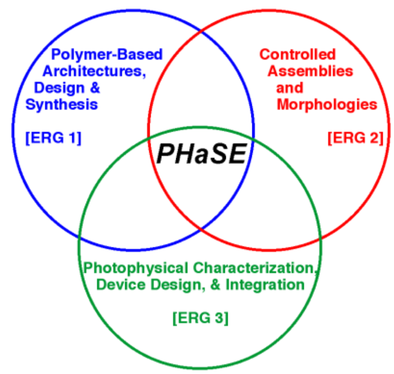
Polymer-Based Materials for Harvesting Solar Energy (PHaSE)
EFRC Directors: Thomas P. Russell and Paul M. Lahti
Lead Institution: University of Massachusetts Amherst

Mission Statement: *To carry out fundamental photovoltaic-oriented research on the use of 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.*

Center Research Portfolio:

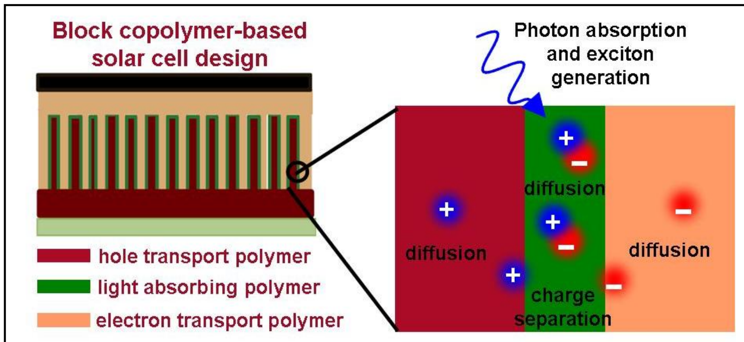
The University of Massachusetts EFRC integrates investigators from multiple departments and institutions into three distinct but interlinked Energy Research Groups or ERGs: ERG 1 *Polymer Based Architecture: Design and Synthesis*, ERG 2 *Controlled Assemblies and Morphologies*, ERG 3 *Photophysical Characterization, 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 Laboratory 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 The Pennsylvania State University. Inorganic nanoparticle/nanorod synthesis and assembly at UMass Amherst is enhanced by collaborations at the World Premier Institute, Advanced Institute of Materials Research at Tohoku University.



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 new p-type and n-type semiconductor polymers for light harvesting and photocurrent generation that can be used as active electronic layers in solar cells. Synthetic strategies focus on molecular self-assembly for morphological control, with structure-tunable photophysical characteristics that assist charge movement in a polymer solar cell. A unifying objective of all work is to provide a range of polymer and nanocomposite materials for assembly and behavior testing in ERGs 2 and 3.

ERG 2. The design and fabrication of a high-efficiency photovoltaic (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, theory, and engineering of polymers; all work together to devise means to control self-assembly and morphology of individual polymer chains in thin films. A major ERG 2 centered focus is the development of general strategies of polymer and molecular nano-scale assembly that work for a range of promising electronic materials. This will allow faster comparisons of efficacy for new materials, using the same assembly and testing process. This strategy also is being used to control morphology and structure of polymer-based and polymer/inorganic-based hybrid materials to optimize PV efficiency. The lessons gained from these studies can then be applied in test device fabrication.

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 charges across organic-electrode interfaces (see figure). All of these processes must be understood to design higher efficiency solar cells. Causes of detrimental effects – like charge carrier recombination and trapping – need to be assessed to avoid structures or morphologies that lead to them. State-of-the-art optical and microscopy techniques are being developed and utilized to study lifetimes and mechanisms of these processes.



Schematic of various processes ongoing in a generic organic-based photovoltaic cell.

A primary goal of ERG 3 is to elucidate photophysical details of charge and energy transport within photovoltaic composite films composed of polymers and molecules assembled on the nano-scale by methods developed in ERG 1 and ERG 2. Single-molecule and time-resolved spectroscopies provide valuable mechanistic insight about the electronic effects of synthetic building block variation and assembly on the fundamental processes in PV systems. A "feedback loop" of design ✶ synthesis-assembly ✶ physical process evaluation ✶ test device evaluation allows identification of the most promising materials and strategies for more rigorous charge mobility test and photovoltaic device fabrication in PHaSE's Photovoltaic & Optical Spectroscopy Facility, and in collaboration with UMass Lowell and Penn State. Computational modeling of these processes, including collaborative work at RPI and Oak Ridge, is also important to predict which materials and assembly schemes are most effective.

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