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Solar Energy Technologies Program

National Solar Technology Roadmap:

Multiple-Exciton-Generation PV

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DRAFT

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DRAFT VERSION

National Solar Technology Roadmap: Multiple-Exciton-Generation PV

Scope

This roadmap addresses the development of solar cells based on inorganic semiconductor nanocrystals (NCs)—such as spherical quantum dots (QDs), quantum rods (QRs), or quantum wires (QWs)—focusing on their potential to improve upon bulk semiconductor cell efficiencies by efficient multiple-exciton generation (MEG). The generation of multiple excitons (i.e., electron-hole pairs) for each absorbed photon of sufficient energy raises the thermodynamically attainable power conversion efficiency of a single-junction photovoltaic (PV) solar cell from 33.7% to 44.4%. Semiconductor NCs are produced at much lower temperatures than their bulk counterparts, enabling significantly lower production cost. Several possible implementations of semiconductor NC-based solar cell devices may be realized.

Technology development stage: The current state of this technology is in the fundamental and exploratory research phase, and is focused on (1) pursuing an experimental and theoretical understanding of the MEG mechanism—i.e., how NCs enhance charge-carrier pair production for high photon energies, (2) materials selection and characterization, and (3) efficient charge separation for photocurrent collection from MEG-active NCs. The research at the National Renewable Energy Laboratory (NREL) on MEG was initiated in 2000, and basic research on MEG is still currently funded by the Office of Science, Office of Basic Energy Sciences (BES). The cooperation and synergism between the basic research funded by BES and the translational research funded by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) in this area will continue in the future.

Target applications: The long-term target application consists of the inexpensive generation of solar electricity and fuels (e.g., H_2) at very high efficiency—third-generation solar cells. Multiple-exciton generation is based on processes observed to occur in colloidal, solution-based inorganic semiconductor nanocrystals. A MEG-active solar cell would allow for inexpensive solution-based processing of solar cells with efficiencies exceeding the Shockley-Queisser limit for conventional solar cells of ~34%. Therefore, the target market for MEG solar electricity production could include virtually any solar PV market, including the generation of hydrogen fuel by solar-powered electrolysis.

Background

All single-junction solar cells in operation today suffer substantial loss due to the thermalization of charge carriers with the crystal lattice. That is, solar photons with energy in excess of the semiconductor bandgap produce electron-hole pairs with excess energy above their respective band edges; the electron and hole generate thermal energy (i.e., heat) as they relax toward the band edges. A thermodynamically attainable device using the full energy of photons within the solar spectrum would convert sunlight to electricity at an efficiency of ~66%. Multiple-exciton generation has demonstrated a route to *reducing* thermalization loss by generating multiple excitons (electron-hole pairs) *per absorbed photon* in semiconductor quantum dots. Highly efficient MEG in semiconductor NCs was first predicted at NREL in 1997, and was first demonstrated experimentally in 2004 at Los Alamos National Laboratory (LANL) and NREL. Subsequently, efficient MEG has been reported in quantum dots of many semiconductors, including PbSe, PbS, PbTe, InAs, CdSe, and Si. MEG can also play an essential role in other R&D efforts such as sensitized nanocrystalline and organic-hybrid solar cells. Considerable opportunity exists to rapidly advance this very promising approach toward third-generation solar cells.

Roadmap Overview

2007: Multiple-exciton generation represents a concept for significantly enhancing the power conversion efficiency of solar cells using semiconductor NCs. The MEG process has been well-documented experimentally in quantum dots of several different semiconductor materials. Additional experimental, theoretical, and modeling work are needed to fully understand the MEG mechanism and attain predictive capabilities; many aspects of the fundamental research will be supported by DOE-BES. Solar cell devices based on NCs have been produced with efficiencies of 1%–3%, although no devices have been shown to exploit MEG. Several possible NC solar cell designs have been identified, and work has begun to demonstrate MEG-enhanced photocurrent from a working device. Possible implementations of NCs include dye replacement in sensitized nanocrystalline metal-oxide solar cells, a blended heterojunction organic-inorganic device in which the NCs replace C_{60}-PCBM, or a QD solar cell based on a *p-i-n* structure.

A significant barrier to producing high-efficiency solar cells that incorporate NCs is to extract the electrons and holes from the NCs without losing the beneficial quantum confinement inherent in the NCs. Thus, among the main scientific challenges are the following: (1) Fully understand the interfacial charge separation in a variety of media; and (2) Achieve efficient long-range charge transport through arrays of coupled NCs. Nanocrystal-sensitization of TiO_2 and NC-conducting polymer bulk heterojunction designs are two strategies for charge separation and collection. Close-packed arrays of NCs that allow for the formation of extended states enable efficient charge transport. Although a detailed understanding of the basic interactions between NCs and their surroundings is lacking, much progress can still be achieved within these proposed PV structures.

2010: Reasonable estimations of progress on MEG devices yield a NC solar cell conversion efficiency of > 8%. Key advancements necessary to achieve this goal include (1) reduced recombination loss by improved material surface and interface, (2) improved coupling between neighboring QDs to facilitate charge transport, and (3) improved cell design to reduce the electron and hole collection time and improve open-circuit photovoltage (V_{oc}). Based on these key advances, a clear demonstration of wavelength-dependent MEG-enhanced photocurrent in a prototype cell will be achieved.

Metrics

MEG-Specific Parameters	Present Status (2007)	Future Goal (2015)
MEG quantum yield at $h\nu = 2.5 \times E_g$	105%–110%	180%
IPCE at $h\nu > 2E_g$	45%	>100%

NC Solar Cell Parameters	Present Status (2007)	Future Goal (2015)
Champion NC solar cell efficiency	1%–3%	25%
AM1.5 photocurrent density at V_{oc}=1.0 eV	~1 mA/cm^2	36 mA/cm^2
Carrier mobility (DC value for coupled NC array)	~1 cm^2/(V·s)	100 cm^2/(V·s)

Identified Needs

Need	Significance	University	Nat'l Lab			Industry		
			NREL	LANL	Sandia	TPP	Incubator	Other
Determine experimentally and theoretically the mechanism driving MEG	Understand the mechanism that drives material-selection for optimizing the combination of MEG effect and bandgap to drive device design.	x	x	x				
Develop theoretical framework for materials design	Establish predictive capability for MEG quantum yield based on parameters such as semiconductor type, surface chemistry, and nanoscale architecture; avoid random exploration for materials.	x	x					
Select materials	Develop semiconductor NCs that are abundant, inexpensive, of low toxicity, and exhibit highly efficient MEG.	x	x					
Design cells for using MEG	Efficient collection of photocurrent such that MEG contributes to conversion efficiency		x					
Investigate contacting materials	Reduce contact losses to improve V_{oc}; generate a large built-in potential.	x	x					
Mass-production of NC materials	Reduce cost and enable wide-scale production.							x
Conduct life-cycle cost analysis	Evaluate potential economics of MEG-NC solar cells; determine component cost targets for NCs and other materials.		x					
Investigate scaling deposition to mass-production	Research deposition techniques (spray, inkjet, screen) for possible use in production.	x	x					