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DOE/NREL Fundamental and Exploratory Research into Solar Cells

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DOE/NREL FUNDAMENTAL AND EXPLORATORY RESEARCH INTO SOLAR CELLS

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ABSTRACT

The U.S. Department of Energy / National Renewable Energy Laboratory supports fundamental and exploratory research into solar cells. The purpose of the following set of research projects is twofold: (1) to provide fundamental experimental and theoretical foundations to existing photovoltaic (PV)/solar cell technologies, and (2) to explore whole new possibilities in PV/solar cell technologies, however revolutionary or nonconventional they might be. As surely as a number of revolutionary new solar cell technologies will most likely involve high-risk, long-term R&D to bring them to fruition, and may also well be needed as a complement to a future energy portfolio, so we also need timely results. As such, one of the primary driving motives for this effort is the possibility of developing one or more "leapfrog" technologies. These are technologies that have the distinct possibility of "leaping ahead" of existing technologies rather than taking the more characteristic development time of 10 to 20 years.

INTRODUCTION

To some extent, success in R&D is based on sheer statistics: fund enough very good groups and with good ideas, and if there is a good solution to be found, it most likely will be. Although not a formal DOE program, collectively these projects function as a program of directed research with the end goal of combined high-efficiency (≥40%) and low-cost (≤50¢/watt) device technologies. Consisting essentially of 34 leading research teams, the projects span a wide range of investigations. In an effort to more clearly distinguish the conventional versus the new, perhaps exotic or non-conventional technologies, both here and in the future, we will propose a categorization scheme to track the basic physics involved for any given device type.

In this context, "nonconventional" solar cells include: (1) quantum-structure solar cells based on nanometer-scale geometries such as "tetrapods," dots, cylinders, and fullerenes; (2) organic cells including molecules of low molecular weight (less than 10,000 amu), such as molecular chromophores and liquid crystals, and polymers of high molecular weight (10,000 to 1,000,000 amu or more); and (3) hybrids of the first two categories, such as dye-sensitized solar cells and polymer/quantum concepts. Next, in terms of high-efficiency conventional devices, studies are being conducted on GeC, GeSi substrates for III-Vs, hot-carrier devices, and III-V nitrides. Advanced analysis techniques such as positron annihilation spectroscopy, femtosecond spectroscopy, and synchrotron studies are being developed and applied to different materials as part of both the fundamental and exploratory studies. Given limited space and numerous projects, we will indicate succinctly the nature of the research, the corresponding research group, and a reference for further inquiry into their work with the reference itself indicating the project principal investigator(s).

Now, more than ever, there is a national mandate for a sustainable and independent energy future. As such, every plausible possibility for solar-powered electricity should be investigated and, as appropriate, developed just as efficiently as possible. Such technologies are deployable over different time frames—e.g., the present, near term (3-5 yr), medium term (5-10 yr), and long term (10-20 yr)—but even the seemingly "long-term" future will arrive all too soon. In the U.S. solar cell arena, such a mandate calls for an intense domestic fundamental and exploratory research program in solar cell-related technologies. Given the gravity of the matter, it is time—past time, actually—to evaluate rigorously all plausible possibilities.

In response to this need, two fundamental research projects were initiated during the last 3 years: the Future Generation project and the Beyond the Horizon project. Some of the projects are directed, high-risk, long-term research; other research focuses on existing technologies in which "knotty" problems have prevented nearly mature technologies from becoming commercially viable.

These projects are primarily university based because universities represent our single greatest repository of scientific knowledge and innovation. As the birthplace of bold new ideas, new energy, and the next generation of technologists, our universities have been, and will continue to be, instrumental in reaching our national energy objectives. This paper provides an overview of the current landscape of solar cell technologies being investigated by various research teams.

Before beginning with particular projects, let's distinguish between two fundamental categories of solar cells that may be useful to both present and future discourse regarding solar cell technologies.

In the first category, we have "conventional" inorganic technologies, or those solid-state semiconductor devices historically regarded as PV materials and devices, such as Si, a-Si, III-Vs (e.g., GaAs, GaAs nitrides), II-VIs (e.g., CdTe), and I-III-VIs (e.g., $CuInSe_2$). We will simply designate these as conventional solar cells. A second major, and distinguishable, category of solar cells includes organic, dye-sensitized, "plastic," polymeric, and nanostructured solar cells. These "nonconventional" solar cells could be generically and reasonably referred to as organic solar cells, or even plastic solar cells. Although the

term “plastic solar cell” could itself be reasonably associated with a solar cell on a flexible plastic substrate, it can only be justifiably used to include any polymer solar cell that includes an organic semiconductor as at least one of the active elements. However, a more fundamental distinction would be predicated on differences in their fundamental operating principles—for example, the mechanism by which photons generate charges or by which the charges are separated and collected. Conventional solar cells rely on photon-generated electron-hole pairs that are subsequently separated by a field caused by band bending between n- and p-type materials and thereby collected as a current. In contrast, cells in the organic category rely on photon-generated excitons (bound electron-hole pairs) whose charges are separated as they encounter local differences in electrochemical potentials, typically at interfaces within the cell structure. Hence, we propose using the term “excitonic solar cells” when referring to this category of solar cell. The physics related to the distinction between these categories of solar cells has been quite effectively addressed in a recent work by Gregg [1]. Using this distinction, we can now speak of fundamental versus exploratory research within the categories of conventional versus excitonic devices. The reason this distinction has become important is the relatively recent dramatic increase in interest in excitonic solar cells, their very real potential to use low-cost, nontoxic organic materials with corresponding low production costs and moderate-to-high conversion efficiencies. This potential for high energy conversion rates is most dramatically shown by the technological progress of organic light-emitting devices (OLEDs), now used in an array of display applications such as cellular phone displays. A recent Nobel Prize awarded for the discovery of this phenomenon and an implicit set of technologies highlight the significance of these organic semiconductors.

FUTURE GENERATION PROJECT

Initiated in 1998, the Future Generation Photovoltaic Technologies Project resulted from a consensus at a 1997 international meeting—often referred to as “The Leapfrog Conference”—specifically convened to review the viability of existing PV technologies and to present and discuss possibilities that might conceivably “leapfrog” current technologies into the future [2]. Photovoltaic technology as a whole was only seeing incremental performance increases, with diminishing hope for a dramatic breakthrough that would lead to a much more commercially viable position in the energy marketplace. As a result, there was a request for proposals and a rigorous competition, with 18 university groups selected and funded to explore possible future-generation PV and conduct fundamental research on conventional solar cell technologies.

Using new characterization techniques and materials studies, five groups focused on the debilitating Staebler-Wronski effect, which has hindered the full potential of terrestrial a-Si cells. Within this area, University of Illinois (Champaign) researchers studied the problem of light-induced instability, medium-range order, and light-induced changes in long-range disorder in a-Si as a function of temperature and deposition method, using fluctuation transmission electron microscopy [3]. Two sophisticated and complementary characterization techniques were developed and applied to the study of microcrystalline a-Si (or what has come to be known as “protocrystalline Si,” in which thin-film a-Si also contains crystallites and is on the verge of extensively crystallizing from those points out). One technique, femtosecond spectroscopy, characterizes the ultrafast carrier dynamics occurring in a-Si in its transition from amorphous to microcrystalline Si [4]. The other technique, positron annihilation spectroscopy, uses antimatter to characterize the corresponding defect states in the same sample [5]. These techniques have been extended to characterizing other PV materials, as well. Researchers at Cornell have examined the intrinsic elastic properties of a-Si using their unique double-paddle oscillator characterization technique as another signature of the physics of the material under different growth and treatment conditions [6]. A group at the University of Minnesota has been studying light-induced changes in long-range disorder in a-Si [7]. Finally, Wronski and Collins at Pennsylvania State University have developed quite useful methods for monitoring the optical properties, and modeling the growth, of prototype Si in real time, which is of much interest to the a-Si community [8,9].

In other thin-film devices, two groups at the University of Oregon are working on thin-film copper indium gallium diselenide (CIGS). One group is developing monolayer deposition of CIGS, and the other has applied photocapacitance techniques to probe the number and type of defect states at the junction [10]. Kao’s group at the State University of New York-Buffalo have used the National Synchrotron Light Source at Brookhaven National Laboratory for GIXS, XAFS, ADXRF, XRD, and AXS analyses to characterize the microstructure of interfaces in a number of thin-film cadmium telluride (CdTe), CIGS, and III-V materials [11].

In the high-efficiency device arena of III-V materials, four universities are investigating different facets of innovative growth methods and characterization of III-V nitrides, with the attendant possibilities for bandgap engineering and the goal of 40%-efficient devices. In particular, the University of California-San Diego [12] and North Carolina State University [13] are combining varying N content in GaInNAs and strained superlattices for bandgap engineering for high-efficiency devices. A collaboration between the University of California-Santa Barbara (for metal-organic chemical vapor deposition and molecular-beam epitaxial growth of GaInAsN) and Harvard (spectroscopic investigations of the subsurface interface electronic structure by ballistic-electron-emission microscopy) has led to increased understanding of the band structure through clear correlation between the predicted band structure and experimentation at layer interfaces within the GaAs nitrides [14].

In terms of Si itself, low-temperature, high-throughput processes for thin, large-grained Si using hot-wire chemical vapor deposition and modeling of the corresponding processes involved are being rigorously pursued at the California Institute of Technology [15]. In a spin-off of their work on porous polycrystalline Si solar

cells, the University of Rochester has created an effective antireflective coating and textured surface using porous-Si surfaces for light trapping that is already of interest to industry [16].

Another project that is both scientifically and commercially significant is the variety of p-type transparent conductive oxide (TCO) films, produced at Northwestern University, that have both high transparency and low resistivity with tunable bandgaps [17]. Within the domain of complex chemistry and obvious practicality is the modeling of chemical reactions between the encapsulant and PV devices in PV modules under field test conditions at Pennsylvania State University [18]. Finally, a West Virginia University team has developed nanostructure-arrays for potentially cost-effective multijunction solar cells, with unanticipated spin-off applications already at hand [19].

Within the Future Generation excitonic materials and device work, the University of California-Berkeley group has developed a number of unique, nano-crystalline composites, some recently reported in *Science*, along with a current efficiency of 2.7% and, more importantly, vital increases in the fundamental understanding and control of these material systems [20]. This reporting, in turn, has received considerable attention from the news media. Concurrently, Vanderbilt has been working on nanocrystalline-based polymer solar electric devices with fullerenes being incorporated to improve charge transport [21].

These Future Generation groups first presented papers at a special symposium, "Photovoltaics for the 21st Century," at the Electrochemical Society Meeting held in Seattle, Washington, in May 1999 [22]. An update of these research results were presented 2 years later at the "Symposium on Photovoltaics for the 21st Century, II," as part of the Electrochemical Society meeting held in Washington, D.C., in March 2001 [23].

BEYOND THE HORIZON PROJECT

Begun in mid-to-late 2001, the Beyond the Horizon initiative was a step beyond the Future Generation project, with much greater emphasis on exploratory research—exploration "beyond the horizon" of our current knowledge and our current paradigm. Considered "directed blue sky research" and still aiming at the same program goal, this initiative involved 11 universities and 5 companies and was intended to explore more of this uncharted territory.

We begin our discussion again with the familiar PV material systems. One California Institute of Technology group is probing the extremes of PV, namely, ultrahigh efficiency (≥40%) and very low cost. The former goal will be realized by "cut and paste," that is, by implantation-induced layer splitting ("cut") and transfer followed by III-V growth on bonded layers ("paste"). The low-cost device portion involves work on relatively low-cost techniques for the hot-wire chemical vapor deposition growth of thin-film c-Si [24]. Still within Si, there is the nanoscale design of thin-film heterogeneous Si solar cells at Iowa State [25] and microcrystalline Si solar cell work at United Solar Systems Corp. Under the heading of thin films, but moving away from Si, there are two projects in low-cost copper indium diselenide (CIS). The first project involves investigating lower cost, low-temperature processing of CIGS devices [26], and the second is a bold attempt at low-temperature, nonvacuum processing of CIGS and, therefore, dramatically lower production costs [27].

In the high-efficiency regime, we also have GeSi buffer layers on Si substrate for III-V solar cells at Ohio State University [28], and the synthesis and nanometer-scale characterization of GaInNAs for high-efficiency solar cells at the University of Michigan [29].

Within the category of excitonic solar cells, quite promising work is underway among different groups. Princeton is working on very high-efficiency solar cells via double-heterostructure and tandem organic solar cells with integrated concentrators. Critical components of this work will be in increasing the excitonic diffusion length, multiple series-connected organic molecule cells in a tandem PV cell, and a clever design for an integrated solar concentrator [30]. Polymer photovoltaic, multilayered devices have already been produced at the University of California-Santa Cruz [31]. The University of Arizona is developing liquid-crystal, molecular organic-based PV devices. Capable of being processed in large areas, these materials have high charge-generation efficiency (large surface area), high charge mobilities, and good photostability; in addition, they are "self-repairing" [32]. In molecular-chromophore solar cell work, joint efforts between North Carolina State and Johns Hopkins are focusing on electron transfer mechanisms in a next-generation dye-cell concept that is totally organic [33], and another Cal Tech group is investigating a number of mechanisms for improving efficiency in dye-sensitized solar cells using a hybrid inorganic/organic exciton concept [34]. Though not yet under contract, DuPont is interested in joining forces with the National Renewable Energy Laboratory (NREL) to develop organic solar cells.

Finally, an eclectic group of projects within this Beyond the Horizon program includes broad-band rugate filters for high-performance solar electric concentrators and a 1-year preliminary inquiry into the possibility of using optical rectenna solar cells as solar cells [35].

CONCLUSION

Our brief discussion mentions only about half of the overall set of 58 projects falling under this fundamental and exploratory research program but we hope we have provided a sense of the overall direction and content of the program and the wide spectrum of investigations of both existing and futuristic solar cells. Much more than a number of isolated scientific investigations, this program consists of directed projects in basic research that represent work performed in concert with other university groups and industry wherever possible. The whole set of projects, including all of the activities at NREL, is regarded as one network, one effort, one ensemble—all directed to finding solar cells that can make a significant and timely contribution to the nation's clean energy needs.

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