

## Polymer-Based Materials for Harvesting Solar Energy (PHaSE)

EFRC Directors: Thomas P. Russell and Paul M. Lahti

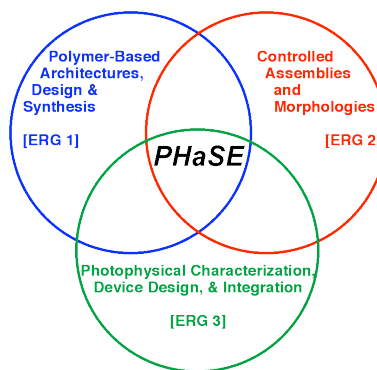
Lead Institution: University of Massachusetts Amherst

### **Mission Statement.**

The goal of the EFRC led by the University of Massachusetts Amherst is to carry out fundamental photovoltaic-oriented research using organic-based polymers and related materials to maximize efficiency in the collection and harvesting of energy over a broad frequency range of the solar spectrum. The center's strongly-networked, interdisciplinary teams of researchers seek ways to minimize charge-quenching exciton recombination, to maximize electron transport across inorganic/organic interfaces, and to optimize design and fabrication strategies for making inexpensive photovoltaic devices.

### **Center Research Portfolio:**

The University of Massachusetts EFRC integrates investigators from multiple departments and institutions into three distinct but cooperating Energy Research Groups or ERGs: ERG 1 *Polymer Based Architecture: Design and Synthesis*, ERG 2 *Controlled Assemblies and Morphologies*, ERG 3 *Photophysical Characterization, Device Design and Integration*. Synthetic work in ERG 1 is complemented by collaborations with the Global Research Laboratory at Seoul National University, the University of Bayreuth and the Heeger Institute at the Gwangju Institute of Science and Technology. Morphological studies in ERG 2 are augmented by theoretical studies of hierarchical ordering with the University of Pittsburgh, and by theoretical studies of exciton dissociation at organic-organic and organic-inorganic interfaces with the Oak Ridge National Laboratories and with Rensselaer Polytechnic Institute. Physico-chemical and test-device work in ERG 3 is augmented by collaborations at the University of Massachusetts Lowell and Konarka. Preparation of anatase titania nanorods and nanotubes is done at The Pennsylvania State University. Inorganic nanoparticle/nanorod synthesis and assembly is pursued at the World Premier Institute, Advanced Institute of Materials Research at Tohoku University. In appropriate cases, the efficiencies of test devices produced by this EFRC will be evaluated and benchmarked at the National Renewable Energy Laboratory.

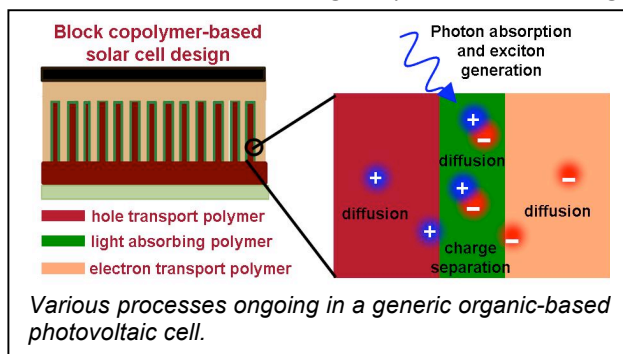


**ERG 1.** The primary research thrusts of this group fall into two main areas. The first is the synthesis of conjugated homopolymers, block copolymers, segmented structures and materials with well-defined structural architectures, with control over component energy levels using electron withdrawing and donating functionality. The second is the preparation of p-type conjugated polymers with end-groups suitable for functionalization of n-type nanoparticles and nanorods, leading to effective dispersion of the particles and rods, and the preparation of hierarchically oriented nanomaterial assemblies for devices. Most of these targets are designed for light harvesting and photocurrent generation, for integration into the active layers of photovoltaic (PV) devices. Synthetic strategies focus on molecular self-assembly for morphological control, plus processibility of polymer and molecular species with structure-tunable photophysical characteristics that can aid more efficient PV behavior. A unifying objective of all work is to provide a range of polymer and nanocomposite materials for morphological and PV device studies undertaken in ERGs 2 and 3.

**ERG 2.** The design and fabrication of a high-efficiency PV device requires precise control over the nanoscale morphology, molecular ordering, and interfacial properties of all components comprising the device. While easy to state, these tasks are practically challenging; most research on polymer-based PV devices to date typically studies just one such task in detail. ERG 2 integrates researchers with well-established expertise in synthesis, as well as theory and engineering of polymers to control self-

assembly of polymers and to manipulate polymer morphologies and individual chains in thin films. This expertise will be used to develop routes to control morphology and structure of polymer-based and polymer/inorganic-based hybrid materials so as to optimize photovoltaic efficiency. The knowledge gained from these studies can then be used in device-fabrication strategies.

**ERG 3.** In an organic solar cell, the conversion of light energy to electric current involves several fundamental processes: (1) absorption of light to create excitons, (2) diffusion of excitons to a region of high electric potential mismatch where charge separation can occur, (3) charge separation, (4) charge transport of holes and electrons to their respective electrodes, and (5) transport of the carriers across the respective organic-electrode interfaces (see figure to right). All of these processes need to be understood to optimize them for higher efficiency solar cells. Detrimental effects – like charge carrier recombination and trapping – need to be assessed to identify structures that inhibit these effects. By state-of-the-art time-resolved optical techniques it is possible to distinguish and quantify the lifetimes and evolution mechanisms of these processes.



A primary goal of ERG 3 is to elucidate photophysical details of charge and energy transport within nanostructured photovoltaic composite films. Single-molecule and time-resolved spectroscopies provide valuable mechanistic insight about the behavior of the synthetic building blocks and their molecular architecture on the primary processes in PV systems. The “feedback loop” of design ↔ synthesis-assembly ↔ physical process evaluation ↔ test device evaluation and back again allows identification of the most promising strategies for more rigorous PV device fabrication and testing in collaboration with UMass Lowell and industrial collaborator Konarka Technologies Inc.

<b>Polymer-Based Materials for Harvesting Solar Energy (Lead Personnel)</b>	
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