NSTC COMMITTEE ON TECHNOLOGY

SUBCOMMITTEE ON NANOSCALE SCIENCE, ENGINEERING, AND TECHNOLOGY

National Nanotechnology Initiative Signature Initiative:

Nanotechnology for Solar Energy Collection and Conversion

Final Draft, July 2010

Collaborating Agencies[1]: *DOE*, *NIST*, *NSF, DOD, IC, USDA/NIFA*

National Need Addressed

The President's Agenda calls for the development of carbon-neutral alternative energy sources to mitigate global climate change, reduce dependence on foreign oil, improve the economy, and improve the environment. The specific targets specified by the President's Agenda state that 10 percent of electricity generated should be derived from renewable sources by 2012 and 25 percent by 2025.

Solar energy is a promising alternative energy source that can address these challenges. It is a resource readily available in every country around the world, and is not a threat to the environment through pollution or to the climate through greenhouse gas emission. The development of a solar energy infrastructure will not only help ensure U.S. energy independence but also represents an unparalleled economic opportunity if the United States can maintain scientific and industrial leadership in this field.

Today, the Levelized Cost of Energy of solar technology is not yet economically competitive with conventional fossil fuel technologies without subsidies. Therefore, new innovations and fundamental breakthroughs can help accelerate the development of economical solar energy technologies that overcome the limits of existing technologies.

Nanotechnology can help overcome current performance barriers and substantially improve the collection and conversion of solar energy. At the nanoscale, a number of physical phenomena have been identified that can improve the collection and conversion of solar energy. Nanoparticles and nanostructures have been shown to enhance the absorption of light, increase the conversion of light to electricity, and provide better thermal storage and transport. However, current demonstrations of these technologies fall short of potential performance because of poor control over feature size and placement, unpredictable micro/nanostructure, poor interface formation, and in many cases short lifetime of laboratory devices. Critical to exploiting the benefits of nanotechnology is a deeper theoretical understanding of conversion and storage phenomena at the nanoscale, improvements in the nanoscale characterization of electronic properties, and developments that enable economical nanomanufacturing of robust devices. Achieving product lifetime and reliability of technologies incorporating nanotechnology that meet or exceed the performance of conventional technologies, which can be 25 years or longer in the case of photovoltaic systems, is also critical to the success of this initiative. The nation has the opportunity to be a world leader in applying nanotechnology to solar energy and harvest the rewards of economic impact and manufacturing jobs by being the early leader.

[1] Please note that "collaborating agencies" is meant in the broadest sense and does not necessarily imply that agencies provide additional funds or incur obligation to do so. Agencies leading this effort and responsible for proposed initiatives are underlined.

Technical Program

This initiative has three R&D thrust areas listed in order of "most advanced" (i.e. industry exists) to "least advanced" (i.e. emerging technologies):

Thrust 1: ***Improve photovoltaic solar electricity generation with nanotechnology***

The thermodynamic limit of 80% efficiency is well beyond the capabilities of current photovoltaic technologies, whose laboratory performance currently approaches only 43%. An integrated, multidisciplinary, experimental and theoretical effort is now needed to drive transformational changes in the way solar cells are conceived, designed, implemented, and manufactured. Nanotechnology provides a promising way to reach these goals. In particular, significant increases in photovoltaic efficiency and reductions in cost may be realized through engineered devices that exploit spatial and compositional inhomogeneities such as surfaces, interfaces, and nanostructures.

The key research goals for Thrust 1 include the following:

1A. Improve the efficiency of photovoltaic (PV) devices.

Nanotechnology can contribute to the improvement of PV device efficiency in a number of ways, including but not limited to the following:

Enhanced light coupling: Increasing the amount of light that reaches the active light sensitive material will improve the efficiency of PV devices. Nanostructured antireflection coatings can dramatically reduce reflection losses, and light capture can be significantly improved by exploiting photonic crystals, plasmonic guiding, and other nanoscale coupling structures. Developing methods for economically incorporating such structures into multilayer heterostructure devices is an important area of research.

Engineered interfaces: Appropriately engineered interfaces can enhance the collection and trapping of light, control the flow of photocarriers, and play a major role in a number of technologies. However, interfaces can be a source of interdiffusion, defects, and impurities that degrade performance. Improving the understanding of carrier dynamics at interfaces is critical, as is the ability to control interfaces between dissimilar materials. There is evidence that integration of carbon nanotubes and other nanowires into the solar cell junction interface as a bonding agent has the potential to improve multijunction solar light transmission and energy conversion efficiency.

Bandgap engineering: Many current-generation photovoltaic devices utilize a single energy bandgap that cannot perfectly match the energies of sunlight photons, so some energy is absorbed but is lost to heat rather than being converted to electricity. New structures must be designed and fabricated that exploit multiple junctions, multi-exciton generation, multiple energy levels, hot-carrier junctions and intermediate band solar cells (IBSC) and other techniques/ phenomena to maximally convert light energy to electricity. Better theoretical and experimental understanding and control of quantum confinement is needed, and the development of semiconductor nanostructures (quantum dots, quantum rods, quantum wires) as well as carbon nanotubes to enhance generation while minimizing thermal loss also is needed.

1B. Develop improved measurement and characterization techniques to support Thrust 1A (Higher Efficiency) and Thrust 1C (Advanced Manufacturing).

Realization of the goals in Thrust 1A and 1D will require better understanding of interfaces and phenomena enhanced by interfaces, inhomogeneities, and nanostructures. New measurement techniques that are spatially resolved at appropriate scales matched with appropriate simulation and modeling can help achieve that goal. New multifunctional techniques combining nanoscale spatial resolution with ultrafast time resolution are needed to measure fundamental carrier dynamics in individual 3D nanoscale structures and in nanostructured arrays. New electromagnetic measurement methods that probe photoinduced carrier generation; carrier scattering processes that lead to energy relaxation, trapping, and recombination; as well as carrier transport and localization in individual nanostructures and heterogeneous assemblies of nanostructures (such as organic materials, nanowires, and quantum dots) are needed.

<u>1C. Advance the fabrication/manufacturing technology of photovoltaic devices.</u>

The promise of new high efficiency photovoltaic devices incorporating nanotechnology will not be commercially realized until scalable low-cost fabrication and manufacturing technologies are developed. For example, well-ordered nano-scale arrays capable of efficiently generating and transporting carriers will be required to maximize photon absorption and minimize electron-hole recombination. Current laboratory-scale fabrication and manufacturing methods to realize such nano-architectures, including self-assembly, nucleation and growth, growth and etch, are cost prohibitive today on the large scale required to meet the nation's renewable energy goals. Development of fabrication methods that are economical and scalable to mass-production is required. Candidate approaches which use nanocoatings or Atomic Layer Deposition (ALD) approaches are applicable and potentially scalable technologies These include consideration of manufacturing techniques that maximize use of readily available materials and minimize need for recycling and end of life-time waste issues.

<u>1D. Improve the stability and longevity of nanotechnology-based photovoltaic devices</u>

Some novel photovoltaic devices that have been proposed utilize nanostructured materials that offer promise of improved efficiency and/or reduced manufacturing cost compared to conventional single, multi-, or micro crystalline devices, but some may also have limited useful lifetimes under exposure to radiation (i.e., sunlight including UV) and other environmental factors (e.g., temperature variations, oxygen, moisture, dirt, etc.). Understanding why degradation occurs is a first step in developing solutions to prevent such degradation. There is a need for new approaches to improving the stability and lifetimes , or new approaches for renewing these materials *in situ* after they have been deployed in photovoltaic arrays. Overall improvement in cost/performance of nanotechnology-enabled photovoltaics may involve a balance between cost-reduction and efficiency and stability improvements. All costs should be considered, including long-term costs due to the environmental impact of the manufacturing of nanotechnology-based materials and devices. Wherever possible, earth-abundant materials should be used. In addition, the unique environmental impact (cost) of the nanomaterials used in these devices needs to also be considered.

- ***Expected Outcomes*Laboratory demonstration of next-generation photovoltaics that close the gap halfway between current best laboratory and theoretical maximum efficiencies by 2020. Examples include:**
  - Multi-junction concentrating photovoltaic (CPV) devices with improvements such as nanostructured antireflection coatings, which together will reach efficiencies of 52% (theoretical max 63%, best to date 42%).
  - Copper Indium Gallium Diselenide (CIGS) and CdTe devices with improvements such as better engineered interfaces and fine-tuned band gap engineering at the nanoscale, when taken together will reach efficiencies 24% and 23%, respectively (theoretical max 27% and 30%, best to date 20% and 17%)
  - Single junction silicon devices with improvements as such better band gap engineering at the nanoscale which will reach efficiencies of 28% (theoretical max 33%, best to date 25%).

  - Photovoltaic devices for demanding applications with nano-engineered improvements which will allow unattended, zero-maintenance operations (space and other) with high reliability, 25 year lifetimes with non-concentrated efficiencies up to 47%.
- **Fabrication and manufacturing technologies (including "green manufacturing" to minimize lifecycle waste) that by 2020 close the performance gap halfway between best laboratory PV devices and production PV modules in a cost-effective manner. The engineering challenges to incorporating the results of nanotechnology research into production systems is significant. While welcoming the potential for revolutionary changes in production, examples of targets for engineering nanotechnology developments into current PV technologies are:**
  - Production triple junction CPV cells achieving 40% efficiency, halfway from today's 38% in production and best laboratory cell result of 42%
  - Production CIGS modules achieving 15% efficiency, halfway from today's 10% in production and best laboratory cell result of 20%
  - Production CdTe modules achieving 14% efficiency, halfway from today's 11% in production and best laboratory cell result of 17%
  - Production silicon modules achieving 22% efficiency, halfway from today's 19% in production and best laboratory cell result of 25%
- **Fabrication and measurement infrastructure supporting advances in nanosolar device development and nanomanufacturing,**

Thrust 2: ***Improve solar thermal energy generation and conversion with nanotechnology***

As a broadband converter of solar radiation to thermal energy, concentrating solar thermal technologies (CSP) offer advantages over current photovoltaics for utility-scale power generation. The advantages are that CSP uses existing energy storage technologies and conventional electric power generating plants (e.g. steam plants) that historically have been interfaced to the grid and distribution networks. Even higher efficiencies and reduced infrastructure costs may be achieved by exploiting recent advances in nanotechnology. Specifically, significant improvements in CSP technology can be achieved in parabolic trough, solar tower and dish collectors. These can be impacted through the use of innovative liquid heat transfer fluids that contain nanoparticles and high solar optical absorption materials and coatings that operate at high temperatures under high solar concentration fluxes. Depending on the characteristics of the nanoparticles and textured surfaces, dramatic improvements in thermal conductivity, boiling point, freezing point, time stability, optical absorption and other physical properties can be achieved. With these gains in performance, a heat exchanger's footprint and required volume of heat transfer fluid can be reduced while still increasing the overall system efficiency. Combined, these factors can lead to considerable improvements in the Levelized Cost of Energy (LCOE). In addition, thermal energy can be directly converted to electricity through the use of thermoelectric materials, but those in use today have low conversion efficiencies. Increased efficiencies will enable opportunities beyond present low-grade heat energy recovery applications. Nanoengineered thermoelectric materials have the potential to dramatically improve this conversion of thermal energy to electricity, but significant experimental and theoretical research is still needed in order to understand and optimize the energy conversion processes in these systems.

The key research goals for Thrust 2 include the following:

<u>2A. Develop new engineered nanofluids for optimized solar-to-thermal conversion and energy storage</u>

Efficiencies of grid-scale concentrating solar thermal electric plants that use heat transfer fluids (CSP parabolic troughs for example), can potentially be significantly increased by exploiting the complex thermodynamic properties of nanoparticle-based liquids. Appropriately designed nanofluids could increase thermal conductivity, increase temperature dependence of thermal conductivity, and increase critical heat flux leading to higher Carnot efficiency and reduce infrastructure footprint. Nanoparticle material composition, size, shape, functionalization, and concentration are currently being assessed and recent experimental reports suggest that solar to thermal conversion efficiencies could be enhanced by approximately an order of magnitude or more by using magnetic nanoparticles in a certain concentration range.

Properties of nanofluids are being experimentally verified to the point Based on such research on nanofluids properties, fields of application are being identified. Consequently Agency activities are focusing on commercially-relevant R&D Programs while others are being scaled back or eliminated. R&D efforts to develop and optimize nanofluids for CSP electric power generation can potentially have significant translational benefit.

2B. Develop advanced high optical absorbance nanocomposite coatings for high solar flux CSP collector systems.

Solar towers have very high fluxes incident on an opaque, metallic vessel (boiler) which converts sunlight to thermal energy and heats a transfer fluid inside. The efficiency of solar to thermal conversion in CSP systems improves as heat transfer fluid temperatures increase above 550 °C. New high temperature, high solar absorbance and low thermal emittance materials and coatings are needed for advanced boilers. Optical and thermal properties of nanomaterials could provide a path toward realizing such high efficiency systems.

Achieving materials and coatings with such properties is very challenging as the two materials properties are seemingly mutually exclusive and trade-offs need to be assessed. Furthermore, these materials must be stable under environmental operating conditions of high temperature and flux, repeated temperature cycling, mechanical stress, moisture, dust and corrosives. Coating delamination must be minimal over long periods of time; preferably years. Approaches using nanocomposites and photonic lattice structures have been proposed and are in early stages of research. Although solar-to-thermal conversion efficiency improvements highly depend on systems design, advanced materials and coatings are estimated to provide approximately a 10% increase over present efficiencies offering a significant increase in solar plant generating capacity and reduced footprint.

2C. Develop efficient thermoelectric convertors

Increasing the overall system efficiency of large-scale solar power plants will yield significant increases in electricity generated over their lifetime and lower LCOE. One approach is to harvest thermal energy in waste heat created during solar power generation by highly efficient thermoelectric devices. Nanoengineered materials may be a key to achieving high-performance bulk thermoelectric materials. Experimental and theoretical research suggest that nanotechnology could improve thermoelectric device efficiencies from approximately ZT=4 in bulk materials to ZT= 20 and higher in nanostructured devices. Device efficiency depends on temperatures found in specific applications so over absolute efficiencies over 10% will have an impact in military and aerospace while over 20% will in automotive and industrial waste heat recovery. Nanomaterials and associated manufacturing processes can significantly reduce the cost to enable highly cost-sensitive markets such as automotive.

Essential to reaching the performance and cost targets is theoretical and experimental understanding of the role and stability of the interface between the nanomaterials and the matrix into which they are embedded. An effective interface must be thermally stable and promote electron transport while impeding phonon transport, so that the material exhibits high electrical conductivity and low thermal conductivity respectively. Interface issues such as diffusion and segregation, doping and composition of the nanostructures, differential thermal expansion, and chemical contrast are essential topics for investigation. As an example, functionalized carbon nanotube (CNT) films are being explored as potential thermoelectric materials with exceptional properties, but deeper understanding of the electrical and thermal properties of these films at the nanoscale is critical for their optimization and eventual incorporation into power-generation devices.

Expected Outcomes:

- Demonstrate viability of and optimum material nanofluid systems for efficient solar to thermal energy conversion in CSP collector systems.
- Develop high optical absorbance and low emittance nanocomposite coatings and materials operating at temperatures found in high solar flux CSP collector systems
- Develop new nanostructured materials with high electrical conductivity and low thermal conductivity for high-efficiency thermoelectric conversion of heat to electricity

Inter-Agency Collaborations:

Synergistic Inter-Agency collaborative Programs will fill gaps in programmatic areas. Activities include serving on each others' existing Grantee Program Reviews Panels and proposal selection panels. An effective mechanism for collaborating is to establish Memoranda of understanding (MOUs) to release joint Program announcements. One example is where DOE and NSF (Le and Maracas) are creating a joint MOU in the Solar Energy/Power area and serving on each others' Program Review Panels (e.g. SETP) and grant proposal Review Panels.

Thrust 3: ***Improve solar-to-fuel conversions with nanotechnology***

Conversion of solar energy into chemical fuels, no matter the system, requires the coupling of photon-driven, single-electron transfer events with fuel-forming, multi-electron catalytic processes. As these processes occur on very disparate temporal scales, their coupling is a significant challenge. Nevertheless, the photosynthetic apparatus, which is essentially composed of a series of nanoscale molecular machines, provides clear proof-of-concept that such coupling can be achieved. Natural photosynthesis produces "biological fuel" in the form of sugars and other reduced carbon-containing compounds (e.g., lipids, starches and proteins) that are derived from atmospheric carbon dioxide. The plants themselves may be used as primary fuel if directly combusted, or secondary fuels (such as ethanol or butanol) may be generated from biomass fermented in reactors. Due to a number of factors, these routes to fuel formation are inefficient. Artificial photosynthetic systems that are inspired by the natural system's nanocomponents are attractive alternate options. Production of useful chemical fuels directly from sunlight with significantly higher efficiencies than the natural system is possible because such artificial systems need not devote captured energy to the maintenance of life processes. Artificial photosynthetic systems, however, remain in the laboratory stage where increased scientific effort is needed to understand structure-function relationships of components, as well as to develop basic principles for component assembly and integration. Rapid advances are foreseeable because emerging nanotechnology capabilities allow for unprecedented manipulation of the nanoscale structures involved in both natural and artificial solar fuel production systems.

The key research goals for Thrust 3 include the following:

3A. Leverage natural photosynthesis for sustainable production of solar fuels

Enhanced understanding regarding the nanoscale architecture of the photosynthetic apparatus, along with enzymes and cofactors involved in carbon dioxide reduction and hydrogen formation, will impact both natural and artificial solar fuel production schemes. Specific goals are to (1) increase our knowledge pertaining to the complex protein structures and catalytic mechanisms that control and optimize energy flow in natural photosynthesis, as well as mechanisms for component repair and assembly; (2) combine nanotechnology and biotechnology to engineer plants that more efficiently convert solar energy into biomass; (3) elucidate the nanoarchitecture of the plant cell wall to understand how it can be modified for enhanced energy storage and/or materials usage; (4) engineer photosynthetic microorganisms to cost-effectively produce simple fuels such as dihydrogen or more advanced carbon-containing biofuels; (5) fully understand the active site chemistry and influence of surrounding proteinaceous nanostructure on catalytic function of multielectron transfer enzymes and enzymes involved in proton-coupled electron-transfer reactions.

3B. Develop highly efficient artificial photosynthetic systems

The overarching goal is to construct man-made components (from organic or inorganic molecules, or inorganic semiconductor nanoparticles) that, as an assembly, convert solar energy into chemical fuels. Efficient solar fuel generation requires three coordinated events—photon absorption, charge separation, and use of the separated charges in fuel-forming reactions. Since the field of photovoltaics is also concerned with light absorption and charge separation, some specific goals to achieve solar fuels are similar to those outlined in Thrust 1. Additional specific goals for this thrust include to (1) develop new electrodes or electrode combinations using nanotechnology to enable a robust, efficient system for direct solar-induced water splitting; (2) generate new nanoscale structures and catalysts derived from earth – abundant materials for photocatalytic water oxidation and photocatalytic carbon dioxide reduction; (3) develop innovative architectures for integration of component machinery to produce a functional, efficient photo-electrochemical reactor; (4) increase fundamental understanding regarding electronic and molecular interactions that would allow for self-assembly of a nanoscale solar fuel system.

Expected Outcomes:

- New technology that will allow for solar-driven advanced biofuel and bio-based chemical production strategies
- Robust sunlight-driven reactors that convert water and carbon dioxide into a high-energy-density fuel and related bio-based chemicals

Agency Roles and Contributions

The challenges of realizing a sustainable solar energy economy are significant; the goals can only be met through transformational science and technology that will be achieved by a concerted, interagency effort that addresses challenges spanning multiple diverse disciplines including materials science, chemistry, biology, engineering, and advanced measurement and characterization science.

Table 1. Agency Contributions by Thrust Area

Thrust Area	DOE	NIST	NSF	DOD	Intel Community	USDA/ NIFA
1. Solar-Electric	•	•	•	TBD	•	•
2. Solar-Thermal	•	•	•	TBD	•	

3. Solar Fuels	•	•	•	TBD		•

Table 1 illustrates agency contributions to each of the key thrust areas. The expertise and perspective that each participating agency will bring to this effort is as follows:

DOE: The Department of Energy financially supports an extensive portfolio of research projects that incorporate nanoscale materials and devices for solar energy collection and conversion. This research is accomplished at DOE labs, universities, and private industry throughout the country. As the nation's leading supporter of energy-related research and development, DOE is in the unique position to be at the hub of this diverse effort. The National Renewable Energy Laboratory along with the five DOE Nanoscale Science Research Centers, provide state-of-the-art fabrication and characterization capabilities for the development of nanoscale materials and structures. The DOE synchrotron light sources, neutron scattering facilities, and electron microscopy centers provide exceptional characterization at short length and time scales. Integration of scientific advances into commercial scale processes is enabled through a technology pipeline that includes Research, Development, Demonstration, and Deployment.

NIST: As the nation's metrology institute, NIST offers a broad capability in the areas of both nanoscale measurements and fabrication for a variety of applications. These measurement tools and facilities can be leveraged to accelerate the development of the next generation of nanoscale materials. NIST's strong coupling with industry ensures that the measurement methods that are developed are quickly disseminated to industry researchers as well as to government partners.

NSF: The National Science Foundation supports interdisciplinary efforts by groups of researchers to address the scientific challenges of highly efficient harvesting, conversion, and storage of solar energy. The main goal is to create a new modality of linking the mathematical and engineering tools with the chemical and materials sciences to develop transformative paradigms in an area of much activity but mainly incremental advances. NSF aims at potentially transformative projects and new concepts based on the integrated expertise and synergy from the various relevant disciplinary communities. A primary emphasis is on the education at all levels of highly trained scientific and technical workforce.\

Intel Community: The Intelligence Community supports research projects on nanoscale materials, devices, and transition to manufacturing for solar and thermal energy collection, conversion, and storage. Foundational technology development is aimed at high-efficiency and high-reliability devices for unattended, zero-maintenance operations. R&D programs are designed to provide initial feasibility funding for a wide range of ideas, with the goal of selecting the most promising ideas for further development and eventual transition to the U.S. manufacturing infrastructure.

USDA/NIFA: The agency supports broad research, education, and extension in agricultural crops and natural plant systems. Direct solar conversion to electricity using nanoscale protein photosynthesis units harvested from leafy vegetables is an example of novel energy technology research. Using new knowledge gained in nanoscale science and engineering to improve biomass yield and fuel conversion efficiency can aid the national biofuel strategy. Value-added uses of agricultural products strengthen the national economy while providing new energy supplies.

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