A national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy

NREL National Renewable Energy Laboratory

Innovation for Our Energy Future

Director's Discretionary Research and Development Program

Annual Report Fiscal Year 2005

December 2005 NREL/MP-700-38759
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Director's Discretionary Research and Development Program

Annual Report Fiscal Year 2005

National Renewable Energy Laboratory

1617 Cole Boulevard
Golden, Colorado 80401-3393

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NREL/MP-700-38759
December 2005

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Introduction

Technical innovation is central to the National Renewable Energy Laboratory's mission. Innovative discretionary research maintains the scientific and technical vitality of the Laboratory, enhances the Laboratory's ability to address future DOE missions, and serves as a proving ground for new and potentially high-value mission enhancing activities. Discretionary research can provide technology pathways for the Office of Energy Efficiency and Renewable Energy (EERE) to attain the Department of Energy's long-term goals, and can accelerate progress on existing technology pathways. The Director's Discretionary Research and Development (DDRD) Program enables researchers to explore novel opportunities within the Laboratory's assigned mission areas, pursue more speculative ideas, and thereby move the science from the realm of imagination to creation and toward application. Research supported by the DDRD Program augments DOE's research and development capabilities, enhances the reputation of the Laboratory, encourages new partnerships that can advance EERE and DOE missions, and can result in technology breakthroughs.

This report highlights NREL's investment in innovation and the value of that investment to the Laboratory and to DOE and EERE.

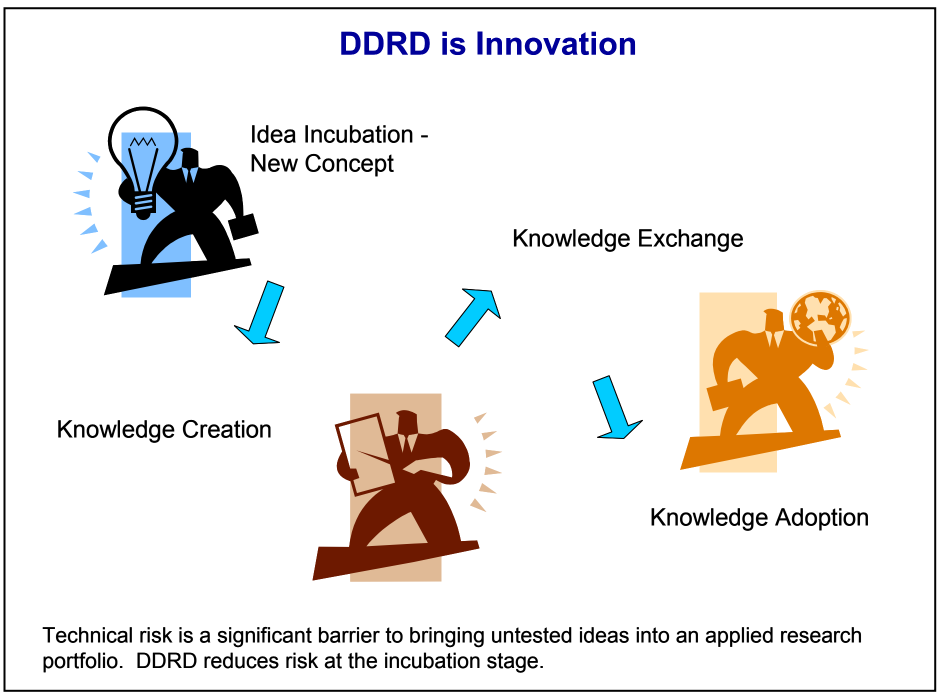

Figure 1. DDRD funds innovative projects within NREL's mission areas. It also provides the tools necessary to move resulting concepts to applications. NREL's 23 active projects cover six technology areas.

Program Overview

The DDRD Program funded 23 projects in fiscal year 2005. The duration of DDRD projects ranges from 2 to 3 years. The projects fall in six technical disciplines, which crosscut the Laboratory's mission areas:

- Advanced Analytic Methodologies and Systems
- Advanced Measurement and Characterization Techniques
- Advanced Materials
- Biotechnology, Chemistry
- Computational Sciences.

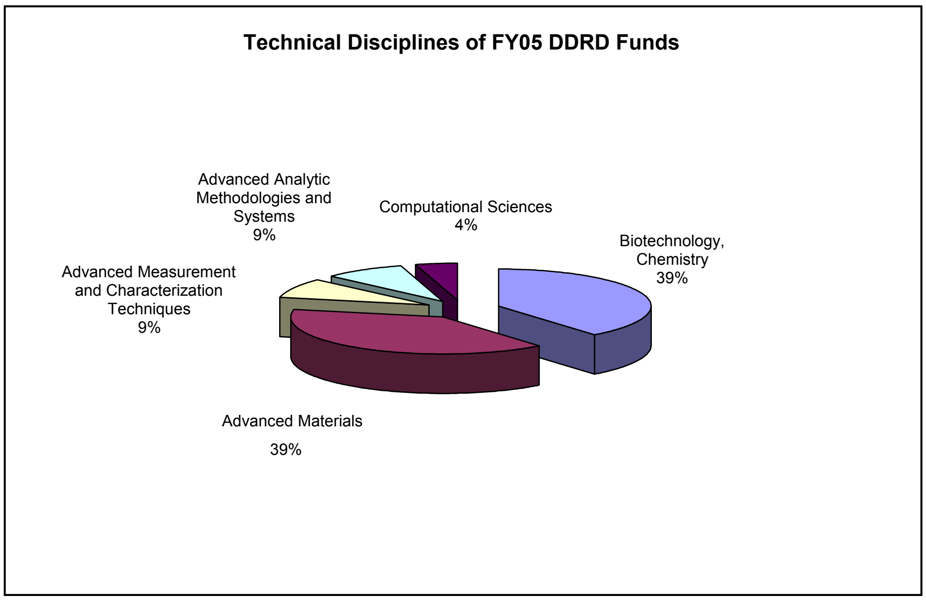

Figure 2. NREL's 23 active projects cover six technical disciplines.

Projects within the aforementioned cross-cutting technical disciplines have the potential to provide new research pathways for DOE programs in the following energy application areas:

- Biomass conversion, bioenergy
- Distributed energy systems and storage
- Hydrogen generation
- Buildings, national security
- Energy system analysis
- Photovoltaics, solid state lighting.

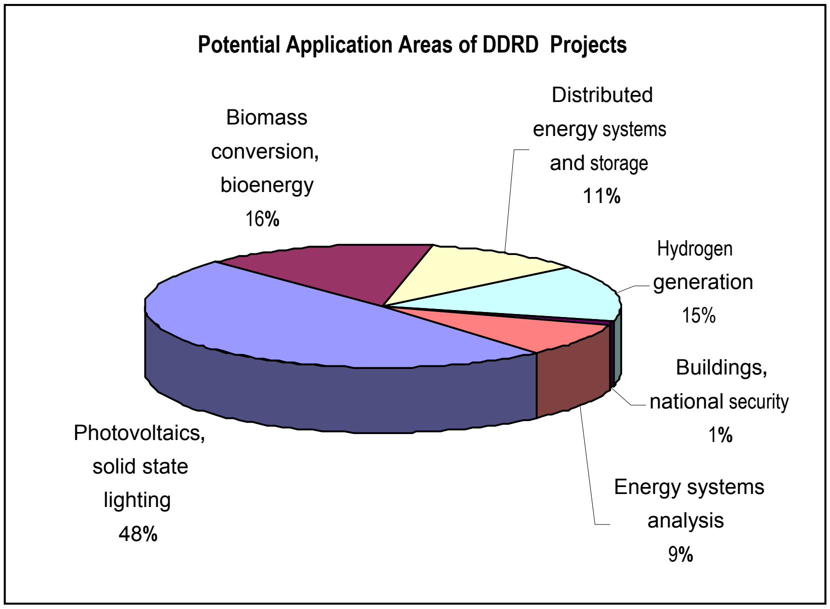

Figure 3. DDRD projects are yielding many potential renewable energy and energy efficiency innovations. DDRD efforts are strongly aligned with efforts in photovoltaics, solid state lighting, biomass conversion, and hydrogen.

Twenty eight proposals were submitted in response to the call for proposals in April 2004, of which 10 new projects were selected for funding in FY05. In all, 23 DDRD projects were executed in FY05.

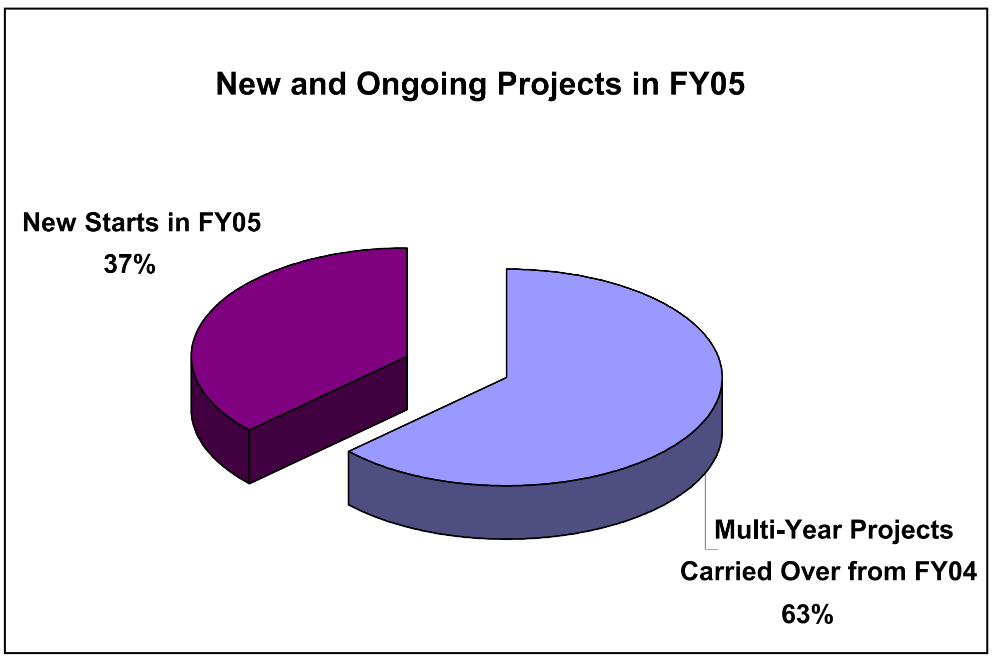

Figure 4. Funding in the amount of $1.4 million was available for new projects in FY05.

FY05 Program Successes

The DDRD program continued to yield innovations and new capabilities in FY05 that strengthen the future value NREL can bring to DOE programs. The following outcomes are illustrative of the value gained from DDRD research in FY05. These examples and additional ones are described in more detail in the ***Program Investments and Value*** section of this report.

- NREL DDRD research confirmed a very novel alternative approach for producing hydrogen from biomass that combines biomass steam pretreatment and anaerobic digestion. Though yields are lower than for thermochemical methods, this strategy can be applied to both dry and wet biomass. As a result of this research the DOE Hydrogen, Fuel Cells, and Infrastructure Program decided to further study anaerobic fermentation of lignocellulosic biomass as a potential low-cost technology for producing hydrogen from waste biomass.

- NREL DDRD research developed new optical microscopy tools to study photoluminescence quenching in thin films of conjugated polymers. The results enable an understanding of the quenching process efficiency and the range over which it can operate, and is being applied to support both photovoltaic and bioenergy investigations.

- NREL DDRD research developed new capabilities in fabricating and characterizing organic light-emitting diodes and synthesizing organic semiconductors such as dendrimers, oligimers, and polymers. These capabilities support the goal of producing low cost, high efficiency solid state indoor lighting from organic white light emitting diodes.

Program Investments and Value

Advanced Analytic Methodologies and Systems

Expert System for the Modeling of Renewable Energy Use

Principal investigator: Walter Short
Award: $142,000
Period of Performance: May 2003 to September 2005
Status: Completed

Goal

This effort will ultimately result in improvements in existing energy market models and help inform policy makers who rely on these models and analysis for insight. Most existing energy market forecasting models were built with a focus on conventional energy technologies. As such, they do a poor job of estimating the potential for most renewable energy technologies to address the nation's energy and environmental goals.

The modeling projects underway at NREL not only provide better estimates of wind and photovoltaics (PV) potential, they also translate the findings in a way that can be used by existing macro models, which cannot delve into the same level of detail with respect to renewables. The scientific/technical problem that was resolved is how to best transfer NREL's reduced-form supply curves to macro models.

Investment Outcome

For the first time, NREL specific market issues with respect to wind, concentrating solar power (CSP) and hydrogen can be modeled. As such, DOE can now examine different scenarios, and authoritatively estimate the impact of these technologies in the marketplace.

The project team accomplished this by developing reduced-form versions of NREL's wind model that could be used in other models to represent the extra-generational costs associated with wind including the additional costs of transmission access and the cost of additional capacity to cover the intermittency of wind, etc. Curves of the above-busbar cost ($/kW of additional wind) versus the total national wind capacity were generated after reviewing other models and reduced-form methodologies, and experimenting with various calculation methods to determine the additional cost.

Because of the complexity of NREL's wind deployment system (WinDS) model, it is not computationally practical to incorporate it into other models. Thus, a reduced-form representation derivable from the WinDS model is required to capture the sensitivity of the driving variables without the full representation of the physical realities. Other model developers can now use NREL graphs in their models to more accurately represent the costs of wind transmission and wind intermittency and calculate their impact on market penetration.

NREL has implemented this reduced-form approach in the single-region Stochastic Energy Development Systems (SEDS) model which uses the WinDS-derived supply curve to capture the wind transmission and intermittency costs and constraints. The implementation of these wind supply curves in other models will improved the quality of EIA's Annual Energy Outlook for wind through its NEMS model. Currently several other models – IPM, NEMS-GPRA (Government Performance Results Act), and Haiku – use the EIA's cost correction factors that severely limit wind and have no analytic basis. The work provides superior support tools for DOE to Model renewable energy markets.

Value of the Outcome
Local, national, and international decision makers depend heavily on the energy projections provided by various macroeconomic models including the U.S. EIA's NEMS model, the MARKAL model, and others. However, up to now it was difficult for these models to provide accurate information on the potential of renewable energy because of historical focus on conventional power sources and very limited special disaggregation; for example, NEMS includes only 13 regions within the United States.

For the first time, DOE can use quantitative methods to accurately model important market issues related to renewable energy, including transmission access and intermittency impacts, instead of using crude approximations. The use of reduced-form output supply curves combined with dissemination of other WinDS results will greatly improve DOE’s renewable energy forecasts and analysis from all energy models and enhance EERE’s ability to model the outcomes of renewable program efforts.

Advanced Materials for Renewable Energy and Energy Efficiency Technologies

Hot-Wire Chemical Vapor Deposition of Metal Oxide Nanorods

Principal Investigators: Anne Dillon and Harv Mahan
Award: $300,000
Period of Performance: October 2004 to September 2006
Status: In Progress

Goal
To investigate production of metal oxide nanorods and nanoparticles for use in electrochromic windows and batteries.

Investment Outcome
The team's preliminary tests are very promising. There is a crystalline molybdenum trioxide powder containing nanoparticles/nanorods at high density that, when fashioned into a film, is ideal for incorporation into a lithium-ion battery. These films have been tested as anodes in lithium-ion batteries, and the reversible capacity for several films vastly exceeds that of the currently employed technology (graphite).

The team is investigating other applications for the high surface area tungsten trioxide nanoparticle materials. GVD Corporation in Cambridge, Massachusetts has expressed interest in testing this material in a hydrogen sensor device. An informal collaboration agreement is in process.

High surface area crystalline metal oxides may have applications beyond those that are currently under investigation.

Value of the Outcome
This work provides a potential new technical approach for DOE’s research in electrochromic windows and energy storage. Tungsten-oxide nanoparticles significantly improve the state-of-the-art electrochromic (EC) technologies as they are significantly more stable in an acid

electrolyte solution. This could allow for EC technologies to be used in display applications. Preliminary results suggest that molybdenum-oxide nanostructures could profoundly advance the negative electrodes employed in Li+ batteries.

Knowledge Transfer

- "Deposition of Small, Highly Crystalline WOx Nanoparticles and Nanotubes by Evaporation of a W filament in an Oxygen Atmosphere," by A.H. Mahan, P.A. Parilla, K.M. Jones, and A.C. Dillon, Chem. Phys. Lett. 413 (2005) 88-94.
- "Crystalline WO3 Nanoparticles Electrochromic Breakthrough," by S.H. Lee, R. Deshpande, P. A. Parilla, K. M. Jones, B. To, A. H. Mahan, and A. C. Dillon, Advanced Materials (under review).
- A follow-up paper to this rapid communication is in preparation.
- "Novel Nanostructured Materials for a Variety of Applications," invited talk presented at the August 2005 SPIE meeting in San Diego.
- "Metal-oxide Nanostructures for Electrochromic and Battery Applications," invited talk presented at the October 2005 National Institute of Standards and Technology (NIST) Nanoscience Workshop in Boulder.
- Two abstracts have been accepted for oral presentations at the fall 2005 Materials Research Society (MRS) Conference.
    - "Hot-wire Chemical Vapor Deposition of Crystalline Tungsten Oxide Nanoparticles," presented by A. H. Mahan.
    - "Electrochromic WO3 Nanoparticles Consisting of Nanorods and Nanospheroids," presented by R. Deshpande.
- This team has been invited to submit a white paper on these early results to the Naval Research Laboratory (NRL) in Arlington, Virginia.

Next Steps

The principal investigators have started exploring metal-oxide structures for battery applications. The work has the potential to significantly improve lithium ion battery technologies, which could lead to the development of a more efficient battery for the next generation hybrid electric vehicles, supporting the goals of DOE's Freedom Car Program.

Improved Thermoelectric Materials Based on Quantum Dot Superlattices

Principal Investigator: Mark Hanna
Award: $200,000
Period of Performance: May 2003 to April 2005
Status: Completed

Goal

To investigate a new concept for improving the thermoelectric figure of merit of III-V semiconductor thin films (with potential applications in electronic and optoelectronic devices), namely the use of quantum dot superlattices to enhance the Seebeck coefficient and reduce the cross-plane thermal conductivity.

Investment Outcome

Mark Hanna's team developed a new crystal growth capability to produce high-quality quantum dot superlattices (QDSL). This new growth capability gives NREL the ability to produce novel structures and devices based on QDSL for both fundamental and device studies.

The team implemented an experimental setup for measuring the thermal conductivity of thin films based upon AC-modulated sample heating and temperature detection, called the 3-omega technique. With this setup, NREL now has a new capability to measure the thermal conductivity of new materials used in thermoelectric and photovoltaic applications.

The 3-omega setup was then used to measure the cross-plane thermal conductivity of a number of QDSLs with different structures. The team found that the cross-plane thermal conductivity of indium gallium arsenide/gallium arsenide (InGaAs/GaAs) QDSLs was reduced by a factor of two to eight below that of GaAs depending upon the superlattice structure and doping level. The large reduction in the thermal conductivity by a factor of eight shows that QDSLs are an effective means to reduce the lattice thermal conductivity of a material – thereby achieving one of the main goals of the project.

Value of the Outcome
This work provides a potential new approach for developing QDSL devices which could provide innovative technologies to meet DOE's PV program goals.

Solid-State Nano-Composite Materials for Supercapacitor Applications

Principal Investigator: Se-Hee Lee
Award: $240,000
Period of Performance: March 2003 to February 2005
Status: Completed

Goal
To develop a new class of solid-state supercapacitor based on novel nano-composites of polycrystalline particles embedded within an amorphous electrolyte matrix.

Investment Outcome
The team successfully synthesized nano-structured nickel oxide thin films employing a method called reactive sputtering, and demonstrated that the defective nature of nickel oxide could be utilized to improve the specific capacitance for supercapacitor application. Although the specific capacitance of the nickel oxide supercapacitor was affected by the fabrication process, the relationship between specific capacitance and nonstoichiometry is not understood. Therefore, the team is proposing further study of the mechanism underlying this relationship.

The electrochemical performance of single wall carbon nanotube (SWNT)/Nafion composite electrodes have been examined in sulfuric acid solutions. The electrochemical capacitance of the composite electrode increases significantly after an oxidation-reduction cycle. The team has shown that electrochemical oxidation of SWNT/Nafion composite electrodes, at high potentials in a strong acidic media, provides a new method of chemical modification of the SWNTs. The electrochemical oxidation and reduction treatment of the SWNT/Nafion composite is potentially useful for modifying the SWNT sidewalls, which results in an enhancement of the electrochemical capacitance.

The team has successfully demonstrated electrochemical capacitive behavior of the Nickel oxide/Tantalum oxide (NiO/Ta_2O_5) nano-composite films in an aqueous solution for the first time. These nano-composite materials promise great potential for fabricating complete solid-state supercapacitors. This unique nano-composite material construction exhibits a substantial electrochromic (EC) optical modulation and may lead to the establishment of a new class of EC materials based on a supercapacitance effect.

The team has performed in-situ Raman spectroscopy measurements on amorphous hydrous ruthenium oxide thin films during the charging/discharging cycles in an effort to elucidate the physical and chemical changes that accompany the electrochemical cycles. Amorphous hydrous ruthenium oxides ($RuO_2{\cdot}xH_2O$) have attracted much interest with respect to the possibility of using this material in electrochemical supercapacitors. The cause of the physical and chemical changes that occur when hydrogen is inserted or extracted from this material during the charging/discharging cycles is not clear. However, based on the Raman spectroscopic studies of these materials, the major effect upon intercalation of hydrogen is reduction of Ru^{4+} ions to Ru^{3+}, and not the creation of new chemical bonds.

Value of the Outcome

The electrochemical capacitor (ECC) is an attractive device for high power density applications. When combined with secondary batteries, electrochemical capacitors provide additional versatility and efficiency in the management of portable power sources. Recent accomplishments pertaining to both inorganic nano-composite material (nickel oxide/tantalum oxide) and organic-inorganic nano-composite material (SWNT/Nafion) directly impact two important areas of energy-related research: energy storage, and nano-science/nano-technology. Based on the team's recent development of these nano-composite supercapacitor materials, the possibility exists to fabricate complete solid-state supercapacitors with properties that rival liquid/gel electrolyte-type devices. Technical innovation in energy storage can facilitate the deployment of the variety of renewable power sources being pursued through DOE research.

Knowledge Transfer

- "Electrochemical transformation of single-walled carbon nanotube/Nafion composite," by P. Liu, S.-H. Lee, Y. Yan, T. Gennett, B. J. Landi, A. C. Dillon, and M. J. Heben, Electrochemical and Solid-State Letters, 7(11) A421 (2004).
- "Effect of non-stoichiometry of nickel oxides on their supercapacitor behavior," by S.-H. Lee, C. E. Tracy, and J. R. Pitts, Electrochemical and Solid-State Letters, 7(10) A299 (2004).
- "Effect of O_2 flow concentration during reactive sputtering of Ni oxide thin films on their electrochemical and electrochromic properties in KCl and KOH electrolytes," by Y. Abe, S.-H. Lee, E. O. Zayim, C. E. Tracy, J. R. Pitts, and S. K. Deb, J. Electrochem. Soc., (submitted).
- "Electrochromic properties of sputtered Ni oxide thin films in neutral KCl electrolytes," by Y. Abe, S.-H. Lee, C. E. Tracy, and J. R. Pitts, Electrochemical and Solid-State Letters, (in press).
- "In-situ Raman spectroscopy of $RuO_2{\cdot}xH_2O$," by H. C. Jo, K. M. Kim, H. Cheong, S.-H. Lee, and S. K. Deb, Electrochemical and Solid-State Letters, 8(4) E39 (2005).
- "Nanophase nickel oxide electrodes with ruthenium oxide additions for supercapacitor applications," by R. Smith, S.-H. Lee, C. E. Tracy, and R. Pitts, J. Electrochem. Soc., (Submitted).
- "Solid-state nano-composite electrochromic pseudocapacitors," by S.-H. Lee, C. E. Tracy, Y. Yan, J. R. Pitts, and S. K. Deb, Electrochemical and Solid-State Letters, 8(4) A188 (2005).

CgMgTe Thin Films for Light Emitting Diodes

Principal Investigator: Kannan Ramanathan
Award: $300,000
Period of Performance: October 2004 to September 2006
Status: In Progress

Goal
To fabricate blue and blue-green light emitting diodes (LED) out of a novel material, Cadmium Magnesium Telluride (CdMgTe).

Investment Outcome
Kannan Ramanathan and his team fabricated the first polycrystalline thin films made of CdMgTe—overcoming equipment and staffing problems. They set up a new fabrication facility that uses effusion cells. The fabricated films are a fine example of multi-component alloy preparation using combinatorial synthesis. With two depositions, they can cover the composition range of 1.4 eV to 2.2 eV. They have established the basic properties of the alloys such as energy gap vs. composition and they are sending a paper to Applied Physics Letters.

Value of the Outcome
Significant progress has been made to achieve the objective of LED device fabrication. This work can potentially provide a new avenue for DOE's research in solid state lighting.

Next Steps
Kannan's team plans to fabricate the LED's in FY06. A side benefit is that this same material can be used to develop a wide bandgap solar cell out of the 1.7 eV material.

OWLEDs: Next Generation Indoor Lighting Using Organic White Light Emitting Diodes

Principal Investigator: Sean Shaheen
Award: $500,000
Period of Performance: April 2003 to March 2005
Status: Completed

Goals

- To perform fundamental research on organic semiconductors and organic/inorganic hybrid nanostructured materials with the end goal application of low cost, high efficiency solid state indoor lighting from organic white light emitting diodes (OWLEDs).
- To develop a core competency at NREL in the area of organic semiconductors and nanostructured materials, including the development of personnel and staffing at NREL, as well as the construction of laboratory tools necessary to carry out research in this area at a high level.

Investment Outcome
NREL now has a new capability: to fabricate and characterize organic light emitting diodes (OLEDs). This capability did not exist before this project. The organic semiconductor synthesis, purification, and characterization laboratory facility is suitable for the fabrication of many types of organic semiconductor devices, such as dendrimers, oligomers, and polymers.

These new capabilities allow NREL researchers to develop novel materials, better understand structure-property relations, and to optimize device performance. The team collaborated with NREL's Computational Sciences team to model the structure-property relations of new materials via computational chemistry modeling, which aides the design of novel organic semiconductors.

Value of the Outcome
NREL's newly developed high-efficiency organic semiconductor device laboratory, which is on par with leading labs in the world, can help advance DOE's goals in solid state lighting. The knowledge base at NREL has been greatly increased in the field of organic semiconductors,

including synthesis and characterization of new materials and fabrication and characterization of new devices. The results will be published in the Journal of Materials Chemistry.

Low Band-Gap Materials for Organic Third Generation Photovoltaics

Principal Investigator: Sean Shaheen
Award: $450,000
Period of Performance: December 2004 to September 2006
Status: In Progress

Goals

- To develop a competency in the fabrication of organic semiconductor based photovoltaic devices, including facilities and personnel to establish NREL as a world-class Laboratory in the field.
- To develop low band gap materials that have optimized transport properties for use in organic photovoltaics; and improve the scientific understanding of the structure-property relation of these materials.
- To improve the understanding of the physics of the operation of these devices and develop models to guide their advancement.

Investment Outcome

Sean Shaheen's team synthesized and characterized a family of dendrimeric organic semiconductors with a variety of molecular structures based on thiophenes. This first set of materials is helpful in understanding the structure-property relations of dendrimers. Fabrication and characterization of devices from initial materials demonstrate the efficient charge transfer and charge transport in these new dendrimer materials. Clear trends in device efficiencies can be seen in relation to the molecular structures of the dendrimers. Results of this work have been submitted for publication.

The team has started synthesizing the next iteration on dendrimers that possess reduced optical band gaps. The first family of dendrimers had optical band gaps ranging from 2.5 eV to 2.7 eV in solution, and 2.3 eV to 2.6 eV in film. NREL's new dendrimer has a band gap of about 2.0 eV in solution and 1.8 eV in film. This data is shown in the attached figures.

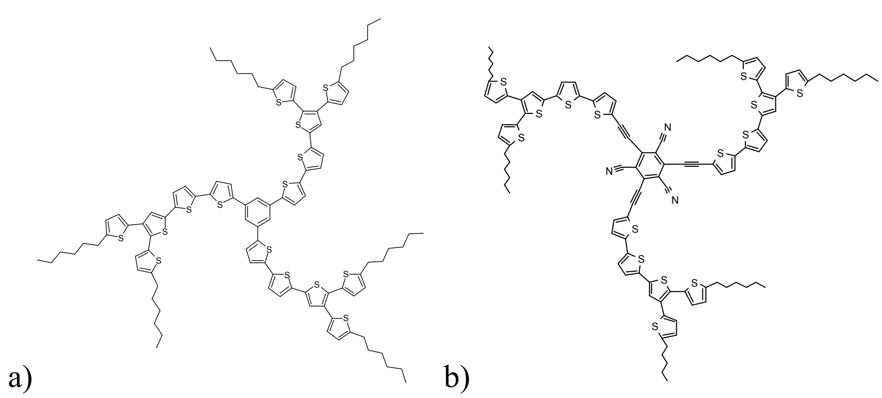

Figure 5 a, b. Computational modeling. With the help of the Computational Sciences Center, the team is running computational chemistry calculations to further understand the structure-property relations of the dendrimers being synthesized. Computer modeling will be a powerful resource in the development of future materials.

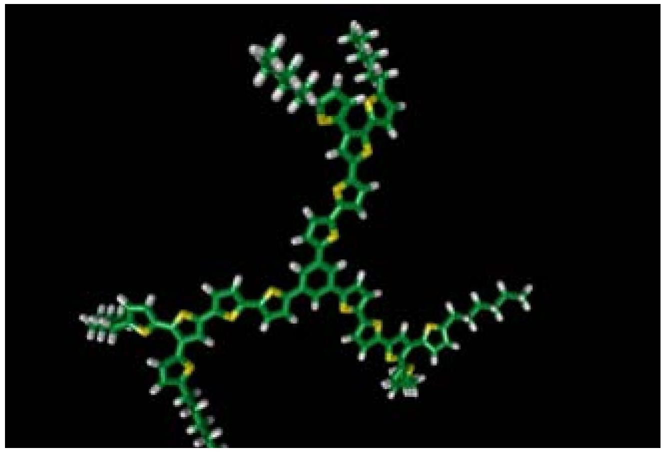

Figure 6. This figure is a three-dimensional structure of the dendrimer depicted in figure 5a.

The team performed Preliminary time-resolved microwave conductivity measurements on dendrimers. Preliminary results show very long-lived charge carriers in some of the dendrimers. This agrees with the premise that these materials are very pure and have few defects that can act as charge traps.

NREL, in partnership with the University of Minnesota, was selected for a competitive research award under the Xcel Energy renewable development fund. This project will enable exploring various avenues of improving organic photovoltaic devices.

Two carrier mobility measurement setups are comlete: Time-of-Flight (TOF) and Current Extraction by Linearly Increasing Voltage (CELIV). Having two techniques available provided a more robust and substantiated measurement of a given material's mobility.

After characterizing the first family of dendrimers in terms of optical properties and device performance, the first module of the next iteration has been synthesized. This module has a significantly reduced optical band gap compared to the first family. The process of characterizing the transport and device properties of this material is underway.

Value of the Outcome

Overall, this program is helping NREL develop novel organic semiconductors for photovoltaic and other applications in support of DOE's Solar Program goals.

Knowledge Transfer

- "Bulk heterojunction organic photovoltaic devices based on phenyl-cored thiophene dendrimers," by N. Kopidakis, W. Mitchell, D. Ginley, G. Rumbles, S. Shaheen, Thin Solid Films (submitted).
- "The Synthesis and Properties of Solution Processable Phenyl Cored Thiophene Dendrimers," by W. Mitchell, N. Kopidakis, G. Rumbles, D. Ginley and S. Shaheen, Journal of Materials Chemistry, 15(42) 418 (2005).
- Collaborations with Prof. C. Daniel Frisbie, University of Minnesota; and with Delft University resulted in shared insights on organic photovoltaics and basic materials characterizations on new dendrimer materials.

Next Steps
The new dendrimer has a reduced band gap compared to the first family of materials. The next step is to fully characterize this material in terms of its carrier mobility and device performance. This molecule utilized just one technique available to the team for reducing the band gap. The team also has several other approaches available, which they will begin to explore as well.

Single Molecule Fluorescence Detection and Imaging

Principal Investigator: Steve Smith
Award: $240,600
Period of Performance: March 2003 to April 2005
Status: Completed

Goal
To develop an optical microscopic tool for the detection of single, isolated molecules and for the development of a near-field optical microscope with a spatial resolution below the diffraction limit of optical radiation. The tool would be applied to the study of photoluminescence quenching in thin films of conjugated polymers, where the process could be attributed to photoinduced electron transfer to an inserted dopant species such as C60. This polymer/C60 combination can be found in the bulk heterojunction excitonic solar cell, and the results are, therefore, pertinent to the understanding of the efficiency of the quenching process and, most importantly, the range over which it can operate.

Investment Outcome
The team developed a microscope with sub-wavelength and single-species resolution. This is a new tool for NREL. Isolated dye molecules and colloidal quantum dots have been detected and fluorescence correlation spectroscopy developed. This is critical to understanding isolated species in their environment and how they are responding.

The team also visualized and modeled novel systems: single-molecule Raman detection of dye molecules adjacent to metal nanoparticles; and detection of colloidal quantum dots (QD) bound to a genetically modified protein. These results demonstrate the capability of the techniques, provide new data that has been published, and serve as a foundation on which new proposals can be developed.

Value of the Outcome
New spectroscopic tools, new expertise, new collaborations, and new proposals emerging from this work are supporting both photovoltaic and bioenergy investigations. These newly developed capabilities catalyzed a new project in bioenergy to look at QD-labeled proteins moving on a cellulose surface. The cross-fertilization resulting from this project has the potential to advance DOE goals in both the PV and Biomass Programs.

Electronic Communication in Assemblies of Semiconductor Nanoparticles

Principal Investigator: Jao van de Lagemaat
Award: $300,000
Period of Performance: May 2003 to September 2005
Status: Completed

Goal
To provide a framework for connecting electronic communication in a macroscopic film of interconnected nanoparticles with the energetic structure of isolated quantized nanoparticles.

Investment Outcome
NREL is now well positioned in the field of conversion technology because of its ability to visualize, model, and study the energy structure of nanomatter. Jao van de Lagemaat's team was able to precisely visualize individual quantum dots and to determine their charging spectrum. Quantum dots are a non-traditional type of semiconductor with potential applications as an enabling material across many industries. Quantum dots enable semiconductors with tunable bandgaps, allowing for unique optical and electronic properties. Knowledge of the charging spectrum of individual dots is of paramount importance to understanding charge conduction in large arrays of dots–a system that can potentially create third generation high efficiency, low cost photovoltaics.

The team developed a computer model of charge transport (i.e. electronic communication) using tunneling spectroscopy to calculate the charging spectrum of individual quantum dots or direct measurement results. Providing a framework to connect electronic communication in a macroscopic film of interconnected nanoparticles with the energetic structure of isolated quantized nanoparticles was the overriding goal of this project. The computer model successfully accomplishes this goal and illustrates the success of the DDRD project. It also shows that NREL is well positioned to model and predict the properties of large-scale assemblies of nanoscaled matter. This is of major importance in guiding the design of solar energy conversion and storage technologies based on such systems. The computer model was also adapted to describe another nanoparticle array system, the titanium dioxide (TiO_2) nanoparticle layer employed in dye-sensitized solar cells to show that a similar effect owing to energetic disorder, is active there even though the particles in this case are not quantized. In cooperation with Art Frank's group, the team showed that the predictions of the model were correct. The results were submitted to Physical Review B during FY 05.

Value of the Outcome
The fundamental knowledge obtained in this project is applicable to all systems that have a degree of energetic disorder and/or long-range interactions. This includes diverse systems such as organic solar cells, amorphous silicon, the dye-sensitized solar cell, thin-film systems, and much more.

Knowledge Transfer

- "Einstein relation for electron diffusion on arrays of weakly coupled quantum dots," by J. van de Lagemaat, Phys. Rev. B (Submitted 29Aug. 2005).
- Peer-review publications and presentations of fundamental results at conferences are expected to lead to new collaborations and contribute to NREL's strong image as a steward of good science. It has already led to one collaboration with the group of Prof. J. Bisquert at the University Jaume I in Castello Spain. He has spent time at NREL discussing the science of these systems and is sending one of his collaborators over for a few months in FY06.
- One other collaboration being discussed, is with Prof. D. Vanmaekelbergh of Utrecht University, The Netherlands; he is a pioneer in this field.

Fundamental Properties and Applications of Novel Crystalline Inorganic-Organic Hybrid Semiconductor
Principal Investigator: Yong Zhang/Brian Fluegel
Award: $450,000
Period of Performance: October 2004 to September 2007
Status: In Progress

Goal
To obtain and understand the basic electronic and optical properties of single layer structures.

Investment Outcome
In the first year of this project, the team made major progress in understanding the fundamental properties of the hybrid materials. They demonstrated the vertical conductivity of hybrid thin-films (double-layer structures) deposited on indium tin oxide (ITO) substrates using flexible top gold (Au) contacts; and observed that the conductivity exhibits rectification behavior. A number of interesting properties have been revealed and a preliminary device operation has been demonstrated. NREL is now better prepared to synthesize hybrid materials and test realistic devices either for photovoltaics (PV) or solid state light (SSL) applications.

Collaborations resulting from this project have significantly expanded NREL's capability in researching novel materials.

Value of the Outcome
Hybrid inorganic-organic semiconductor materials are new materials that exhibit unique optical and electrical properties that constitute the most recent development in materials science. The acquisition of expertise in these materials can open up new and exciting materials and device research opportunities for photovoltaic applications. Collaboration with a university provides added value in graduate level education for future scientific manpower for the nation.

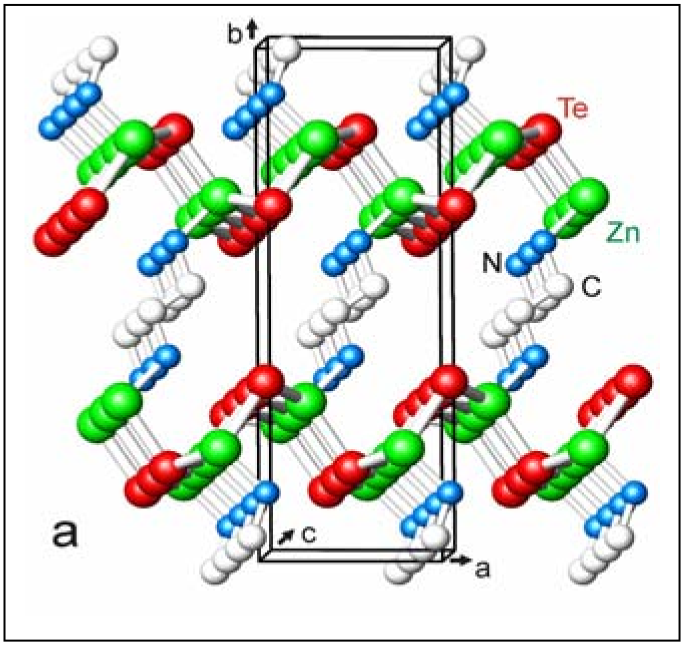

Figure 7. Crystal structure of an organic-inorganic hybrid semiconductor, β-$ZnTe(en)_{0.5}$, determined by X-ray diffraction: multiple ZnTe layers (green and red atoms) interconnected by ethylenediamine molecules (white C and blue N atoms, hydrogen atoms omitted) at Zn atoms.

Next Steps
- Carefully study the thermal and vibrational properties of the hybrid materials.
- Perform electronic and band structure calculations for the double-layer structures.
- Continue to test realistic device structures.
- Attempt to synthesize selected types of hybrid materials.
- Propose follow on work to the DOE Solid-State Lighting program.

Advanced Measurement and Characterization Techniques

Shape and Crystallography of III-V Semiconductor Nanoparticles

Principal Investigator: Phil Ahrenkiel
Award: $120,000
Period of Performance: October 2004 to September 2006
Status: In Progress

Goal
To develop new methods for imaging and diffraction of colloidal nanoparticles.

Investment Outcome
Work on this project has generated a tomogram of titanium dioxide (TiO2) nanoparticles and improved three dimensional rendering capabilities. TiO2 was indicated as a system to which improved imaging methods could be applied.

Value of the Outcome
Nanostructured TiO2 is the electro-optically active semiconductor used in a range of solar energy technologies, from solar dissociation of toxic materials for waste remediation to the backbone of dye-sensitised, nanostructured solar cells. TiO2 nanoparticles are also used in numerous device applications involving transparent, conducting thin films. The optoelectronic properties are affected by the particle shape, and the full 3-D shape is often nearly impossible to determine from conventional microscopy. The team was able to generate tomograms that allow direct analysis of the 3-D particle shape and determination of the physical dimensions of the particles.

Tomography is also being used to determine the shapes and arrangements of semiconductor nanoparticles. Some applications require the assembly of the nanoparticles into ordered 3-D arrangements for charge transport. Tomography allows visualization of the particle arrangements in high-symmetry orientations that would otherwise remain inaccessible. This detailed structural information aids the chemists who synthesize the particles and facilitates improved theoretical understanding.

Knowledge Transfer
A poster will be presented at the Materials Research Society (MRS) fall meeting, and is a great opportunity for exposure to numerous groups in the nanotechnology fields.

Next Steps
The team will gain experience or seek assistance assembling tomograms into animations that are annotated for distribution and presentation.

Single-Crystal X-Ray Diffraction Facility (Capability)

Principal Investigator: Phil Parilla
Award: $130,000
Period of Performance: August 2002 to July 2005
Status: Completed

Goal
Strengthen core competencies in x-ray diffraction and establish a new capability to use single-crystal diffraction.

Investment Outcome
The project team became familiar with the concepts of analysis techniques required to determine atomic positions based on x-ray diffraction (XRD) data. This expertise is valuable for interpreting and analyzing data from existing x-ray diffraction equipment and even more valuable when in use with a single-crystal diffractometer.

Value of the Outcome
NREL researchers gained valuable experience and knowledge about single-crystal diffraction. Single-crystal x-ray studies are key research techniques for advanced materials development for energy-related applications.

Bioenergy, Biotechnology, Chemistry

Integrating Steam Pretreatment and Anaerobic Digestion: A Flexible Strategy for Biomass Conversion to Methane and Hydrogen (H_4, H_2) and Co-Products

Principal Investigator: Stefan Czernik
Award: $324,000
Period of Performance: March 2003 to April 2005
Status: Completed

Goal
To prove the concept that steam-exploded biomass can be fermented by microbes, yielding hydrogen and methane.

Investment Outcome
This project produced two outcomes. First, there is direct production of hydrogen from liquid hemicellulose-rich fraction obtained by steam explosion of corn stover. Using a natural inoculant obtained from the heated sludge of a local wastewater treatment plant, Stefan Czernik's team demonstrated that indigenous microbes were capable of fermenting the aqueous hydrolyzates derived from the hemicellulose fraction of the steam-pretreated corn stover. Biogas contained equal amounts of hydrogen and carbon dioxide. In addition to glucose, the natural inoculant could also utilize other sugars equally well, resulting in nearly 87% to 94% utilization of the glucan and xylan. Hydrogen molar yields of 2.84 and 3.0 per mole of sugar were obtained with hydrolyzate from neutral and acidic steam explosion, respectively. Overall, neutral steam explosion of the corn stover at 220°C-3 min yielded the best hydrogen production amongst the other conditions under investigation. Higher severity treatment resulted in excessive losses of sugars and formation of unwanted by-products (furfural and hydroxyl-methyl-furfural). This finding strongly suggests that steam explosion is a suitable pretreatment technology for biomass fermentation to hydrogen.

Second, there is direct production of hydrogen from solid lignocellulose fraction of steam-pretreated corn stover. Initially, using the sewage sludge consortium, the team did not succeed in generating hydrogen from lignocellulose within a three-week reaction time. Findings suggested that the inability of those microbes to produce hydrogen from the lignocellulosic solids was not due to the inhibition by the lignin component or other inhibitory products, but rather to the lack of cellulolytic microbes in the consortium, which were either not present initially, or became inactive during the inoculant baking process. Eventually, it was discovered that a thermophilic bacterium Clostridium thermocellum is able to ferment most of the lignocellulosic solids obtained by steam explosion of corn stover and, most likely other steam-treated biomass, thereby producing hydrogen. The hydrogen yields based on total sugar content were comparable to those from anaerobic fermentation of free glucose; the latter is a more favorable substrate, yet costly. This finding meets the goal of this DDRD project.

Value of the Outcome
The most significant outcome is that the team proved that hydrogen could be produced from biomass by integrating biomass steam pretreatment and anaerobic digestion. This strategy can be applied to both dry and wet biomass. This project develops core competency in the anaerobic digestion area using fermentative organism to directly produce hydrogen. As a result of this research, the DOE Hydrogen, Fuel Cells, and Infrastructure Program supported further study of anaerobic fermentation of lignocellulosic biomass as a potential technology for producing hydrogen from waste biomass.

Knowledge Transfer
- "Hydrogen production from the fermentation of corn stover biomass pretreated with a steam explosion process," by R. Datar, J. Huang, P-C. Maness, A. Mohagheghi, S. Czernik, and E. Chornet, Environmental Science and Technology (submitted).
- A second paper is being prepared.

Nitrogen Conversion to NO_x in Biomass Thermochemical Processes
Principal Investigator: David Dayton
Award: $406,907
Period of Performance: June 2002 to May 2005
Status: Completed

Goal
To develop a fundamental understanding of the forms of nitrogen in biomass, and insights into the mechanism and kinetics of how fuel-bound nitrogen transforms to nitrogen oxide emissions (NOx) in biomass thermochemical conversion processes.

Investment Outcome
The project team's experiments using isotopically-labeled plant samples, advanced the understanding of the transformation of nitrogen during biomass pyrolysis and gasification. Combustion experiments provided the first direct determination of the relative release of nitrogen oxide (NO2) and nitric oxide (NO) during biomass combustion under idealized laboratory conditions. Fundamental measurements like these can be used to help predict changes in NOx emissions during biomass/coal cofiring.

This project has improved understanding of the forms of nitrogen in biomass, and insights into the mechanism of how fuel-bound nitrogen transforms to NOx in thermochemical conversion processes. The project team developed a way to quantitatively measure how much fuel-bound nitrogen is released as molecular nitrogen and NO. The team is determining how fuel-bound nitrogen in biomass transforms during the initial stages of pyrolysis. The hope is to expand these measurements to gasification/reducing conditions to see how the high temperature chemistry changes. Ultimately, these results can be used to help develop and validate chemical kinetic mechanisms to explain and predict NOx release from biomass thermochemical processes.

Value of the Outcome
Thermochemical conversion is one of the promising technologies for expanded biomass use being pursued through DOE R&D. Transformation of fuel-bound nitrogen during thermochemical conversion is the genesis of undesired emissions in biomass processes for heat, power, and liquid fuels production.

Increased understanding of the emissions from thermochemical conversion will provide a basis for improving emission abatement and control strategies, facilitating achievement of DOE Biomass Program goals.

Localized Carrier Dynamics in Organic Semiconductor Probed via Time-Resolved THz Photoconductivity (TRTP)

Principal Investigator: Randy Ellingson
Award: $309,412
Period of Performance: October 2004 to September 2006
Status: In Progress

Goal

Organic semiconductors are expected to play a large role in future solar cell applications. The goal of this work was to develop a competent and advanced terahertz (THz) spectroscopy project at NREL, which would place the Laboratory at the forefront of this important new field. In addition, a flexible time-resolved THz photoconduction spectrometer will strengthen many of NREL's current core programs. Developing an understanding of their microscopic carrier dynamics will contribute significantly to this endeavor.

Investment Outcome

Randy Ellingson's team was able to implement improvements to time-resolved THz photoconductivity (TRTP) apparatus to improve frequency coverage and sensitivity in this first year, and have achieved a factor of 5-10 improvement since initially setting up the experiment. Work will continue on polyacenes to provide detailed understanding of the localized conductivity, and compare temperature dependent mobility measurements to previous time-of-flight (TOF) results.

Time-resolved photoconductivity was measured in a sample of indium phosphide (InP) semiconductor nanocrystals embedded in a poly-(3-hexylthiophene) (P3HT) polymer host. This was a demonstration of NREL's ability to measure the complex conductivity of an arbitrary polymer. In addition, this work will provide a foundation for studying energy and/or charge transfer in hybrid QD/polymer systems or other molecular/polymer systems, such as single-walled carbon nanotube and polymer systems.

This project has clearly made progress on the ability to prepare poly-acene crystals, and to perform straightforward optical characterization of the materials; however, there was a delay due to the class IV laser shutdown from January through April 2005. The ultrafast time-resolved measurements were not possible without the use of the laser. The laser system is now functioning properly and the measurement systems are set up and able to acquire data.

New knowledge includes:

- The ability to grow tetracene-doped anthracene crystals. Such a material system has not been previously studied, and while this material will not be addressed as a first priority, it offers the potential for unique properties with regard to free carrier formation in organic semiconductors.
- The ability to measure THz signals from both pure polymer as well as a C_{60}-polymer blend has been demonstrated (C_{60} is the most common carbon buckyball, and when functionalized as [6,6]-phenyl C_{61}-butyric acid methyl ester, is commonly referred to as PCBM). This ability allows further investigation of the effects of sample composition and quality on the free carrier yield and lifetimes, and should enable correlation between these properties and the solar cell efficiencies measured in complete cells. The recent success in demonstrating the PCBM concentration dependence of the apparent free carrier yield in the polymer blend provides a foundation for broad application of the technique. It is the principal investigator's opinion that the results to date have already established, in principle, the merit of this approach as complementary to slower characterization methods such as time-resolved microwave conductivity.

Value of the Outcome
The team has made excellent progress toward a reliable and powerful analytical technique for quantitative assessment of blended materials systems (organic/organic or inorganic/organic) for use in solar energy conversion. Advances in blended materials systems may provide new paths to advance DOE's Solar Program goals.

Next Steps

- Access is available to a series of samples of P3HT/C_{60} with varying C_{60} concentrations. This will allow study of the concentration dependence, enabling NREL to determine whether the apparent yield of free carriers is linear with concentration (further work is in progress here).
- Annealing these samples gives better conductivity along the polymer chain, apparently due to improved ordering and crystallinity.
- The team would like to take a more in-depth look at the effects of annealing on the THz conductivity signature.The team expects to resume characterization of the polyacenes in pressed-powder form, the results of which will provide information important to this project as well as to projects involving charge transfer in small-molecules interacting with inorganic semiconductor nanocrystals or single-walled carbon nanotubes.

Nanostructured PbTe/PbSe Thermoelectric Materials

Principal Investigator: Mark Hanna
Award: $190,000
Period of Performance: October 2004 to March 2006
Status: In Progress

Goal
To develop a process to make a high ZT nanostructured lead telluride/lead selenide (PbTe/PbSe) thermoelectric material with colloidal precursors that can be scaled up to produce large-area thick thermoelectric devices.

Investment Outcome
The x-ray diffraction (XRD) and x-ray photoelectron spectroscopy (XPS) measurements indicate that the lead tellurium (PbTe) nanocrystals contain free metallic lead and iodine. These impurities may be detrimental to the thermoelectric properties of PbTe devices made from these nanocrystals, so the project team investigated other nanocrystal synthesis routes. A promising synthesis has been identified which produces cleaner material and will be used to make PbSe and PbTe/PbSe core shell particles in the next quarter.

Value of the Outcome
Major advances in the development of nanostructured materials show promising results for significantly enhancing thermoelectric energy conversion efficiency as compared to more traditional BiTe-type materials. Development of this capability opens up new research opportunities for efficient energy conversion.

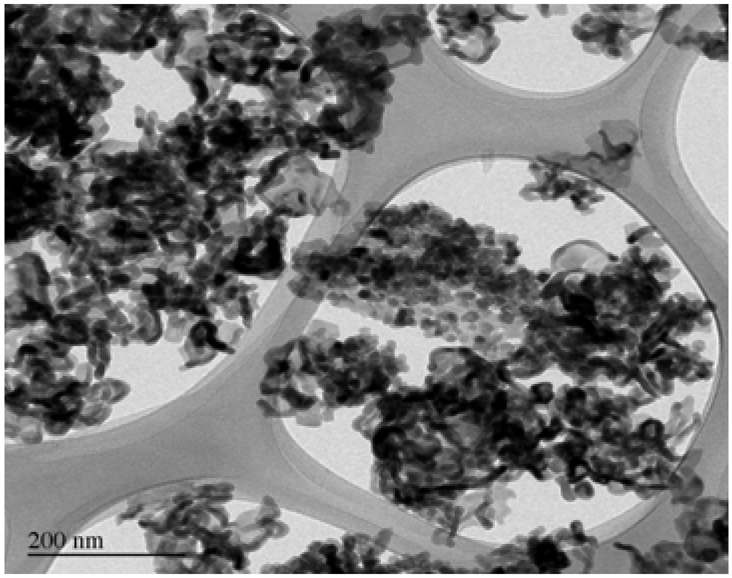

Figure 8. Transmission electron micrograph of PbSe nanoparticles synthesized from PbI2 and Na2Se in methanol.

Next Steps

Make and characterize core-shell PbTe/PbSe nanoparticles. These nanoparticles will be used to fabricate pellets and their mechanical and thermoelectric properties will be studied.

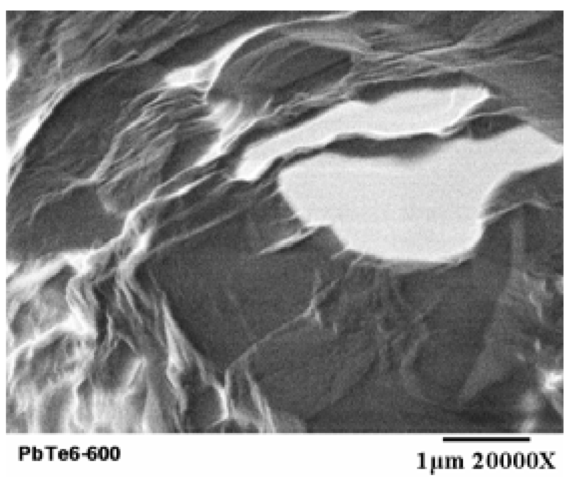

Figure 9. Pressed PbTe nanoparticle pellet after annealing at 600C for 30 minutes. The crystal facets of the grains have rounded edges due to the higher annealing temperature.

Biomass-Derived Nitrogen-Containing Slow Release Soil Amendments

Principal Investigator: Kimberly Magrini-Bair
Award: $150,000
Period of Performance: November 2003 to March 2005
Status: Completed

Goal

To develop a slow release nitrogen-containing soil amendment derived from biomass chars. If successful, these materials would provide a new market for renewable biomass-derived materials, increase soil fertility to protect water from chemical (fertilizer) runoff, and to provide long-term storage of carbon in soils.

Investment Outcome

The project team demonstrated that biomass-derived chars (chemically reacted with urea and pyrolysis oil to add nitrogen) enhance plant growth similar to the addition of rich nitrogen, phosphorous, potassium (NPK) fertilizer. They also found that adding char (raw and functionalized) to soil significantly enhances root growth and that char can support the growth and subsequent release of nitrogen-fixing bacteria into soils.

Value of the Outcome

These promising results provide the basis to design renewable time-release fertilizers for promoting above and below ground plant growth that additionally sequester carbon in the soil. Sustainable benefits of using these materials as targeted agricultural fertilizers are: producing fertilizers from renewable biomass; eliminating conventional fertilizer nitrate runoff into watersheds (a severe and growing water quality problem); increasing soil organic matter accumulation from enhanced root growth; and sequestering carbon in soils. If developed further, the impact of this work is a sustainable and renewable agricultural system based on biomass-derived fertilizers. This approach could revolutionize traditional agricultural practices, minimizing envirnmental impacts of conventional fertilizer use. This approach could also create a new market for biomass-derived materials, and enhance the economics of biorefineries – thus supporting DOE's goal to create a bioindustry.

Transition Metal Catalysis: Experiment and Theory

Principal Investigator: Mark Nimlos
Award: $412,756
Period of Performance: October 2004 to September 2007
Status: In Progress

Goals

- To use a close collaboration between laboratory measurements and quantum mechanical molecular modeling to improve our understanding of catalytic processes that are important in renewable energy production and utilization.
- To develop hydrogenolysis catalysts that are capable of converting alcohols into alkanes. This novel chemical process is thermodynamically favored, seldom observed, and would introduce a new simple approach to a chemical transformation that is usually quite difficult. The technology could be used to convert glycerol, a byproduct of biodiesel production, to a high value compound. The technology could also be useful for converting sugars for polysaccharides into diesel fuel. Novel complexes, which have been developed at NREL, should be capable of catalyzing this hydrogenolysis reaction. The focus of this project is to demonstrate the feasibility of catalytic hydrogenolysis of alcohols, and perhaps more important, to demonstrate that high level quantum mechanical calculations can be useful in guiding the development of these catalysts.

Investment Outcome
Mark Nimlos' team obtained reasonable relative hydricites for palladium and nickel diphosphine complexes with ethyl (depe) and propyl bridges (depp). They also obtained reasonable geometries for the diethyl phosphines. Experiments showed that the methyl phosphines provide fairly accurate models of the diethyl compounds. However, when these calculations were extended to the larger ligands, accurate hydricites could not be obtained. As the bite angle of these ligands increases from xylenyl (depx) to diphenylether (depPE) to xanthenyl (EtXan), experiments showed that the hydricites increased. Calculations showed decreasing hydricites for complexes with these ligands. The problem is believed to arise from the large number of possible conformers that exist for these large ligands. In the last quarter of the fiscal year, model ligands were used in order to reduce the possible conformers and make the calculations more tractable. Diphosphine ligands were replaced with two PH3 or PMe3 ligands frozen at bite angles similar to the angles of the large ligands.

The first milestone: "prepare $[Pt(EtXantphos)_2]^{2+}$ and $[Pd(EtXantphos)_2]^{2+}$ and perform alcohol (C-O) hydrogenolysis studies with benzyl alcohol" has been completed. The second milestone, "perform same hydrogenolysis studies with other alcohols and optimize conditions for selective hydrogenolysis", is underway.

Value of the Outcome
Encouraging results to date indicate that this technology has the potential to provide a simple chemical transformation to convert glycol, a bioproduct of biodiesel production, to a high value compound, and to convert sugars or polysaccharides into diesel fuel. If positive results continue, the project may improve the economies of biodiesel. This project supports DOE goals in bioenergy, biofuels, which are to reduce dependence on petroleum and create a bioindustry.

Next Steps
Continue work on milestones, test catalysts, and conduct more detailed computations of model systems.

Rapid Assignment of Metabolic Function to Genes of Saccharomyces cerevisiae *Using Metabonomics*

Principal Investigators: Arjun Singh and Mark Davis
Award: $380,265
Period of Performance: June 2003 to June 2005
Status: Completed

Goal

- To develop a rapid method to assign function to genes by analyzing the metabolic profiles.
- Identify and assign at least three biomarkers and their gene function relationships.
- Develop a proof of concept for using nuclear magnetic resonance (NMR) and/or pyrolysis molecular beam mass spectrometer (PyMBMS) to rapidly assay changes in metabolic activity caused by genetic manipulation.
- Identify a change in gene expression due to changes in growth conditions.
- Two publications in refereed journals and one proposal submission in the area of metabonomics and gene function.

Investment Outcome
The team completed experiments using MBMS to analyze intact yeast cells and to classify three different pathway mutations. Experimental reproducibility was poor and much time was spent identifying the sources or errors. The result of these experiments indicated that it was going to be difficult to grow yeast strains to perform the high throughput screening experiments that were originally envisioned. However, Arjun Singh and Mark Davis demonstrated the utility of the method for identifying yeast mutations.

The team used electrospray mass spectrometry (ESMS) to analyze cell extracts. This approach was chosen to increase selectivity and sensitivity and it allowed the team to focus on primary metabolites. The intent was to prove reproducibility of the experiment by focusing on the primary metabolites. This approach suffered from many of the same problems as in the MBMS approach. However, several sources of experimental reproducibility were identified and new experiments were designed to improve the high-throughput approach.

In the last year of this project, the team started classifying multiple yeast mutations using the ESMS analysis of the yeast extracts. They classified 13 strains from three different metabolic pathways including cell wall mutations, aromatic amino acid mutations, and sulfur amino acid mutations. The data was encouraging because it appeared to classify the mutations as well as the metabolic pathway. This result was important because it demonstrated that the observed difference was due to changes in the metabolic pathways and not due to the yeast mutations being grown in a different flask. While there are still problems with day-to-day reproducibility, The principal investigators overcame many of the reproducibility problems with growth and extraction conditions.

This approach showed that day-to day variability could be removed by performing binary comparisons. This method will be explored further in future work.

Value of the Outcome
Advances in metabolomics and metabolic profiling will enable a greater basic understanding of plant and single cell metabolic and biosynthetic networks especially when used in conjunction with other "omic" data. The high-throughput analytical methods developed during this project could be used to develop a more complete understanding at a molecular and genetic level of plant cell wall formation and deconstruction allowing the development of more efficient microorganisms and biomass feedstocks. The techniques developed also could be used to reveal interactions between microbes, enzymes, and plant constituents enabling an understanding of how diverse genomes interact providing for a comprehensive systems biology approach to understanding biological biomass conversion.

The expertise developed under this DDRD proposal is being applied in projects with the Office of Science, Biological and Environmental Research (OS-BER), National Science Foundation (NSF), and industry pertaining to metabolic and genetic screening of plant materials.

Pentose Transport and Assay Development
Principal Investigator: Min Zhang
Award: $356,618
Period of Performance: June 2003 to March 2006
Status: In Progress

Goals

- To establish methodologies to study structure and function relationships of xylose transport proteins.
- To establish rapid and reliable assays for analysis of the kinetics of sugar transport.

Investment Outcome

Xylose is the second most abundant sugar available in the world and could potentially produce one third of the ethanol from plant biomasss feedstocks. Microbial utilization of xylose suffered from its low utilization rate and low product yield. Efficient utilization of xylose is the key to economical production of liquid transportation fuels from biomass feedstocks**.** This is critically important to EERE's strategic goals to reduce or end dependence on foreign oil and to create a bioindustry (based on biorefineries).

Results, thus far, suggested that xylE was expressed on plasmind, and that a high level of expression could be toxic to the cell. This is an essential step for testing xylE function. The team developed a growth assay method that offers high throughput screening of transport mutants. They also created a promoter mutant library that contains various growth rates. Characterization of this library is in progress. Once the library and other aspects of the system have been established, NREL will be able to learn the structure and function relationships of this important sugar transporter.

Value of the Outcome

Efficient utilization of xylose, the second most abundant sugar in the world, could tremendously expand the biomass ethanol industry. This technology is critical to the economical production of liquid transportation fuels from biomass feedstocks. The work potentially supports DOE goals in creating a bioindustry and reducing dependence on petroleum.

Next Steps

- Characterize the promoter mutant library.
- Conduct site-directed mutagenesis using alanine scanning and its characterization.
- Submit a proposal to DOE's Office of Science Program.

Computational Sciences

Study of Fundamental Protein/Protein Interactions Involved in Biological Energy Generation

Principal Investigator: Kwiseon Kim
Award: $381,000
Period of Performance: October 2004 to September 2007
Status: In Progress

Goal

Study via computational modeling the mechanisms governing competing protein/protein interactions involved in biological energy-generating processes and understand their impact on the rate of hydrogen production.

Investment Outcome

Kwiseon Kim and her team are working on establishing and documenting the method for studying protein interactions computationally by molecular docking. The work consists of building protein models, docking and screening complexes, analyzing interfaces and calculating binding free energies using molecular dynamics techniques. They established a method to calculate binding free energies, taking into account the translational, rotational, and vibrational components of binding entropy, polar and apolar solvation energy, and complex interaction enthalpy. They have also determined improved force field parameters for the metalloclusters in ferredoxin and hydrogenase using density functional theory and Natural Bond Orbital methods.

Value of the Outcome
Interprotein surface analysis combined with further computational analysis can be used to screen proposed mutations to yield a rational enzyme engineering strategy. The parameterization method developed here can be used to establish more accurate force fields for other molecules of general technological interest. A computational biochemist post doc has been hired, thus increasing computational modeling capability in biological sciences.

Developing efficient means of producing hydrogen (H2) from renewable sources is a compelling challenge on the path toward national energy security. Photobiological H2 generation promises to be a clean, cost-effective means of meeting that challenge. This project addresses an important aspect of this nascent technology by significantly enhancing our fundamental understanding of protein interactions, with the goal of improved electron transport essential to efficient algal H2 production.

Next Steps

- Complete quantum mechanical parameterization of metalloclusters involved in the system and testing in molecular dynamical simulations.
- Further develop the method for calculation of binding free energy. Refine solvation model and protein structural features for consistent interfacial engineering.
- Analyze Brownian dynamics simulations of *C. reinhardtii* ferredoxin and hydrogenase model proteins for the estimates of association rate constants.

Electric and Hydrogen Technologies and Systems

Electrical Model Development and Validation for Distributed Resources

Principal Investigator: Ben Kroposki
Award: $149,998
Period of Performance: October 2004 to September 2005
Status: Completed

Goals

- To conduct research necessary for developing and validating advanced models for multiple distributed resources (DR).
- To develop the in-house capability to understand and model the electrical effects of multiple distributed resources on the distribution system, and determine the impacts of large penetrations for DR.
- To develop collaboration with the Colorado School of Mines (CSM) in electrical engineering research.

Investment Outcome
Ben Kroposki's team completed:

- A literature search of electrical models for distributed resources. This information adds to NREL's knowledge base on the types of models for electric power systems and distributed resources.
- Evaluation and selection of software programs for simulating electrical performance of distributed resources and electric power systems. This work allowed NREL to invest significantly in a new modeling tool for understanding electric power systems operation.
- Model development for a variety of distributed resources at the NREL DER test facility. This accomplishment established new models for understanding the electrical performance of DR. Some of these models are not available in the literature and will be valuable for understanding the performance and operations of inverter based DR.

Value of the Outcome
This project developed new capabilities in conducting electrical modeling of distributed resources and electric power systems using power system computer design software (PSCAD). This model allows for advanced simulation of electric power systems and allows users to develop models of individual components. New models were developed for inverter based DR (i.e. PV, wind, fuel cell). This project also established a new collaborative effort between NREL and CSM in electrical power systems.

As a result of this work, follow on work to develop models for advanced power electronics and electrical interfaces will be supported in FY06 through the DOE Distributed Energy Program and the California Energy Commission Public Interest Energy Research Program.

Prototype Renewable Planning Model (RPM)

Principal Investigator: Ben Kroposki
Award: $500,000
Period of Performance: May 2005 to July 2007
Status: In Progress

Goal
To develop a preliminary assessment tool, the Renewable Planning Model (RPM), to integrate basic resource availability (i.e. solar irradiation, wind resource, and biomass feedstocks) with infrastructure elements (i.e. power distribution system, roads) and constraints onto a single geographic interface.

Investment Outcome
The project team created a basic web-based geographic information system (GIS) map viewer and interface with HOMER program, received distribution system load data from Xcel Energy, and added overlay capability to GIS mapper. They also developed a tool that will show basic resource availability–solar irradiation and wind resource. NREL has sought technical expertise, and data from a utility on its distribution system to ensure that the tool is a usable product.

Near-term, the project will establish a more complete prototype before the product is shared on a larger scale. Long-term, this project could be expanded to work with a variety of utilities and energy analysis.

Value of the Outcome
This tool will allow DOE and other decision makers to assess the deployment potential of a range of renewable energy sources based on geographic resources as well as transmission and distribution capacities, road proximity, terrain suitability, regional incentives, etc. It will be an efficient tool for the evaluation of local, regional, or national impacts of technical and economic goals as well as regulatory and demand-based influences.

Next Steps
The next step is to focus on a specific example situation (siting commercial PV systems) and to develop a protoype that will examine the specifics of that issue.

Appendix A: Acronyms and Symbols

AC – Alternating Current

ANL – Argonne National Laboratory

Au – Gold

AWEA – American Wind Energy Association

BNL – Brookhaven National Laboratory

BSCL – Biomass Surface Characterization Laboratory

CdMgTe – Cadmium Magnesium Telluride

CEC – California Energy Commission

CELIV – Current Extraction by Linearly Increasing Voltage

CH_4 – Methane

C-O – Alcohol

CSM – Colorado School of Mines

CSP – Concentrating Solar Power

CSU – Colorado State University

C60 – (The most common carbon buckyball)

DDRD – Director's Discretionary Research and Development (program)

depPE – Diphenylether

depx – Xlenyl Diphenylether

DER – Distributed Energy Resources

DOE – Department of Energy

DR – Distributed Resources

EC – Electrochromic

ECC – Electrochemical Capacitor

EIA – Energy Information Administration

En – Ethylenediamine

EPA – Environmental Protection Agency

ESMS – Electrospray Mass Spectrometry

Etxan – Xanthenyl

eV – Electron Volt

FAD – Flavin Adenine Dinucleotide

GaAs – Gallium Arsenide

GIS – Geographic Information System

GPC – Gel Permeation Chromatography

GPRA – Government Performance and Results Act

HPLC – High Pressure Liquid Chromatography

H_2 – Hydrogen

ICF – Integrated Planning Model

InGaAs – Indium Gallium Arsenide

InP – Indium Phosphide

IPM – Integrated Planning Model

ITO – Indium Tin Oxide

K – Potassium

LCMS – Liquid Chromatography Mass Spectrometry

LEDs – Light Emitting Diodes

MARKEL – (EPA's wind model)

MBMS – Molecular Beam Mass Spectrometer

MIT – Massachusetts Institute of Technology

MRS – Materials Research Society

N – Nitrogen

NADP – Nicotinamide Adenine Dinucleotide Phosphate

Na2Se – Sodium Selenide

NBO – Natural Bond Orbital

NEMS – National Energy Modeling System

NiO – Nickel Oxide

NIST – National Institute of Standards Technology

NMR – Nuclear Magnetic Resonance

NO – Nitric Oxide

NOx – (Encompasses all nitrogen oxide emissions: NO, N2O, and NO2)

NPK – Nitrogen, Phosphorous, Potassium

NRL – Naval Research Laboratory

NSF – National Science Foundation

NSOM – Near-field Scanning Optical Microscope

N2 – Nitrogen Oxide

OLEDs – Organic Light Emitting Diodes

OPV – Organic Photovoltaic

OS-BER – Office of Science, Biological and Environmental Research

P – Phosphorous

P3HT – Poly-(3-hexylthiophene)

PbI2 – Lead Iodide

PbSe – Lead Selenide
PbTe – Lead Telluride

PCBM – (C_{60} is the most common carbon buckyball, and when functionalized as: [6,6]-phenyl C_{61}-butyric acid methyl ester; it's commonly referred to as PCBM.)

PECVD – Plasma Enhanced Chemical Vapor Deposition

PNNL – Pacific Northwest National Laboratory

PSCAD – Power Systems Computer Aided Design (software)

PyMBMS – Pyrolysis Molecular Beam Mass Spectrometer

PV – Photovoltaics

QD – Quantum Dot

QDSL – Quantum Dot Superlattices

RFF – Resources for the Future

RPM – Renewable Planning Model

RuO_2 x H_2O – Amorphous Hydrous Ruthenium Oxides

SEDS – Stochastic Energy Development Systems

SERF – Solar Energy Research Facility

SiO2 – Silicon Dioxide

SSL – Solid State Light

SWNT – Single-Walled Nanotubes

Ta_2O_5 – Tantalum Oxide

TEM – Transmission Electron Microscope

THz – Terahertz

TiO2 – Titanium Dioxide

TOF – Time-of-Flight

TRTP – Time-Resolved THz Photoconductivity

U of W – University of Wisconsin

WFO – Work for Others

WinDS – Wind Deployment System

WO3 – Substoichemetric (The W is not fully oxidized.)

XPS – X-ray Photoelectron Spectroscopy

XRD – X-ray Diffraction

ZnTe – Zinc Telluride

ZT – (A dimensionless figure of merit for thermoelectric materials. $ZT=S^2\sigma T/k$ – *S is the Seebeck coefficient, σ is the electrical conductivity, k is thermal conductivity, and T is the temperature.)*

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The Director's Discretionary Research and Development (DDRD) program is designed to encourage technical innovation and build new research and development capabilities at the National Renewable Energy Laboratory (NREL). Technical innovation is critical to the long-term viability of NREL (also referred to as the Laboratory) and to the success of the U.S. Department of Energy (DOE). The strategic value of DDRD is being continuously enhanced by expanding the opportunities to propose and pursue innovative ideas for building new and enhanced capabilities. DOE-EE's (Office of Energy Efficiency and Renewable Energy) policy for the DDRD program enables NREL's Director to: "…approve for funding, projects put forth by Laboratory staff which propose to explore and/or develop innovative or creative opportunities within mission areas assigned to the Laboratory. Projects should advance research and development directed toward solving present scientific or technical problems; or should be experiments and analysis directed toward determining the merit and utility of new ideas or concepts."

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