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Recovery Act –EFRC: Solar Energy Conversion in Complex Materials (SECCM)

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Executive Summary

Researchers at the University of Michigan designed and synthesized new materials for high efficiency photovoltaic (PV) and thermoelectric (TE) devices, predicated on new fundamental insights into equilibrium and non-equilibrium processes, including quantum phenomena, that occur in materials over various spatial and temporal scales.

They developed fundamentally new insights into relationships between synthesis, structures, and properties of inorganic thin films and low-dimensional structures, for thermoelectric and photovoltaic applications. This understanding enabled us to exploit trade-offs between absorption and transport processes in nanostructured materials. Our research enabled, for the first time, the elucidation of fundamental limits & opportunities for solar energy conversion in quantum dots and highly mismatched alloys (HMA)s. The impact of this work is that it provided guidance in the fabrication of advanced PV and TE devices. Moreover, it facilitated the *selection and design of materials for the special class of intermediate band & hot carrier solar cells*.

In another area, the researchers made significant advances into the computational and experimental design of materials for thermoelectric energy conversion. Specifically, through a combination of materials synthesis/processing, often guided by theoretical/computational efforts, they defined fundamental interactions that determine thermoelectric energy conversion efficiency in the following material systems: doped organic semiconductors, single molecules, nanowires, nanostructured bulk thermoelectric (TE) materials and highly

mismatched alloys (HMAs). These accomplishments enabled the identification of new pathways toward new materials design and morphological control for higher ZT. New and deep insights into quantum energy transport at the molecular level for existing and new technologies were gained.

The third major area of accomplishment includes the development of a fundamental understanding of the links between nanostructural morphology, chemical design and charge recombination in organic and hybrid materials. This was enabled through the use of computational tools, chemical design and synthesis, and processing strategies, to create new organic and hybrid materials possessing specific morphologies for energy conversion. An important accomplishment also included the development of the ideal diode equation for excitonic materials. This model not only predicted, for the first time, the thermodynamic limits of OPVs, but it also provided guidance in the molecular (chemical) structural design, morphological design and control of OPVs.

It is noteworthy that some of our accomplishments were predicated on the development and uses of ultrafast spectroscopic and scanning probe tools for investigating the spatial and temporal behavior of the organic, inorganic and hybrid materials. Consequently we were able to elucidate mechanisms of energy (electron, phonon, photon interactions) transport and charge transfer at the sub-picosecond scales and nanometer scales, improving materials selection and design for efficient energy conversion.

These research accomplishments provided new insights and understanding of three important grand scientific challenges posed by the Department of Energy. The first of these is “How do we control materials processes at the level of electrons?” Our work, for example, led to the understanding of the relation between the electronic structure of molecules and their heat dissipation properties. A second grand challenge is: “How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?” The researchers demonstrated the growth of organic thin films with novel crystalline yet smooth morphologies previously found only in nature (e.g. sea organisms). Additionally, they developed a model for multi-phase, multi-scale molecular transport that can predict nano-morphology from molecular properties and process conditions. A third Grand Challenge is “How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?” The researchers developed first-principles physics models of exciton and charge recombination at organic interfaces. This guided the molecular and structural design of materials, leading to higher efficiency solar cells. As a second example, the researchers developed an *ab initio* phase diagram of thermoelectric materials (substituted and filled skutterudites) that were experimentally synthesized. Experiments, for the first time, confirmed the model predictions.

Finally, these accomplishments are documented in over 250 refereed archival publications in high impact factor journals, and 22 patent applications. Moreover, 110 graduate students and Post docs, employed in US industry and academia.

Goals/Objectives and Accomplishments

The goal of the Center was to design and to synthesize new materials for high efficiency photovoltaic (PV) and thermoelectric (TE) devices, predicated on new fundamental insights into equilibrium and non-equilibrium processes, including quantum phenomena, that occur in materials over various spatial and temporal scales.

Our work was organized in three different thrusts below.

Thrust 1: Photovoltaic Applications of Inorganic Thin Films and Low-Dimensional Structures. We developed a fundamental understanding of relationships between synthesis, structures, and properties of inorganic thin films and low-dimensional structures.

Thrust 2: Thermoelectric Energy Conversion. We defined fundamental interactions that determine thermoelectric energy conversion efficiency in: doped organic semiconductors, single molecule systems, nanowires, nanostructured bulk thermoelectric (TE) materials, highly mismatched alloys (HMAs). This included the theoretical/computational design and experimental synthesis of materials for TE conversion.

Thrust 3: Energy Transport In Organic And Hybrid Systems. We developed a fundamental understanding of the links between nanostructural morphology, chemical design and charge recombination in organic and organic based systems.

The objectives and details of the accomplishments are now described for each of the thrusts.

I. Thrust 1: Inorganic Thin Films and Low-Dimensional Structures: Photovoltaic Applications

Objectives:

- A. Develop in-situ structural-optical-electrical characterization of semiconductor PV devices ranging from thin films to branched nanowires.
- B. Calculate the confinement-induced electronic bandgaps of wurtzite InGaN nanowires
- C. 3D phase-field simulations of the influence of buffer layer morphology on single and multi-layer QD growth
- D. Examine the influence of QD aspect ratio on carrier lifetimes and photovoltaic properties under a range of solar concentrations.
- E. Examine the nature of the IB states (extended vs. localized) and carrier lifetimes in highly mismatched alloy systems.
- F. Use density functional and many-body perturbation theory in the GW approximation to calculate the electronic states and optoelectronic properties of highly mismatched alloys.

- G. Examine alternative barrier layers to control carrier dynamics in staggered type II band offset QD heterostructures
- H. Examine ultrafast laser induced nanostructuring of ZnSe and its impact on the wavelength and angular dependence of absorption.

Accomplishments:

- **Mechanisms of Quantum Dot Formation during Annealing of Metallic Islands**

Provides new insights into the mechanisms of quantum dot formation which are likely to be applicable to a wide range of semiconductors. Semiconductor quantum dots have been proposed for a wide variety of solid state devices, including solar cells and light-emitting diodes. During annealing of In islands, crystalline InAs quantum dots form via either droplet epitaxy or solid phase epitaxy. For surfaces with metastable Ga-As dimers, one-to-one conversion from In island to InAs quantum dot occurs by droplet epitaxy. For surfaces with amorphous As cap, quantum dots nucleate by solid phase epitaxy, leading to more quantum dots than In islands. (Goldman, Pan)

- **What is the Band Alignment of GaSb/GaAs Quantum Dots?**

This investigation reveals the surface termination-independence of effective bandgaps and band offsets at GaSb/GaAs QD interfaces. Capped GaSb/GaAs QDs were grown by MBE on both Sb- and As- terminated surfaces. TEM reveals both coherent and semi-coherent clusters, as well as misfit dislocations, independent of surface termination. X-STM and STS reveal clustered QDs with “nested” type I band offsets at the GaSb/GaAs interfaces, consistent with those expected for unstrained GaSb/GaAs systems. (Goldman, Millunchick)

- **InGaN Nanostructures for Hot Carrier Solar Cells**

The energy band width of nanostructures grown using selective area epitaxy has been much broader than expected, reducing device efficiency in applications such as hot carrier solar cells. This work explains the origin of this energy state broadening. InGaN active layers were embedded in GaN nanopyramids grown by selective area epitaxy. A phase-field model was developed to simulate growth. The photoluminescence (PL) spectrum calculated from simulation showed good agreement with the measured PL spectrum. (Ku, Thornton)

- **Quantum-Confined InN for Visible-Wavelength Optoelectronics**

InN nanostructures may be used to fabricate solar cells, light-emitting diodes, and lasers that convert visible light to electricity and vice versa more efficiently. Atomistic first-principles calculations used to predict the electronic and optical properties of 1nm-wide InN nanowires. Quantum confinement in the nanowires substantially increases the band gap and the exciton binding energy compared to bulk InN, leading to efficient optical emission and absorption in the visible range. Quantum-confined InN nanostructures are a promising alternative to InGaN alloys for optoelectronic applications at green/cyan wavelengths, where efficient light emitting devices are currently unavailable. (Kioupakis)

II. Thermoelectric Energy Conversion

Objectives:

- A. Use MBE to grow $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ thin films and study their carrier and lattice dynamics by transport studies and by ultra-fast optical measurements.

- B. Carry out simulation studies on the new energy conversion mechanism incorporating potential barriers and hot carrier transport, and attempt to grow and explore relevant semiconducting structures.
- C. Explore contributions to the temperature-independent lattice conductivity of Cu_2Se and B_{13}C_2 from the short and long-range acoustic phonon transport.
- D. Explore the influence of embedded indium nanocrystals on thermoelectric properties of GaAs.
- E. Explore a possibility of shifting the position of the peak of the thermoelectric phonon-drag effect by the strength of the film-substrate interaction.
- F. Continue experiments on single molecular junctions with different molecules and their various terminations to elucidate heat dissipation and Peltier cooling.
- G. Pursue further improvements in the Seebeck coefficient of organic semiconductors.

Accomplishments

• **Influence of Embedded Metallic Nanocrystals on Thermoelectric Properties of Semiconductors:** This approach provides a possible path toward improvements in the thermoelectric properties of compound semiconductors. Low-dimensional structures, including embedded metallic NCs are predicted to enhance the thermoelectric figure of merit. Using In^+ ion implantation into GaAs with various annealing temperatures, we have identified conditions necessary for the formation of In NCs. We show these NCs act as electron donors, while the Seebeck coefficient is enhanced and grain boundary scattering reduces the thermal conductivity. Application of this approach to more heavily doped GaAs will likely lead to further increases in the Seebeck coefficient. (Goldman, Uher, Clarke)

• **Understanding Heat-Dissipation in Atomic-Scale Junctions**

This work establishes the formalism necessary for understanding heat dissipation in several mesoscopic systems where transport is predominantly elastic. Such systems include semiconductor nanowires, two-dimensional electron gases, semiconductor heterostructures, carbon nanotubes, and graphene, among others. Heat dissipation and transport nanoscale devices remain poorly characterized due to experimental challenges. In this study, using custom-fabricated scanning probes with integrated nanoscale thermocouples, it is shown that heat dissipation in the electrodes of molecular junctions, whose transmission characteristics are strongly dependent on energy, is asymmetric, *i.e.* unequal and dependent on both the bias polarity and the *thermoelectric properties of atomic-scale junctions*. In contrast, atomic junctions whose transmission characteristics show weak energy dependence do not exhibit appreciable asymmetry. These results unambiguously relate the electronic transmission characteristics of atomic-scale junctions to their heat dissipation properties. (Reddy)

• **Thermoelectric Properties of High Mismatched Alloys – Case of ZnTe:N**

Highly mismatched alloys (HMAs) have been predicted to exhibit enhanced TE properties. By changing the nitrogen concentration, a measurable improvement of the TE performance was demonstrated in the HMA system ZnTe:N . Thin films of ZnTe:N materials were grown on GaAs substrates layer by layer. TE properties were measured over a large range of temperatures 5 – 300 K. A greatly enhanced Seebeck coefficient at low temperatures was observed, which corresponded with a plateau in electrical resistivity. (Uher, Phillips)

• **“Adding” Electrons in Bismuth Telluride through Thallium Doping**

The presence of thallium atoms has been proved to be a more elegant and much easier way of controlling the electrical properties of bismuth telluride. The right number of thallium atoms can help making advanced electronic materials. Single crystals of $\text{Bi}_{2-x}\text{Tl}_x\text{Te}_3$ have been grown with $x = 0 - 0.30$. Microscopy and spectroscopy techniques have been used to analyze the structure and

chemical composition. Electrical and thermal properties have been characterized at different temperatures. Experimental data have been examined by theoretical model. (Uher)

- **Phonon Drag in Thin Films Tuned by the Choice of Substrate**

Our experiments provide a way to study the nature of the phonon spectrum in thin films, which is rarely probed but clearly important for a complete understanding of thin film properties and the interplay of the substrate and films. Bi_2Te_3 films were grown on BaF_2 and sapphire, substrates with vastly different physical properties. The magnitude of the phonon-drag peak strongly depends on the film thickness while the temperature where the peak occurs is thickness independent. (Uher)

- **Improving Thermoelectric Efficiency via Low Thermal Boundary Conductance**

Provides novel design principle for enhancing thermoelectric figure-of-merit (ZT) which could help achieve $\text{ZT} > 1$ for organic semiconductors. Low thermal boundary conductance (G_b) between organic semiconductor copper phthalocyanine (CuPc) and silver (Ag) proved to be beneficial to thermoelectric material design. Measurements showed thermal conductivity decreases initially as silver nanoparticle (NP) concentration ($x_{\text{Ag}}\%$) rises while electrical conductivity continues to grow, resulting in optimization in ZT at specific concentrations. Finite Element Modeling indicates that ZT values of organic-inorganic nanocomposites can be potentially enhanced 10-fold around the optimized filler concentrations ($x_f\%$) with interfacial engineering and particle size (radius r) control. (Shtein, Pipe)

- **A General Strategy to Enhance Thermoelectric Efficiency in Organic Semiconductors**

Since reducing dopant volume leads to a substantial increase in carrier mobility, this strategy can be applied to improve the performance of organic optoelectronic or electronic devices in which highly conductive OSCs are required. Removing excess poly(styrenesulphonate) (PSS) dopant from poly(3,4-ethylenedioxythiophene) (PEDOT) was shown to simultaneously increase both the Seebeck coefficient (S) and electrical conductivity (σ), leading to a significant increase in $S^2\sigma$. Thermal conductivity (k) was also decreased by removing PSS. As a result, all parameters constituting ZT ($= S^2\sigma/k$) vary so that ZT increases, leading to $\text{ZT} = 0.42$ at room temperature. (Pipe)

III. Thrust 3: Energy Transport In Organic And Hybrid Systems

Objectives:

- A. Design, fabricate, and characterize optical microcavity OPVs utilizing high luminescence quantum yield molecules – a new design principle for OPVs.
- B. Demonstrate algorithms and simulation procedures for the prediction of electron and hole transport properties in disordered structures, including interfaces.
- C. Achieve highly oriented morphologies (and tunable energy levels) of polymer-based solar cells (spherulites etc.) and correlate with carrier transport processes and device performance.
- D. Confirm and elucidate templating effects of deposition order & conditions.
- E. Show high efficiency OPV structures incorporating exciton dissociation layer (EDL) at the acceptor/cathode interface, and OPVs with two EDLs in addition to the donor/acceptor heterojunction already present.
- F. Develop complementary fully quantum-mechanical methodology for calculating exciton transfer rates within the donor and acceptor layers.

- G. Develop molecular design criteria (e.g. controlled HOMO-LUMO levels and gap sizes, long-range ordered morphologies with high electron and hole mobilities) in small-, macro-molecular, and organic-inorganic systems.
- H. Develop hybrid structures involving silsesquioxanes functionalized with brominated phenyl groups, with the goal to create 3-D conductive networks with tailored HOMO-LUMO gaps, and hence, exhibiting target light absorption properties.

Accomplishments

• **A predictive approach for calculating electron charge transfer within molecules**

Provides a rigorous scheme to obtain the electron transfer rate constant in OPV systems by taking into account nuclear tunneling effect. Charge transfer and transport rates determine photovoltaic cell efficiencies. Our computational scheme obtains charge transfer (CT) rate constants within the framework of Fermi's golden rule (FGR), with no empirical parameterization invoked. CT rate constants were calculated for two benchmark donor-acceptor systems: phenylacetylene-bridged carbazole-naphthalimide and C60-aniline (N,N-dimethylaniline). The results demonstrate the validity of FGR approach for calculating CT rate constants in solid-state organic photovoltaic materials where intramolecular degrees of freedom would dominate the CT process. (Dunietz, Geva)

• **Silicon Caged Macromolecules for Solar Applications at Reduced Cost**

Organic/hybrid photovoltaic cells offer multiple opportunities to improve PV flexibility, tunability, and cost. The creation of new silica based synthetic materials offers the opportunity to exploit advantages found in carbon based systems but with more control of size, molecular structure, optical properties and ultimately cost to manufacture. Photophysical properties were characterized using single photon absorption, two-photon absorption, fluorescence emission and fluorescence lifetime kinetics. Fluorescence efficiency decreases in going to larger cages, unexpected for an increasing number of chromophores. 10 stilbenevinylSQ offers up to a 10-fold increase in two-photon absorption cross-section per chromophore over a free chromophore, signifying an increased ability to separate charges in the absorption process. (Laine, Goodson)

• **Stretchable Nanoparticle Conductors with Self-Organized Conductive Pathways**

Stretchable conductors from self-organized nanoparticles show great potential for bio-implantable devices, photovoltaics, and flexible electronics with electro-tunable mechanical properties. Well-established conduction pathways are an essential requirement for good stretchable conductors. Stretchable conductors from spherical nanoparticles, despite their minimal aspect ratio showed excellent properties: 5xLBL had conductivity of $11,000 \text{ S cm}^{-1}$ and $2,400 \text{ S cm}^{-1}$ at 0% and 110% strain, while 5xVAF revealed record conductivity of 35 S cm^{-1} at 480% strain. Solid composites with electro-tunable mechanical properties could enable a new generation of implantable devices or soft robotics. (Uher, Kotov)

• **Improved measurements of ultrafast pulses of light**

Ultrafast pulse measurements are important for obtaining high time resolution measurements of energy and charge transfer in photovoltaics. The method will also find applications in nonlinear microscopy and other types of spectroscopic measurements. It is possible to measure the time-duration of a fs pulse by making two copies of the pulse with a controllable relative time-delay, and measuring the second-harmonic spectrum of the pulse-pair as a function of the relative time-delay. The above method takes a long time because you need to remove several interfering signals from the desired signal. If you add a controllable phase to one of the pulse-copies, then you can remove the interfering signals using much less data. (Ogilvie)

• **Recovering lost excitons in organic photovoltaics using a transparent dissociation layer**

Photocurrent generation in organic solar cells requires the diffusion of excitons to a heterojunction (HJ) for dissociation. If excitons recombine before reaching a HJ, their energy is lost and they don't contribute to photocurrent. In this work, the EDL creates a second HJ so that excitons don't have to travel as far to dissociate. The increase in photocurrent could lead to significant improvements in power efficiency for future devices. EQE is the efficiency of converting absorbed photons to collected free electrons. We show that MoO₃ (a common anode buffer layer) parasitically quenches excitons. The EDL converts the anode/donor interface from quenching to exciton-dissociating. Photocurrent from both heterojunctions are perfectly additive when no electrical bias is applied. (Shtein, Kim, Green)

- **Reduction of open circuit voltage loss in a polymer photovoltaic cell via interfacial molecular design**

May aid in the design of materials which overcome charge recombination loss to the open circuit voltage leading to inexpensive, high efficiency organic photovoltaic cells. Multiple monolayer spacers are placed at the donor-acceptor junction in a planar polymer solar cell. Open circuit voltage rises from 0.43 to 0.9 V, while fill factor and current density fall. Diode current and temperature dependent measurements suggest that the interfacial spacer suppresses deleterious charge recombination. (Kim, Green, Shtein)

- **Improved ultrafast two-dimensional electronic spectroscopy**

Advanced ultrafast spectroscopies like 2DES offer high time resolution measurements of energy and charge transfer in photovoltaics, and can additionally reveal coupling between states and the impact of "hot states" on charge transfer. The present method makes 2DES measurements on photovoltaics feasible. In 2DES, there are two pump pulses with a variable time delay and a probe pulse. Generating the two pump pulses with a pulse-shaper allows for efficient removal of interfering signals. The traditional way to perform 2DES with a pulse shaper uses "pump-probe" geometry where the two pumps are collinear and the signal is emitted in the same direction as the probe. By adding a diffractive optic element to split the pump pulses into two beams, the signal can be emitted in a "background-free" direction enabling a large increase in S/N while maintaining the advantages of pulse-shaped 2DES. (Ogilvie)

- **Confining light to metal's surface greatly enhances absorption in organic photovoltaics (OPVs)**

Using surface plasmons (SPPs), oscillations of charges on a metal surface, can enhance absorption and efficiency in thin OPVs and enable improved light detection for integrated, nanoscale optics. Wavelength and angle-resolved photocurrents are measured for different light polarizations to compare SPP and normal excitation schemes across the visible spectrum. Computational simulations of optics and current generation in devices confirm that performance improvements in experiments are a result of up to a 9x enhancement in light absorption. (Shtein, Green)

- **Role of Domain Size and Phase Purity on Carrier Transport in Organic Solar Cells**

Provides morphological design principles that enable the fabrication of the active material morphologies of that would maximize OPV device efficiency. Used a combination of thermal energy, organic solvent and super critical carbon dioxide (sc-CO₂) processing strategies to create morphologies of PHT/PCB₆₁M with different domain sizes and average phase purities. scCO₂ processing improves phase purities without coarsening domains, leading to: (1) 40% increase in initial charge carrier density (n_0); (2) increased carrier by a factor of 2; (3) decreased mobility (μ) and recombination coefficient (α); (4) short circuit currents (J_{SC}) and power conversion efficiencies (PCE) of devices are enhanced by a factor of 3, compared to solvent-cast devices. Thermal annealing increases domain size phase purity, as well as : (1) smaller n_0 and α ; (2) 1400% increase in μ , J_{SC} and fill factor.

- **Surprisingly high electron conductivity and efficient exciton blocking**

Working with the group of Prof. Green, we investigated our novel exciton filtering buffer layers developed under CSTECH sponsorship, and comprised of mixtures of C60 with the wide energy gap, small molecular weight semiconductor bathophenanthroline (BPhen). These mixtures exhibit a combination of surprisingly high electron conductivity and efficient exciton blocking when employed as buffer layers in organic photovoltaic cells. Photoluminescence quenching measurements show that a 1:1 BPhen/C60 mixed layer has an exciton blocking efficiency of $84 \pm 5\%$ compared to that of 100% for a neat BPhen layer. This high blocking efficiency is accompanied by a 100-fold increase in electron conductivity compared with neat BPhen. Transient photocurrent measurements show that charge transport through a neat BPhen buffer is dispersive, in contrast to nondispersive transport in the compound buffer. Interestingly, although the conductivity is high, there is no clearly defined insulating-toconducting phase transition with increased insulating BPhen fraction. Thus, we infer that C60 undergoes nanoscale (<10 nm domain size) phase segregation even at very high (>80%) BPhen fractions.

- **Critical Domain Sizes for Efficient Exciton Transport and Dissociation in Small-Molecular Organic Solar Cells**

Although bulk heterojunction (BHJ) organic solar cells devices often exhibit enhanced performance over planar devices, the volumetric distribution of materials in BHJs makes it difficult to characterize active layer morphology and separate the individual steps of the photoconversion process. Thus, while the impact of nanostructure on charge and exciton management remains critical to improving OPV performance, it is poorly understood. We used a two-dimensionally distributed mixed layer inserted at the heterojunction of planar-mixed heterojunction small-molecule OPVs. By constraining the nanostructure to two-dimensions, we were able to directly quantify the dependence of morphology on composition and determine the critical domain sizes necessary for efficient exciton diffusion and dissociation. These results provide a much-needed framework for optimizing morphology with respect to exciton transport and dissociation in the design and processing of future small molecular OPVs.

- **Role of Interlayer Förster Resonant Energy Transfer in Single- and Multi-Junction OPVs**

Interlayer Förster resonant energy transfer (FRET) can occur over larger distances than the typical exciton diffusion length (L_D), OPV structures supporting FRET has been considered to improving exciton diffusion efficiency (η_{Diff}). Prior work assumed 100% harvesting of excitons undergoing FRET, whereas we show those assumptions to be inaccurate in many common OPV material combinations. We showed how the diffusion efficiency of the Förster acceptor (FA) layer determines the overall diffusion efficiency of the device. We used modeling and experiments of the FRET process in single- and multi-junction devices to properly design layer structures and material selection based on known material properties to achieve higher efficiency devices.

Summary of Project Activities and Overall Accomplishments

University of Michigan researchers made revolutionary advances toward the design and synthesis of functional materials for low cost, high efficiency photovoltaic (PV) and thermoelectric (TE) devices. New fundamental insights into equilibrium and non-equilibrium charge transport and generation processes that occur in materials over various spatial and temporal scales (website <http://cstec.engin.umich.edu>) were developed.

Specifically, they accomplished the following: (1) developed a fundamental understanding of charge and exciton dynamics in organic heterojunctions, (2) developed new insights into quantum dot material physics in inorganic structures, and (3) developed an understanding of thermal transport in single molecules in thermoelectric materials. A summary of the accomplishments follows.

- a. Fundamental origins of thermoelectric energy conversion in: i) doped organic semiconductors, ii) single molecule systems, iii) nanowires, iv) nanostructured bulk thermoelectric (TE) materials and v) highly mismatched alloys (HMAs).
- b. Elucidated the fundamental limits & opportunities for energy conversion in quantum dot nanostructures and HMAs via intermediate band & hot carrier solar cells.
- c. Developed new means of circumventing the trade-off between absorption and transport processes in nanostructured energy conversion systems.
- d. Developed and used ultrafast spectroscopic and scanning probe tools to elucidate mechanisms of energy transport and charge transfer at the nanometer and sub-picosecond scales.
- e. Developed computational tools, chemical synthesis, and processing strategies to create new organic and hybrid materials for energy conversion.
- f. Developed the ideal diode equation for excitonic materials to understand the fundamental energy conversion processes in OPVs and guide molecular design.
- g. Demonstrated thermal and photon energy conversion in HMA systems.

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