

# Novel Materials for Photovoltaic Technologies

## Preprint

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## NOVEL MATERIALS FOR PHOTOVOLTAIC TECHNOLOGIES

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While existing photovoltaic technologies continue to advance, there are still many exciting opportunities in the area of novel materials. These opportunities arise because there is a substantial need for reducing the costs associated with the preparation and processing of photovoltaics, and because the theoretically possible photovoltaic efficiencies have yet to be achieved in practical devices. Thus it remains reasonable to continue photovoltaic research activity aimed at entirely new approaches to processing and at entirely new materials as the active media. This group identified three areas for further consideration:

1. Nano/molecular composites and hierarchical structures
2. Organic semiconductors
3. Hot carrier devices

## **Nano/molecular composites and hierarchical structures**

One of the greatest areas of opportunity in novel photovoltaics arises from developments in the physics and chemistry of nanometer scale components. Over the last decade there have been dramatic improvements in our understanding of the physical properties of nanocrystals, nanotubes, and nanorods; in parallel, there has been a great deal of progress in methods for the preparation and assembly of these objects into functional assemblies. Photovoltaics based upon the assembly of nanometer scale components may be advantageous for the following reasons:

1. Charge generation and separation take place on the nanometer scale, and thus assembly of components on the same length scale may permit detailed tailoring of properties;
2. Size dependent scaling laws allow for control of fundamental properties, for instance the optical density is enhanced in small semiconductor particles, as compared to the bulk, due to quantum confinement effects;
3. The use of nanoscale components can lead to many of the advantages observed in MBE grown systems (tandem cells), but with very inexpensive processing. Isolated nanoscale building blocks can be produced cheaply, with almost no defects; Nanoscale components can be compatible with the elimination of toxic materials, and processing of large areas at low temperature.

There are several indications that these ideas are reasonable. Foremost among these is the recent development of the Graetzel cell, which is inexpensively assembled from nanoscale components, and which displays an efficiency of 10-12%. In this cell, the individual components are assembled in a crude manner, and there is a great deal that could be gained by further systematic design. For instance, well-defined nanorods of two different semiconductors could be assembled in bundles, so that charge separation can take place at the interface between the rods, and then the individual charges can be conducted along the rods to the appropriate electrodes. By stacking layers of such devices, each layer with a different diameter of rod, a multi-band gap cell could be constructed, due to the quantum size effect.

While the realization of such cells may still be a decade or more in the future, even in the short term there are potentially significant advantages to processing with nanoscale components now. Nanometer size crystals melt at lower temperatures than bulk crystals. Thus it is possible to spray nanocrystals onto a hot substrate, where they will fuse and form a thin film, at temperatures far lower than where thin films are grown by alternate methods. Further, such spray pyrolysis does not require vacuum, and thus is compatible with large area processing.

There are numerous areas of research that need to develop further before photovoltaic cells based on the assembly of nanoscale components can be realized. These include the ability to assemble components on multiple, hierarchical length scales, and the study of the physics of charge separation, electrical contact, band offsets, and electrical transport in composites of nanoscale components. This requires parallel developments in theory and experiment, in physics, chemistry, and materials science.

### **Organic Photovoltaics**

Photovoltaics based on organic crystals, polymers, and molecules represent a potentially attractive approach to solar energy conversion. Organic materials offer the possibility of providing low cost, flexible, light weight, easily processed, environmentally friendly photovoltaics. The low power output realized from existing organic photovoltaic technologies has rendered them commercially non-viable. However, the wide range of materials that can be prepared and processed provides immense variability in composition that may one day be exploited to rationally design efficient organic photovoltaics.

The recent advent of commercially available light-emitting-diodes based on organic polymers and the development of processable semiconducting polymers with improved quality provide proof that organic materials can be used in photonic devices. If these or related materials are made to be viable in the photovoltaic industry, improved solar conversion efficiencies are urgently needed. Organic solar cells reported to date have less than 1 % efficiencies under solar irradiation which compares poorly with 10-15 % of silicon photovoltaics. It is likely that new organic materials with small band gaps

and high electron/hole mobilities are required for a future generation of efficient organic solar cells.

Organic materials may also provide applications in composite solar cells. One such application is in the sensitized nanocrystalline solar cells described in this chapter. Organic dyes with high oscillator strengths may be used in place of the widely used Ru(II) polypyridyl compounds. Furthermore, organic polymers or gels ('hole conductors') may be used in place of the iodide/triiodide electrolyte currently employed in the nanocrystalline solar cells. Other niche markets of organic materials already exist, and progress in these areas could help to lower costs and alleviate environmental problems for organic derived photovoltaic technologies.

In summary, organic solar cells offer many potential advantages over existing technologies but suffer from low power conversion efficiencies. The development of an efficient organic photovoltaic would provide the proof-of-concept required for industrial support and eventual commercialization. Organic materials may also find applications as components in more traditional photovoltaic devices.

### **Hot Carrier PV Cells**

The maximum thermodynamic efficiency for converting solar radiation into electrical or chemical free energy is 32% for a single bandgap absorber if the photogenerated charge carriers (electrons and holes) are allowed to come to complete equilibrium with the lattice vibrations of the system (phonons in semiconductor materials). Carriers produced by absorption of photons with energies above the bandgap have excess kinetic energy and are called hot carriers; they have an electron or hole temperature greater than the lattice temperature. For solar radiation absorbed by semiconductors the initial photogenerated electron temperature is 3000K.

The equilibration (cooling) of the photogenerated carriers in semiconductors occurs via electron-phonon scattering and results in carrier cooling; in bulk semiconductor materials the process is very fast (a few picoseconds at solar intensities). Hence, the assumption of complete carrier-phonon equilibration in PV cells based on bulk semiconductor p-n junctions is usually valid. This means that the excess kinetic

energy of carriers created by absorption of photons having energies in excess of the bandgap is dissipated as heat by carrier-phonon interactions.

The optimum bandgap for single bandgap PV cells is 1.2-1.4 eV; since solar photons have an energy range of 3.5 to 0.6 eV, a large fraction of the energy of absorbed supra-bandgap photons is lost as heat, resulting in the 32% limit on conversion efficiency. If this energy loss to lattice vibrations can be avoided, the thermodynamic efficiency of converting solar radiation to free energy is increased and reaches 66% in the limiting case of no carrier cooling loss. To reduce the thermalization loss in PV cells, the conventional approach has been to utilize tandem multi-bandgap structures to more closely match the absorption characteristic of the PV cell to the solar spectrum. The larger bandgap region absorbs the bigger photons and the smaller bandgap region absorbs the smaller photons. For 2- and 3-bandgap tandem structures the theoretical thermodynamic efficiencies are increased to 42 and 50%, respectively.

Another way to avoid carrier cooling losses is to utilize the excess kinetic energy directly. This can be done in two ways: (1) extract the photogenerated carriers before they cool to produce a higher photovoltage; and (2) utilize the excess kinetic energy of hot carriers to produce a second electron-hole pair via an impact ionization process (reverse-Auger recombination).

The first approach requires that the rate of carrier transport and collection in the PV device be faster than carrier cooling; if the carrier cooling can be slowed this, of course, makes this process more competitive. Large reductions in carrier cooling rates have been observed in quantized semiconductor structures at high photoexcitation intensities. The second approach requires that the rate of impact ionization be greater than the rate of hot carrier cooling.

Since successful hot carrier processes in PV cells can produce much higher theoretical conversion efficiencies in single bandgap materials, their structure could be more simple than tandem solar cells and a research effort on these types of new PV cells

is warranted. The problems that need to be addressed are: (1) how to slow hot carrier cooling in semiconductors at solar light intensities; (2) how to collect hot carriers efficiently at the contacts in hot carrier PV cells; and (3) how to enhance reverse-Auger processes to make them competitive with carrier cooling.