Editorial

Molecular Design of Thin Film Optoelectronic Materials for Solar Cells

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Chemistry is expected to play a prominent role in advancing the discoveries needed to unlock the promise of alternative and renewable energy sources. Building on the analogy of the late Nobel Laureate Richard Smalley, who described chemists in this pursuit as "nurturers of the garden of science and engineering", the pages of the *Journal of the American Chemical Society* have become a showcase where harvests of the field are put on display. The abundance of recent progress in photovoltaic materials makes now an appropriate time to collect and arrange the fruits of these labors into a cornucopia we call *JACS* Select, the name visitors to the *JACS* Beta Web site (http://pubs.acs.org/JACSbeta) have chosen for the Journal's virtual issues.

This particular *JACS* Select brings together a fascinating assortment of science in the theme of "Molecular Design of Thin Film Optoelectronic Materials for Solar Cells". This title may, at first glance, sound narrowly defined; however, skimming through the contents will reveal an amazing breadth of topics that squarely hits on all four of chemistry's traditional disciplines and extends into materials topics such as solid state, polymer, supramolecular, and nano sciences. The research that you will read is melded with theory, synthesis, processing, device fabrication, and measurement. Finally, you will see that the publications address fundamental issues such as our understanding of hole−electron transfer or the interaction of light with molecular matter, as well as technologically relevant discoveries like the invention of new transparent conductors.

High efficiency of power conversion is the benchmark sought after in the solar cell field. This term quantifies the power collected and converted from light to electricity. While the efficiencies of silicon-based solar cells now exceed 22%, their high cost of production and inflexibility present a unique opportunity for molecular-based devices. Even though the efficiencies of solar cells based on molecular materials are presently lower than efficiencies of silicon by a factor of 2 or more, molecular materials offer the promise of easy processing and the ability to conform to large-area substrates of complex shape, simply being applied as a coating or ink.

Two main approaches are commonly used to fabricate molecular-based photovoltaic devices. One tactic is the dye-sensitized solar cell (DSC or DSSC), the efficiency of which currently tops out at ca. 11%. The second approach is the concept of bulk heterojunction (BHJ) materials, where blends of organic components such as a semiconducting polymer (usually an electron donor) and an electron acceptor phase-separate on the nanoscale, enabling photoinduced electron transfer at the interface. The best BHJ materials currently have efficiencies of only 5%, but this low number is almost certain to rise, just as rapid progress was made during the past decade on closely related materials—the organic light-emitting diodes.

Many of the issues that limit the practical utility of solar cells based on both DSSCs and BHJs are examined in this *JACS* Select collection, along with new materials such as flexible conductors that may play critical roles in novel applications such as easily deployable solar canopies. The first eight publications in the virtual issue address limitations in DSSCs or related device concepts, highlighting critical factors that must be optimized to achieve higher power conversion efficiencies and greater stabilities. The latest developments on designing robust, highly efficient sensitizers are described in a pair of publications, the first reported by **Wang**, **Zakeeruddin**, and **Grätzel**[1] and the second by **Hagfeldt** and **Sun**.[2] Next, a pair of contributions by **O'Regan** and **Torres**[3] and **Yanagida**[4] describe new aspects related to the chemistry of the redox electrolyte. The remaining four Articles and Communications in this group report on novel building blocks for DSSCs, starting with the use of hyperbranched conjugated

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polyelectrolytes by **Schanze** and **Reynolds**,[5] followed by **Pyun** and **Armstrong**'s use of nanoparticle composites[6] and **Kamat**'s quantum dot solar cells.[7] Finally, **Matsuo** and **Nakamura** communicate a photocurrent-generating interface, beautifully illustrating how molecular details such as the geometric configuration of the photoactive acceptor and donor can strongly influence the functional characteristics of the system.[8]

The next six publications describe recent advances in BHJ thin film materials. One of the emerging themes in this area of research is that the morphology of the blend—the size and shape of the phase-separated domains—plays a critical role in device performance. Methods of manipulating the morphology are clearly important, e.g., through the use of additives as reported by **Heeger**[9] or by carefully selecting conditions to deposit a three-dimensional network of preassembled polymer−semiconductor nanowires blended with a fullerene acceptor, as reported by **Jenekhe**.[10] Fundamental processes such as charge generation and the lifetime of photogenerated radical ion pairs are also essential to enhance device performance in molecular-based systems. The topic is investigated at the molecular level by **Ratner** and **Wasielewski** using time-resolved spectroscopic methods and a donor (D)−bridge (B)−acceptor (A) model, yielding a set of observations that can only be described by hole transfer involving the highest occupied molecular orbitals of the D−B−A system.[11] Complementing this time-resolved molecular-level description is a report on spatially resolved photovoltaic activity by **Palermo**, **Müllen**, and **Samorì**, in which the behavior of phase-segregated acceptor−donor blend architectures is revealed by Kelvin probe force microscopy.[12] A subsequent contribution by **Janssen** details a photophysical study of a BHJ polymer−fullerene blend, quantifying the electron−hole dissociation kinetics and its dependence on electric field and blend composition; the data support the hypothesis that fullerene clusters are crucial for efficient generation of free charge carriers in photovoltaic devices.[13] An article by **Leclerc** rounds out this group by highlighting some of the challenges of rationally designing new BHJ polymers, revealing that factors like polymer molecular weight and solid-phase organization weigh heavily into solar cell performance.[14]

The final six contributions report exciting new molecular materials relevant to solar cells. Two of the publications describe intriguing molecular approaches to donor−acceptor heterojunctions, one by **Campidelli**, **Guldi**, and **Torres** which involves "click chemistry" and single-wall carbon nanotubes[15] and another by **Fukushima** and **Aida** that involves supramolecular coassembly.[16] While polythiophenes have been a workhorse among the semiconducting polymers for photovoltaics, theoretical studies have indicated that the polyselenophenes may offer superior properties. This issue of *JACS* Select includes a Communication by **Bendikov** on poly(3,4-ethylenedioxyselenophene) (PEDOS), the first highly conductive selenium analogue to one of the most important polythiophenes.[17] Although PEDOS has yet to be tested in photovoltaics, the reported properties suggest exciting promise for this material. The next two contributions, one by **Peng**[18] and one by **Sun**,[19] describe molecular materials that produce transparent conductive films, possibly paving the way to new substrates for flexible solar cells and other

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applications. The final article, by **Köse**, gives a detailed theoretical account of a light harvesting, π-conjugated dendritic macromolecule.[20]

We hope these contributions provide our readers with an up-to-date view of molecular photovoltaic materials. What is most exciting about this issue is the recognition that, for all the progress realized to this point, we are certain to see many new, exciting developments in the coming months and years. The overarching problem being addressed is clearly an important one to solve, and we are certain that the pages of *JACS* will be filled with many of the important breakthroughs that will ultimately contribute to harnessing and delivering the energy needed to sustain our world.

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