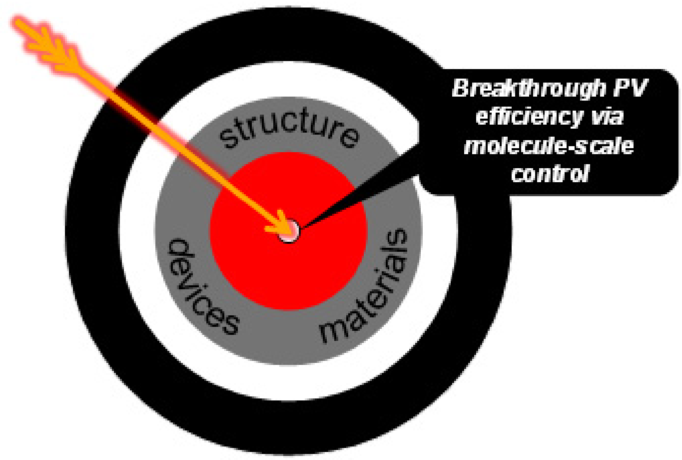
Re-Defining Photovoltaic Efficiency Through Molecule Scale Control (RPEMSC)
EFRC Director: James Yardley
Lead Institution: Columbia University

Mission Statement*: To develop the enabling science needed to realize breakthroughs in the efficient conversion of sunlight into electricity in nanometer sized thin films.*

The primary approach of the EFRC is to develop new fundamental understanding that will enable the development of revolutionary highly-efficient inexpensive photovoltaic solar cells. The EFRC will focus its expertise in chemical synthesis, fabrication, manipulation, and characterization of nanoscale materials and materials theory in order to: (1) systematically develop fundamental understanding of the primary photovoltaic processes in organic and hybrid materials needed to advance the efficiency of inexpensive solar cells toward the well-known Shockley-Queisser efficiency limit; and (2) develop and quantitatively investigate new nanostructured materials with potential for extracting multiple electrical charges from a single absorption event thus establishing a scientific basis for moving the efficiency of these solar cell devices well beyond the Shockley-Queisser efficiency limit. The new understanding and novel nanomaterials developed by this research team are playing a key role in enabling the development highly-efficient solar energy technologies. The research program of the EFRC centers around four multi-disciplinary and interlocking research thrusts. Each thrust represents an integrated effort incorporating theory, materials, and measurement.



Thrust 1 examines aspects of “Charge Transport Fundamentals in Layered Systems.” In this thrust we are exploring new materials suitable for examination of the fundamental physics in solar cell devices building upon expertise in growing and fabricating structures based on ordered molecular layers one molecule thick including conductors (graphene), semiconductors (molybdenum sulfide) and insulators (hexagonal boron nitride). We are developing methodology for the study of charge creation, dissociation, diffusion, and charge separation in specifically-fabricated layered structures. These materials offer opportunity for fundamental understanding, but also have practical implications. Thus we are examining the efficacy of these new carbon-based conductor materials including graphene for use as transparent conducting materials for efficient extraction of charge from thin film photovoltaic devices. For example we have demonstrated a functioning novel “transparent” solar cell prototypical structure using transparent graphene electrodes for both cathode and anode.

Thrust 2 explores “Multiple Carrier Generation.” Our program is working to identify clear experimental signatures for multi-exciton generation (MEG) processes which are capable of producing multiple pairs of charge carriers with a single photon absorption event. This involves systematic exploration of MEG and related phenomena in quantum dot and carbon-based systems such as graphene nano-ribbons or carbon nanotubes using direct charge carrier detection as well as a variety of spectroscopic techniques. In addition we are exploring theoretically generic concepts for carrier multiplication processes. We are examining entirely new mechanisms for the fission of a single excited state into two excited triplet state molecules, which in turn generate two hole-electron charge pairs. This program will allow us to establish a quantitative and predictive understanding for a number of MEG and related carrier multiplication concepts. This theory will guide our experimental program in terms of systems under study and materials used in these systems.

Thrust 3 is dedicated to "New Materials for Solar Energy." In this thrust we are developing entirely new, and chemically well-characterized, nanoscale materials. These include new quantum dots materials and novel chemical compounds that we call "molecular clusters." In addition we have discovered a new class of charge-transfer molecular crystals that open up new solar energy opportunities. We are quantifying the dynamics and effectiveness of fundamental photophysical processes in these materials, using modern tools of Nanoscale science including ultrafast and single molecule spectroscopies. We are studying the structure of interfaces of these new and novel materials with other semiconductors as well as with metals. Based on these interfaces, we are correlating the charge transport characteristics at interfaces with the observed structure. We are also building a theoretical framework to model kinetic processes of charge transport, with input from atomic scale calculation of local bonding, structure, and electronic states. We are measuring the effectiveness of charge transport across interfaces using a variety of techniques including photoemission.

Thrust 4 represents a cross-cutting research platform which integrates concepts developed within the EFRC program into solar cell device prototype structures for quantitative demonstration of the efficacy of the technological developments within the Center. We are examining a concept called UTOP (Ultra-Thin Organic Photovoltaics) which is designed to achieve high photo conversion efficiency in very thin organic layers using new optical trapping techniques to efficiently absorb solar radiation. We are exploring prototypical solar cell structures built from unique molecules containing inorganic moieties useful for absorption of solar radiation and generation of excited electron-hole pairs. We hypothesize that these molecular analogs of quantum dots can effectively generate excitons in configurations where exciton transport, charge separation, and charge collection will be highly efficient. We are also actively characterizing prototype structures incorporating graphene electrodes.

Center for Re-Defining Photovoltaic Efficiency Through Molecule Scale Control	
Columbia University	James Yardley (Managing Director), Louis Brus (Scientific Director), Tony Heinz (Scientific Director), Simon Billinge, Ronald Breslow, Luis Campos, Dirk Englund, George Flynn, Irving Herman, James Hone, Laura Kaufman, Philip Kim, Ioannis Kymissis, Colin Nuckolls, Richard Osgood, Jonathan Owen, Abhay Pasupathy, David Reichman, Kenneth Shepard, Michael Steigerwald, Latha Venkataraman, Chee Wei Wong, Xiaoyang Zhu
Purdue University	Ashraf Alam
Brookhaven National Laboratories	Charles Black, Mark Hybertsen, Matt Sfeir

Contact: James T. Yardley
Professor, Electrical Engineering
jy307@columbia.edu
212-854-3839
www.cise.columbia.edu/efrc/