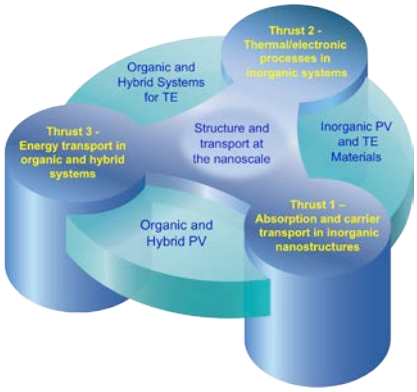
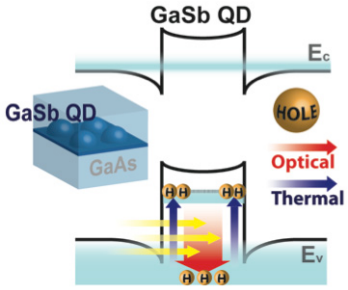
Center for Solar and Thermal Energy Conversion (CSTEC)
EFRC Director: Peter F. Green
Lead Institution: University of Michigan, Ann Arbor

***Mission Statement**: To study complex material structures on the nanoscale to identify key features for their potential use as materials to convert solar energy and heat to electricity.*

Research in CSTEC falls in three synergistic and collaborative thrusts, under a unifying concept: *structure and transport at the nanoscale.* Energy conversion processes in materials are the result of a complex interplay between structure (which includes aspects of symmetry and dimensionality) over different length scales, while the dynamic processes that occur over a wide range of time scales. The basic challenge is to access the wide range of length and time scales in order to understand and then overcome the trade-offs associated with the complex energy conversion processes involved. Achieving our objectives requires a team with diverse expertise working closely together in a highly collaborative manner on different aspects of the problem.

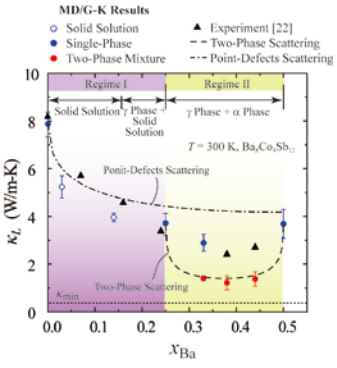


The objective of the first thrust, **CSTEC Thrust 1**, is to exploit unique quantum effects at the nanoscale to understand and to maximize the absorption of energy from sunlight and to minimize energy losses, associated with carrier transport, using nanostructured inorganic materials, including highly mismatched Alloys (HMAs) and quantum dots, to achieve high efficiency solar energy conversion. We synthesize nanostructured materials architectures for solar energy conversion such that the *optical absorption* and *electronic transport are tailored to achieve* properties not available in the bulk, circumventing, for example the trade-off between absorption and transport efficiency of bulk systems. Specific systems under investigation include the following: (a) **Intermediate band concepts exploiting** nanostructures involving QD: Type-I and II, to control carrier life times and absorption (b) **highly mismatched alloys** (GaAs:N, GaAs:Bi, and ZnTe:O) with tailored band gaps, lattice spacings and densities of states in order to control electron and phonon transport.



Energy band diagram of a quantum dot with a type II band line-up

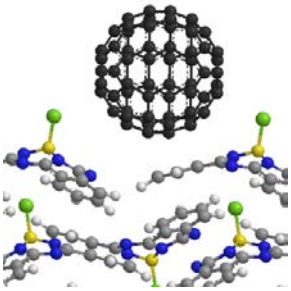
The objective of **CSTEC Thrust 2** is to understand and to exploit fundamental mechanisms and processes associated with electron and hole transport, as well as electron-phonon coupling, in materials, with the goal of achieving high figures of merit in thermoelectric (inorganic, hybrid or molecular) materials. Current research problems include: (a) understanding electronic and phonon transfer at metal-organic molecule-metal junctions (MMMJ), (b) modifying carrier and phonon dynamics through judicious manipulation of structure in thin films and nanostructured materials, and (c) investigating



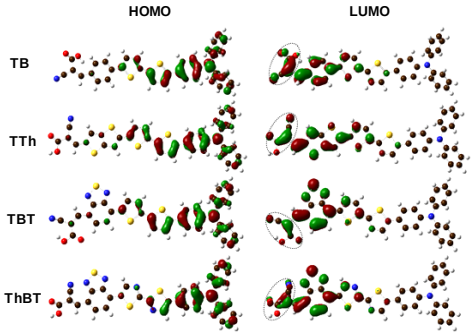
Theoretical predictions of the thermal conductivity in different phases of a skutterudite thermoelectric material

structural order-disorder transitions and phonon conductivity of partially filled skutterudites using combined experimental and theoretical methods to improve the thermoelectric figure-of-merit.

In **CSTEC Thrust 3** we investigate the molecular and structural origins of energy conversion (absorption, carrier generation and recombination, transport) phenomena in organic and hybrid material systems with the goal of producing highly efficient materials and morphological structures for OPVs. Our efforts to develop and to maximize the performance/efficiency of OPVs include: (1) a combined experimental / computational approach to the molecular design and synthesis of new materials; (2) the design and development of processing strategies to control morphology at the nanoscale; (3) the measurement and prediction of structure and carrier transport, and (4) materials and nanoscale photonics optimization to enhance absorption.



Simulations of molecular configurations in C_{60}/SubPc



Homo/Lumo levels calculated for molecules synthesized for solar energy conversion

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