper (Cu) in CuF_2 diffuses much faster, forming large particles that cannot be easily dissolved. ▪ Theoretical studies on a structure-retaining cathode ($CuTi_2S_4$) predicted that Ti_2S_4 will form and the copper will very slowly re-insert into the lattice. ▪ Developed unique *in situ* transmission electron microscopy/ scanning tunneling microscopy characterization that showed, in real-time, the formation of iron nanoparticles, < 5 nm, on reaction of lithium with FeF_2. ▪ Determined that large capacity fade is predominantly due to surface decomposition of certain electrolytes and subsurface diffusion of the reaction products.

Website: http://necces.chem.sunysb.edu/

Five-Year Goals and 2012 Progress

Photosynthetic Antenna Research Center | Energy Frontier Research Centers
Director: Robert E. Blankenship | Basic Energy Sciences
Lead Institution: Washington University in St. Louis | DOE Office of Science

Mission: To maximize photosynthetic antenna efficiency in living organisms and to fabricate robust micron-scale biohybrid light-harvesting systems to drive chemical processes or generate photocurrent.

Partner Institutions: Los Alamos National Laboratory; New Mexico Consortium; North Carolina State University; Oak Ridge National Laboratory; Sandia National Laboratories; University of California, Riverside; University of Glasgow (UK); University of Pennsylvania; University of Sheffield (UK)

Award: $20.0 M

Senior Investigators: 17 **Postdoctoral Staff:** 32 **Graduate Students:** 28 **Technical Staff:** 11
Publications: 51 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Enhance photosynthetic efficiency by determining and tailoring antenna size, composition, and spectral coverage.	▪ Assessed the role of antenna size and composition in cyanobacteria and green algae using molecular biology and advanced imaging technologies. - Determined that effects of changing antenna size differs between organisms; e.g., decreasing antenna size may increase photosynthetic efficiency in algae but not in cyanobacteria. ▪ Developed tools including new mutant strains to extend spectral coverage of native antennas.
Design and construct light-harvesting assemblies based on synthetic or mixed synthetic and native-like components with customized absorption of visible and near-infrared photons, delivering the energy to a target site with a high quantum yield.	▪ Constructed biohybrid and bioinspired antennas that contain tunable chromophores and designer or engineered native-like peptide scaffolds. ▪ Developed an antenna complex based on self-assembly of synthetic chromophores without scaffolding.
Achieve the expertise and tools to exercise comprehensive molecular- to nano- to micro-scale control over light-harvesting systems *in vivo* and *in vitro,* leading to tailored arrays for efficient solar light harvesting, energy transfer and trapping that can be used to generate chemical fuels or photocurrent.	▪ Developed nanopatterned antenna on surfaces for controlled migration pathways of harvested energy. ▪ Applied novel characterization tools to better understand light-harvesting system: - Characterized global pigment distribution in antenna using Atomic Force Microscopy (AFM). - Characterized antenna structure using neutron and small angle scattering techniques. - Developed combined AFM/optical, total internal reflection fluorescence, and scanning near-field microscopy techniques for evaluating the energy trapping of light harvesting arrays. ▪ Assessed energy transfer dynamics in antenna.

Website: http://parc.wustl.edu

Five-Year Goals and 2012 Progress

Polymer-Based Materials for Harvesting Solar Energy (PHaSE) Energy Frontier Research Centers
Director: Thomas P. Russell and Paul M. Lahti Basic Energy Sciences
Lead Institution: University of Massachusetts, Amherst DOE Office of Science

Mission: To carry out fundamental photovoltaic-oriented research on the use of organic-based polymers and related materials to maximize efficiency in the collection and harvesting of energy over a broad frequency range of the solar spectrum.

Partner Institutions: University of Massachusetts, Lowell; University of Pittsburgh; Pennsylvania State University; Rensselaer Polytechnic Institute; Oak Ridge National Laboratory

Award: $16.0 M, ARRA
Senior Investigators: 22 **Postdoctoral Staff:** 18 **Graduate Students:** 13 **Technical Staff:** 3
Publications: 54 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Develop new electronic materials to harvest solar light over a wide spectral range, and create charge separation.	▪ Created multiple new polymers able to absorb light in 600-1000 nm region not utilized by present "plastic" solar cells; hole and electron carrier systems made; test solar cells are under development. ▪ Created new "push-pull" and polymer molecular systems that give charge-separated excited states upon photo-excitation; solid state charge transport testing underway.
Develop novel design strategies to optimize device efficiency.	▪ Induced "superhighway"-like, multi-lane assemblies for a conductive polymer, P3HT, with attached semiconductor nanorods and side-chain altered P3HT. ▪ Developed structured polymer materials using nanoparticles and nanorods containing photoactive polymers, such as P3HT.
Limit exciton recombination to give more electrical charges for harvesting.	▪ Performed spectral analysis of semiconductor polymer nanofibers/ nanoparticles to reveal previously unseen details of inter-polymer organization; on-going tests to correlate spectral results with x-ray scattering structure determination and with charge transport. ▪ Developed analytical spectroscopic /microscopic studies to probe absorption and structural characteristics of polymeric nanoparticles that influence charge-pair recombination in solar cells.
Maximize electron transport to get more electrical charges through a device.	▪ Started unraveling the complexity of solvent-based processing conditions that underpin the ordering and performance of active layers in device fabrication, for instance that appropriate solvent choice for P3HT precipitation yields narrow size-distribution nanoparticles.
Optimize fabrication strategies that maximize photoconversion efficiency.	▪ Achieved new insights into nanoparticle morphology from structural studies on P3HT-based systems; important for improving photovoltaics. ▪ Developed strategies to optimize photoconversion efficiency of low-band-gap polymers via basic studies of their structure and morphology. ▪ Fundamental experimental and theoretical studies provided new insights about transport processes in conjugated polymers and across organic/organic and organic/inorganic hybrid interfaces. ▪ Correlated structure (aggregate and crystalline) with the spectroscopic characteristics of photoactive polymers, and the ultimate relationship of polymer organization to efficiency.

Website: http://www.cns.umass.edu/efrc

Re-Defining Photovoltaic Efficiency Through Molecule Scale Control Energy Frontier Research Centers
Director: James Yardley Basic Energy Sciences
Lead Institution: Columbia University DOE Office of Science

Mission: To develop the enabling science needed to realize breakthroughs in the efficient conversion of sunlight into electricity in nanometer sized thin films.

Partner Institutions: University of Texas at Austin; Purdue University, Brookhaven National Laboratory

Award: $16.0 M, ARRA
Senior Investigators: 26 **Postdoctoral Staff:** 33 **Graduate Students:** 35 **Technical Staff:** 0
Publications: 47 **Invention Disclosures:** 5 **Patents/Applications:** 5 **Patents Licensed:** 0
Companies using EFRC research: Chromation Partners, LLC

5 Year Research Goals	Progress
Provide demonstrated advances in fundamental understanding of charge creation, separation, and extraction in organic and hybrid nanoscale systems.	▪ Evaluated graphene materials as transparent electrodes for solar cells and demonstrated "ohmic" contact behavior with organic semiconductors, an important step for lowering losses in the extraction of charge. ▪ Demonstrated transparent solar cells that use graphene as both cathode and anode, a key step in making efficient tandem solar cells that can exceed the theoretical 34% single junction solar cell efficiency limit (the Shockley-Queisser limit).
Develop materials and structures that will dramatically improve the efficiency of charge separation and extraction in organic or hybrid systems, seeking a demonstrated quantum yield of charge carriers that approaches unity.	Created new semiconducting materials and structures that offer improvement in photovoltaic device characteristics: ▪ Engineered reticulated junctions between organic phases based on a ball and socket interaction which serve as the charge separation interface in organic devices. ▪ Synthesized new inorganic molecular cluster compounds that should mimic the performance of quantum dots, but which should allow processing into novel device structures. ▪ Invented novel co-crystals of inorganic clusters with organic electron acceptors that exhibit unusual metallic or semiconducting behavior. ▪ Discovered that a single molecular layer of molybdenum disulfide (MoS_2) is a direct bandgap semiconductor which has an ideal bandgap for solar energy conversion.
Develop and study new device concepts including structures and architectures for thin film solar cells capable of operation at efficiencies approaching the Shockley-Queisser limit of 34%.	▪ Built solar cell devices based on a "projected electrode" concept that gives improved collection efficiency. ▪ Developed and started to implement a concept based on ultra-thin organic photocells that should provide excellent efficiency approaching the 34% limit.
Demonstrate thin film solar cell devices, concepts, and corresponding materials that allow optimal generation and extraction of multiple excitons per photon absorbed.	▪ Experimentally demonstrated the generation of multiple charge pairs per photon absorbed using a new "Exciton Fission" scheme in pentacene. Currently developing a theoretical understanding to enable the design of more effective systems.

Website: http://www.cise.columbia.edu/efrc/

Five-Year Goals and 2012 Progress

Revolutionary Materials for Solid State Energy Conversion
Director: Donald T. Morelli
Lead Institution: Michigan State University

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To investigate the underlying physical and chemical principles of advanced materials for the conversion of heat into electricity.

Partner Institutions: Northwestern University; The Ohio State University; University of Michigan; University of California, Los Angeles; Wayne State University; Oak Ridge National Laboratory

Award: $12.5 M
Senior Investigators: 15 **Postdoctoral Staff:** 10 **Graduate Students:** 14 **Technical Staff:** 1
Publications: 60 **Invention Disclosures:** 3 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: ZT Plus, Inc; BSST, Inc.

5 Year Research Goals	Progress
Use advanced computational techniques to understand how to design materials with tailored thermal and electronic properties.	▪ Learned how to employ *ab initio* density functional theory and molecular dynamics simulations to understand the thermodynamic driving forces for phase separation in thermoelectric (heat to electricity) nanocomposites. ▪ Used computational techniques to investigate the lattice dynamics of thermoelectric semiconductors and reveal the important relationship between anharmonicity and minimal thermal conductivity in solids. ▪ Developed computational techniques for quantitatively predicting the thermal conductivity of solids based on their structure and bonding.
Understand the influence of structure and nanostructure on phonon transport in solids.	▪ Showed that in nanostructured solids, additional thermal conductivity reduction can be achieved by scattering lattice vibrational waves [phonons] from interfaces with spacings on the nanoscale. Reducing thermal conductivity improves the thermoelectric performance. ▪ Experimentally showed that solids with large anharmonicity in their lattice vibrational spectrum can exhibit minimal thermal conductivity. ▪ Synthesized a variety of new bulk homogeneous and nanostructured materials based on computational predictions and characterized their thermoelectric properties.
Understand how to maintain charge transmission in poorly thermally conducting solids.	▪ Demonstrated that coherent nanoprecipitates introduced into the matrix of a thermoelectric semiconductor can allow charge transmission at the nanoparticle-matrix interface, resulting in improved charge carrier transport and better overall thermoelectric performance. ▪ Showed that "decoration" of grain boundaries by metallic phases can significantly enhance electrical conductivity across grain boundaries without degrading other important properties, such as the Seebeck coefficient (a measure of the induced thermoelectric voltage in response to a temperature difference), leading to a better thermoelectric material.

Website: http://science.energy.gov/bes/efrc/centers/rmssec/

Five-Year Goals and 2012 Progress

Solid State Solar Thermal Energy Conversion
Director: Gang Chen
Lead Institution: Massachusetts Institute of Technology

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To create novel, solid-state materials for the conversion of sunlight into electricity using thermal and photovoltaic processes.

Partner Institutions: Boston College; Oak Ridge National Laboratory; Rensselaer Polytechnic Institute

Award: $17.5
Senior Investigators: 19 **Postdoctoral Staff:** 18 **Graduate Students:** 26 **Technical Staff:** 10
Publications: 85 **Invention Disclosures:** 0 **Patents/Applications:** 9 **Patents Licensed:** 0
Companies using EFRC research: GMZ Energy

5 Year Research Goals	Progress
Understand electron and phonon transport in thermoelectric materials and identify promising materials and nanostructures.	▪ Developed first-principles based simulation tools to compute phonon thermal conductivity and interface transmission. ▪ Developed three-dimensional modulation doping concept to increase electronic power factor. ▪ Predicted that ABO_2 minerals (delafossites such as $PtCoO_2$) can have opposite signs of the Seebeck coefficient in different crystallographic directions and large thermal power.
Probe the details of phonon and electron transport experimentally.	▪ Developed two thermal conductivity spectroscopy techniques to measure phonon mean free path distributions: a pump-probe and a transient grating technique. ▪ Observed strong anharmonic interactions between phonon modes in lead telluride (PbTe) using inelastic neutron scattering. ▪ Observed coherent phonon heat conduction in superlattice structures.
Develop materials synthesis methods and structural and property characterization tools to enhance the thermoelectric figure-of-merit (ZT, a higher value indicates better thermoelectric performance).	▪ Achieved a ZT over 1.5 in copper selenide ($CuSe_2$), and high ZT values in lead selenide (PbSe) and half heusler compounds. ▪ Demonstrated effectiveness of modulation doping in 3D nanostructures in improving thermoelectric performance. ▪ Developed microwave-based bottom-up approach to synthesize nanostructured bismuth telluride (Bi_2Te_3) with good ZT values. ▪ Identified mechanisms of alloy formation in the ball-milling synthesis of Bi_2Te_3.
Control the absorption and re-emission of light.	▪ Designed, fabricated and characterized 2D photonic crystals with high wavelength selectivity at high temperatures. ▪ Developed concept of an angular selective photonic crystal. ▪ Invented an approach to make an incandescent lamp with a theoretical efficiency of nearly 40%.
Demonstrate the potential impact of the proposed solar-to-heat-to-electricity approaches.	▪ Demonstrated solar thermoelectric generators at 4.8% efficiency without any optical concentration, seven to eight times more efficient than comparable devices. ▪ Built a test bed to validate the solar thermo-photovolatic concept. ▪ Conducted fundamental studies on methods to fabricate interfacial contacts in thermoelectric devices.

Website: http://s3tec.mit.edu/

Five-Year Goals and 2012 Progress

Understanding Charge Separation and Transfer at Interfaces in Energy Materials
Director: Peter Rossky
Lead Institution: University of Texas at Austin

Energy Frontier Research Centers
Basic Energy Sciences
DOE Office of Science

Mission: To pursue fundamental research on charge transfer processes that underpin the function of highly promising molecular materials for photovoltaic and electrical energy storage applications.

Partner Institutions: Sandia National Laboratories

Award: $15.0 M, ARRA
Senior Investigators: 16 **Postdoctoral Staff:** 16 **Graduate Students:** 9 **Technical Staff:** 10
Publications: 32 **Invention Disclosures:** 0 **Patents/Applications:** 0 **Patents Licensed:** 0
Companies using EFRC research: none

5 Year Research Goals	Progress
Establish fundamental relationships between molecular-level charge separation and transfer (CST) processes and the function of these processes in organic photovoltaic (OPV) and electrical energy storage (EES) materials	Key mechanistic findings include: ▪ Atomic/molecular level understanding of nanoscale morphology critical to OPV and EES materials, ▪ Discovery of hot charge transfer states as key intermediates in OPV function, and ▪ Presence of defects and dimensional confinement of EES materials influences lithium-ion diffusion.
Evaluate these newly discovered relationships for the design and assembly of interfaces in OPV and EES materials with CST functions	▪ Determined that energy efficiency is strongly dependent on morphological order in OPV and EES materials. ▪ Used information gained from mechanistic studies to design and synthesize new OPV and EES materials.
Promote key materials innovations through the introduction of novel chemical syntheses, fabrication approaches and analytical methodologies based on our fundamental discoveries	Materials innovations include: ▪ Two-molecule model systems that mimic bulk OPV films, ▪ New, efficient polymer coupling and chain-growth polymerization methodologies, and ▪ Stable, low-cost EES materials (metal oxides and polymorphs, silicon-based structures) with improved energy storage capacity.
Integrate the experimental study of these materials with theoretical concepts and models that accurately incorporate various electronic, chemical, morphological, and physical degrees of freedom in a description of interfacial CST processes	Computational methods reveal: ▪ 2D lithium-ion diffusion is correlated with the presence of anti-site defects, which can be monitored in real-time experimentally, ▪ Crystal chemistry and cationic substitutions directly influence atomic structure and stability for charge storage materials, ▪ Charge transfer states predicted by theory can be directly observed experimentally, and ▪ Molecular orientation affects charge transfer in OPVs.
Support excellence in energy technology by promoting the technological impact of our center's scientific innovations	▪ Developed unique methodologies to study solar cell degradation mechanisms in commercially relevant materials.

Website: http://www.efrc.nano.utexas.edu