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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 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-Confining 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  $(Bi_{1-x}Sb_x)_2Te_3$  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<sub>2</sub>Se and B<sub>13</sub>C<sub>2</sub> 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<sup>+</sup> 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 Bi<sub>2-x</sub>Tl<sub>x</sub>Te<sub>3</sub> 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.  $\text{Bi}_2\text{Te}_3$  films were grown on  $\text{BaF}_2$  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  $ZT > 1$  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 ( $s$ ), leading to a significant increase in  $S^2s$ . Thermal conductivity ( $k$ ) was also decreased by removing PSS. As a result, all parameters constituting  $ZT (= S^2s/k)$  vary so that ZT increases, leading to  $ZT = 0.42$  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  $35 \text{ S cm}^{-1}$  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  $\text{MoO}_3$  (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-CO<sub>2</sub>) processing strategies to create morphologies of PHT/PCB<sub>61</sub>M with different domain sizes and average phase purities. scCO<sub>2</sub> 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 ( $\mu$ ) and recombination coefficient ( $\alpha$ ); (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  $\alpha$ ; (2) 1400% increase in  $\mu$ ,  $J_{SC}$  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 CSTECC 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 ( $\eta_{\text{Diff}}$ ). 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.

## Publications

1. "Surprisingly High Conductivity and Efficient Exciton Blocking in Fullerene:Wide-Energy-Gap Small Molecule Mixtures", K. J. Bergemann, J. Amonoo, B. Song, P. Green, S. R. Forrest, *Nano Lett.*, **15**, 3994 DOI: 10.1021/acs.nanolett.5b00908 (2015).
2. Wilcox D. E., Lee M. H, Sykes M. E., Niedringhaus A., Geva E., Dunietz B. D., Shtein M and Ogilvie J. P. "Ultrafast charge-transfer dynamics at the boron

subphthalocyanine chloride / C<sub>60</sub> heterojunction: Comparison between experiment and theory" *J. Phys. Chem. Lett.* **6** 569–575 (2015)

3. Lee M. and Geva E. and Dunietz B., "Donor-to-donor vs. donor-to-acceptor interfacial charge transfer states in phthalocyanine-fullerene organic photovoltaic system" *J. Phys. Chem. Lett.* **5** 3810-3816 (2014)
4. Z. Zheng, A. Manna, H. Phillips, M. Hammer, C. Song, E. Geva and B. Dunietz, "Molecular structure, spectroscopy and photo induced kinetics in tri-nuclear cyanide bridged complex in solution: A first principle perspective" *J. Am. Chem. Soc.* **136** 16954–16957 (2014)
5. S. Chang, E. S. Zech, J. Walrath, T.W. Kim, Yen-Hsiang Lin, L. J. Mawst, and R. S. Goldman, "Influence of Sb Incorporation on InGaAs(Sb)N/GaAs Band Alignment" *Appl. Phys. Lett.* **105**, 142105 (2014).
6. M. J. Abere, C.-Y. Chen, D.R. Rittman, M. Kang, R.S. Goldman, J.D. Phillips, B. Torralva, and S.M. Yalisove, "Nanodot Formation Induced by Femtosecond Laser Irradiation", *Appl. Phys. Lett.* **105**, 163103 (2014).
7. Y.W. Li, V.A. Stoica, K. Sun, W. Liu, L. Endicott, J. C. Walrath, Y.H. Lin, K.P. Pipe, R.S. Goldman, C. Uher, and R. Clarke, "Ordered Horizontal Sb<sub>2</sub>Te<sub>3</sub> Nanowires Induced by Femtosecond Lasers", *Appl. Phys. Lett.* **105**, 201904 (2014).
8. M.V. Warren, J.C. Canniff, H. Chi, F. Naab, V.A. Stoica, R. Clarke, C. Uher, and R.S. Goldman, "Influence of Embedded Bismuth Nanocrystals on GaAs Thermoelectric Properties," *J. Appl. Phys.* **117**, 065101 (2015).
9. J.C. Walrath, Y.-H. Lin, S. Huang, and R.S. Goldman, "Profiling the local carrier concentration across a semiconductor quantum dot", *Appl. Phys. Lett.* **106**, 192101 (2015).
10. M. Luengo-Kovac, M. Macmahon, S. Huang, R. S. Goldman, and V. Sih, "g-factor modification in a bulk InGaAs epilayer by an in-plane electric field," *Phys. Rev. B* **91**, 201110(R) (2015).
11. K. T. Lee, J.Y. Lee, S.-Y. Seo, and L. J. Guo, "Colored ultra-thin hybrid photovoltaics with high quantum efficiency," *Light: Science & Applications*, **3**, e215 (2014).
12. Gun-Ho Kim<sup>+</sup>, Dongwook Lee<sup>+</sup>, Apoorv Shanker<sup>+</sup>, Lei Shao, Min Sang Kwon, David Gidley, Jinsang Kim\* and Kevin Pipe\* "High thermal conductivity in amorphous polymer blends by engineered interchain interactions" *Nature Materials* **2015**, *14*, 295.

13. Kyeongwoon Chung, Min Sang Kwon, Brendan Leung, Antek Wong-Foy, Min Su Kim, Jeongyong Kim, Shuichi Takayama, Johannes Gierschner, Adam Matzger, Jinsang Kim “Shear-triggered Crystallization and Light Emission of a Thermally Stable Organic Supercooled Liquid” *ACS Central Science* 2015, **1**, 94.
14. David Bilby, Bradley Frieberg, Shobita Kramadhati, Peter Green, Jinsang Kim “Design Considerations for Electrode Buffer Layer Materials in Polymer Solar Cells” *ACS Appl. Mater. & Interfaces* 2014, **6**, 14964.
15. Hyoungchul Kim, Sedat Ballikaya,<sup>c,d</sup> Hang Chi,<sup>c</sup> Jae-Pyung Ahn,<sup>e</sup> Kiyong Ahn,<sup>b</sup> Ctirad Uher and Massoud Kaviani, Ultralow thermal conductivity of b-Cu<sub>2</sub>Se by atomic fluidity and structure distortion *Acta Materialia* 86 (2015) 247–253
16. D. Bayerl and **E. Kioupakis**, Theoretical limits of thermoelectric figure of merit in n-type TiO<sub>2</sub> polymorphs, *Physical Review B* **91**, 165104 (2015).
17. S. Toulouse, B. P. Isaacoff, G. Shi, M. Matuchová, **E. Kioupakis**, and R. Merlin, Frenkel-like Wannier-Mott excitons in few-layer PbI<sub>2</sub>, *Physical Review B* **91**, 165308 (2015).
18. G. Shi and **E. Kioupakis**, Electronic and optical properties of nanoporous silicon for solar-cell applications, *ACS Photonics* **2** (2), 208–215 (2015).
19. G. Shi and **E. Kioupakis**, Quasiparticle band structures and thermoelectric transport properties of p-type SnSe, *Journal of Applied Physics* **117**, 065103 (2015).
20. Olvera, G. Shi, H. Djieutedjeu, A. Page, C. Uher, **E. Kioupakis\***, and P. F. P. Poudeu\*, Pb<sub>7</sub>Bi<sub>4</sub>Se<sub>13</sub>: A Lillianite Homologue with Promising Thermoelectric Properties, *Inorg. Chem.* **54**, 746–755 (2015)
21. G.-H. Kim, D. Lee, A. Shanker, L. Shao, M. S. Kwon, D. Gidley, J. Kim, and K. P. Pipe, “High thermal conductivity in amorphous polymer blends by engineered interchain interactions”, *Nature Mater.* **14**, 295 (2015)
22. Wilcox, DE (Wilcox, Daniel E.); Lee, MH (Lee, Myeong H.); Sykes, ME (Sykes, Matthew E.); Niedringhaus, A (Niedringhaus, Andrew); Geva, E (Geva, Eitan); Dunietz, BD (Dunietz, Barry D.); Shtein, M (Shtein, Max); Ogilvie, JP, “Ultrafast Charge-Transfer Dynamics at the Boron Subphthalocyanine Chloride/C-60 Heterojunction: Comparison between Experiment and Theory” *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*, **6** (2015) Pages: 569-575
23. Shalev, Olga; Biswas, Shaurjo; Yang, Yongsoo; Eddir, Tareq; Ahanotu, Onye; Lu, Wei; Clarke, Roy; Shtein, M. “Growth and modelling of spherical crystalline

morphologies of molecular materials.” NATURE COMMUNICATIONS **5** (2014) 5204

24. “Phase-Field Simulations of GaN Growth by Selective Area Epitaxy from Complex Mask Geometries”, L.K. Aagesen, M.E. Coltrin, J. Han, K. Thornton, *J. Appl. Phys.*, **117**, 194302 (2015).
25. C. M. Andres, J. Zhu, T. Shyu, C. Flynn, N. A. Kotov, “Shape-Morphing Nanocomposite Origami,” *Langmuir* **30**, 5378-5385 (2014).
26. B. X. Dong , B. Huang, A. Tan , and Peter F. Green, “Nanoscale Orientation Effects on Carrier Transport in a Low-Band-Gap Polymer,” *J. Phys. Chem. C* **118**, 17490-17498 (2014).
27. Y. Jin, C. Shao, J. Kieffer, M. L. Falk, and M. Shtei, “Spatial nonuniformity in heat transport across hybrid material interfaces,” *Phys. Rev. B* **90**, 054306 (2014).
28. X. Mao, J.-G. Kim, J. Han, H. Suk Jung, S. G. Lee, N. A. Kotov, and J. Lee, “Phase-Pure FeSex (x=1, 2) Nanoparticles with One- and Two-Photon Luminescence,” *JACS* **136**, 7189-7192 (2014).
29. X. Xiao, K. J. Bergemann, J. D. Zimmerman, K. Lee, S. R. Forrest, “Small-Molecule Planar-Mixed Heterojunction Photovoltaic Cells with Fullerene-Based Electron Filtering Buffers,” *Adv. Energy Mater.* **4**, 1301557 (2014).
30. S. Huang, S. J. Kim, X. Q. Pan, and R. S. Goldman, “Origins of interlayer formation and misfit dislocation displacement in the vicinity of InAs/GaAs quantum dots,” *Appl. Phys. Lett.* **105**, 032107 (2014).
31. F. D. Fuller, J. Pan, A. Gelzinis, V. Butkus, S. S. Senlik, D. E. Wilcox, C. F. Yocom, L. Valkunas, D. Abramavicius & J. P. Ogilvie, "Vibronic coherence in oxygenic photosynthesis," *Nat. Chem.* **6**, 706–711 (2014).
32. C. K. Renshaw and S. R. Forrest, “Excited state and charge dynamics of hybrid organic/inorganic heterojunctions. I. Theory,” *Phys. Rev. B* **90**, 045302 (2014).
33. Panda, C. K. Renshaw, A. Oskooi, K. Lee, and S. R. Forrest, “Excited state and charge dynamics of hybrid organic/inorganic heterojunctions. II. Experiment,” *Phys. Rev. B* **90**, 045303 (2014).
34. D. Wilcox, J. Ogilvie, M. Shtei, M. Sykes, and A. Niedringhaus, “Heterodyne-detected and ultrafast time-resolved second-harmonic generation for sensitive measurements of charge-transfer,” *Opt. Lett.* **39**, 4274 (2014).

35. J. Hwang, K. Lee, A. Teran, S. Forrest, J. D. Phillips, A. J. Martin and J. Millunchick, "Multiphoton Sub-Band-Gap Photoconductivity and Critical Transition Temperature in Type-II GaSb Quantum-Dot Intermediate-Band Solar Cells", *Physical Review Applied* **1**, 051003 (2014).

36. H. Chi, H. Kim, J. C. Thomas, G. Shi, K. Sun, M. Abeykoon, E. S. Bozin, X. Shi, Q. Li, X. Shi, E. Kioupakis, A. Van der Ven, M. Kaviani, and C. Uher, "Low-temperature structural and transport anomalies in Cu<sub>2</sub>Se," *Phys. Rev. B* **89**, 195209 (2014).

37. Li, J. Amonoo, B. Huang, P. K. Goldberg, A. J. McNeil, and P. F. Green, "Enhancing photovoltaic performance using an all-conjugated random copolymer to tailor bulk and interfacial morphology," *Adv. Funct. Mater.*, DOI: 10.1002/adfm.201401058 (2014).

38. D. E. Wilcox and J. P. Ogilvie, "Comparison of pulse compression methods using only a pulse-shaper," *J. Opt. Soc. Am. B* **31**, 1544 (2014).

39. O. L. Griffith and S. R. Forrest, "Exciton Management in Organic Photovoltaic Multi-donor Energy Cascades," *Nano Lett.* **14**, 2353 (2014).

40. M. Kang, I. Beskin, A. A. Al-Heji, O. Shende, S. Huang, S. Jeon, and R. S. Goldman, "Evolution of ion-induced nanoparticle arrays on GaAs surfaces," *Appl. Phys. Lett.* **104**, 182102 (2014).

41. M. Lee, E. Geva, and B. Dunietz, "Calculation from First-Principles of Golden Rule Rate Constants for Photoinduced Subphthalocyanine/Fullerene Interfacial Charge Transfer and Recombination in Organic Photovoltaic Cells," *J. Phys. Chem. C* **118**, 9780 (2014).

42. Barito, M. E. Sykes, B. Huang, D. Bilby, B. Frieberg, J. Kim, P. F. Green, and M. Shtein. "Universal Design Principles for Cascade Heterojunction Solar Cells with High Fill Factors and Internal Quantum Efficiencies Approaching 100%," *Adv. Energy Mater.*, DOI: 10.1002/aenm.201400216

43. H. Phillips, Z. Zheng, E. Geva, B. D. Dunietz, "Orbital gap predictions for rational design of organic photovoltaic materials, *Org. Electron.* **15**, 1509 (2014).

44. J. I. Park, T. D. Nguyen, G. de Queiros Silveira, J. H. Bahng, S. Srivastava, G. Zhao, K. Sun, P. Zhang, S. Glotzer, and N.A. Kotov, "Terminal Supraparticle Assemblies from Similarly Charged Protein Molecules and Nanoparticles," *Nat. Commun.* **5**, 3593 (2014).

45. J. M. Foley, S. M. Young, J. D. Phillips, "Symmetry-Protected Mode Coupling Near Normal Incidence for Narrowband Transmission Filtering in a Dielectric Grating", *Phys. Rev. B* **89**, 165111 (2014).

46. J. Zhang, R. Liu, N. Cheng, Y. Zhang, J. Yang, C. Uher, X. Shi, L. Chen, and W. Zhang, "High-Performance Pseudocubic Thermoelectric Materials from Non-Cubic Chalcopyrite Compounds," *Adv. Mater.* **26**, 3848 (2014).

47. C. Chen, J. Zheng, K. Nguy, F. Naab, and J. D. Phillips, "Distinguishing Optical Behavior of Oxygen States and Native Deep Level Emission in ZnTe", *J. Elec. Mater.* **43** 879 (2014).

48. M. DeJarld, D. Nothern, and J. M. Millunchick, "Droplet destabilization during Bi catalyzed vapor-liquid-solid growth of GaAs," *J. Appl. Phys.* **115**, 114307 (2014).

49. J. Y. Lee, K.-T. Lee, S. Seo, and L. J. Guo, "Decorative power generating panels creating angle insensitive transmissive colors," *Sci. Rep.* **4**, 4192 (2014).

50. B. Song, C. Rolin, J. D. Zimmerman, and S. R. Forrest, "Effect of mixed layer crystallinity on the performance of bulk heterojunction organic photovoltaic cells," *Adv. Mater.*, **26**, 2914 (2014).

51. Y. Zheng, S. Wang, W. Liu, Z. Yin, X. F. Tang, H. Li, and C. Uher, "Thermoelectric Transport Properties of p-type Silver-doped PbS with in-situ Ag<sub>2</sub>S Nanoprecipitates," *J. Physics D: Appl. Phys.* **47**, 115303 (2014).

52. D. Bayerl and E. Kioupakis, "Visible-Wavelength Polarized Light Emission with Small-Diameter InN Nanowires," *Nanolett.* **14**, 3709 (2014).

53. M. E. zotti, A. Barito, J. A. Amonoo, P. F. Green, and M. Shtein, "Broadband Plasmonic Photocurrent Enhancement in Planar Organic Photovoltaics Embedded in a Metallic Nanocavity," *Adv. Energy Mater.* DOI: 10.1002/aenm.201301937

54. H. Kim, M. H. Kim, and M. Kaviani, "Lattice Thermal Conductivity of UO<sub>2</sub> Using Ab-initio and Classical Molecular Dynamics," *J. Appl. Phys.* **115**, 123510 (2014).

55. S. Biswas, N. Geva, Y. Yang, R. L. Headrick, R. Pindak, R. Clarke, and M. Shtein, "Spatial mapping of morphology and electronic properties of air-printed pentacene thin films," *Adv. Funct. Mater.* **24**, 3907 (2014).

56. B. Huang, J. A. Amonoo, A. Li, X. C. Chen, P. F. Green, "Role of Domain Size and Phase Purity on Charge Carrier Density, Mobility and Recombination in P3HT:PC61BM devices," *J. Phys. Chem. C* **118**, 3968 (2014).

57. M. Kang, J. H. Wu, W. Ye, Y. Jiang, E. A. Robb, C. Chen, and R. S. Goldman, "Formation and evolution of ripples on ion-irradiated semiconductor surfaces", *Appl. Phys. Lett.* **104**, 052103 (2014).

58. F. D. Fuller, D. E. Wilcox, J. P. Ogilvie, "Pulse shaping based two-dimensional electronic spectroscopy in a background free geometry," *Opt. Express* **22**, 1018 (2014).
59. L. A. Zotti, M. Burkle, F. Pauly, W. Lee, K. Kim, W. Jeong, Y. Asai, P. Reddy, J. C. Cuevas, "Heat dissipation in and its relation to thermopower in single-molecule junctions," *New J. Phys.* **16**, 015004 (2014).
60. Z. M. Gibbs, H. Kim, H. Wang, R. L. White, F. Drymiotis, M. Kaviany, and G. J. Snyder, "Temperature dependent band gap in PbX (X = S, Se, Te)," *Appl. Phys. Lett.* **103**, 262109 (2013).
61. L.K. Lee, L.K. Aagesen, K. Thornton, and P.-C. Ku, "Origin of broad luminescence from site-controlled InGaN nanodots fabricated by selective-area epitaxy," *Phys. Stat. Sol. A* **211**, 531 (2014).
62. D. Bilby, J. Amonoo, M. Sykes, B. Frieberg, B. Huang, J. Hungerford, M. Shtein, P. Green, J. Kim "Reduction of Voc Loss in a Polymer Photovoltaic Cell via Interfacial Molecular Design: Insertion of a Molecular Spacer" *Appl. Phys. Lett.* **103**, 203902 (2013).
63. Y. Jin, S. Nola, K. P. Pipe, and M. Shtein, "Improving thermoelectric efficiency in organic-metal nanocomposites via extra-low thermal boundary conductance," *J. Appl. Phys.* **114**, 194303 (2013).
64. S. Ballikaya, C. Uher, "Enhanced thermoelectric performance of optimized Ba, Yb filled and Fe substituted skutterudite compounds," *J. Alloys Compd.* **585**, 168 (2014).
65. Y. J. Cho, J. Y. Lee, and S. R. Forrest, "Polymer photovoltaic cells with a graded active region achieved using double stamp transfer printing," *Appl. Phys. Lett.* **103**, 193301 (2013).
66. X. Tong , N. Wang , M. Slootsky , J. Yu, and S. R. Forrest , " Intrinsic burn-in efficiency loss of small-molecule organic photovoltaic cells due to exciton-induced trap formation," *Sol. Energy Mater. Sol. Cells* **118**, 116 (2013).
67. Kargar, Y. Jing, S. J. Kim, C. T. Riley, X. Pan, and D. Wang, "ZnO/CuO Heterojunction Branched Nanowires for Photoelectrochemical Hydrogen Generation," *ACS Nano* **7**, 11112 (2013).
68. J. H. Jung, K. Chou, J. C. Furgal, and R. M. Laine, "Synthesis of acetoxyphenyl- and hydroxyphenyl-terminated polyfunctional T-8, T-10, T-12 silsesquioxanes and initial studies on their use in the formation of highly crosslinked polyesters," *Appl. Organomet. Chem.* **27**, 666 (2013).

69. M. H. Lee, B. D. Dunietz, and E. Geva, "Calculation From First Principles of Intramolecular Golden-Rule Rate Constants for Photo-Induced Electron Transfer in Molecular Donor-Acceptor Systems," *J. Phys. Chem. C*, **117**, 23391 (2013).

70. W. Ma, H. Kuang, L. Xu, L. Ding, C. Xu, L. Wang, and N. A. Kotov, "Attomolar DNA detection with chiral nanorod assemblies," *Nat. Commun.* **4**, 2689 (2013).

71. S. Shin, C. Melnick, and M. Kaviani, "Phonon Recycling," *JSME Mech. Engr. Rev.* **1**, TEP0002-1-10 (2014).

72. J.-Y. Kim and N. A. Kotov, "Charge Transport Dilemma of Solution-Processed Nanomaterials," *Chem. Mater.* **26**, 134 (2014).

73. H. Zhou, J.-P. Kim, J. H. Bahng, N. A. Kotov, and J. Lee, "Self-Assembly Mechanism of Spiky Magnetoplasmonic Supraparticles," *Adv. Funct. Mater.* **24** 1439 (2014).

74. S. J. Kim, J. Jokisaari, A. Kargar, D. Wang, X. Pan, "Mechanical Effects on Electrical Properties of CuO Nanowires", *Microscopy & Microanalysis* 19 (suppl 2), 1496-1497 (2013).

75. S. Huang, S. J. Kim, R. Levy, X. Q. Pan, and R. S. Goldman, "Mechanisms of InAs/GaAs quantum dot formation during annealing of In islands," *Appl. Phys. Lett.* **103**, 132104 (2013).

76. X. Wu, L. Xu, L. Liu, W. Ma, H. Yin, H. Kuang, L. Wang, C. Xu, and N. A. Kotov, "Unexpected Chirality of Nanoparticle Dimers and Ultrasensitive Chiroplasmonic Bioanalysis," *J. Am. Chem. Soc.* **135**, 18629 (2013).

77. B. Yeom, H. Zhang, H. Zhang, J.I. Park, K. Kim, A. O. Govorov, and N. A. Kotov, "Chiral Plasmonic Nanosstructures on Achiral Nanopillars," *Nano Lett.* **13**, 5277 (2013).

78. H. Zhang, P. R. Patel, Z. Xie, S. D. Swanson, X. Wang, and N. A. Kotov, "Tissue-Compliant Neural Implants from Microfabricated Carbon Nanotube Multilayer Composite," *ACS Nano* **7**, 7619 (2013).

79. B. E. Lassiter, J. D. Zimmerman, S. R. Forrest, "Tandem organic photovoltaics incorporating two solution-processed small molecule donor layers," *Appl. Phys. Lett.* **103**, 123305 (2013).

80. J. Furgal, J. H. Jung, S. Clark, T. Goodson III, and R. Laine, "Beads on a Chain (BoC) Phenylsilsesquioxane (SQ) Polymers via F-Catalyzed Rearrangements and ADMET or Reverse Heck Cross-coupling Reactions: Through Chain,

Extended Conjugation in 3-D with Potential for Dendronization," *Macromolecules* **46**, 7591 (2013).

81. M. Kang, A. A. Al-Heji, J.-E. Lee, T. W. Saucer, S. Jeon, J. H. Wu, L. Zhao, A. L. Katzenstein, D. L. Sofferman, V. Sih, and R. S. Goldman, "Ga Nanoparticle enhanced Photoluminescence of GaAs," *Appl. Phys. Lett.* **103**, 101903 (2013).

82. J. H. Jung, J. C. Furgal, S. Clark, M. Schwartz, K. Chou, R. M. Laine, "Beads on a chain (BoC) polymers with model dendronized beads. Copolymerization of [(4-NH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>SiO<sub>1.5</sub>)<sub>6</sub>(IPhSiO<sub>1.5</sub>)<sub>2</sub>] and [(4-CH<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>SiO<sub>1.5</sub>)<sub>6</sub>(IPhSiO<sub>1.5</sub>)<sub>2</sub>] with 1,4-diethynylbenzene (DEB) gives through chain, extended 3-D conjugation in the excited state that is an average of the corresponding homopolymers," *Macromolecules* **46**, 7580 (2013).

83. Kargar, K. Sun, S. J. Kim, D. Lu, Y. Jing, Z. Liu, X. Pan, and D. Wang, "Three-dimensional ZnO/Si broom-like nanowire heterostructures as photoelectrochemical anodes for solar energy conversion," *Phys. Status Solidi A* **210**, 2561 (2013).

84. Ryan D. Murphy, Michael J. Abere, Keegan J. Schrider, Ben Torralva, and Steven M. Yalisove, "Nanoparticle size and morphology control using ultrafast laser induced forward transfer of Ni thin films," *Appl. Phys. Lett.* **103**, 093113 (2013).

85. J. D. Zimmerman, B. E. Lassiter, X. Xiao, K. Sun, A. Dolocan, R. Gearba, D. A. Vanden Bout, K. J. Stevenson, P. Wickramasinghe, M. E. Thompson, and S. R. Forrest, "Control of Interface Order by Inverse Quasi-Epitaxial Growth of Squaraine/ Fullerene Thin Film Photovoltaics," *ACS Nano*, **7** 9268 (2013).

86. H. Liu, X. Yuan, F. Xu, X. Shi, P. Lu, Y. He, Y. Tang, S. Bai, W. Zhang, L. D. Chen, H. Lin, X. Gao, X. Zhang, H. Chi, and C. Uher, "Ultrahigh Thermoelectric Performance by Electron Critical Scattering in Cu<sub>2</sub>Se," *Adv. Mater.* **25**, 6607 (2013).

87. J. Martin, A. H. Hunter, T. W. Saucer, G. V. Rodriguez, V. Sih, E. Marquis, J. Millunchick, "Atom probe tomography analysis of different modes of Sb intermixing in GaSb quantum dots and wells." *Appl. Phys Lett.* **103** 122103 (2013).

88. G. Tan, W. Liu, H. Chi, X. Su, S. Wang, Y. Yan, X. Tang, W. Wong-Ng, and C. Uher, "Realization of high thermoelectric performance in p-type unfilled ternary skutterudites FeSb<sub>2+x</sub>Te<sub>1-x</sub> via band structure modification and significant point defect scattering," *Acta Materialia* **61**, 7693 (2013).

89. S. Ballikaya, H. Chi, J. R. Salvador, and C. Uher, "Thermoelectric Properties of Ag-Doped Cu<sub>2</sub>Se and Cu<sub>2</sub>Te," *J. Mater. Chem. A* **1**, 12478 (2013).

90. M. Kang, J. H. Wu, D. L. Sofferman, I. Beskin, H. Y. Chen, K. Thornton, and R. S. Goldman, "Origins of Ion Irradiation-Induced Ga Nanoparticle Motion on GaAs Surfaces," *Appl. Phys. Lett.* **103**, 072115 (2013).

91. G. Tan, W. Liu, S. Wang, Y. Yan, H. Li, X. F. Tang, and C. Uher, "Rapid Preparation of CeFe<sub>4</sub>Sb<sub>12</sub> Skutterudite by Melt Spinning: Rich Nanostructures and High Thermoelectric Performance," *J. Mater. Chem. A* **1**, 12657 (2013).

92. P. Sahoo, Y. Liu, J. P. A. Makongo, X.-L. Su, S. J. Kim, N. Takas, H. Chi, C. Uher, X. Pan and P. F. P. Poudeu, "Enhancing thermopower and hole mobility in bulk p-type half-Heuslers using full-Heusler nanostructures," *Nanoscale* **5**, 9419 (2013).

93. J. M. Foley, S. M. Young, and J. D. Phillips, "Narrowband mid-infrared transmission filtering of a single layer dielectric grating," *Appl. Phys. Lett.* **103**, 071107 (2013).

94. G-H. Kim, L. Shao, K. Zhang, and K. P. Pipe, "Engineered doping of organic semiconductors for enhanced thermoelectric efficiency," *Nature Mater.*, **12**, 719 (2013).

95. Y. Kim, J. Zhu, B. Yeom, M. Di Prima, X. Su, J.-G. Kim, S. J. Yoo, C. Uher, and N. A. Kotov, "Stretchable nanoparticle conductors with self-organized conductive pathways," *Nature* **500**, 59-U77 (2013).

96. G. Tan, W. Liu, S. Wang, Y. Yan, H. Li, X. F. Tang, and C. Uher, "Rapid Preparation of CeFe<sub>4</sub>Sb<sub>12</sub> Skutterudite by Melt Spinning: Rich Nanostructures and High Thermoelectric Performance," *J. Mater. Chem. A* **1**, 12657 (2013).

97. E.S. Zech, A. S. Chang, A. J. Martin, J. C. Canniff, Y.H. Lin, J. M. Millunchick, and R. S. Goldman, "Influence of Quantum Dot Atomic Structure and Strain Relaxation on GaSb/GaAs Band Offsets" *Appl. Phys. Lett.* **103**, 082107 (2013).

98. D. E. Wilcox, F. D. Fuller, and J. P. Ogilvie, "Fast second-harmonic generation frequency-resolved optical gating using only a pulse shaper," *Opt. Lett.* **38**, 2980 (2013).

99. G. Wang, L. Endicott, H. Chi, P. Lošt'ák, and C. Uher, "Tuning the Temperature Domain of Phonon Drag in Thin Films by the Choice of Substrate", *Phys. Rev. Lett.* **111**, 046803 (2013).

100. H. Chi, C. Chen, J. D. Phillips, and C. Uher, "Transport properties of ZnTe:N thin films", *Appl. Phys. Lett.* **103**, 042108 (2013).

101. H. Chi, W. Liu, K. Sun, X. Su, G. Wang, P. Lošt'ák, V. Kucek, Č. Drašar, and C. Uher, "Low-temperature transport properties of Tl-doped Bi<sub>2</sub>Te<sub>3</sub> single crystals", *Phys. Rev. B* **88**, 045202 (2013).

102. B.-G. Kim, E. J. Jeong, J. W. Chung, S. Seo, B. Koo, J. Kim "A Molecular Design Principle of Lyotropic Liquid Crystalline Conjugated Polymers with Directed Alignment Capability for Plastic Electronics" *Nature Materials* **12**, 659 (2013).

103. G. Ma, Y. Zhou, X. Li, K. Sun, S. Liu, J. Hu, and N. A. Kotov, "Self-Assembly of Copper Sulfide Nanoparticles into Nanoribbons with Continuous Crystallinity," *ACS Nano* **7**, 9010 (2013).

104. J. Zhu, H. Zhang, and N. A. Kotov, "Thermodynamic and Structural Insights into Nanocomposites Engineering by Comparing Two Materials Assembly Techniques for Graphene," *ACS Nano* **7**, 4818 (2013).

105. H. J. Park, H. Kim, J. Y. Lee, T. Lee and L. J. Guo, "Optimization of polymer photovoltaic cells with bulk heterojunction layers hundreds of nanometers thick: modifying the morphology and cathode interface," *Energy Environ. Sci.* **6**, 2203 (2013).

106. M. V. Warren, J. C. Canniff, H. Chi, E. Morag, F. Naab, V. A. Stoica, R. Clarke, C. Uher, and R. S. Goldman, "Influence of embedded indium nanocrystals on GaAs thermoelectric properties," *J. Appl. Phys.* **114**, 043704 (2013).

107. S. Ballikaya, N. Uzar, S. Yildirim, H. Chi, X. Su, G. Tan, X. Tang, and C. Uher, "Lower Thermal Conductivity and Higher Thermoelectric Performance of Fe-Substituted and Ce, Yb Double-Filled p-Type Skutterudites," *J. Elec. Mater.* **42**, 1622 (2013).

108. N. Bartynski, C. Trinh, A. Panda, K. Bergemann, B. E. Lassiter, J. D. Zimmerman, S. R. Forrest, and M. E. Thompson, "A Fullerene-Based Organic Exciton Blocking Layer with High Electron Conductivity," *Nanolett.* **13**, 3315 (2013).

109. J. Furgal, J. H. Jung, T. Goodson III, and R. Laine, "Analyzing Structure-Photophysical Property Relationships for Isolated T8, T10 and T12 Stilbenevinyl Silsesquioxanes," *J. Am. Chem. Soc.* **135**, 12259 (2013).

110. W. Lee, K. Kim, W. Jeong, L. A. Zotti, F. Pauly, J. C. Cuevas, and P. Reddy, "Heat dissipation in atomic-scale junctions," *Nature* **498**, 209 (2013).

111. W. Ma, H. Kuang, L. Wang, L. Xu, W.-S. Chang, H. Zhang, M. Sun, Y. Zhu, Y. Zhao, L. Liu, C. Xu, S. Link, and N. A. Kotov, "Chiral plasmonics of self-assembled nanorod dimmers," *Sci. Rep.* **3**, 1934 (2013).

112. Barito, M. E. Sykes, D. Bilby, J. Amonoo, Y. Jin, S. E. Morris, P. F. Green, J. Kim, and M. Shtein, "Recovering lost excitons in organic photovoltaics using a transparent dissociation layer," *Appl. Phys. Lett.*, **113**, 203110 (2013).

113. M. Luengo-Kovac, T. W. Saucer, A. J. Martin, J. Millunchick, and V. Sih, "Analyzing pattern retention for multilayer focused ion beam induced quantum dot structures," *J. Vac. Sci. Tech. B* **31**, 031208 (2013).

114. R. D. Murphy, B. Torralva, and S. M. Yalisove, "The role of an interface on Ni film removal and surface roughness after irradiation by femtosecond laser pulses," *Appl. Phys. Lett.* **102**, 181602 (2013).

115. H. J. Park, J. Y. Lee, T. H. Lee, L. J. Guo, "Advanced Heterojunction Structure of Polymer Photovoltaic Cells Generating Ultrahigh Photocurrent with Internal Quantum Efficiency Approaching 100 %," *Adv. Energy. Mater.* **3**, 1135 (2013).

116. J. Chen, M. Trigo, S. Fahy, É. D. Murray, Y. M. Sheu, T. Gruber, R. Henning, Y. J. Chien, C. Uher, and D. A. Reis, "Time- and momentum-resolved probe of heat transport in photo-excited bismuth," *Appl. Phys. Lett.* **102**, 181903 (2013).

117. J. Martin, T. W. Saucer, V. Sih, and J. M. Millunchick, "Effects of pre-determined lateral separation on quantum dot size and dissolution," *Appl. Phys. Lett.* **102**, 182105 (2013).

118. Y. Liu, P. Sahoo, J.P. A. Makongo, X. Zhou, S.-J. Kim, H. Chi, C. Uher, X. Pan, and P. F. P. Poudeu, "Large Enhancements of Thermopower and Carrier Mobility in Quantum Dot Engineered Bulk Semiconductors," *JACS* **35**, 7486 (2013).

119. H. Yang, E. Glynnos, B. Huang, P. F. Green, "The Out-of-Plane Carrier Transport in Conjugated Polymer Thin Films: Role of Morphology," *J. Phys. Chem. C* **117**, 9590 (2013).

120. H. Kim and M. Kaviany, "Coupled Polaron-Phonon Effects on Seebeck Coefficient and Lattice Conductivity of  $B_{13}C_2$  from First Principles," *Phys. Rev. B* **87**, 155133 (2013).

121. K. J. Zhang, A. Yadav, K. H. Kim, Y. Oh, M. F. Islam, C. Uher, and K. P. Pipe, "Thermal and Electrical Transport in Ultralow Density Single-Walled Carbon Nanotube Networks", *Adv. Mater.* **25**, 2926 (2013).

122. Y. Yacoby, N. Elfassy, S. K. Ray, R. K. Singha, S. Das, E. Cohen, S. Yochelis, R. Clarke, and Y. Paltiel, "Morphology and Growth of Capped Ge/Si Quantum Dots" *J. Nanopart. Res.* **15**, 1608 (2013).

123. C. Chen, S. J. Kim, X. Pan, and J. D. Phillips, "Epitaxial Growth of ZnTe on GaSb(100) using in situ ZnCl<sub>2</sub> Surface Clean," *J. Vac. Sci. Technol B* **31**, 03C118 (2013).

124. B.-G. Kim, K. Chung, J. Kim, "Molecular Design Principle of All-organic Dyes for Dye-sensitized Solar Cell" *Chem. Eur. J.* **19**, 5220 (2013).

125. L. Xu, W. Ma, L. Wang, C. Xu, H. Kuang, N. A. Kotov, "Nanoparticle assemblies: dimensional transformation of nanomaterials and scalability," *Chem. Soc. Rev.* **42**, 3114 (2013).

126. R. L. Field III, Y. Jin, H. Cheng, T. Dannecker, R. M. Jock, Y. Q. Wang, C. Kurdak, and R. S. Goldman, "Influence of N incorporation on persistent photoconductivity in GaAsN alloys," *Phys. Rev. B* **87**, 155303 (2013).

127. J. Martin, J. Hwang, E. A. Marquis, E. Smakman, T. W. Saucer, G. V. Rodriguez, A.H. Hunter, V. Sih, P. M. Koenraad, J. D. Phillips, J. Millunchick, "The disintegration of GaSb/GaAs nanostructures upon capping," *Appl. Phys. Lett.* **103**, 113103 (2013).

128. Y. Bai, J. Yeom, M. Yang, S. Cha, K. Sun, N. A. Kotov, "Universal Synthesis of Single-Phase Pyrite FeS<sub>2</sub> Nanoparticles, Nanowires, and Nanosheets," *J. Phys. Chem. C* **117**, 2567 (2013).

129. K. L. Agrawal, M. E. Sykes, K. H. An, B. Frieberg, P. F. Green, and M. Shtein, "Influence of Exciton Lifetime on Charge Carrier Dynamics in an Organic Heterostructure" *Appl. Phys. Lett.* **102**, 113304 (2013).

130. H. Liu, X. Shi, M. Kirkham, H. Wang, Q. Li, C. Uher, W. Zhang, and L. D. Chen, "Structure-Transformation-Induced Abnormal Thermoelectric Properties in Semiconducting Copper Selenide," *Mater. Lett.* **93**, 121 (2013).

131. S. Shin, C. Melnick, and M. Kaviani, "Heterobarrier for converting hot-phonon energy to electric potential," *Phys. Rev. B* **87**, 075317 (2013).

132. H. Sun, V. Stoica, M. Shtein, R. Clarke, and K. P. Pipe, "Coherent control of GHz resonant modes by an integrated acoustic etalon," *Phys. Rev. Lett.* **110**, 086109 (2013).

133. H. S. Ji, H. Kim, C. Lee, J.-S. Rhyee, M. H. Kim, M. Kaviany, and J. H. Shim, "Vacancy-suppressed lattice conductivity of high-ZT  $\text{In}_4\text{Se}_{3-x}$ ," *Phys. Rev. B* **87**, 125111 (2013).

134. X. Xiao, J. D. Zimmerman, B. E. Lassiter, K. J. Bergemann, and S. R. Forrest, "A hybrid planar-mixed tetraphenyldibenzoperiflanthene/C70 photovoltaic cell," *Appl. Phys. Lett.* **102**, 073302 (2013).

135. X. Liu, H. Kim, and L. Jay Guo, "Optimization of thermally reduced graphene oxide for an efficient hole transport layer in polymer solar cells," *Org. Electron.* **14**, 591 (2013).

136. B.-G. Kim, X. Ma, C. Chen, Y. Ie, E. W. Coir, H. Hashemi, Y. Aso, P. F. Green, J. Kieffer, J. Kim, "Energy Level Modulation of HOMO, LUMO, and Band-Gap in Conjugated Polymers for Organic Photovoltaic Applications" *Adv. Funct. Mater.*, **23**, 439 (2013).

137. S. Zheng, E. Geva, B. Dunietz, "Solvated charge transfer states of functionalized anthracene and tetracyanoethylene dimers: A computational study based on a range separated hybrid functional and charge constrained self-consistent field with switching Gaussian polarized continuum models" *J. Chem. Theory Comput.*, **9**, 1125 (2013).

138. L. Zhou, P. Qiu, C. Uher, X. Shi, L. Chen, "Thermoelectric properties of p-type  $\text{Yb}_x\text{La}_y\text{Fe}_{2.7}\text{Co}_{1.3}\text{Sb}_{12}$  double-filled skutterudites," *Intermetallics* **32**, 209 (2013).

139. X. Lu, D. T. Morelli, Y. Xia, F. Zhou, V. Ozolins, H. Chi, X. Zhou, and C. Uher, "High Performance Thermoelectricity in Earth-Abundant Compounds Based on Natural Mineral Tetrahedrites," *Adv. Energy Mater.* **3**, 342 (2013).

A. Lin and J. D. Phillips, "Resolving Spectral Overlap Issue of Intermediate Band Solar Cells using Non-uniform Subbandgap State Filling," *Prog. Photovoltaics*, accepted December 2012.

140. M. H. Kuo, Taesu Oh, and P. C. Ku, "MOCVD growth of vertically aligned InGaN nanowires," *J. Cryst. Growth* **370**, 311 (2013).

141. A.-M. Yousefi, Y. Zhou, A. Querejeta-Fernandez, K. Sun, and N. A. Kotov, "Streptavidin Inhibits Self-Assembly of CdTe Nanoparticles," *J. Phys. Chem. Lett.* **3**, 3249 (2012).

142. G. Tan, S. Wang, X. Tang, H. Li, C. Uher, "Preparation and thermoelectric properties of Ga-substituted p-type fully filled skutterudites  $\text{CeFe}_{4-x}\text{Ga}_x\text{Sb}_{12}$ ," *J. Solid State Chem.* **196**, 203 (2012).

143. H. Chi, H. Kim, J. C. Thomas, X. Su, S. Stackhouse, M. Kavany, A. Van der Ven, X. Tang and C. Uher, "Configuring Pnicogen Rings in Skutterudites for Low Phonon Conductivity," *Phys. Rev. B* **86**, 195209 (2012).

144. R. D. Murphy, M. J. Abere, H. Zhang, H. Sun, B. Torralva, J. F. Mansfield, N. A. Kotov, and Steven M. Yalisove, "Ultrafast Laser Orthogonal Alignment and Patterning of Carbon Nanotube-Polymer Composite Films" *Appl. Phys. Lett.* **101**, 203301 (2012).

145. Y. Ganjeh, B. Song, K. Pagadala, K. Kim, S. Sadat, W. Jeong, K. Kurabayashi, E. Meyhofer, and P. Reddy, "A Platform to Parallelize Planar Surfaces and Control their Spatial Separation with Nanometer Resolution," *Rev. Sci. Instrum.* **83**, 105101 (2012).

146. L.K. Aagesen, L.K. Lee, P.-C. Ku, K. Thornton, "Phase-Field Simulations of GaN/InGaN Quantum Dot Growth by Selective Area Epitaxy," *J. Cryst. Growth* **361**, 57 (2012).

147. M. Yang, Ming; Hou, Ying; Kotov, Nicholas A, "Graphene-based multilayers: Critical evaluation of materials assembly techniques," *Nano Today*, **7**, 430 (2012)

148. J. A. Amonoo, E. Glynos, X. C. Chen, and P. F. Green, "An Alternative Processing Strategy for Organic Photovoltaic Devices Using a Supercritical Fluid," *J. Phys. Chem. C* **116**, 20708 (2012).

149. C. M. Andres, I. Larraza, T. Corrales, and N. A. Kotov, "Nanocomposite Microcontainers," *Adv. Mater.* **24**, 4597 (2012).

150. B. Huang, E. Glynos, B. Frieberg, H. Yang, and P. F. Green, "Effect of Thickness-Dependent Microstructure on the Out-of-Plane Hole Mobility in Poly(3-Hexylthiophene) Films," *ACS Appl Mater. Interfaces* **4**, 5204 (2012).

151. W. J. Yan, L. G. Xu, C. L. Xu, W. Ma, H. Kuang, L. B. Wang, N. A. Kotov, "Self-Assembly of Chiral Nanoparticle Pyramids with Strong R/S Optical Activity," *JACS* **134**, 15114 (2012).

152. J. Zhu, C. M. Andres, J. Xu, A. Ramamoorthy, T. Tsotsis, N. A. Kotov, "Pseudonegative Thermal Expansion and the State of Water in Graphene Oxide Layered Assemblies," *ACS Nano*, **6**, 8357 (2012).

153. J. Balachandran, P. Reddy, B. D. Dunietz and V. Gavini, "End group induced charge transfer in molecular junctions: Effect on thermopower," *J. Phys. Chem. Lett.*, **3** 1962 (2012).

154. D. M. N. M. Dissanayake, Brian Roberts, and P.-C. Ku, "Angular selective backreflector for semitransparent photovoltaics," *Appl. Phys. Lett.* **101**, 063302 (2012).

155. M. Kang, T. W. Saucer, M. V. Warren, J. H. Wu, H. Sun, V. Sih, R. S. Goldman, "Surface plasmon resonances of Ga nanoparticle arrays," *Appl. Phys. Lett.* **101**, 081905 (2012).

156. M. Kang, J. H. Wu, S. Huang, M. V. Warren, Y. Jiang, E. A. Robb, and R. S. Goldman, "Universal mechanism for ion-induced nanostructure formation on III-V compound semiconductor surfaces," *Appl. Phys. Lett.* **101**, 082101 (2012).

157. G.-H. Kim and K. P. Pipe, "Thermoelectric model to characterize carrier transport in organic semiconductors," *Phys. Rev. B* **86**, 085208 (2012).

158. C. K. Renshaw, J. D. Zimmerman, B. E. Lassiter, and S. R. Forrest, "Photoconductivity in donor-acceptor heterojunction organic photovoltaics," *Phys. Rev. B* **86**, 085324 (2012)

159. S. Sadat, E. Meyhofer, and P. Reddy, "High resolution resistive thermometry for micro/nanoscale measurements," *Rev. Sci. Instrum.* **83**, 084902 (2012).

160. H. Kim, M. Kaviani, "Effect of thermal disorder on high figure of merit in PbTe," *Phys. Rev. B* **86**, 045213 (2012)

161. H. Zhang, J. Shih, J. Zhu, N. A. Kotov, "Layered Nanocomposites from Gold Nanoparticles for Neural Prosthetic Devices," *Nano Letters*, **12**, 3391 (2012)

162. J. D. Zimmerman, X. Xiao, C. Kyle Renshaw, S. Wang, V. V. Diev, M. E. Thompson, and S. R. Forrest, "Independent Control of Bulk and Interfacial Morphologies of Small Molecular Weight Organic Heterojunction Solar Cells," *Nano Lett.* **12**, 4366 (2012).

163. H. Phillips, E. Geva, and B. D. Dunietz, "Calculating Off-Site Excitations in Symmetric Donor–Acceptor Systems via Time-Dependent Density Functional Theory with Range-Separated Density Functionals," *J. Chem. Theory Comput.* **8**, 2661–2668 (2012).

164. X. Su, H. Li, Y. Yan, H. Chi, X. Tang, Q. Zhang and C. Uher, "The role of Ga in  $\text{Ba}_{0.30}\text{Ga}_x\text{Co}_4\text{Sb}_{12+x}$  filled skutterudites," *J. Mater. Chem.* **22**, 15628 (2012).

165. S. J. Kim, B. C. Juang, W. Wang, J. R. Jokisaari, C. Chen, J. D. Phillips and X. Pan, "Evolution of self-assembled Type-II ZnTe/ZnSe nanostructures: Structural and electronic properties", *J. Appl. Phys.* **111**, 093524 (2012).

166. Querejeta-Fernández, J. C. Hernández-Garrido, H. Yang, Y. Zhou, P. F. Green, A. Varela, M. Parras, J.J. Calvino-Gámez, J. M. González-Calbet and N. A. Kotov, "Unknown Aspects of Self-Assembly of PbS Microscale Superstructures," *ACS Nano* **6**, 3800 (2012).

167. L. Wang, L. Xu, H. Kuang, C. Xu, N. A. Kotov, "Dynamic Nanoparticle Assemblies," *Acc. Chem. Res.* **45**, 1916 (2012).

168. Y. Bai, S. Ho, N. A. Kotov, "Direct-Write Maskless Lithography of LBL Nanocomposite Films and Its Prospects," *Nanoscale* **4**, 4393 (2012).

169. J. Hwang, A. J. Martin, J. M. Millunchick, J. D. Phillips, "Thermal emission in type-II GaSb/GaAs quantum dots and prospects for intermediate band solar energy conversion," *J. Appl. Phys.* **111**, 074514 (2012).

170. J. H. Jung, J. C. Furgal, T. Goodson III, T. Mizumo, M. Schwartz, K. Chou, J.-F. Vonet, R. M. Laine, "3-D molecular mixtures of catalytically functionalized [vinylSiO<sub>1.5</sub>]<sub>10</sub>/[vinylSiO<sub>1.5</sub>]<sub>12</sub>. Photophysical characterization of third generation derivatives," *Chem. Mater.* **24**, 1883 (2012).

171. B-G. Kim, C-G Zhen, E. J. Jeong, J. Kieffer, J. Kim, "Organic Dye Design Tools for Efficient Photo-Current Generation in Dye Sensitized Solar Cells; Exciton Binding Energy and Electron Acceptor" *Adv. Funct. Mater.* **22**, 1606 (2012).

172. J.-E. Lee, T. W. Saucer, A. J Martin, D. Tien, J. M. Millunchick, and V. Sih, "Ground-state exciton emission of InAs quantum dots produced by Focused-Ion-Beam-directed nucleation," *J. Lumin.* **133**, 117 (2013).

173. X. Su, H. Li, Y. Yan, G. Wang, H. Chi, X. Zhou, X. F. Tang, Q. Zhang, and C. Uher, "Microstructure and Thermoelectric Properties of CoSb<sub>2.75</sub>Ge<sub>0.25</sub>-<sub>x</sub>Te<sub>x</sub> Prepared by Rapid Solidification," *Acta Mater.* **60**, 3536 (2012).

174. S. Zheng, H. Phillips, E. Geva, and B. D. Dunietz, "Ab Initio Study of the Emissive Charge-Transfer States of Solvated Chromophore-Functionalized Silsesquioxanes," *J. Am. Chem. Soc.* **134**, 6944 (2012).

175. H. Liu, X. Shi, F. Xu, L. Zhang, W. Zhang, L. Chen, Q. Li, C. Uher, T. Day, and G. J. Snyder, "Copper Ion Liquid-Like Thermoelectrics," *Nature Mater.* **11**, 422 (2012).

176. J. Martin, T. W. Saucer, G. V Rodriguez, V. Sih, J. Millunchick, "Lateral patterning of multilayer InAs/GaAs(001) quantum dot structures by in vacuo focused ion beam," *Nanotechnology* **23**, 135401 (2012).

177. M. V. Warren, A. W. Wood, J. C. Canniff, F. Naab, C. Uher, and R. S. Goldman, "Evolution of Structural and Thermoelectric Properties of Indium-ion-implanted Epitaxial GaAs," *Appl. Phys. Lett.* **100**, 102101 (2012).

178. X. Xiao, G. Wei, S. Wang, J. D. Zimmerman, C. K. Renshaw, M. E. Thompson, and S. R. Forrest, "Small-Molecule Photovoltaics Based on Functionalized Squaraine Donor Blends," *Adv. Mater.* **24**, 1956 (2012).

179. C. M. Andres, M. L. Fox, N. A. Kotov, "Traversing Material Scales: Macroscale LBL-Assembled Nanocomposites with Microscale Inverted Colloidal Crystal Architecture," *Chem. Mater.* **24**, 9 (2012).

180. B. Roberts, D. M. Nanditha M. Dissanayake, and P.-C. Ku, "Angular selective semi-transparent photovoltaics," *Opt. Express* **20**, 045315 (2011).

181. P. R. Tekavec, K. L. M. Lewis, J. A. Myers, F. D. Fuller, and J. P. Ogilvie, "Towards broad bandwidth two-dimensional electronic spectroscopy: correction of chirp from a continuum probe," *IEEE J. Sel. Top. Quant.* **PP**, 1 (2011).

182. J. Martin, T. W. Saucer, K. Sun, S. J. Kim, G. Ran, G. V Rodriguez, X. Pan, V. Sih, J. Millunchick, "Analysis of defect-free GaSb/GaAs(001) quantum dots grown on the Sb-terminated (2x8) surface," *J. Vac. Sci. Technol. B* **30**, 02B112 (2012).

183. J. H. Wu and R.S. Goldman, "Mechanisms of Nanorod Growth on focused-ion-beam irradiated Semiconductor surfaces: Role of Redeposition," *Appl. Phys. Lett.* **100**, 053103 (2012).

184. K. Bergemann and S. R. Forrest, "Measurement of exciton diffusion lengths in optically thin organic films," *Appl. Phys. Lett.* **99**, 243303 (2011).

185. L. K. Lee, L. Zhang, H. Deng, and P.-C. Ku, "Room-Temperature Quantum-Dot-Like Luminescence from Site-Controlled InGaN Quantum Disks," *Appl. Phys. Lett.* **99** 263105 (2011).

186. H. Phillips, S. Zheng, A. Hyla, R. Laine, T. Goodson, III, E. Geva, and B. D. Dunietz, "Ab Initio Calculation of the Electronic Absorption of Functionalized Octahedral Silsesquioxanes via Time-Dependent Density Functional Theory with Range-Separated Hybrid Functionals," *J. Phys. Chem. A* **116**, 1137 (2012).

187. G. Wei, X. Xiao, S. Wang, K. Sun, K. J. Bergemann, M. E. Thompson and S. R. Forrest, "Functionalized Squaraine Donors for Nanocrystalline Organic Photovoltaics," *ACS Nano* **6**, 972 (2011).

188. L. Xu, H. Kuang, C. Xu, W. Ma, L. Wang, N. A. Kotov, "Regiospecific Plasmonic Assemblies for in-situ Raman Spectroscopy in Live Cells," *J. Am. Chem. Soc.* **134**, 1699 (2012).

189. E. Cohen, N. Elfassy, G. Koplovitz, S. Yochelis, S. Shusterman, D. P. Kumah, Y. Yacoby, R. Clarke and Y. Paltiel, "Surface X-Ray Diffraction Results on the III-V Droplet Heteroepitaxy Growth Process for Quantum Dots: Recent Understanding and Open Questions," *Sensors* **11**, 10624 (2011).

190. J. P. A. Makongo, D. K. Misra, J. R. Salvador, N. J. Takas, G. Wang, M. R. Shabetai, A. Pant, P. Paudel, C. Uher, K. L. Stokes, and P. F. P. Poudeu, "Thermal and electronic charge transport in bulk nanostructured  $Zr_{0.25}Hf_{0.75}NiSn$  composites with full-Heusler inclusions," *J. Sol. State Chem.* **184**, 2948 (2011).

191. J. P. A. Makongo, D. K. Misra, X. Zhou, A. Pant, M. R. Shabetai, X. Su, C. Uher, K. L. Stokes, and P. F. P. Poudeu, "Simultaneous Large Enhancements in Thermopower and Electrical Conductivity of Bulk Nanostructured Half-Heusler Alloys," *J. Am. Chem. Soc.* **133**, 18843 (2011).

192. S. Huang, A. V. Semichaevsky, L. Webster, H. T. Johnson, and R. S. Goldman, "Influence of wetting layers and quantum dot size distribution on intermediate band formation in InAs/GaAs superlattices," *J. Appl. Phys.* **110**, 073105 (2011).

193. R. R. Collino, A. W. Wood, N. M. Estrada, B. B. Dick, H. W. Ro and C. L. Soles, Y. Q. Wang, M. D. Thouless, R. S. Goldman, "Formation and transfer of GaAsN nanostructure layers," *J. Vac. Sci. Technol. A* **29**, 060601 (2011).

194. D. M. N. M. Dissanayake, B. Roberts, and P. C. Ku, "Plasmonic Backscattering Enhanced Inverted Photovoltaics," *Appl. Phys. Lett.* **99**, 113306 (2011).

195. J. H. Jung and R. M. Laine, "Beads on a Chain (BOC) Polymers Formed from the Reaction of  $NH_2PhSiO_{1.5}^x[PhSiO_{1.5}]_{10-x}$  and  $[NH_2PhSiO_{1.5}]_x[PhSiO_{1.5}]_{12-x}$  Mixtures ( $x = 2-4$ ) with the Diglycidyl Ether of Bisphenol A," *Macromolecules* **44**, 7263 (2011).

196. Y. Li, V. A. Stoica, L. Endicott, G. Wang, H. Sun, K. Pipe, C. Uher, and R. Clarke, "Femtosecond laser-induced nanostructure formation in  $Sb_2Te_3$ ," *Appl. Phys. Lett.* **99**, 121903 (2011).

197. Y. Xia, T. D. Nguyen, M. Yang, B. Lee, A. Santos, P. Podsiadlo, Z. Tang, S. C. Glotzer, and N. A. Kotov, "Self-assembly of self-limiting monodisperse supraparticles from polydisperse nanoparticles," *Nat. Nanotechnol.* **6**, 580 (2011).

198. R. Liu, J. Yang, X. Chen, X. Shi, L. Chen, and C. Uher, "p-Type skutterudites  $R_xM_yFe_3CoSb_{12}$  ( $R$ ,  $M$  = Ba, Ce, Nd, and Yb): Effectiveness of double-filing for the lattice thermal conductivity reduction," *Intermetallics* **19**, 1747 (2011).

199. G. Wang, L. Endicott, and C. Uher, "Recent Advances in the Growth of Bi-Sb-Te-Se Thin Films," *Sci. Adv. Mater.* **3**, 539 (2011).

200. W. Wang, J. D. Phillips, S. J. Kim and X. Pan, "ZnO/ZnSe/ZnTe heterojunctions for ZnTe-based solar cells", *J. Electron. Mater.* **40**, 1674 (2011).

201. Brian E. Lassiter, Guodan Wei, Siyi Wang, Jeramy D. Zimmerman, Viacheslav V. Diev, Mark E. Thompson, and Stephen R. Forrest, "Organic photovoltaics incorporating electron conducting exciton blocking layers," *Appl. Phys. Lett.*, **98**, 243307 (2011).

202. C. K. Renshaw, C. W. Schlenker, M. E. Thompson, S. R. Forrest, "Reciprocal carrier collection in organic photovoltaics," *Phys. Rev. B* **84**, 045315 (2011).

203. M. Yang, K. Cao, L. Sui, Y. Qi, J. Zhu, A. Waas, E. M. Arruda, J. Kieffer, M. D. Thouless, and N. A. Kotov, "Dispersions of Aramid Nanofibers: A New Nanoscale Building Block," *ACS Nano* **5**, 6945 (2011).

204. S.-H. Jung, C. Chen, S.-H. Cha, B. Yeom, J. H. Bahng, S. Srivastava, J. Zhu, M. Yang, S. Liu, and N. A. Kotov, "Spontaneous Self-Organization Enables Dielectrophoresis of Small Nanoparticles and Formation of Photoconductive Microbridges," *J. Am. Chem. Soc.* **133**, 10688 (2011).

205. E. L. Lanni, J. R. Locke, C. M. Gleave, and A. J. McNeil, "Ligand-based steric effects in Ni-catalyzed Hain-Growth polymerizations using bis(dialkylphosphino)ethanes," *Macromolecules* **44**, 5136 (2011).

206. G. D. Lilly , A. Agarwal , S. Srivastava , and N. A. Kotov, "Helical Assemblies of Gold Nanoparticles," *Small* **7**, 2004 (2011).

207. S. Sulaiman, J. Zhang, T. Goodson III, and R. M. Laine, "Synthesis, characterization and photophysical properties of polyfunctional phenylsilsesquioxanes: [o-RPhSiO<sub>1.5</sub>]<sub>8</sub>, [2,5-R<sub>2</sub>PhSiO<sub>1.5</sub>]<sub>8</sub>, and [R<sub>3</sub>PhSiO<sub>1.5</sub>]<sub>8</sub> compounds with the highest number of functional units/unit volume," *J. Mater. Chem.* **21**, 11177 (2011).

208. N. C. Giebink, G. P. Wiederrecht, M. R. Wasielewski, and S. R. Forrest, "Thermodynamic efficiency limit of excitonic solar cells," *Phys. Rev. B* **83**, 195327 (2011).

209. J. Hwang and J. D. Phillips, "Band structure of strain-balanced GaAsBi/GaAsN super-lattices on GaAs", *Phys. Rev. B* **83**, 195327 (2011).

210. M. F. Roll, J. W. Kampf, R. M. Laine, "Crystalline hybrid polyphenylene macromolecules from octaalkynylsilsesquioxanes, crystal structures, and a potential route to 3-D graphenes," *Macromolecules* **44**, 3425 (2011).

211. N. Sergueev, S. Shin, M. Kaviany, and B. Dunietz, "Efficiency of thermoelectric energy conversion in biphenyl-dithiol junctions: Effect of electron-phonon interactions," *Phys. Rev. B* **83**, 195415 (2011).

212. X. Su, H. Li, G. Wang, H. Chi, X. Zhou, X. Tang, O. Zhang, and C. Uher, "Structure and transport properties of double-doped  $\text{CoSb}_{2.75}\text{Ge}_{0.25-x}\text{Te}_x$  ( $x = 0.125-0.20$ ) with in situ nanostructure," *Chem. Mater.* **23**, 2948 (2011).

213. Tan, J. Balachandran, S. Sadat, V. Gavini, B. D. Dunietz, S-Y. Jang, and P. Reddy, "Effect of length and contact chemistry on the electronic structure and thermoelectric properties of molecular junctions," *J. Am. Chem. Soc.* **133**, 8838 (2011).

214. J. Zhu, B. S. Shim, M. Di Prima, and N. A. Kotov, "Transparent Conductors from Carbon Nanotubes LBL-Assembled with Polymer Dopant with  $\pi-\pi$  Electron Transfer," *J. Am. Chem. Soc.* **133**, 7450 (2011).

215. V. D. Dasika, A. Semichaevsky, J.P. Petropoulos, A.M. Dangewicz, J.C. Dibbern, M. Holub, P.K. Bhattacharya, J.M.O. Zide, H.T. Johnson, and R.S. Goldman, "Influence of Mn dopants on InAs/GaAs quantum dot electronic states," *Appl. Phys. Lett.* **98**, 141907 (2011).

216. C.-H. Kim, S.-H. Cha, S. C. Kim, M. Song, J. Lee, W. Shin, S.-J. Moon, J. H. Bahng, N. A. Kotov, and S.-H. Jin, "Silver Nanowire Embedded in P3HT:PCBM for High-Efficiency Hybrid Photovoltaic Device Applications," *ACS Nano* **5**, 3319 (2011).

217. R. M. Laine and M. F. Roll, "Polyhedral phenylsilsesquioxanes," *Macromolecules* **44**, 1073 (2011).

218. J. Lee, T. W. Saucer, A. J. Martin, D. Tien, J. M. Millunchick, and V. Sih, "Photoluminescence imaging of focused-ion-beam induced individual quantum dots," *Nano Lett.* **11** 1040 (2011).

219. G. Wei, S. Wang, K. Sun, M. E. Thompson and S. R. Forrest, "Solvent-annealed crystalline squarine: PC70BM (1:6) solar cells," *Adv. Energy Mater.* **1**, 184 (2011).

220. B-G. Kim, E. J. Jeong, H. J. Park, D. Bilby, L. J. Guo, J. Kim, "Effect of polymer aggregation on the open circuit voltage in organic photovoltaic cells: aggregation induced conjugated polymer gel and its application for preventing open circuit voltage drop," *ACS Appl. Mater. Interfaces* **3**, 674 (2011).

221. G.-H. Kim, M. Shtein, K. P. Pipe, "Thermoelectric and bulk mobility measurements in pentacene thin films," *Appl. Phys. Lett.* **98**, 093303 (2011).

222. H. Phillips, A. Prociuk, B. D. Dunietz, "Bias effects on the electronic spectrum of a molecular bridge," *J. Chem. Phys.* **134**, 054708 (2011).

223. T. W. Saucer, J.-E. Lee, A. J. Martin, D. Tien, J. M. Millunchick, and V. Sih, "Photoluminescence of patterned arrays of vertically stacked InAs/GaAs quantum dots," *Solid State Commun.* **151**, 269 (2011).

224. D. Bilby, B. Kim, J. Kim, "Recent design strategies for polymer solar cell materials," *Pure Appl. Chem.* **83**, 127 (2011).

225. D. P. Kumah, J.H. Wu, N.S. Husseini, V.D. Dasika, R.S. Goldman, Y. Yacoby, and R. Clarke, "Correlating structure, strain, and morphology of self-assembled InAs quantum dots on GaAs", *Appl. Phys. Lett.* **98**, 021903 (2011).

226. J. Bludska, I. Jakubec, S. Karamazov, J. Horak, and C. Uher, "Lithium ions in the van der Waals gap of  $\text{Bi}_2\text{Se}_3$  single crystals," *J. Solid State Chem.* **183**, 2813 (2010).

227. H. Kim, M. Kaviani, J. C. Thomas, A. van der Ven, C. Uher, and B. Huang, "Structural order-disorder transitions and phonon conductivity of partially filled skutterudites," *Phys. Rev. Lett.* **105**, 265901 (2010).

228. J. Martin, T. Tritt, and C. Uher, "High temperature Seebeck coefficient metrology," *J. Appl. Phys.* **108**, 121101 (2010).

229. C. Drasar, A. Hovorkova, P. Lostak, S. Ballikaya, C.-P. Li, and C. Uher, "Figure of Merit of  $(\text{Sb}_{0.75}\text{Bi}_{0.25})_{2-x}\text{In}_x\text{Te}_{2.8}\text{Se}_{0.2}$  Single Crystals," *J. Elec. Mater.* **39**, 1760-1763 (2010).

230. J. R. Locke and A. J. McNeil, "Syntheses of gradient  $\pi$ -conjugated copolymers of thiophene," *Macromolecules* **43**, 8709 (2010).

231. Yadav, Y. Jin, P. K. L. Chan, M. Shtein, and K. P. Pipe, "Intermolecular electronic coupling in organic molecular thin films measured by temperature modulation spectroscopy", *Appl. Phys. Lett.* **97**, 203307 (2010).

232. M. Andres, N. A. Kotov. "Inkjet deposition of layer-by-layer assembled films." *J. Am. Chem. Soc.* **132**, 14496 (2010).

233. Ding, Washington, B. D. Dunietz, "On the conditions for enhanced transport through molecular junctions based on metal centers ligated by pairs of pyridazino-derived ligands," *Mol. Phys.* **108**, 2591 (2010).

234. N. C. Giebink, G. P. Wiederrecht, M. R. Wasielewski, and S. R. Forrest, "Ideal diode equation for organic heterojunctions. I. Derivation and application," *Phys. Rev. B* **82**, 155305 (2010).

235. N. C. Giebink, B. E. Lassiter, G. P. Wiederrecht, M. R. Wasielewski, and S. R. Forrest, "Ideal diode equation for organic heterojunctions. II. The role of polaron pair recombination," *Phys. Rev. B* **82**, 155306 (2010).

236. M-G. Kang, T. Xu, H. J. Park, X. Luo, and L. J. Guo, "Efficiency enhancement of organic solar cells using transparent plasmonic Ag nanowire electrodes," *Adv. Mater.* **22** 4378 (2010).

237. J. Kim and M. Kaviani, "Phonon-coupling enhanced absorption of alloyed amorphous silicon for solar photovoltaics," *Phys. Rev. B* **82**, 134205 (2010).

238. Y. Li, V. A. Stoica, L. Endicott, G. Wang, C. Uher, and R. Clarke, "Coherent optical phonon spectroscopy studies of femtosecond-laser modified  $\text{Sb}_2\text{Te}_3$  films," *Appl. Phys. Lett.* **97**, 171908 (2010).

239. M. Yang, R. Alvarez-Puebla, H-S. Kim, P. Aldeanueva-Potel, L. M. Liz-Marzan, and N. A. Kotov, "SERS-active gold lace nanoshells with built-in hotspots," *Nano Letters* **10**, 4013 (2010).

240. T. Dannecker, Y. Jin, H. Cheng, C. F. Gorman, J. Buckeridge, C. Uher, S. Fahy, C. Kurdak, and R. Goldman, "Nitrogen composition dependence of electron effective mass in  $\text{GaAs}_{1-x}\text{N}_x$ ," *Phys. Rev. B* **82**, 125203 (2010).

241. B. E. Lassiter, R. R. Lunt, C. K. Renshaw, and S. R. Forrest, "Structural templating of multiple polycrystalline layers in organic photovoltaic cells," *Opt. Express* **18**, A444 (2010).

242. Prociuk and B. D. Dunietz, "Photo-induced absolute negative current in a symmetric molecular electronic bridge," *Phys. Rev. B* **82**, 125449 (2010).

243. L. Huang and M. Kaviani, "Filler-reduced phonon conductivity of thermoelectric skutterudites: ab initio calculations and MD simulations," *Acta Mater.* **58**, 2516 (2010).

244. G. D. Lilly, Y. Chen, X. Pan and N. A. Kotov , "Effect of CdSe nanoparticles on the growth of Te nanowires: greater length and tortuosity and nonmonotonic concentration effect," *J. Phys. Chem. C* **114**, 2428 (2010).

245. S. Sadat, A. Tan, Y. J. Chua, and P. Reddy, "Nanoscale thermometry using point contact thermocouples," *Nanoletters* **10**, 2613 (2010).

246. G. Wei, S. Wang, K. Renshaw, M. E. Thompson, and S. R. Forrest, "Solution processed squaraine bulk heterojunction photovoltaic cells," *ACS Nano* **4**, 1927 (2010).

247. K. H. An, M. Shtein, and K. P. Pipe, "Surface plasmon mediated energy transfer of electrically-pumped excitons", *Opt. Express* **18**, 4041 (2010).

248. M-G. Kang, H. J. Park, S.-H. Ahn, T. Xu, and L. J. Guo, "Towards low-cost, high efficiency, and scalable organic solar cells with transparent metal electrode and improved domain morphology," *IEEE J. Sel. Top. Quantum Electron.* **PP(99)**, 1 (2010).

249. B-G. Kim, M-S. Kim, Jinsang Kim, "Ultrasonic assisted nano-dimensional self-assembly of poly-3-hexylthiophene for organic photovoltaic cells" *ACS Nano* **4**, 2160 (2010).

250. G. D. Lilly, J. Lee, and N. A. Kotov, "'Cloud' assemblies: quantum dots form electrostatically bound dynamic nebulae around large gold nanoparticles." *Phys. Chem. Chem. Phys.* **12**, 11878 (2010)

251. H. J. Park, M. G. Kang, S.-H. Ahn and L. J. Guo, "A Facile Route to Polymer Solar Cells with Optimum Morphology Readily Applicable to a Roll-to-Roll Process without Sacrificing High Device Performances," *Adv. Mater.* **22**, E247 (2010).

252.

253. Tan, S. Sadat, P. Reddy, "Measurement of thermopower and current voltage characteristics of molecular junctions to Identify orbital alignment." *Appl. Phys. Lett.* **96**, 013110 (2010).

254. M. Yang, K. Sun and N. A. Kotov, "Formation and assembly-disassembly processes of ZnO hexagonal pyramids driven by dipolar and excluded volume interactions," *J. Am. Chem. Soc.* **132**, 1860 (2010).

255. W. Wang, A. Lin, J. D. Phillips and W. Metzger, "Generation and recombination rates at ZnTe:O intermediate band states", *Appl. Phys. Lett.* **95**, 261107 (2009).