

SYMPOSIUM TP03

Emerging Low-Temperature Thermal Energy Conversion Technologies
November 26 - November 29, 2018

Symposium Organizers

Michael Chabynyc, University of California, Santa Barbara
Terry Hendricks, California Institute of Technology
Kedar Hippalgaonkar, Institute of Materials Research and Engineering
Shannon Yee, Georgia Institute of Technology

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* Invited Paper

SESSION TP03.01: Organic and Polymer Thermoelectrics I

Session Chairs: Christian Muller and Shannon Yee

Monday Morning, November 26, 2018

Sheraton, 3rd Floor, Gardner AB

8:00 AM *TP03.01.01

PEDOT-Based Thermoelectric Materials and Devices Qingshuo Wei; National Advanced Institute of Science and Technology, Tsukuba, Japan.

In this talk, we are going to focus on two topics. The first one is understanding of the doping mechanism of poly(3,4-ethylenedioxythiophene). We have shown that PEDOT was doped by protons. The doping and de-doping processes using protonic acid and base are fully reversible. We are going to demonstrate that the use of protonated EDOT moieties as an end group to prepare organic conductors is a promising approach toward highly conductive organic materials. In the second part, we are going to present proof-of-concept studies of organic thermoelectric devices fabricated by thermal lamination. With an air-cooled heat sink, the device exhibited a power output of ca. 100 microwatt, which is sufficient to power practical devices.

8:30 AM TP03.01.02

Thermoelectric Polymer Films with High Power Factor Arising from the Significant Seebeck Coefficient Enhancement by Surface Energy Filtering Guan Xin, Zeng Fan and Jianyong Ouyang; Materials Science and Engineering, National University of Singapore, Singapore, Singapore.

Thermoelectric (TE) materials are important for sustainable development because they can be used to directly convert heat into electricity. Compared with inorganic TE materials, polymers have advantages of low cost, high abundance, high mechanical flexibility and low or no toxicity. However, the Seebeck coefficient of polymers are much lower than their inorganic counterparts. In this work, we find that the Seebeck coefficient of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) can be enhanced by coating second layer materials. The Seebeck coefficient enhancement is ascribed to the surface energy filtering induced by these materials. The surface energy filtering can increase the mean electron energy and thus the Seebeck coefficient of the PEDOT:PSS films. After coating second layer on PEDOT:PSS films sequentially treated with acid and base can give rise to a power factor of $401.2 \mu\text{W m}^{-1} \text{K}^{-2}$ with the Seebeck coefficient of $47.2 \mu\text{V K}^{-1}$ and electrical conductivity of 1801 S cm^{-1} .

8:45 AM TP03.01.03

Analyzing the Effect Preferred Orientation and Doping on the Transport Properties of $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ Alloys for Thermoelectric Power Generation Applications Omer Meroz and Yaniv Gelbstein; Material Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel.

When attempting to find new alternative energy resources new technological developments must be made to bring society one step closer to a cleaner environment. Thermoelectric devices take thermal heat, either directly from solar energy or as a byproduct of fuel burn, and transform it to electricity. At its core is to prepare high performance TE nanocomposites, both p- and n-type, in a time and energy efficient way.

The performance of thermoelectric devices is assessed by the dimensionless figure of merit ZT of the material, defined as $ZT = \alpha^2 \sigma T / k$, where α , σ , k and T are the Seebeck coefficient, the electrical and thermal conductivities, and the absolute temperature, respectively. The thermal conductivity is a combination of thermal conductivity via electrons, κ_e , and via phonons, κ_l . The main difficulty in improvement of the efficiency of a thermoelectric device is due to the complex relation between σ , α and k . Improving the performance of thermoelectric materials is usually done either by improving the power factor, $\alpha^2 \sigma$, or by applying phonon scattering methods in order to lower the thermal conductivity.

Bismuth-telluride-based alloys are of great importance not only as the best thermoelectric materials with the maximal ZT values close to unity near room temperature, but also due to the potential for further performance improvement.

In this study $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ compositions were electronically optimized by various CHI_3 doping levels, preferred alignment of the crystallographic orientation, and lattice thermal conductivity minimization. The synthesis route included rocking furnace melting, energetic ball milling and hot pressing under optimal conditions for enhancement of the thermoelectric figure of merit, ZT commonly applied in low temperature power generation applications. The transport properties in perpendicular to the pressing direction were examined.

9:00 AM TP03.01.04

OpenBTE—An Open-Source Solver for the Phonon Boltzmann Transport Equation in Multi-Dimensional Structures Giuseppe Romano; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Over the last decades, Fourier's law has been challenged by measurements of heat transport at small length and time scales. In fact, when the mean free

path (MFP) of heat carriers (i.e. phonons) becomes comparable to the characteristic length, heat travels quasi-ballistically, therefore deviating from standard diffusive theory. The Boltzmann transport equation (BTE) has been the mainstream model of non-diffusive heat transport and has been applied successfully to simple cases, such as thin films and nanowires. However, as complex geometries become increasingly accessible experimentally, a more flexible BTE solver is needed. In this talk, we will present OpenBTE [1], an open-source solver for the space-dependent phonon BTE in three-dimensional structures. The code is interfaced to first-principles calculations from which bulk-related data is collected, and to a Fourier's solver to model low-MFP phonons, so that the framework is entirely parameter-free across all the scales. Furthermore, thanks to its finite-volume formulation, OpenBTE can easily handle complex-shaped geometries, offering a unique capability of thermal conductivity tuning. OpenBTE groups phonons based on their MFPs, an approach that boosts the computational efficiency, especially for complex-unit cell materials [2]. We will also describe the adopted parallelization scheme and its scaling performances. Finally, we will show a few examples, including porous materials and thin films. [1] www.openbte.org [2] G. Romano and J. C. Grossman. "Heat conduction in nanostructured materials predicted by phonon bulk mean free path distribution." *Journal of Heat Transfer* 137.7 (2015): 071302.

9:15 AM TP03.01.05

Chain Morphology Effect on Thermal Conductivity of Polymer-Based Materials Faisal Almana^{1,2}, Weidong Tang³, Oliver Fenwick³, Martyn A. McLachlan¹ and Natalie Stingelin^{4,1}; ¹Imperial College London, London, United Kingdom; ²SABIC, Riyadh, Saudi Arabia; ³Queen Mary University of London, London, United Kingdom; ⁴Georgia Institute of Technology, Atlanta, Georgia, United States.

Polymers are an attractive alternative to inorganic thermoelectric materials as they are lightweight, generally of low cost to manufacture, offer freedom-of-design as well as having low thermal conductivity. However, our fundamental understanding of thermal transport in polymeric systems needs to be drastically improved to gain the capability to design systems for thermal applications from the outset. The abundance of variety of polymers systems renders this task highly challenging. For instance, while blending is a well-known route for the manipulation of polymer properties, little is known how various blending options affect the thermal conductivity of the blend components and the overall blend. Here, we use polymers with model functional groups and discuss the effect of blending on chain conformation and how, in turn, this changes the thermal transport of the overall material. We draw comparisons to other multicomponent systems such as organic/inorganic hybrid materials and present data that start allowing us to establish design rules and how structural features – both in blends and inorganic/organic hybrids – affect thermal conductivity. Ultimate goal is to provide a general understanding on a broad range of systems that can be used to tune the thermal conductivity of polymers to the final required properties.

9:30 AM *TP03.01.06

Thiophene Polymers for Thermoelectric Blends and Composites Howard E. Katz and Hui Li; Johns Hopkins University, Baltimore, Maryland, United States.

The ability to control the carrier energy levels, functional group polarity, and film morphology make organic and polymeric semiconductors (OSCs) especially attractive for various energy interconversions. Their mechanical flexibility, low temperature processing, potential printability, capability of blending to form composites, and use of common elements are additional attractive features. In this presentation, we focus on thiophene polymers blended with dopants and Fermi level-setting additives for thermoelectric applications. Two thiophene polymers, poly(bisdodecylquaterthiophene) and poly(bisdodecyl thioquaterthiophene) (PQT12 and PQTS12, respectively), were used in active layers. From measurements of cyclic voltammetry and the electronic characteristics, we found that the introduction of sulfurs into the side chains induces traps in films of the PQTS12. Doping the polymer with sulfur in side chains (PQTS12) with the strong oxidant nitrosonium tetrafluoroborate (NOBF₄), we obtained a very high conductivity up to 350 S cm⁻¹, which is the highest reported nonionic conductivity among films made from dopant-polymer solutions. We found the combination of efficient charge transfer, tighter π - π stacking and strong intermolecular coupling is responsible for the high conductivity. Furthermore, the high conductivity is stable in air without extrinsic ion contributions that are associated with the polymer most often used for high conductivity, poly(ethylenedioxythiophene) (PEDOT:PSS). The thermoelectric power factor compared favorably with prior reports for p-type polymers that were made by the alternative process of immersion of polymer films into dopant solutions, and fit the established models for thermoelectric polymers. Additional data obtained from thiophene copolymers containing the ethylenedioxythiophene subunit supported these conclusions. The applicability of these polymers in hybrid composites will also be considered.

10:00 AM BREAK

SESSION TP03.02: Organic and Polymer Thermoelectrics II

Session Chair: Howard Katz

Monday Afternoon, November 26, 2018

Sheraton, 3rd Floor, Gardner AB

1:30 PM *TP03.02.01

Bulk Doping Strategies for Plastic Thermoelectrics Christian Muller; Chalmers University of Technology, Goteborg, Sweden.

Molecular doping of conjugated polymers is a widely explored tool for the preparation of highly conducting materials for organic thermoelectrics. While doping of thin films is well understood, there is a lack of doping strategies that can be applied to bulk materials. Hence, the up to millimeter thick architectures, which are needed to construct the legs of a thermoelectric generator, are more challenging to realize. In this talk two bulk doping strategies are presented. Foams of poly(3-hexylthiophene) can be sequentially doped without compromise in thermoelectric performance. Further, conjugated polymers with more polar oligo ethylene glycol side chains show improved compatibility with the dopant. As a result, thermally stable p-doped films with a high electrical conductivity of 100 S/cm can be prepared. The same concept is also applicable to n-type polymers, with conductivities reaching 0.3 S/cm.

2:00 PM TP03.02.02

Intrinsically Conductive Polymers with a Power Factor of >700 $\mu\text{W}/(\text{m K}^2)$ Jianyong Ouyang; National University of Singapore, Singapore, Singapore.

Organic thermoelectric materials have drawn great interest because of their advantages including mechanical flexibility, easy availability, non-toxicity and low thermal conductivity. Thermoelectric materials with high ZT are required for highly efficient thermoelectric conversion. But the electrical conductivity

and Seebeck coefficient of thermoelectric materials are interdependent. Hence, the power factor of organic thermoelectric materials is remarkably lower than their inorganic counterpart.

Here, I will present some of our works in developing intrinsically conductive polymers with high thermoelectric power factors. We developed methods to enhance both the Seebeck coefficient and electrical conductivity of intrinsically conductive polymers. We observed an ultrahigh power factor of $>700 \mu\text{W}/(\text{m K}^2)$ on intrinsically conductive polymers.

2:15 PM TP03.02.03

Polymer Morphology Dominates Over Energy-Dependent Scattering in Organic-Inorganic Hybrid Thermoelectrics Pawan Kumar¹, Edmond Zaia^{2,4}, Erol Yildirim³, D V M. Repaka¹, Shuo-Wang Yang³, Jeffrey Urban^{2,4} and Kedar Hippalgaonkar¹; ¹IMRE, Singapore, Singapore; ²Chemical Engineering, University of California, Berkeley, Berkeley, California, United States; ³IHPC, Singapore, Singapore; ⁴Lawrence Berkeley National Laboratory, Berkeley, California, United States.

Hybrid (organic-inorganic) materials have emerged as a promising class of thermoelectric materials, achieving power factors ($S^2\sigma$) exceeding those of either constituent. The mechanism of this enhancement is still under debate, and pinpointing the underlying physics of transport has proven difficult. In this work, we combine transport measurements with extensive theoretical simulations and first principles calculations on a prototypical PEDOT:PSS-Te(Cu_x) nanowire hybrid material system to understand the effect of templating and charge transfer at inorganic-organic interface on the observed high thermoelectric performance. Further, we apply the framework of the recently developed Kang-Snyder universal charge transport model to show that scattering of holes in the hybrid system, defined by the energy-dependent scattering parameter (s), remains the same as in the host polymer matrix; performance is instead dictated by polymer morphology manifested in an energy-independent transport coefficient. We build upon this universal language to explain thermoelectric behavior in a variety of PEDOT and P3HT based hybrids.

2:30 PM TP03.02.04

Effect of Process Conditions on the Thermoelectric Properties of Wet-Spun PEDOT:PSS Fibers Ruben Sarabia and Matthew Weisenberger; Center for Applied Energy Research, Lexington, Kentucky, United States.

New smart or electronic textiles cross conventional uses to include functionalities such as light emission, health monitoring, climate control, sensing, storage and conversion of energy, etc. Here, thermoelectric textiles not only hold great promise in becoming the power source of next generation wearable electronics, but also could become on-spot climate control devices. Further, thermoelectric textiles are also interesting from an industrial perspective since their flexibility and conformability make them suitable for energy recovery from curved surfaces in the mid to low temperature range. For example, a thermoelectric textile could be designed to be wrapped around a steam pipe to harvest waste heat.

Intrinsically conductive polymers have gained attention in the field of thermoelectric textiles because they are made of earth-abundant elements, they show, in general, good mechanical properties and flexibility, they can be processed using low cost large-scale methods such as solution processing and they have an intrinsically low thermal conductivity.

Aqueous dispersions of PEDOT:PSS can be processed into fibers using a traditional wet-spinning process where the polymer solution (dope) is coagulated using a non-solvent (Okuzaki et al. 2003). In this work, we study how the variation of typical wet-spinning parameters such as the dope concentration, composition of the coagulation bath, applied draw, flow rate, etc., affect the thermoelectric properties of PEDOT:PSS wet-spun fibers. Additionally, we also explore possible post-treatments to enhance further the thermoelectric properties of these fibers.

2:45 PM BREAK

3:15 PM *TP03.02.05

Quantum-Interference-Enhanced Thermoelectricity in Single-Molecule Junctions Colin Lambert; Lancaster University, Lancaster, United Kingdom.

Experimental evidence of the effect of quantum interference on the room-temperature electrical conductance of single-molecules¹ opens the possibility of exploiting quantum interference in single molecules and self-assembled molecular layers.

In this talk, I will present a brief outline of current understanding of quantum interference in single-molecules² and then discuss how quantum interference can be exploited to increase the thermoelectric performance of single molecules and assemblies of molecules connected to nano-gap electrodes³. Results will be presented for the thermoelectric properties of metallo-porphyrins, endohedral fullerenes and oligoynes.

1. *J. Am. Chem. Soc.*, 2011, **133**, 11426; *Nature Nano.* 2012, **7**, 305; *Nat. Nano.*, 2012, **7**, 663; *Phys. Rev. Lett.* 2012, **109**, 056801; *Nano. Lett.* 2012, **6**, 1643-1647; *JACS* 2012, **134**, 5262; *Beilstein J. Nanotech.* 2011, **2**, 699 and refs. therein

2. Lambert, *Chem. Soc. Rev.* **44**, 875-888 (2015); Geng, et al., *J. Am. Chem. Soc.* **137**, 4469 (2015); Sangtarash et al., *J. Am. Chem. Soc.* **137** 11425 (2015); D. Manrique, et al., *Nature Comm.* **6** 6389 (2015); Berritta et al, *Nanoscale* **7** 1096 (2015)

3. Evangeli et al., *Nano Letters* **13**, 2141-2145 (2013); Garcia-Suarez et al, *Nanotechnology* **25**, 205402 (2014); Sadeghi et al, *Nano Lett.* **15**, 7467-7472 (2015); Manrique et al., *Nano. Lett.* **16**, 1308-1316 (2016); Ismael et al, *Nanoscale* **7** 17338 (2015); Rincón-García et al, *Nature Materials*, **15**, 289-293 (2016); Han et al., *Nature Comm.* **7** 11281 (2016); M. Noori et al, *Nanoscale* **9** (16), 5299-5304 (2017); Q. Al-Galiby et al, *Nanoscale* **9** (14), 4819-4825 (2017)

3:45 PM TP03.02.06

Disordered Transport in Highly Doped Materials—Vapor Doping of a Model Small Molecule System Kelly A. Peterson¹, Ashlea Patterson², Alejandro Vega-Flick³, Bolin Liao³ and Michael L. Chabinye¹; ¹Materials, University of California, Santa Barbara, Santa Barbara, California, United States; ²The University of Utah, Salt Lake City, Utah, United States; ³Mechanical Engineering, University of California, Santa Barbara, Santa Barbara, California, United States.

Amorphous small molecule semiconductor films are widely used in organic light emitting displays and have promising applications in solar cells and thermoelectric devices. Smooth, consistent films can be easily fabricated using vapor deposition or spin casting. Adding dopants increases the conductivity of organic semiconductors, but high concentrations of dopants can disrupt the film structure, alter the shape of the density of states in the material, and increase the effects of Coulomb interactions on charge transport. Understanding how these factors affect disordered charge transport is an important component of a broader picture of charge transport in organic semiconductors.

We chose to use the small molecule spiro-OMeTAD, commonly used as a hole transport layer in OLEDs and solar cells, and dopant F₄TCNQ as the model

system. Doping spiro-OMeTAD films with F₄TCNQ vapor allowed us to control the carrier concentration and to reach higher doping ratios, up to 1:2 dopant:host molecules, than possible through mixing the two in solution for casting. Structural characterization confirmed that films remain amorphous even at the highest doping levels with no apparent phase separation. We quantitatively determined the carrier concentration using UV-Vis and electron paramagnetic resonance (EPR) spectroscopy to interpret the evolution of the electrical conductivity. UV-Vis spectra show the presence of high concentrations of F₄TCNQ⁻ and spiro-OMeTAD⁺ ions in the films. In this range of carrier concentrations (10¹⁹ – 10²⁰ 1/cm³), the electrical conductivity was linear with carrier concentration, while Seebeck coefficient stayed relatively constant. The cause of this unexpected trend in Seebeck coefficient with carrier concentration was investigated in relation to the shape of the density of states and spiro-OMeTAD's electronic structure, which has degenerate HOMO and HOMO-1. Temperature-dependent conductivity and thermopower measurements were used to further analyze the transport mechanism. We also determined the effect of high dopant concentration and ionic effects on in-plane thermal conductivity measured by a transient grating technique.

4:00 PM *TP03.02.07

Controlling Electrostatic Interactions in Organic Thermoelectrics Lambert Jan Anton Koster; Zernike Institute for Advanced Materials, University of Groningen, Groningen, Netherlands.

Careful control of the doping level is required to capitalize on the unique benefits of organic semiconductors. Most studies in this field focus on the influence of backbone structures on the thermoelectric properties while the effects of side chains are less explored.

In this contribution, we describe our efforts to improve the thermoelectric properties of fullerene derivatives and conjugated polymers by modifying their electrostatic interactions. This is accomplished by tailoring their side chains. We find that both the miscibility and doping efficiency are improved by using polar side chains.

A fullerene derivative with a hydrophilic triethylene glycol type side chain (PTEG-1) is used as the host and (4-(1,3-dimethyl-2,3-dihydro-1H benzoimidazol-2-yl)phenyl)dimethylamine (*n*-DMBI) as the dopant. It is found that PTEG-1 molecules readily form layered structures parallel to the substrate after solution processing. The fullerene cage plane is alternated by the triethylene glycol side chain plane; the *n*-DMBI dopants are mainly incorporated in the side chain plane without disturbing the π - π packing of PTEG-1.

Since the polar side chains offer the space for accommodating dopant molecules and influence the molecular order, their length also plays a key role in the doping process. We systematically examine the effects of the side chains of a series of fullerene derivatives by varying their polarity and length. By optimizing the side chains, we find an electrical conductivity of 2.3 S/cm with a power factor of 23.1 μ W/mK² which leads to an estimated *ZT* value of 0.1.

The effectiveness of polar side chains for n-doping conjugated polymers is also verified in the case of the poly{[N,N'-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5'-(2,2'-bithiophene)} (N2200) system. Replacing the alkyl side chains of N2200 with polar side chains causes a 200 times enhancement in electrical conductivity. The underlying charge transport mechanism in molecularly doped fullerene derivatives and n-polymer is also explored. Our work offers insights into the roles of side chains in n-type organic thermoelectrics.

4:30 PM TP03.02.08

The Influence of Dopant Size and Electron Affinity on the Electrical Conductivity and Thermoelectric Properties of Conjugated Polymers Kenneth R. Graham and Zhiming Liang; University of Kentucky, Lexington, Kentucky, United States.

The choice of dopant and the method used to introduce a dopant can greatly influence the resulting electronic and thermoelectric properties of conjugated polymers. Multiple factors contribute to these dopant dependent properties; including how the dopant affects the polymer crystallinity and film morphology, how close the dopant molecule is to the π -conjugated backbone, and how efficiently the dopant creates polarons on the polymer. In this work we investigate the influence of large molybdenum complexes as dopants vs. smaller iron complexes on the electrical conductivity and Seebeck coefficient of several conjugated polymers. For multiple polymers we find that the large molybdenum complexes lead to electrical conductivities that are over an order of magnitude higher than that of the iron complexes at low doping concentrations. With the same number of polarons present based on absorbance measurements, the larger molybdenum complexes lead to higher electrical conductivities than the smaller iron complexes. We attribute the greater electrical conductivity achieved with the molybdenum dopants to lower coulombic attraction energies that result in more delocalized polarons. However, the electrical conductivity of the polymers doped with the molybdenum complexes saturate at lower doping concentrations than the iron complexes. Thus, the iron complexes can lead to overall greater electrical conductivities and higher power factors than the molybdenum complexes. Surprisingly, ferric chloride can dope PDPP-4T efficiently and lead to higher electrical conductivities than with Mo(tf₃)₃, despite the ionization energy of PDPP-4T being 0.4 eV higher than the electron affinity of ferric chloride.

SESSION TP03.03: Composite Thermoelectrics
Session Chairs: Qingshuo Wei and Luisa Whittaker-Brooks
Tuesday Morning, November 27, 2018
Sheraton, 3rd Floor, Gardner AB

8:00 AM *TP03.03.01

Can Polymer-Carbon Nanotube Composites Ever Be Better Thermoelectrics Than Pristine Materials? Mariano Campoy-Quiles; Institute of Materials Science of Barcelona, Bellaterra, Spain.

It has been recently suggested that once the polymer chains have done their role helping to disperse the nanotubes, the thermoelectric properties of a polymer-carbon nanotube (CNT) composite would be better if the polymer is removed altogether. This vision does not, however, consider that the polymer can offer other benefits, such as helping to dope the CNTs, varying the system thermal conductivity, changing the microstructure or serving as binder for the respiratory hazardous CNTs. In this talk I will describe different polymer-CNT combinations and fabrication protocols and show some cases examples in which compositing is a good option.

First I will show the case of nanocellulose-CNTs films grown by bacteria. By introducing the CNT dispersions in the culture media, bacteria produce nanocellulose films in which the CNTs are finely dispersed. The resulting films are thermally stable at least until 500K, can be bended completely, and even wrapped around heat sources of random shapes, greatly enhancing the thermal boundary conductance. Using Raman thermometry, we show a 20-fold reduction of the in-plane thermal conductivity of the composite with respect to the reference bulky paper. The *ZT* of the composites is similar to that of the

reference, while saving about 90% of the expensive component, the CNTs.

Then, I will describe several cases of CNT doping by the polymer, including changing the character from p- to n-type. Finally, I will discuss the properties of polymer-CNT structures in which the polymer is laminated on top of the CNTs.

8:30 AM TP03.03.02

Optimization of Potential Barrier for Enhanced Thermoelectric Performance of PEDOT:PSS/Bi₂Te₃ Composite Films via Polar Solvent Vapor Annealing [Wan Sik Kim](#)¹, Gopinathan Anoop¹, Hyejeong Lee¹, Hyun Bin Kim², Soo Hyeon Kim³, Gi Won Goo¹, Hyunmyung Lee¹, Hyeon Jun Lee¹, Bongjin S. Mun¹, Ji-Woong Park¹, Eunji Lee¹ and Ji Young Jo¹; ¹Gwangju Institute of Science and Technology, Gwangju, Korea (the Republic of); ²Korea Atomic Energy Research Institute (KAERI), Jeongeup, Korea (the Republic of); ³Korea Basic Science Institute (KBSI), Daejeon, Korea (the Republic of).

The efficiency of TE materials can be evaluated by the dimensionless figure of merit $ZT = S^2\sigma T/\kappa$ or power factor $P = S^2\sigma$, where S is the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is absolute temperature. The equations of ZT and P imply that high S , high σ , and low κ are required for achieving a high efficiency from the TE materials. High σ and S reduce Joule heating as well as improve the energy conversion efficiency of heat to electricity, while a low κ prevents thermal shorting between two ends. However, because of the conflicting relationship between S , σ , and κ , it is challenging to enhance the efficiency of a single TE material. For example, an enhancement of σ is usually accompanied by a decrease of S and an increase of κ , which has restricted in achieving a maximized ZT .

To solve these problems, the energy filtering effect, which occurs at an interface between two different components in nanocomposites and superlattices, has been found to be successful in solving the conflicting relationship of TE factors via enhancement of S without significant reduction of σ . However, experimentally, an enhanced P or ZT has not been achieved in many composites. The reason is because, in reality, the σ of the nanocomposites has been significantly reduced by the inappropriate potential barrier at the interface of the component materials. This implies that the introduction of any potential barrier is not the key, but an appropriate barrier to simultaneously enhance S and σ so that to achieve a maximized P or ZT .

Here, we synthesize the poly(3,4-ethylene dioxythiophene) polystyrene sulfonate (PEDOT:PSS)/Bi₂Te₃ nanowires (NWs) composites film treated by polar solvent vapor annealing (PSVA) to systematically investigate the TE factors and optimize potential barrier energy at their interface for enhanced TE performance. The PSVA treatment results in enhancement of σ and variable work function of PEDOT:PSS due to changes in structure and PEDOT to PSS ratio. The composite films are annealed for 10, 30, 60, and 120 min using dimethyl sulfoxide to modulate work function of PEDOT:PSS for variable potential barrier energies of composite films. Enhanced σ is attributed to two different (phase separation and PSS de-doping) structural changes of PEDOT:PSS as PSVA duration. The S is varied by different magnitude of energy filtering effect caused from various potential barrier energies. The highest S , σ , and P at room temperature are 44.7 mV/K, 1015 S/cm, and 203 mW/mK², respectively in 120 min PSVA treatment of PEDOT:PSS/Bi₂Te₃ NWs composite film which exhibits 0.11 eV of potential barrier energy. This work highlights simultaneous enhancement of both S and σ by the energy filtering effect, which is controlled through tuning the potential barrier energy at interface in organic-inorganic composite materials.

8:45 AM TP03.03.03

A New Approach for Enhanced Thermoelectric Performance of Polymer/Inorganic Bulk Composites [Kaya Wei](#)^{2,1} and George Nolas¹; ¹University of South Florida, Tampa, Florida, United States; ²National High Magnetic Field Laboratory, Tallahassee, Florida, United States.

Polymers are currently of great interest for thermoelectric applications, primarily due to a specifically unique combination of properties that are atypical of inorganic material, including mechanical flexibility, low cost, low temperature and cost processing, and general non-toxicity. Moreover, for specific polymer/inorganic composites enhanced thermoelectric performance, as compared to the conducting polymer alone, has been realized. Here we employ PEDOT:PSS/thermoelectric Bi_{0.5}Sb_{1.5}Te₃-alloy p-type composites as a model system to demonstrate a new approach to enhanced performance in polymer/inorganic composites: Ethylene Glycol (EG) treatment of PEDOT:PSS, to enhance conductivity in the polymer, and spark plasma sintering (SPS) processing, to consolidate the composites into dense, bulk materials with less distortion of the polymer chains therefore resulting in even higher electrical conductance. Together with a low thermal conductivity, we achieved greatly enhanced thermoelectric performance as compared to the EG treated polymer alone. Moreover, our approach allows for the preparation of polymer/inorganic thermoelectric composites to be processed in a form that allows these composites to be incorporated in existing applications of current refrigeration devices. In addition, we demonstrate that SPS processing is the only method that can provide such results, since hot pressing, cold pressing or mold forming results in extensive distortion of the polymer chains whereas SPS does not, in part due to the current flowing through the composite material during SPS processing.

9:00 AM *TP03.03.04

Less is More—Thermoelectric Performance Enhancements in Polymer-Free Semiconducting Single-Walled Carbon Nanotube Networks [Andrew J. Ferguson](#) and Jeffrey Blackburn; National Renewable Energy Laboratory, Lakewood, Colorado, United States.

There is growing interest in carbon nanostructures for a variety of electronic and optoelectronic applications. We will present studies aimed at understanding and improving the thermoelectric (TE) performance of single-walled carbon nanotube (SWCNT) thin film networks, built upon polymer-based extraction of semiconducting SWCNTs that eliminates metallic SWCNTs and other impurities. Rational choice of the starting SWCNT material and polymer allows us to sensitively tune the semiconducting SWCNT diameter distributions within the composites. When employed in conjunction with a doping process that allows exquisite control over the charge carrier density, we demonstrate that the peak performance, as determined by the TE power factor, is dependent on the SWCNT diameter.¹

Modification of the extraction process produces semiconducting SWCNT thin films where nanotube bundling is minimized during network formation and the polymer can be completely removed in the solid state, resulting in intimate tube-tube contacts. By controlling the bundle size and extent of polymer remaining in the semiconducting SWCNT network we demonstrate TE power factors that double the performance of semiconducting SWCNT networks previously demonstrated.^{2,3} We trace the improved performance to enhanced electrical conductivity, resulting from improved doping and strongly enhanced charge carrier mobility, and analyze our data within the framework of a recently developed TE transport model. We show that removal of the polymer from the semiconducting SWCNT network has negligible impact on the thermal conductivity, which appears to be limited by dopant-induced phonon scattering processes. Finally, we demonstrate equivalent TE performance in both p-type and n-type semiconducting SWCNT networks, paving a path toward all-carbon TE generators.

1. Avery, A. D. *et al.* Tailored semiconducting carbon nanotube networks with enhanced thermoelectric properties. *Nat. Energy* **1**, 16033 (2016).

2. Norton-Baker, B. *et al.* Polymer-Free Carbon Nanotube Thermoelectrics with Improved Charge Carrier Transport and Power Factor. *ACS Energy Lett.* **1**, 1212–1220 (2016).

3. MacLeod, B. A. *et al.* Large n- and p-type thermoelectric power factors from doped semiconducting single-walled carbon nanotube thin films. *Energy Environ. Sci.* **10**, 2168–2179 (2017).

9:30 AM TP03.03.05

Optimization of the Thermoelectric Figure of Merit in the Conducting Polymer PEDOT:PSS Films Through Incorporating 1-d Nano-Structured BiTe Compound Junyoung Lim, Sangwon Jo and Yongsok Seo; Seoul National University, Seoul, Korea (the Republic of).

Thermoelectric materials can generate electricity from unused waste heat and natural heat sources. To fabricate efficient thermoelectric materials, novel nano-structuring approach of mixing inorganic semiconductors of BiTe alloys with highly conducting polymer (PEDOT: PSS) was devised. This thermoelectric nanocomposite material was prepared through the alloy nanorods forming process in the PEDOT : PSS solution. Two step reduction process allows easy formation of the alloy. Uniform alloy nanorod-PEDOT:PSS composite suspension was obtained which spread well on the substrate with ease of controlling the thickness. High conductivity of PEDOT: PSS provides excellent passage of electrons with low thermal conductivity. The nano-composite has a Seebeck coefficient 48mVK^{-1} and an electrical conductivity of 1300Scm^{-1} at room temperature. The corresponding power factor was $316\text{mWm}^{-1}\text{K}^{-2}$ to yield a figure of merit $[ZT]=0.41$, which makes this nano-composite materials useful for waste energy harvesting at low temperature.

9:45 AM TP03.03.06

Multifunctional Thermoelectric Yarn Based Smart Textiles for Energy Harvesting, Cooling and Tactile Sensing Yuanyuan Zheng, Xinzhi Hu and Kun Zhang; Donghua University, Shanghai, China.

In contrast to thin-strip based thermoelectric generators (or 2D-TEGs), three-dimensional deformable textile-shaped thermoelectric generators (T-TEGs) show great appeal for smart textiles owing to their excellent structural compatibility with textiles and diverse capabilities of powering wearable electronics, microclimate controlling, adaptively temperature and tactile sensing. However, there have been no reported T-TEGs that can simultaneously accommodate the demands for practical application. In this work, we manufacture organic-based T-TEG with multifunctionality by assembling segmentally-doped carbon nanotube yarn (CNTY) with PEDOT: PSS (*P*-type) and polyetherimide (*N*-type) inks into a spacer fabric. As an electricity generator, the T-TEG shows superior voltage and power output of 51.5V/m^2 and $\sim 786\text{ }\mu\text{W/m}^2$ at a temperature difference of 20 K, respectively. Interestingly, applying one-volt electrical input can lead to the surface temperature drop of approximately 2.5 kelvins, causing a typical sensation between cool and cold, showing exceptional potential for human thermoregulation in smart textiles. Moreover, we shows the excellent wearing performance of T-TEG and ultrahigh sensitivity to the tactile touch including pressure (1.388KPa^{-1}) and thermal (11.623K^{-1}) stimuli. [q11] To our knowledge, all these results make the developed T-TEG outperforming all reported organic-based F-TEGs and T-TEGs. The developed strategy can inspire the manufacturing of cost-effective T-TEGs with the well-established industrial processes.

10:00 AM BREAK

SESSION TP03.04: N-Type Organic Thermoelectrics
Session Chairs: Michael Chabinye and Shannon Yee
Tuesday Morning, November 27, 2018
Sheraton, 3rd Floor, Gardner AB

10:30 AM *TP03.04.01

Self-Dopant Design Principles in N-Type Organic Thermoelectrics Daniel Powell, Jonathan Ogle and Luisa L. Whittaker-Brooks; Chemistry, University of Utah, Salt Lake City, Utah, United States.

Small molecule n-type semiconductors are typically doped by blending the semiconductor with extrinsic compounds that readily generate radicals, necessitating that the semiconductor and dopant be co-soluble. In perylene diimides these solubilizing groups, and also the dopants themselves, tend to be sterically bulky and can disrupt the packing structure of organic films; decreasing the electronic coupling between adjacent molecules and hindering charge mobility. The dopants may also aggregate during film casting, decreasing the number of charge carriers available to the system and creating additional grain boundaries. Additionally, the introduction of dopants modifies the density of states near the Fermi-energy such that populated states now exist at some energy relative to the LUMO of the organic semiconductor. Upon charge transfer the energies of these states distort in ways that may be very difficult to predict, leading to a broader density of states. The molecular design of the semiconductor, and also the selection of the proper dopant is a difficult process with several convoluted considerations. These challenges may be mitigated by intrinsically doping the n-type organic semiconductor via a process dubbed self-doping. Herein, we have investigated the effects of self-dopant structure on the processability and doping efficiency in a variety of perylene diimide n-type organic semiconductors. We believe our findings provide fundamental design rules for the fabrication of effective self-dopants geared toward increasing the thermoelectric properties of n-type organic semiconductors.

11:00 AM TP03.04.02

Air-Stable Thermoelectric Materials Based on N-Type Nickel-Coordination Polymers for Energy Harvesting Akanksha K. Menon, Rylan Wolfe, Seth Marder, John R. Reynolds and Shannon Yee; Georgia Institute of Technology, Atlanta, Georgia, United States.

Over 60% of available waste heat is at temperatures below 250 °C. Low cost and large scale thermoelectric devices based on conducting polymers can capture this heat and convert it directly into electricity. Organic materials are suitable for low grade thermal energy harvesting as they can be synthesized from abundant elements and can be processed from solution using low cost fabrication techniques. Furthermore, their low thermal conductivity and flexible nature enable new device architectures and applications. Despite these advantages, polymer-based thermoelectric devices have not made an impact and this is largely attributed to the lack of high performance n-type polymers (power factor $> 10\text{ }\mu\text{W/m-K}^2$), To address this, we investigate metallo-organic polymers (also known as coordination polymers) as a suitable class of n-type polymers that are electrically conducting and maintain their stability in air. First, we present the synthesis, characterization and thermoelectric properties of n-type poly(nickel-ethenetetrathiolate) or NiETT. By modifying the reaction conditions and film post-treatment by annealing, the thermoelectric properties can be simultaneously enhanced to obtain a high performing n-type polymer that maintains its stability under ambient conditions. Specifically, to address challenges with the reproducibility of air-oxidized NiETTs, a chemical oxidant is used to systematically tune the thermoelectric properties. Furthermore, the observations and insight gained from the ETT study are extended to other metallo-organic polymers such as the poly(nickel-tetrathiooxalate) or NiTTO. This is another coordination polymer that is easier to control synthetically as it is polymerized electrochemically. Herein, we present for the first time the thermoelectric properties of NiTTO films in a PVDF matrix, as well as its thermoelectric properties with varying counterions. Finally, temperature-dependent thermoelectric property measurements reveal that these polymers show semiconducting behavior that is consistent with thermally-activated hopping transport. The development of these two high performance and air stable n-type materials enables their application in realistic devices for thermoelectric energy harvesting.

11:15 AM TP03.04.03

Organometallic Coordination Polymers for Thermoelectric Applications Bob C. Schroeder and Zilu Liu; Chemistry, University College London, London, United Kingdom.

Over the decades, scientific evidence has mounted that the emission of anthropogenic greenhouse gases is the main reason for the increase of surface temperatures observed on Earth. Abandoning fossil fuels in the short term, however, is both technologically difficult and economically risky. Therefore, it would be advantageous to use the produced energy more efficiently thereby curbing the overall energy production and ultimately the greenhouse gas emissions. Around 60% of the energy input is lost after conversion as waste heat, of which half is so-called low temperature (<200°C) waste heat. A technology suitable to recover waste heat and transform it into usable electricity is thermoelectric generators. Due to the so-called Seebeck effect, applying a temperature differential across a suitable material will generate an electric voltage. Recovering the low-temperature waste heat however via thermoelectric generators is challenging, mainly because current technologies are based on rare, often toxic elements (*i.e.* tellurium, lead, ...); and as a result, thermoelectric modules are rather expensive and can only be efficiently operated at elevated temperatures. It is therefore paramount to develop new thermoelectric materials, able to harvest low-temperature waste heat efficiently.

The ideal thermoelectric material possesses a high electrical conductivity, while at the same time being an excellent thermal insulator. Whereby it is relatively straightforward to find materials which fulfil one of these critical requirements, it is much more difficult to find a single material accomplishing both. Materials based on organometallic coordination polymers are attractive candidates for thermoelectric materials because they have shown promising electrical conductivities, while at the same time maintaining low thermal conductivities. This paper will discuss several synthetic approaches leading towards different organometallic coordination polymers with various geometries, and will investigate not only the effect of the molecular geometry on the thermoelectric properties, but also the effects of the coordinated metal cations.

11:30 AM TP03.04.04

Anisotropic Thermal Conductivity Measurements of Semiconducting and Thermoelectric Polymers Using a Suspended Film 3-Omega Technique Sampath Kommandur and Shannon Yee; Georgia Institute of Technology, Atlanta, Georgia, United States.

Anisotropic thermal conductivity can complicate the performance of semiconducting polymer thin-films in applications such as thermoelectrics. Anisotropic measurements of low thermal conductivity polymers are challenging and there are a limited number of appropriate measurement techniques. Suspended film 3-omega is an appropriate technique but has often required unfavorable microfabrication. Herein, we report on the utility of the suspended 3-omega technique that uses shadow masking, and no other microfabrication techniques, in performing anisotropic (in-plane and through-plane) thermal conductivity measurements of semiconducting polymers - P3HT and commercially available N2200, and n-type thermoelectric polymers - poly-nickel ethenetetrathiolates (poly(Ni-ETT)) and poly-nickel tetrathioxyates (poly(Ni-TTO)).

The necessary conditions for the validity of a 1D heat transfer model and experimental guidelines for in-plane thermal conductivity measurements of polymer thin-films are developed. Measured thermal conductivities are compared with predictions from the conventional k-min model and a recent empirical model that more accurately predicts the temperature dependence.

11:45 AM TP03.04.05

Soluble Alkali-Metal CNT Salts for N-Type Thermoelectric Composites Bernhard Dorling and Mariano Campoy-Quiles; ICMAB-CSIC, Bellaterra, Spain.

We report on a promising method that allows to simultaneously disperse and n-dope carbon nanotubes (CNTs).

This is achieved by reducing CNTs with Alkali metals like Potassium [1]. The resulting polyelectrolyte salts spontaneously dissolve in polar solvents like DMSO, without requiring any deleterious mechanical methods like sonication, which are known to reduce CNT length. We have explored a range of commercially available CNTs, and show that this method allows to disperse even very long CNT species, which are near-intractable to process without introducing defects otherwise.

Apart from making them soluble, a pleasant side effect of the reduction is that after the solvent has evaporated, the Alkali metals remain in the film and dope the CNTs, resulting in buckypapers that exhibit a negative Seebeck coefficient. The obtained n-type power factors reach hundreds of $\mu\text{Wm}^{-1}\text{K}^{-2}$, on par with the p-type power factors of the neat CNTs.

Furthermore, inspired by previous art [2,3], we show that the CNT solubility can be strongly increased by adding crown ethers to the solution [2], which also improves the doping efficiency and air-stability of the formed films [3].

Finally, we will discuss our results on n-doped CNT-polymer composites prepared using this method.

[1] Pénicaud, A., Dragin, F., Pécastaings, G., He, M. & Anglaret, E. Concentrated solutions of individualized single walled carbon nanotubes. *Carbon* 67, 360–367 (2014).

[2] Jiang, C., Saha, A. & Martí, A. A. Carbon nanotubides: an alternative for dispersion, functionalization and composites fabrication. *Nanoscale* 7, 15037–15045 (2015).

[3] Nonoguchi, Y. et al. Simple Salt-Coordinated n-Type Nanocarbon Materials Stable in Air. *Adv. Funct. Mater.* 26, 3021–3028 (2016).

SESSION TP03.05: Thermoelectrics and Organic Electronics
Session Chairs: Riccardo Di Pietro and Andrew Ferguson
Tuesday Afternoon, November 27, 2018
Sheraton, 3rd Floor, Gardner AB

1:30 PM *TP03.05.01

The Development and Use of Dopants to Modulate the Electrical Properties of Conjugated Polymers Seth R. Marder; School of Chemistry and Biochemistry, School of Materials Science and Engineering and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia, United States.

Conjugated polymers have attracted interest for thermoelectric applications due to their potential for use in low-cost, large-area, devices. In this talk I will discuss the development of n- and p- dopants and the role they can play in modulating the electronic properties of conjugated polymers.

2:00 PM TP03.05.02

Flexible, Multi-Functional Organic-Inorganic Composites for Passive Thermal Management via Conduction and Radiation Luis M. Lozano^{1,2}, Seong Don Hong^{3,4}, Hadi Zandavi¹, Yi Huang¹, Gang Chen¹, Richard M. Osgood³ and Svetlana V. Boriskina¹; ¹Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; ²Escuela de Ingeniería y Ciencias, Tecnológico de Monterrey, Monterrey, Mexico; ³U.S. Army Natick Soldier Research, Development and Engineering Center, Natick, Massachusetts, United States; ⁴Defense Agency for Technology and Quality, Seoul, Korea (the Republic of).

Thermal management is nowadays focused on overcoming several challenges for energy savings in buildings, as well as for improving reliability and preventing premature failure in electronic devices. Passive thermal management strategies that enable cooling without any electricity input could therefore have a significant impact on global energy consumption. Consequently, there are both needs and opportunities for novel materials to help address some of these thermal management challenges, which fuel the research progress on developing new materials with high thermal conductivity and tailored thermal emittance properties. In this regard, polymers continue to infiltrate modern technologies due to their unique combination of properties, such as light weight, durability, flexibility, corrosion resistance, low cost, and ease of processing. However, the application of polymers in thermal management has been largely hampered by their low thermal conductivities. Here we report the fabrication of ultra-drawn polyethylene-based thin films filled with inorganic nanoparticles that show both spectrally-tailored absorptance/emittance properties and lateral heat-spreading functionalities. The high thermal conductivity is achieved by the alignment of polyethylene chains, which have a backbone structure of carbon-carbon bonds, while the inorganic filler provides the means to engineer optical properties of films in the broad spectral range. Furthermore, the filler dispersion within the polymer matrix is improved after the drawing process, which even generates better mechanical properties in the composite film. These results provide a feasible route for large-scale fabrication of passively cooling surfaces for heat management in terrestrial and space-based applications.

This work was supported by the NSRDEC 'Thermal Management of Fibers and Films' program, through ARO sponsored ISN.

2:15 PM *TP03.05.03

Evidence for Low Disorder, Narrow-Band Charge Transport in the Thermoelectric Response of Semicrystalline Polymer Semiconductors Riccardo Di Pietro; Hitachi Cambridge Laboratory, Cambridge, United Kingdom.

Semiconducting polymers possess unique mechanical, thermal and electrical properties that make them interesting candidates for thermoelectric applications. However, the recent development of semicrystalline polymer semiconductors with field-effect mobilities comparable to and sometimes exceeding those of amorphous silicon has exposed the limitations of commonly used disorder-based charge transport models which were developed originally for more disordered, lower mobility materials. This is especially true when including in the picture the thermoelectric properties of this class of materials.

I will present our work on the structural, electric and thermoelectric characterisation of semicrystalline polymers for which we have recently shown a correlation between charge density dependence of mobility and the size of the crystalline domains in the polymer film.[1] We have characterised the temperature and charge carrier dependence of the Seebeck coefficient and found it in contradiction with charge transport models based on energetic and positional disorder. On the very contrary these measurements provide direct experimental evidence for narrow band conduction at the charge densities typically observed in thin film transistors. The comparison with the conductivity measurements highlights an additional aspect which is the need to include electron-electron interactions to consistently explain the measured properties.[2]

Based on these findings, we propose an alternative charge transport model that explicitly accounts for the presence of interspersed crystalline and amorphous regions within the polymer film and for local electron-electron interactions. This approach captures all the unique features observed experimentally and highlights new directions which can lead to a further improvement of both electric and thermoelectric performance of polymer semiconductors.

[1] Di Pietro, R. et al. Adv. Funct. Mater. 26, 8011 (2016).

[2] Statz, M. et al. Comms. Phys. 1, 16 (2018)

2:45 PM TP03.05.04

Additive Printing and Photonic Sintering of High-Performance and Flexible Thermoelectric Materials and Devices Using Colloidal Nanocrystals Yanliang Zhang¹, Tony Varghese², Chaochao Dun¹, Nicholas Kempf¹ and Mortaza Saeidijavash¹; ¹University of Notre Dame, Notre Dame, Indiana, United States; ²Boise State University, Boise, Idaho, United States.

The flexible thermoelectric generator (f-TEG) is a very promising technology for energy harvesting to enable self-powered wireless sensors and wearable devices, an area of exponential growth. Here, we present a scalable and cost-effective additive manufacturing process to fabricate f-TEGs using colloidal nanocrystals, and an innovative and highly efficient photonic sintering method to sinter large areas of printed films using pulsed light. Flexible TE films and devices were printed using screen printing and aerosol jet printing, followed by pulsed photonic sintering process. The pulsed sintering confines the delivered thermal energy within the printed film region without over heating the substrate, enabling TE film sintering on flexible polymer based substrates with relatively low melting point. In addition, the pulsed sintering limits grain size growth due to an ultrafast heating and cooling process, and lower thermal conductivity can be achieved than films sintered by conventional thermal processing.

The p-type and n-type printed films demonstrate peak ZTs of 1 and 0.43 near room temperature along with superior flexibility, which is among the highest reported ZT values in flexible thermoelectric materials. A flexible thermoelectric device fabricated using the printed films produces a high power density above 19 mW/cm² with 80 K temperature difference between the hot side and cold side. The additive printing and photonic sintering can enable a highly scalable and low-cost roll-to-roll manufacturing process to transform high-efficiency colloidal nanocrystals into high-performance and flexible TEG devices for widespread applications.

3:00 PM BREAK

3:30 PM *TP03.05.05

Harvesting Waste Heat Using Ionic Liquid-Based Thermoelectrochemical Cells Jenny Pringle¹, Danah Al-Masri¹, Abuzar Taheri¹, Matthew Russo¹ and Douglas R. MacFarlane²; ¹Institute for Frontier Materials, Deakin University, Burwood, Victoria, Australia; ²School of Chemistry, Monash University, Clayton, Victoria, Australia.

Thermoelectrochemical cells (thermocells) are based on an alternative design to the traditional semiconductor-based thermoelectric devices as they use an electrolyte containing a redox couple. The electrochemical potential of this redox couple depends on temperature, and therefore in a device with two electrodes held at different temperatures a potential difference is created. Thus, these cells allow direct thermal to electrical energy conversion with no carbon emissions.

Until recently, research into thermoelectrochemical cells had primarily focused on aqueous electrolytes, predominantly with the ferri/ferrocyanide redox couple. However, the good thermal and electrochemical stability, non-volatility and non-flammability of many ionic liquids (ILs) makes them promising alternative electrolytes for these devices. Potential advantages include increased thermoelectrochemical device efficiencies, longer lifetimes and the ability to utilise waste heat sources in the 100 – 200 °C temperature range.

The highest power outputs to-date for thermoelectrochemical cells using IL electrolytes have been achieved through our use of a high entropy change $\text{Co}^{\text{III}}/\text{bpy}_3$ redox couple. Here we discuss our research into the use of a range of Fe and Co-based complexes in different IL and IL/solvent mixtures for thermal energy harvesting. The Seebeck coefficient and thermoelectrochemical cell performance is shown to be strongly influenced by the nature of the redox couple and the IL. We also discuss our recent research into the development of quasi-solid state electrolytes using either water-based or IL-based electrolytes.

4:00 PM TP03.05.06

($p \times n$)-type Transverse Thermoelectrics for Refrigeration and Energy Harvesting at Ambient Temperatures Qing Shao¹, Boya Cui¹, Xueting Yan¹, Arun Kumar Mannodi Kanakkithodi², Yi Xia², Xin Li³, Maria K. Chan², Jiong Yang³ and Matthew Grayson¹; ¹Northwestern University, Evanston, Illinois, United States; ²Argonne National Laboratory, Lemont, Illinois, United States; ³Shanghai University, Shanghai, China.

($p \times n$)-type transverse thermoelectrics are introduced as an alternative to conventional or “longitudinal” thermoelectrical materials for applications at room temperature and below. A microscopic theory for such materials is explained, based on a simple two-band anisotropic effective mass model for conduction and valence bands. Such materials are predicted to have performance advantages over standard thermoelectrics in small-scale devices as well as at cryogenic temperatures.

Transverse thermoelectrics drive heat orthogonal to an applied electric current. As such they have the geometric advantage that the heat-flow cross section is independent of the current-flow cross section. As the name suggests, this unique behavior of ($p \times n$)-type transverse thermoelectrics results from having a Seebeck tensor with orthogonal p - and n -type Seebeck behaviors. One feature of such materials is that the bandgap should be of order several kT at the optimal operation temperature, and that the optimal performance occurs near intrinsic doping. Whereas conventional thermoelectrics must be extrinsically doped n -type or p -type to function, these intrinsic materials will not suffer from dopant freeze-out, opening a new cryogenic range of operation for solid state cooling.

Transverse thermoelectrics have the device advantage of having full thermoelectric performance in a single-leg. This single-leg structure makes it trivial to achieve “infinite stages” of Peltier cooling, for example, which can only be achieved with standard thermoelectrics in a cascaded multi-stage structure. Single-leg ($p \times n$)-TTE’s can also be scaled down to microscale devices, giving them niche applications that cannot be addressed by conventional multi-leg thermoelectric coolers or heaters.

Compared earlier transverse thermoelectric paradigms, the transverse Seebeck response in ($p \times n$)-type transverse thermoelectrics is due to structural asymmetry in the band structure of a single crystal. Thus a simple two-band anisotropic effective-mass model is shown to be adequate to explain experimental data on such materials. From such a model, ambipolar resistivity Seebeck and resistivity tensors can be calculated. The predicted transverse thermoelectric behavior is shown to be maximized with the Fermi energy near mid bandgap. A transverse power factor PF is introduced, and from the published literature, we propose the following materials as candidate materials for ($p \times n$)-type TTE: Re_4Si_7 , CsBi_4Te_6 , PdCoO_2 , Na_xCoO_2 ($x = 0.45, 0.55$) and $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$.

4:15 PM *TP03.05.07

Electronic and Ionic Thermoelectric Effects and Energy Conversion and Storage Applications Choongho Yu; Texas A&M University, College Station, Texas, United States.

Thermoelectric effect, which is voltage generation under a temperature gradient, can be induced by electron or/and ion transport. Here the two different transport mechanisms and their thermoelectric properties are discussed, and the transport behaviors in polymer only and polymer composites are compared. While thermoelectric voltage induced mainly by electrons is typically smaller than that of ions, the voltage can be continuously generated. Recently reported thermally-induced ion transport needs to be utilized in a non-continuous manner, but it exhibits extremely large thermally induced voltage. Based on thermally induced ion transport, novel methods have been developed for simultaneously harvesting and storing electrical energy without losing the benefit of solid-state non-moving part devices like conventional thermoelectrics. We called the device thermally chargeable supercapacitor (TCSC), and arrays of TCSC have been batch-fabricated, and connected together to raise the output voltage up to 2.1 V, suggesting excellent suitability for roll-to-roll mass manufacturing and practical implementation of thermal energy harvesting. The outcomes suggest that it may be feasible to eliminate needs for battery replacement and wired connections to power lines for various distributed electronic systems whenever and wherever a temperature gradient is present.

4:45 PM TP03.05.08

Ab Initio Design of a Transparent Thermoelectric Oxide— ZnSb_2O_6 Adam J. Jackson^{1,2}, Alex M. Ganose^{1,2,3}, Winnie Leung¹, Benjamin A. Williamson^{1,2,3} and David O. Scanlon^{1,2,3}; ¹Chemistry, University College London, London, United Kingdom; ²Thomas Young Centre, University College London, London, United Kingdom; ³Diamond Light Source Ltd., Didcot, United Kingdom.

Thermoelectric devices have a range of applications for energy conversion and recovery. As renewable technology reaches more ambitious scales, new requirements and opportunities emerge. Primarily the drive has been to identify materials with a high thermoelectric figure of merit ZT . [1] Metal oxides are appealing due to their high chemical and thermal stability and avoid dependence on the limited supply of heavy anions such as Te. Electrical conductivity has been achieved in many wide-bandgap metal oxides and carrier concentrations can be manipulated by extrinsic doping. These transparent conducting oxide (TCO) materials form a vital component of devices including solar cells and display screens. So far, their thermoelectric performance has been limited by the relatively high lattice thermal conductivity of crystalline oxides, leading to an interest in nanostructuring. [2]

It has been demonstrated that another route to low thermal conductivity lies in the use of materials with an increasing variety of elements. Cation mutation can lower the thermal conductivity even when the underlying structure and mass density remains the same. [3] Two recurring features in successful TCOs have been the presence of post-transition metals (e.g. Sn, Ga, In) and structures containing edge-sharing octahedra. A search space of ternary transition metal oxides with octahedral motifs yields a number of Sb(V)-based compounds, and a high-throughput computational search for materials with low electron effective masses emphasised ZnSb_2O_6 as an interesting candidate. [4,5]

We have performed third-order lattice dynamics calculations to predict the intrinsic lattice thermal conductivity of ZnSb_2O_6 , which is found to be less than half that of ZnO across the whole operating temperature range. We have also examined the defect chemistry of the system, identifying appropriate dopants for an n -type zinc antimonate device. Device modelling identifies an optimal carrier concentration which is found to be achievable based on the study of defect transition levels. The corresponding value of ZT is over 0.5: greater than existing n -type thermoelectrics. We conclude that ZnSb_2O_6 has the potential to form the n -type component of a high-performance transparent thermoelectric device.

1. Bell, L. E. (2008) *Science* **321** 1457-1461
2. Koumoto, K., Wang, Y., Zhang, R., Kosuga, A., Funahashi, R. (2010) *Annu. Rev. Mater. Res.* **40** 363-394
3. Shibuya, T., Skelton, J. M., Jackson, A. J., Yasuoka, K., Togo, A., Tanaka, I., Walsh, A. (2016) *APL Mater.* **4** 104809
4. Mizoguchi, H., Woodward, P. (2004) *Chem. Mater.* **16** 5233-5248
5. Hautier, G., Miglio, A., Waroquier, D., Rignanese, G.-M., Gonze, X. (2014) *Chem. Mater.* **26** 5447-5458

SESSION TP03.06: Poster Session
 Session Chairs: Michael Chabinye, Terry Hendricks, Kedar Hippalgaonkar and Shannon Yee
 Tuesday Afternoon, November 27, 2018
 8:00 PM - 10:00 PM
 Hynes, Level 1, Hall B

TP03.06.01

Graphene-Carbon Nanotube Aerogel as 'Organic' Thermochemical Energy Harvesters—Synthesis, Structure and Properties Sanju Gupta and Romney Meek; Western Kentucky University, Bowling Green, Kentucky, United States.

Three-dimensional scaffolds comprising different ratio of graphene nanosheets and multi-walled carbon nanotubes (GA-CNT, hereon) macro-assemblies. The resulting hydrothermally synthesized hydrogels are freeze-dried and thermally reduced to yield graphene and graphene-carbon nanotube aerogels with ultralow densities and tunable mesoscopic pore sizes. These 'all carbon' aerogels prepared as monolithic solids from suspensions of few-layer graphene oxide nanosheets and small diameter multiwalled carbon nanotubes in which organic wet chemistry is used to cross-link the individual sheets and with carbon nanotubes. In contrast to methods that utilize physical cross-links between graphene oxide nanosheets, this approach with polymeric linkers and organic functionalization provides covalent carbon bonding among the graphene sheets and molecular attachment with carbon nanotubes, respectively, thus facilitating rapid and facile electron transport. As a result they are expected to exhibit improved electrical conductivities, moderate thermal conductivity, highly interconnected multiplexed topology with large internal surface areas thus promoting enhanced surface ion adsorption which makes these mesoporous materials viable candidates for use in harvesting thermo-electrochemical energy and energy storage technologies. Thermoelectric property measurements for both the carbon nanotube aerogels by themselves and for hybrids with graphene nanosheets revealed promising and unprecedented (p-type and n-type) thermopower values, especially with electrolyte with an upper bound to 3.2 mV/K. We used complementary analytical techniques including electron microscopy, temperature dependent electrical property, and Raman spectroscopy while evaluating performance to establish microstructure-processing-property-performance correlations. This work is supported in parts by KSEF-RDE Grant, KY NASA EPSCoR and KY NSF EPSCoR Grants.

TP03.06.02

Investigation for PEDOT:PSS Thermoelectric Properties Changes with Additive Process Won-Tae Park¹, Marco Cassinelli³, Peitro Pandolfini³, Chanil Park², Mario Caironi³, Jung-Hyun Kim² and Yong-Young Noh¹; ¹Dongguk University, Seoul, Korea (the Republic of); ²Yonsei University, Seoul, Korea (the Republic of); ³Istituto Italiano di Tecnologia, Milano, Italy.

Printed electronics have been developed with various synthesized high performance conducting organic materials for flexible devices as display, photovoltaics, memory and sensor applications. Thorough efforts for the development of printed electronics have been made to realize wearable application. Recently, the conductive materials show remarkable conductivity and seebeck coefficient (S), therefore thermoelectric application also rise to new era for wearable energy harvesting devices. Up to date, inorganic materials (e.g. Bi₂Te₃) have shown the best thermoelectric properties. However, such materials are rare with high process cost and are also difficult to achieve flexible applications. On the other hand, organic materials have advantages of processability at low temperature and ambient condition, also good harvesting energy efficiency even at room temperature. Here we demonstrate thermoelectric devices (TED) with PEDOT:PSS conducting polymer prepared with different concentration of dimethyl sulfoxide (DMSO) to investigate the thermoelectric property changes. DMSO is well known as PEDOT:PSS conductivity controlled sulfonic acid, and it can dramatically change PEDOT:PSS conductivity. As-fabricated films conductivity varied from 12.02 to 1179.93 S/cm with different DMSO concentration (0 ~ 10 wt%). Finally, power factor(PF) increased 100 times (0.19 to 24.61 uW/mK²) while seebeck coefficient (S) almost remained stable (12.60 ~ 14.44 uV/K). According to GIWAX and XPS analysis, this difference in thermoelectric properties should be due to better crystallization of the conductor PEDOT: PSS after removing the excess PSS in the PEDOT: PSS solution by adding certain amount of DMSO.

TP03.06.03

Alloying of Rare-Earth Tellurides for Improved Thermoelectric Performance Dean Cheikh¹, Brea E. Hogan^{1,2}, Trinh Vo¹, Paul von Allmen¹, Bruce Dunn², Jean-Pierre Fleurial¹ and Sabah K. Bux¹; ¹Jet Propulsion Laboratory, Pasadena, California, United States; ²Materials Science and Engineering, University of California, Los Angeles, Los Angeles, California, United States.

Thermoelectric generators (TEG) are solid state heat engines which convert thermal energy to electrical energy. The efficiency of thermoelectric materials is related to Carnot efficiency and a material's ability to convert heat into electricity. Thermoelectric efficiency is defined by the dimensionless thermoelectric figure-of-merit, ZT , where $ZT = (S^2/\rho\kappa)T$ where high electrical resistivity(ρ), high Seebeck coefficient (S) and low total thermal conductivity (κ) are essential for a good thermoelectric materials. A rare-earth chalcogenide series of interest, La_{3-x}Te₄, can accommodate vacancies on the rare earth position that provide disorder within the lattice, thus enhancing phonon scattering and lowering lattice thermal conductivity values (~0.8 W m⁻¹ K⁻¹). Additionally the defect concentration controls the electronic properties of the system, allowing metallic behavior at x = 0 and semiconducting behavior when x = 1/3. With an optimized vacancy concentration a peak ZT of 1.1 is attainable at 1275 K. Another isostructural rare-earth telluride, Pr_{3-x}Te₄, was recently demonstrated to be a high-performance thermoelectric material. Band structure calculations indicated that the introduction of the 4f electrons of Pr, which are not present in La, resulted in peak in the density of states (DOS) near the Fermi level and lead to an experimentally observed increase in the Seebeck coefficient. Additionally, Pr_{3-x}Te₄ was found to have a lower total and lattice thermal conductivity compared to La_{3-x}Te₄. The improved electronic and thermal properties resulted in a peak $ZT = 1.7$ at 1200 K with an optimized vacancy concentration. Here we present a study of the alloy (La, Pr)_{3-x}Te₄ to further decrease the thermal conductivity via point-defect scattering on the rare-earth site. The thermoelectric properties of the (La, Pr)_{3-x}Te₄ series were studied; the materials were synthesized using the low-temperature mechanochemical synthesis approach and then compacted through spark plasma sintering (SPS). X-ray diffraction (XRD) and scanning electron microscopy (SEM) were used for structural and phase characterization. The thermoelectric properties will be measured to 1275 K and their impact on ZT will be discussed.

TP03.06.04

Continuous Thermal Tunability of VO₂-SiO₂ Nano-Composite Capacitors Yifei Sun¹, Doug White², Amy Duwel² and Shiram Ramanathan¹; ¹Purdue University, West Lafayette, Indiana, United States; ²Draper Laboratory, Cambridge, Massachusetts, United States.

Thermally tunable dielectrics are of interest for energy-related applications such as thermal energy harvesting, capacitive energy storage and combined heat-power energy systems. Vanadium dioxide (VO₂) displays a sharp temperature-driven insulator-metal transition (MIT) and the dielectric constant of VO₂ varies by few orders of magnitude across the MIT temperature (T_{MIT}) corresponding to changes in carrier density. The increase in dielectric constant with temperature is potentially interesting for capacitive energy harvesting if the leakage in metallic state can be addressed properly. Consequently, VO₂-containing mixed phase systems are promising for thermally tunable applications where insulator-metal transition driven property changes can be harnessed. In this study, we utilize co-sputtering to fabricate VO₂-SiO₂ composite thin films which possess continuous temperature tunability distinct from the sharp transition seen in individual VO₂ crystals. The smooth thermal tunability stems from the MIT of VO₂ inclusions spatially dispersed in SiO₂ matrix. Thin film capacitors with VO₂-SiO₂ dielectric sandwiched between silica layers shows smooth thermal tunability of ~60% between 25 °C to 100 °C at 1 MHz with suppressed current leakage. We further find that thermal hysteresis can be significantly reduced in such nano-composites. We will compare and contrast capacitive properties of individual VO₂ films versus nanocomposite VO₂-SiO₂ structures and their variation with temperature, and contrast their properties with better studied counterparts, namely polymer-metal composites.

TP03.06.05

Enhancement of Electrical and Thermoelectric Properties of a Planar Cyclopentadithiophene-Benzothiadiazole Based Copolymer with sp² Hybridized Bis(alkylsulfanyl)methylene Substituent Yeran Lee, Luan T. Nguyen, Miso Kim and Han Young Woo; Chemistry, Korea University, Seoul, Korea (the Republic of).

Organic thermoelectric(OTE) devices have attracted considerable attention due to its advantages of lightweight, low-cost, and flexible electricity generation modules, etc. Although OTE devices have great advantages, still inorganic thermoelectric devices are currently used for power generation using waste heat because they show better performance than organic ones. Therefore, there is a great need for developing alternative OTE materials. Previously, we synthesized a p-type OTE polymer based on cyclopentadithiophene and benzothiadiazole, poly[(4,4'-(bis(hexyldecylsulfanyl)methylene)cyclopenta[2,1-b:3,4-b']dithiophene)-alt (benzo[c][1,2,5]thiadiazole)] (PCPDTSBT) and investigated its thermoelectric properties using mixing method with tris(pentafluorophenyl)borane(BCF) as a dopant. In here, we checked significantly enhanced both electrical and thermoelectrical properties by using different doping system; immersing the polymer film in the iron trichloride solution. Polaron states were observed by UV/Vis absorbance and electron spin resonance(ESR) spectroscopy. The electrical conductivity was studied by 2 points or 4 points probe methods. The detailed film morphology of the pristine and doped polymer films was investigated by atomic force microscopy (AFM).

TP03.06.06

Exploration of Organic Redox Couples for use in Thermogalvanic Devices Jesse Hinricher, Thomas Carney and Fikile Brushett; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

The U.S. consumed 97.7 quadrillion BTUs of energy in 2017, of which over 68% was rejected as heat, motivating research into conversion technologies that transform this low-grade waste heat into more valuable forms of energy (e.g. electrical energy) [1]. Thermoelectric generators, among the most widely studied devices, utilize inorganic semiconductors (e.g. bismuth telluride, lead telluride, and silicon germanium) with alternating p- and n-type dopants that are selected for their electrical conductivity but have accompanying thermal conductivity which diminishes performance [2]. Additionally, thermal cycling places mechanical stress on the system leading to premature failure [3]. An alternate approach is to use thermogalvanic cells which leverage dissolved electro-active molecules that oxidize and reduce at electrodes held at different temperatures, and consequently different potentials. Though promising, present thermogalvanic devices retain the drawback of coupled ionic and thermal conductivity which limits their conversion efficiency.

Here, we explore the use of organic active species in thermogalvanic cells. Organics are of interest due to their high entropy of reaction and heat capacity resulting in large Seebeck coefficients and open circuit potentials. Additionally, organics have tunable physical and electrochemical properties which expands the materials design space. To this end, we leverage recent technology developments in redox flow batteries (RFB) to improve performance of thermogalvanic generators. The proposed cell retains key advantages of RFBs, namely independent energy and power scaling, durability, and low cost while decoupling the conductive and thermal properties present in solid-state devices. We extend Tester's results on an aqueous copper system [4] to organic active species with a novel reactor design. A range of organic active species are examined by cyclic voltammetry, bulk electrolysis, and other techniques at various temperatures and top-performers are transferred to the thermogalvanic cell for further performance analysis. In addition, we report a few engineering advances to the thermogalvanic cell to mitigate losses and improve cell potential.

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TP03.06.07

Farming Thermoelectric Paper Bernhard Dorling¹, Deyaa Abol-Fotouh^{2,1}, Osnat Zapata-Arteaga¹, Xabier Rodríguez-Martínez¹, Andrés Gómez¹, J. Sebastián Reparaz¹, Anna Laromaine¹, Anna Roig¹ and Mariano Campoy-Quiles¹; ¹ICMAB-CSIC, Bellaterra, Spain; ²City of Scientific Research and Technological Applications, New Borg Al-Arab, Egypt.

This contribution reports on new thermoelectric composites that are prepared by growing bacterial cellulose (BC) in the presence of carbon nanotubes (CNTs) dispersed in an environmentally friendly aqueous medium. The resulting micrometer-thick, free-standing films of finely intermixed BC fibers and CNT bundles can be employed without further substrate. By combining a low-cost and easy to process biopolymer that exhibits intrinsically low thermal conductivity, with carbon nanotubes, which exhibit high mechanical strength and good electrical properties, a new type of thermoelectric composite was obtained. The composite exhibits a thermoelectric performance that is similar or even better than that of neat buckypaper, while containing only about 12 wt.% of CNTs. The films are highly porous, which not only contributes to their low thermal conductivity of only about 0.3 Wm⁻¹K⁻¹, but furthermore facilitates effective n-

doping all throughout the film thickness.

Additionally, the films are flexible, and can be conformally wrapped around heat sources, improving thermal contact.

Importantly, BC/CNT composites are stable up to at least 500 K, which naturally increases ZT as well as allows for a wider range of viable applications.

TP03.06.08

High Thermal Conductivity of Electrospinning PVA Nano-Fiber Film Rulai Guo, Xiandong Chen, Ni Tang, [Xiaoxiang Yu](#), Zhan Peng, Chao Chen, Zhigang Xue, Xiaobo Li, Jianfeng Zang and Nuo Yang; Huazhong University of Science and Technology, Wuhan, China.

Flexible substrates that host electronic components are an essential part of soft electronics. The continuing miniaturization of these electronics requires the substrates with high thermal conductivity to avoid function failure and lifetime reduction. However, soft and mechanically deformable systems have typically low thermal conductivity. Here, we fabricate a flexible polyvinyl alcohol (PVA) nano-fiber film (PVANFF) by the electrospinning technique, which exhibits excellent flexibility and high thermal conductivity simultaneously. We found the effective thermal conductivity of PVANFF along the fiber axis is twice as high as amorphous PVA membrane. This excellent performance is attributed to polymer molecular chain alignment and fibrous structural improvements, which are resulted from the high strain rates during the electrospinning process. Furthermore, we enhance the thermal conductivity of the PVANFF by mingling it with Ag nanowires (AgNWs). And we also measure the PVANFF without the air between the fibers by filling it with amorphous PVA. Our study provides design guidance for flexible substrates.

TP03.06.09

Fabrication and Life Testing of Advanced Skutterudite-Based Unicouples for a Proposed Enhanced Multi-Mission Radioisotope Thermoelectric Generator [Obed Villalpando](#), Ike Chi, Samad Firdosy, Kevin Smith, Brian Phan, Sutinee Sujittosakul, Kevin Yu, Michell Aranda, Thierry Caillat, Jean-Pierre Fleurial, Billy C. Li, Stanley Pinkowski, Chen-Kuo Huang, Jong-Ah Paik, Pawan Gogna and Terry Hendricks; Jet Propulsion Laboratory, Pasadena, California, United States.

Radioisotope Thermoelectric Generators (RTG's) have been used on several NASA missions when they enable or significantly enhance the ability of a mission to meet its objectives. The current state-of-the-art RTG power source, Curiosity rover's Multi-Mission Radioisotope Thermoelectric Generator (MMRTG), has operated for more than three Martian years (2061 earth days) on the red planet. In order to increase the power and conversion efficiency of future MMRTG systems and extend the lifetime of future rover missions, an effort to mature advanced thermoelectric technology for use in a proposed Enhanced Multi-Mission Radioisotope Thermoelectric Generator (eMMRTG) was started in 2013. The conceptual design approach of the eMMRTG is to replace the heritage MMRTG couples in the thermoelectric module assembly with more advanced skutterudite (SKD)-based couples without any significant design changes to the generator. The new SKD thermoelectric materials not only can provide higher thermoelectric performance, but also can operate at higher maximum operating temperatures in comparison to MMRTG thermoelectric materials. As a result, an eMMRTG power system could provide up to a 25% increase in conversion efficiency over the MMRTG at beginning of life (BOL) and about a 50% increase in power output over the MMRTG in a 17-year life span. The proposed eMMRTG would preserve all of the MMRTG's multi-mission capabilities while offering an enhancement in power and potentially lower power degradation rates. Work at the Jet Propulsion Laboratory has focused on developing these advanced SKD unicouples to have long-term stability while still maintaining ample power output. This update will report on the progress for demonstrating manufacturability and validating performance of these advanced SKD unicouples developed and tested by Jet Propulsion Laboratory (JPL).

TP03.06.10

Synthesis and Thermoelectric Performance of Semiconducting-Metallic Ceramic Composites [Julio E. Rodriguez](#)¹ and Adam Sebastian Gutiérrez²; ¹Department of Physics, Universidad Nacional de Colombia, Bogotá, Colombia.

Polycrystalline composites with a nominal composition of $\text{La}_{0.95}\text{Ca}_{0.05}\text{CoO}_3\text{-La}_{1.7}\text{S}_{0.3}\text{CuO}_4$ (La(Ca)CoO-La(Sr)CuO) were fabricated using the solid state reaction method. Thermoelectric properties were studied using Seebeck coefficient $S(T)$, electrical resistivity $\rho(T)$ and thermal conductivity $\kappa(T)$ measurements. These transport properties were studied in the temperature range between 85 and 300K. The thermoelectric performance of La(Ca)CoO ceramics was improved as a consequence of the decreasing of its electrical resistivity with Ca doping and metallic La(Sr)CuO₃ adding. The composite exhibits maximum values for the thermoelectric power factor, PF and the figure of merit ZT close to $28 \mu\text{W/K}^2\text{-cm}$ and 0.5, respectively. Thus, the behavior observed in the transport properties become these composites promising materials for use in thermoelectric devices for low-temperature applications.

TP03.06.11

Transport properties of CNT-PEDOT/PSSA Polymer Composites Sebastian Forest² and [Kofi Adu](#)^{1,2}; ¹Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania, United States; ²Physics, The Pennsylvania State University, Altoona, Altoona, Pennsylvania, United States.

Organic thermoelectric materials are receiving considerable attention due to the fact that they can be potentially used for fabricating flexible, printable, and low cost organic thermoelectric generators (OTEGs). Conjugated polymers such as poly(3,4-ethylenedioxythiophene) (PEDOT), poly(3-hexylthiophene) (P3HT) and polyaniline (PANI) are some examples of organic thermoelectric materials. However, for fabricating the OTEGs, the thermoelectric performance of the conjugated polymers needs to be improved further. Recently, carbon nanotubes (CNTs) have been used as effective additives for improving the thermoelectric performance of conjugated polymers. By adding CNTs to the conjugated polymer matrix, density of the electrical pathways in the nanocomposite increases; thereby, greatly enhancing the electrical conductivity. The enhanced electric conductivity results in enhanced thermoelectric performances of the CNT/conjugated polymer nanocomposite. We present our results on temperature dependence transport properties of CNT-PEDOT/PSS composite and boron doped composites of different CNT loading (0.1wt%, 0.5wt%, 1.0%, 2.0% and 5.0wt%) and correlate the CNT loading with the electrical conductivity.

TP03.06.12

Porous $\text{SnSe}_{1-x}\text{S}_x$ Nanosheets as Promising Ternary Nanocrystals for Thermoelectric Applications [Hyun Ju](#), Taeseob Oh, Dabin Park, Hyunwoo Oh and Jooheon Kim; Chung-Ang University, Seoul, Korea (the Republic of).

Herein we report a higher figure of merit (ZT) in SnSe based thermoelectric materials by markedly reducing the thermal conductivity, which is achieved *via* three promising strategies: substitution with isoelectronic S atoms, exfoliation of nanosheets from a bulk ingot, and chemical transformation of the material into a porous structure. $\text{SnSe}_{1-x}\text{S}_x$ nanosheets are prepared by hydrothermal Li-intercalation and subsequent exfoliation process from bulk $\text{SnSe}_{1-x}\text{S}_x$ ingots. The substitution of S atoms into SnSe and the exfoliation of $\text{SnSe}_{1-x}\text{S}_x$ nanosheets contribute to the scattering of phonons at numerous atomic disorders and nano-sized boundaries, resulting in effective reduction of the thermal conductivity and an enhanced ZT . The introduction of porosity into the $\text{SnSe}_{1-x}\text{S}_x$ nanosheets through the chemical transformation process further reduces thermal conductivity, which leads to a higher ZT . Finally, the porous $\text{SnSe}_{0.8}\text{S}_{0.2}$ nanosheets has an outstanding ZT of 0.12 at 310 K, significantly higher than that of pristine SnSe.

TP03.06.13

Thermal-Charging Electrochemical Cell for Converting Low Grade Heat in Isothermal Operation Xun Wang and Shien Ping Feng; The University of Hong Kong, Hong Kong, Hong Kong.

A tremendous amount of energy is wasted in the form of low grade heat from source below 100 °C. Current thermoelectric or thermoelectrochemical technologies are still facing with low efficiency from limited temperature difference, balance between electric and thermal conduction, and construction on specific scenario such as thermal cycle. Here we proposed a new thermoelectrochemical system with graphene oxide(GO) as positive electrode and polyaniline(PANI) as negative electrode which can operate in isothermal condition to continuously convert low grade heat into electricity. We observed that GO had a high thermal response due to oxygen containing functional groups, and the electrochemical cell with GO as positive electrode and titanium foil as electrode could reach a high temperature coefficient of 3.5 mV/K. When heating up the cell, a heat induced voltage difference can be created and current can be generated by promoting the oxidation reaction of PANI if employing PANI as negative electrode. This system demonstrated a thermal-electricity energy conversion efficiency of 3.92% when operating in 90 °C. The findings show enormous potential to harvest low grade heat via thermo-electrochemical cell.

TP03.06.14

Synthesis of High Conducting and Thermoelectric PEDOT:PSS/Carbon Materials Aerogel for Dual-Sensors Gyung Hyun Yoon, Sang Woo Lee and O Ok Park; Korea Advanced Institute of Science and Technology, Daejeon, Korea (the Republic of).

Poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) is one of the promising conducting polymers which exhibit p-type thermoelectric property, having the various characteristics such as water solubility, flexibility, and commercial availability. In this paper, we fabricated thermoelectric nanocomposite aerogel, composed of PEDOT:PSS and carbon nanotube (CNT) via an easy and reproducible freeze-drying method. CNT could be simply dispersed in PEDOT:PSS aqueous solution, due to the secondary interactions between them, for example, pi-pi interaction and van der Waals interaction. At 140 degrees Celsius, crosslinker, glycidoxypropyl-trimethoxysilane (GOPS) reacted -OH groups and epoxy group in the solution and robust nanocomposite aerogels were successfully formed. These nanocomposite aerogels showed better electrical conductivity and thermoelectric effect than those of pristine PEDOT:PSS aerogels due to embedding CNTs into PEDOT:PSS matrix. As an application of the fabricated aerogel, we also demonstrated highly sensitive pressure/temperature(P/T) dual-sensor using PEDOT:PSS/CNT aerogel. By simply mixing CNT and cross-linking agent in PEDOT:PSS solution, electrical and thermoelectric properties were improved as well as the sensitivity of the P/T dual-sensor.

TP03.06.16

Photo-Seebeck Effects in Doped P3HT Composites Harold O. Lee and Sam-Shajing Sun; Norfolk State University, Norfolk, Virginia, United States.

As the global energy and environmental preservation needs continue to grow, the demand for renewable and clean energy conversion materials and devices continues to rise as well. Thermoelectric (TE) materials and devices can convert waste heat into electricity and therefore it can be a potential renewable and clean energy source. TE materials research and development has been mostly focusing on inorganic semiconductors such as Bi-Te or Sb-Te alloys with thermoelectric figure-of-merits (ZT values) around one at room temperature. Inorganic TE materials generally exhibit high electrical conductivity but also high thermal conductivity that is inversely related to the thermoelectric figure of merit (ZT values). Organic and polymeric materials typically exhibit low electrical conductivities, high Seebeck coefficients, and orders of magnitude lower thermal conductivities as compared to their inorganic counterparts. However, the electrical conductivities of organic/polymeric materials are tunable via doping or molecular engineering. In this study, a series of carefully doped P3HT composites are systematically evaluated for heat as well as light modulated devices. Along with a high absorption coefficient, when the polymer film thickness is less than the penetration depth of the incoming photons, the photo effects are significant and could be very useful for light modulations of thermoelectric functions. With further systematic studies and a better understanding of the mechanisms behind the photo-Seebeck effect, the development of potential high-efficiency multi-function materials and devices appears feasible.

TP03.06.17

Temperature Sensitivity Inversion of GaInP Solar Cells by Thermoelectric Hybridization Bruno Lorenzi^{1,2}, Dario Narducci¹ and Gang Chen²; ¹University of Milano-Bicocca, Milan, Italy; ²Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

It is well known that temperature sensitivity is one of the main drawbacks of photovoltaics (PV). Especially in the case of optically concentrated systems, the solar cell working temperature is always much higher than ambient temperature. High working temperatures increase carrier recombination, therefore decreasing solar cell performance. In this context heat recovery strategies are in principle a solution to balance this loss increasing the overall system efficiency. Among these solutions thermoelectric hybridization has already been shown to be an effective candidate. However, the field of solar cell thermoelectric hybridization is still burgeoning. Often, works in literature are contradictory and in some cases the work reports unphysically large efficiency improvements. It is thought that the false efficiency improvement observed is due to incorrect experimental procedures, such as the implementation of very optimistic cold side temperatures, and the lack of normalization to active area when combining PV and TEG output contributions.

In this communication we report the development and the rigorous characterization of Gallium Indium Phosphide (GaInP) solar cells hybridized with Bismuth Telluride (Bi₂Te₃) thermoelectric generators (TEGs).

The results showed an inversion of the solar cell temperature sensitivity with an absolute efficiency gain of 2% (\approx 15% of the sole PV efficiency) corresponding to an optimal working temperature of around 400 K. We find that the key to this improvement is the use of a wide-gap solar cell and the implementation of thermal strategies that prevent heat dissipation to the environment. In addition, the variation of both gain and optimal temperature as a function of the optical concentration were studied, showing the applicability of this kind of hybridization in different contexts.

These results, which are in excellent accordance with a more general theoretical model already reported by the authors, demonstrate in an accurate fashion the real potential of thermoelectric hybridization of solar cells.

TP03.06.18

Influence of the Mobility Ratio and Density of States Width on the Thermoelectric Properties of Polymer Blends Ashkan Abtahi¹, Yadong Zhang², Xuyi Luo³, Jianguo Mei³, Seth R. Marder² and Kenneth R. Graham¹; ¹University of Kentucky, Lexington, Kentucky, United States; ²Georgia Institute of Technology, Atlanta, Georgia, United States; ³Purdue University, West Lafayette, Indiana, United States.

Conjugated polymers can be used in mechanically flexible and low cost thermoelectric (TE) devices, but their thermoelectric performance must be improved to make them commercially viable. The performance of thermoelectric materials depends on the electrical conductivity, Seebeck coefficient and thermal conductivity. In polymer based TE materials the polymer needs to be doped to become electrically conductive. The higher the doping concentration, the more electrically conductive the material becomes, but generally at the cost of a decrease in the Seebeck coefficient. Blending of π -

conjugated polymers has been proposed as a method to minimize the tradeoff between electrical conductivity and the Seebeck coefficient, thus potentially allowing higher power factors to be reached. By blending polymers, the total density of states (D.O.S.) in the material will be manipulated, which may be used to alter the energy dependence of charge transport in the TE material. Manipulating the D.O.S., particularly by introducing highly conductive states at higher energies with respect to the Fermi energy, allows the energy dependence of charge transport to be enhanced and the Seebeck coefficient increased. The major parameters that we expect to impact the power factor in polymer blends are the mobility ratios between the pure polymer and the shape of D.O.S. Here, we use a model introduced by Bässler and Arkhipov to theoretically probe how the mobility ratio and the shape of the D.O.S. impact the Seebeck coefficient and thermoelectric performance. These calculations are then used to fit experimental data of various polymer blends with varying mobility ratios and D.O.S. distributions. We find that a narrower D.O.S. and higher mobility of the added polymer with respect to host polymer can lead to an enhancement in the Seebeck coefficient of the TE material, but we do not observe increases in the power factor.

TP03.06.19

Thermoelectric Properties of Unsorted and Sorted Single-Walled Carbon Nanotube Sh Tsuyohiko Fujigaya^{1, 2}; ¹Kyushu University, Fukuoka, Japan; ²JST, Saitama, Japan.

Single-walled carbon nanotubes (SWNTs) especially their semiconducting type are promising thermoelectric (TE) materials due to their high Seebeck coefficient. In this study, we measured the electrical conductivity (σ), Seebeck coefficient (S) and thermal conductivity (κ) of sorted semiconducting SWNTs (s-SWNTs) and metallic SWNTs (m-SWNTs) together with their mixture and the unsorted SWNTs to study the effect of sorting for the conversion efficiency, which is often evaluated as the power factor (PF) and figure of merit ($ZT = S^2\sigma T/\kappa$). We found that as the s-SWNT purity increased, ZT increased, mainly due to the increasing of Seebeck Coefficient. Thermal conductivity on the other hand, remains the same with the increase of s-SWNT. Our group is the first to report thermal conductivity and ZT of SWNT sheet with different s-SWNT purity.

TP03.06.20

Dual-Beam Pulsed Laser Deposition of Ga₂Te₃/(Bi_{1-x}Sb_x)₂Te₃ Nanocomposite Films for Thermoelectric Applications Bo-Yao Yu, Chih-Chuan Su, Po-Hung Chen and Chun-Hua Chen; Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan.

Heterogenization of nanomaterials has become one of the most promising strategies for modifying thermoelectric materials. The introduction of heterogeneous dopants could not only selectively improve intrinsically-poor specific properties of the base materials, but potentially break the physically coupled thermoelectric properties due to the created various heterogeneous functional interfaces for further enhancing the overall thermoelectric figure of merit (ZT). In this work, a series of novel Ga₂Te₃/Bi_{0.5}Sb_{1.5}Te₃ heterogeneous nanocomposite films with different compositional ratios were successfully deposited on SiO₂/Si substrates using a dual pulse laser deposition system. The optimized electrical conductivity of 303 S/cm and Seebeck coefficient of 295 μ V/K found with the composition of Ga₂Te₃:Bi_{0.5}Sb_{1.5}Te₃=22:78 is respectively 45% and 40% higher than those reported for Bi_{0.5}Sb_{1.5}Te₃. In overall, the corresponding power factor of 26 μ W/cmK² is approximately two times higher than that found for Bi_{0.5}Sb_{1.5}Te₃.

TP03.06.21

Improving the Thermoelectric Power Factor in 2D Materials Using Periodic Potential Barriers Adithya Kommini and Zlatan Aksamija; University of Massachusetts Amherst, Amherst, Massachusetts, United States.

The conversion of waste heat to electricity using thermoelectric devices has the potential to improve our energy utilization efficiency. Significant research efforts over the past two decades have been devoted to increasing the efficiency of thermoelectric (TE) energy conversion via nanostructuring. One approach to improve the TE efficiency is electron filtering where "cold" (low energy) electrons are restricted from participating in transport by an energy barrier. However, the impact of electron tunneling through thin barriers and resonant states on TE properties, especially in two-dimensional (2D) mono- and few-layer materials, has been given significantly less attention. In our previous work, we simulated the effect of energy filtering and quantum-mechanical (QM) tunneling through a series of potential barriers in silicon and found that tall, sharp barriers can significantly enhance the TE power factor. We extend our previous work to study the effect of energy filtering from a series of potential barriers in 2D materials, such as those arising from lateral or vertical van der Waals heterostructures, superlattices, or when a monolayer is exposed to a series of electrostatic gates. In this work, we develop a comprehensive transport model that includes electron-phonon coupling and electron-impurity scattering alongside with quantum effects arising from the potential barriers. Our model captures the carrier-potential interactions in the Wigner formalism as an additional force term called the "quantum evolution operator", which is added to the semi-classical Boltzmann transport equation (BTE). The resulting Wigner-Boltzmann transport equation is solved using Rode's iterative method, with the electronic structure data being pre-calculated from density functional theory (DFT). We then study the impact of height, width, and shape (smoothness) of the potential barriers on TE properties. Our simulations show a steady increase in TE efficiency with the height of the potential barrier in gated single layer (SL) molybdenum disulfide (MoS₂), reaching a maximum enhancement of approximately 25 percent. Further, we explore the impact of the barrier width and shape and find that, unlike 3D, sharp, narrow barriers are not always better. We attribute this to the unique step-like 2D electronic density of states. This study identifies ways to achieve high TE performance in nanoscale thermoelectric devices with periodic features, such as van der Waals heterostructures and superlattices. The improvement in TE efficiency helps in the development of energy-efficient devices ranging from wearables powered by scavenging body heat, to thermal sensors, and solid-state electronic cooling.

TP03.06.22

Tuning Band Structure and Electronic Transport in Multilayered Semiconductor Nanostructures Sanghamitra Neogi and Vitaly Proshchenko; University of Colorado Boulder, Boulder, Colorado, United States.

When the device size reaches the nanoscale, scattering at interfaces dictate the device functionality. Additionally, dimensional reduction significantly modifies the properties of carriers in the nanostructure. A complete treatment of transport in a multi-interface system requires solving the complex interplay between dimensional confinement and interface scattering. In this work, we investigate electron transport in layered Si/Ge superlattices with imperfect interfaces employing density functional theory in combination with semi-classical Boltzmann transport theory. We demonstrate tunability of electron transport in multilayered nanostructures by the introduction of compositional variability, engineered interface structures and external strain. The structural variability induces strain that strongly influences the bonding environment and therefore, the charge densities in these structures. The modified charge densities directly impact electronic band structures and consequentially, cross-plane electronic transport across the multilayered systems. Our work establishes a direct relationship between the introduction of local and global strain and cross-plane transport in multilayered semiconductor superlattice structures. One representative result from our study is that introduction of positive strain (tension) in the in-plane direction of Si/Ge superlattices leads to significant improvement of the Seebeck coefficient at higher carrier concentrations. Our work establishes strategies to attain a phonon-glass-electron-crystal regime in order to achieve a high ZT for thermoelectric applications. The project is funded by the DARPA (DSO) MATRIX program. This work used XSEDE, which is supported by NSF grant number ACI-1053575.

TP03.06.23

Thermoelectric Properties of MA P-Type BiSbTe-NFC Hydrogel Composite Films Under Applied Pressure Deepa Madan¹, Eunhwa Jang¹, Aswani Poosapati¹, Nathaniel Jang² and Liangbing Hu²; ¹University of Maryland Baltimore County, Baltimore, Maryland, United States; ²University of Maryland College Park, College Park, Maryland, United States.

Flexible Thermoelectric generators (TEGs) are attractive because they can potentially provide higher power density, can have higher aspect ratio elements, and are more scalable than conventional TEGs. Flexible TEG devices are printed on flexible substrates using thermoelectric (TE) inks consisting of TE particles, a suitable binder, and a solvent. Films printed using TE inks typically have much lower performance as compared to commercially available bulk TE pellets. A high amount of insulating binder present in inks deteriorates the electrical properties and overall performance of printed TE films. In this work, we explore a novel binder, synthesize efficient TE particles with suitable dopants, and perform cold-pressing to densify the films to improve the TE performance of p-type TE materials. We chose wood-based nanofiber cellulose (NFC) hydrogel as a binder because a very small amount of hydrogel is sufficient to provide good adhesion strength and flexibility. We initially check the feasibility of use of NFC hydrogel as a binder with commercially available Sb₂Te₃ TE particles. Then, followed by synthesizing various mechanically alloyed (MA) particles using Te as a dopant with the objective of improving the TE performance. For optimizing thermoelectric inks we made films with different weight ratios of the binder and the TE powder (e.g., 1:100, 1:1000, and 1:10000). Unlike most other TE films with thermoset polymers that require high curing temperatures and long curing time, NFC hydrogel TE composite films are cured at the room temperature in a short time to achieve good properties. These films were then subjected to a range of uniaxial pressure (10 Mpa to 1000 Mpa) for 5 minutes to densify the films. A significant improvement in the electrical conductivity was achieved by varying the applied pressures. Optical microscope and SEM images showed that (1) the number of pores in the NFC hydrogel phase with particles decreased with an increase in the weight ratio of the TE powder, and (2) the NFC hydrogel phase and particles were compacted and densified. Because the particles aggregate with each other, the grain boundaries and scattering were reduced, helping improve the electrical conductivity. SEM cross-section images revealed that with higher TE particles concentration, the TE films have more uniform and denser surfaces. The best sample among various MA BiSbTe samples was 1:10000 binder to MA Bi_{0.46}Sb_{1.34}Te_{3.2} (which consists 8% extra Te) at 600 Mpa applied pressure. Its power factor of 1338.8 $\mu\text{W}/\text{mK}^2$ is approximately 15 times that of MA Bi_{0.5}Sb_{1.5}Te₃ sample for which no pressure was applied. Overall, the low mass loading of binder to particles ratio, the application of external applied pressure, and the addition of extra Te to MA Bi_{0.5}Sb_{1.5}Te₃ improved the power factor by approximately 130 times (1:10000, 600Mpa, MA Bi_{0.46}Sb_{1.34}Te_{3.2}, 1338.8 $\mu\text{W}/\text{mK}^2$) as compared to Sb₂Te₃-NFC composite films without any external pressure.

TP03.06.24

The Transverse Seebeck Effect Oded Rabin¹, Stuart Laurence¹ and Nicholas Tiliakos²; ¹University of Maryland, College Park, Maryland, United States; ²Innoveering LLC, Ronkonkoma, New York, United States.

In anisotropic single crystal materials the Seebeck coefficient tensor may contain non-zero off-diagonal elements. With proper crystal alignment, a unidirectional heat flux generates EMFs both parallel (normal Seebeck voltage) and perpendicular (transverse Seebeck voltage) to the temperature gradient. This presentation will highlight the theoretical and practical advantages and challenges in utilizing the transverse Seebeck effect in miniature high-speed heat flux sensors. Compatible with large scale microfabrication, this technology is suitable for microcalorimetry and fast thermal analysis of materials and processes.

TP03.06.25

Nanoporous V–VI Chalcogenides Nanoplates for Efficient Thermoelectrics with Preferential Interfacial Scattering Chaochao Dun¹, Jian Wang², Kirill Kovni², David L. Carroll³ and Yanliang Zhang¹; ¹Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, Indiana, United States; ²Department of Chemistry, Iowa State University, Ames, Iowa, United States; ³Physics Department, Wake Forest University, Winston Salem, North Carolina, United States.

Nanoporous architectures are known to have low thermal conductivities thanks to the enhanced phonon scattering at pore interfaces. In this paper, instead of the chemically engineered interface, we adopted the morphology engineered interface in V-VI systems to realize an electron-transmitting but phonon-blocking structure using preferential energy carrier scatterings determined by the modulation of geometric factors. The synthetic nanopore in the nanoplates offers superior control of both the pore size and the porosity in the consolidated nanostructured bulk pellets. Such versatility offers an additional degree to improve the thermoelectric properties. The effective multi-frequency phonon scattering along with minimal charge carrier scattering lead to a substantial reduction of lattice thermal conductivity and a slight increase of Seebeck coefficient. Thanks to the existence of pore boundaries, effectively multiter preferential scatterings were achieved, which involves more phonons scattering than that of charge carries, more low-energy charge carries scattering than high-energy carries, leading to an improved figure of merit of the V-VI systems.

TP03.06.26

Investigation of Thermoelectric Performance of MoS₂ Nanostructure Along with Its Secondary Phase Pratisha Gangwar, Sunil Kumar and Neeraj Khare; Physics, Indian Institute of Technology Delhi, New Delhi, India.

Thermoelectric materials have been the subject of intense research from both theoretical and technological point of view due to their ability to directly convert waste heat into the electricity and can provide an alternative approach to deal with the future energy crisis [1]. The energy conversion efficiency of thermoelectric material is evaluated from the figure of merit ($zT = S^2\sigma T/\kappa$), a dimensionless quantity, where S is the Seebeck coefficient, σ is the electrical conductance, T is the absolute temperature and κ ($\kappa = \kappa_e + \kappa_p$) is the thermal conductance composed of the contributions from electrons (κ_e) and phonons (κ_p) [2]. For efficient energy conversion, the figure of merit should be greater than 1. The conventional thermoelectric materials possess low value of zT thus cannot be used for thermoelectric applications [1]. Thus to improve the zT value, materials which possess high Seebeck coefficient and high electrical conductivity or low thermal conductivity are required.

Recently, layered transition metal dichalcogenides (TMDCs) have gained a lot of research attention for thermoelectric applications due to the advantage of low thermal conductivity possessed by these materials [3]. Among TMDCs, molybdenum disulfide (MoS₂) has been demonstrated as a good thermoelectric material due to its high value of thermo-EMF (or thermoelectric voltage) and low value of thermal conductivity [3]. But, low electrical conductivity limits its thermoelectric conversion efficiency [4]. So, the challenge is to increase its electrical conductivity without compromising the low thermal conductivity. One of the way is to enhance its electrical conductivity is by incorporating metal nanostructures in the semiconducting host matrix [1].

In the present work, we demonstrate thermoelectric properties of MoS₂ by incorporating Mo₂S₃, a semi-metallic secondary phase of MoS₂. The presence of semi-metallic Mo₂S₃ in MoS₂ matrix enhances its electrical conductivity. Further, enhancement in Seebeck coefficient is also observed due to the filtering of low energy charge carriers. For this study, we have synthesised MoS₂ nanosheets (pristine and secondary phase incorporated) via hydrothermal method. By varying the growth time, 16 hours and 36 hours, we are able to get pristine MoS₂ (labelled as M36) and MoS₂ with secondary phases (labelled as M16). The structural and morphological analysis of as-synthesized MoS₂ is performed with X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Furthermore, thermoelectric performance of the MoS₂ samples (M16 and M36) is studied and analysed.

TP03.06.27

Effect of In as a Substitute and not a Filler on Thermoelectric Properties of CoSb₃ Skutterudites Keshav P. Dabral and Satish Vitta; Indian Institute of Technology Bombay, Mumbai, India.

CoSb₃ with an open structure which can accumulate several fillers has been extremely studied due to its phonon glass electron crystal character. In the earlier studies In has been added to CoSb₃ as a filler to reduce thermal conductivity due to its large size compared to both Co and Sb. In the present work however its effect on the thermoelectric properties when used as substitute for Sb has been investigated in detail. The substituted alloys, Co₄Sb_{12-x}In_x with $x = 0.5, 1$ and 1.5 were synthesised by standard technique and hot pressed at 600°C under a pressure of 60Mpa for 12 minutes into circular pellets. Structure characterization by X-ray diffraction shows that for $x=0.5$ and 1.0 , the alloys consist of essentially single phase indicating that In has gone into solution as substitute for Sb. The alloy with $x=1.5$ however shows phase segregation. The skutterudite phase, CoSb₃ is present along with CoSb₂ and Sb. Hence this alloy was not investigated further. The variation of electrical conductivity with temperature shows a weak metallic behaviour for $x=0.5$ while that of $x=1.0$ exhibits a weak semiconducting behaviour. Both the alloys show very weak temperature dependence with conductivity varying between 9×10^6 and $1.1 \times 10^7 \text{ sm}^{-1}$ when the temperature increased from 300K to 800K. The Seebeck coefficient of the alloys in the complete temperature range is negative indicating electrons to be the dominating charge carriers. The Seebeck coefficient of $x=0.5$ alloy is found to be higher varying from $150 \mu\text{VK}^{-1}$ to $200 \mu\text{VK}^{-1}$ compared to $x=1.0$ alloy in which it varies from $125 \mu\text{VK}^{-1}$ to $175 \mu\text{VK}^{-1}$. At $\sim 600\text{K}$ bipolar transport begins in the both alloys clearly showing the presence of very small gap between the majority and minority carriers. The high Seebeck coefficient and electrical conductivity of $x=0.5$ alloy results in a large power factor of $3.7 \text{ mWm}^{-1}\text{K}^{-2}$ at $\sim 650\text{K}$. The thermal conductivity of both compound $x=0.5$ and $x=1.0$ alloys is found to be low in the complete temperature range, 300K to 800K varying between $2.5 \text{ Wm}^{-1}\text{K}^{-2}$ and $3.5 \text{ Wm}^{-1}\text{K}^{-2}$. The thermal conductivity of $x=0.5$ alloy however is found to be lower than that of $x=1$ alloys at almost all the temperatures. The relatively low thermal conductivity and extremely large power factor of $x=0.5$ alloy results in a high figure-of-merit of 0.82 at 773K. These results clearly show that low levels of substitution of Sb with In is highly beneficial in increasing the power factor substantially compared to the reduction in the thermal conductivity.

TP03.06.28

Gaussian Process Regression of Electron-Phonon Coupling Matrix Elements with Applications in Thermoelectric Materials Research Jeeyoun Kim, Semi Bang and Daehyun Wee; Ewha Womans University, Seoul, Korea (the Republic of).

Electronic transport coefficients in semiconductors can be obtained by solving the semiclassical Boltzmann transport equation within the relaxation time approximation. The main task is the evaluation of the inverse of the electron energy relaxation time induced by the electron-phonon (el-ph) interaction. Here, we investigate a method, the electron-phonon averaged via Gaussian process regression (EPA-GPR) method, of predicting the Seebeck coefficient and electrical conductivity by estimating the electron-phonon coupling. This method results from the combination of the electron-phonon averaged (EPA) method and the Gaussian process regression (GPR) strategy. With the electron-phonon averaged (EPA) method, the momentum-dependent electron-phonon coupling matrix, $|g_{mnv}(\mathbf{k}, \mathbf{q})|^2$, is approximated by its energy-dependent equivalent, $g^2_{\nu}(\epsilon_1, \epsilon_2)$. $g^2_{\nu}(\epsilon_1, \epsilon_2)$ is modeled as a Gaussian process which is a collection of random variables, any finite number of which have a joint Gaussian distribution. During the regression, the characteristic length-scale of the covariance function of the Gaussian process can be estimated within the type two maximum likelihood (ML-two) approximation. To reduce the computational cost, we use the KISS-GP (Kernel Interpolation for Scalable Structured Gaussian Processes) method, in which the evaluation of the covariance function is replaced with interpolation from a well-defined grid. The calculation on the grid can exploit its underlying Kronecker-Toeplitz structure to boost the calculation speed. A potential thermoelectric half-Heusler compound, HfCoSb, is considered as a test case. Thermoelectric properties, including the Seebeck coefficient and the electrical conductivity, are estimated. The results of the two different approaches are compared in order to show the advantages of the EPA-GPR method as a practical method for estimating thermoelectric properties of materials.

TP03.06.29

Accelerating Evaluation of Converged Lattice Thermal Conductivity Guangzhao Qin and Ming Hu; University of South Carolina, COLUMBIA, South Carolina, United States.

Designing materials with specific properties is a long-term goal in materials science. High-throughput *ab-initio* materials screening and design is a new and rapidly growing area in computational materials research. The application of high-throughput calculations has recently made formidable progress and led to novel insights in this field. The lattice thermal conductivity (κ) is a crucial physical property of crystalline materials for enormous practical implications, such as electronic cooling, thermoelectrics, phase change memories, and *etc.* Therefore, the fast evaluation of reliable κ for variety of materials plays a key role in identifying suitable materials for targeted applications. Currently, first-principles based anharmonic lattice dynamics (ALD) method coupled with phonon Boltzmann transport equation (BTE) is one of the most featured methods to obtain the κ , which involves calculation of interatomic force constants (IFCs). Especially, the anharmonic IFCs are evaluated based on the third order derivatives of the total energy with respect to the atomic displacements, which requires huge computational costs. However, severe problem arises for choosing an appropriate (usually not large enough) cutoff distance (r^{cutoff}) when calculating the anharmonic IFCs. Thus, the high-throughput evaluation of reliable κ remains a challenge due to the large resources costs and time-consuming procedures in calculating the anharmonic IFCs for the convergence test. In this work, based on the analysis of the harmonic (second order) IFCs, we propose a concise strategy to efficiently accelerate the evaluation process of obtaining accurate and converged κ by solving the cutoff distance problem. The proposed strategy is efficient for directly determining when the κ converges with respect to r^{cutoff} and how to fast get satisfactorily converged κ . With this strategy, we study the divergence problem of thermal conductivity of graphene, a long debate of two-dimensional heat conduction in literature. The feasibility of the method is also confirmed by other systems. In addition, the computing speed with our approach could be one order of magnitude faster compared to the traditional method in most situations, where the $\sim 20^{\text{th}}$ nearest neighbors are considered. The quantitative strategy proposed herein can be a good candidate for fast evaluating the reliable κ and thus provides useful tool for high-throughput materials screening and design with targeted thermal transport properties.

SESSION TP03.07: New Directions in Low Temperature Electrochemical and Thermal/Thermoelectric Properties

Session Chair: Colin Lambert

Wednesday Morning, November 28, 2018

Sheraton, 3rd Floor, Gardner AB

8:00 AM *TP03.07.01

Non-Covalent Interactions in Electrochemical Reactions and Implication in Clean Energy Applications Botao Huang, Sokseiha Muy, Shuting Feng, Jame Sun, Carl V. Thompson and Yang Shao-Horn; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Understanding non-covalent interactions in the electrified interfaces is critical to design energy-conversion and energy-storage devices. Tuning non-covalent interactions associated with solvent molecules and redox-inactive ions provides new opportunities to enhance the reaction entropy changes and reaction kinetics of metal redox centers, which can increase the thermodynamic efficiency of energy conversion devices such as thermo-electrochemical cells and fuel cells. In this work, the contribution of non-covalent interactions in one electron transfer reactions (e.g. ferri/ferrocyanide and aquo iron) and multi-electron transfer reactions (such as HOR/HER, ORR and OER) was studied, where different structure making/breaking ions were employed. These structure making/breaking ions were found to tune reaction entropy by altering the solvation shell of redox active species and modifying the interfacial water structure of electrode surface, where kinetics is faster at higher reaction entropy.¹ New sights for electrochemical reaction mechanisms have been provided. At device level, we developed charge-free thermo-electrochemical devices. Instead of operating under temperature gradient for thermoelectric generators (TEG), charge-free devices work at isothermal condition and cycled between hot and cold conditions.² Transition metal (e.g. Fe and Co) complexes based charge-free cell has shown a cycle-average power output of 5.5 $\mu\text{W}/\text{cm}^2$ by optimizing electrode materials and redox concentration.

References:

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8:30 AM TP03.07.02

Thermodynamics of Atom Motion and Metal Deposition in Mixed Ionic Electronic Conductors Matthias T. Agne¹, Pengfei Qiu², Xun Shi² and Jeffrey G. Snyder¹; ¹Northwestern University, Evanston, Illinois, United States; ²Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China.

The possibility of decomposition in superionic mixed ionic-electronic conductors (MIEC) has limited their engineering applications. Specifically, high efficiency MIEC thermoelectric materials have not been utilized due to decomposition under large electronic currents and large temperature gradients. Herein, we derive the critical condition for decomposition, which corresponds to a critical chemical potential difference defined from linear non-equilibrium thermodynamics. This analysis leads to the conclusion that voltage, not current density, is the relevant design parameter. Consequently, the decomposition condition is independent of the geometry of the device; whereby, a strategy is presented for improving stability in devices subjected to electrical and temperature gradients. By using a series of electronically conducting, but ion-blocking barriers to reset the chemical potential it is possible to keep the material below the threshold for decomposition. Experimentally, the thermodynamic theory is validated in the Cu_{2-x}Se MIEC system.

8:45 AM TP03.07.03

Thermal Transport Across Organic-Inorganic Heterojunctions Through Subpicosecond- and Atomically-Resolved Temperature Monitoring of Vibration Modes Yuexiang Yan and Yee Kan Koh; National University of Singapore, Singapore, Singapore.

Understanding heat transfer across organic-inorganic heterojunctions is important for emerging applications such as photothermal cancer therapy and organic-inorganic hybrid thermoelectric materials. In this study, we employ a new integrated approach to study heat dissipation from gold nanorods (GNRs) conjugated with organic ligands and suspended in water, with an atomic spatial resolution. In the integrated approach, we employ the picosecond transient absorption to monitor the time-resolved temperature evolution of GNRs after being heated by ultrafast laser pulses. In addition, we employ the time resolved Raman spectroscopy to monitor the temperature evolution at multiple locations along ligands (i.e., 4-Nitrothiophenol and 4-Aminothiophenol) conjugated to gold nanorods. We find that the bonds in the conjugated ligands are heated almost instantaneously and reach a peak temperature within ~ 1 ps after heating by the laser pulses, suggesting that the bonds are directly heated by hot electrons across the Au-thiol heterojunction the bonds. We also found that the bonds cool a lot faster than the gold nanorods, with a relaxation time of only ~ 3 ps (vs 300 ps for the gold nanorods). This indicates that coupling of Au-thiol heterojunctions is much stronger than coupling of the ligands to water. Our work facilitates better understanding of heat transfer at atomic scale.

9:00 AM TP03.07.04

Magnetically Driven Heat Transport in Field-Induced Weyl Semimetals Dung Vu, Koen Vandaele, Nandini Trivedi and Joseph P. Heremans; The Ohio State University, Columbus, Ohio, United States.

Theory predicts^[1] that the Fermi arcs in Weyl semimetals (WSM) induce entropy transport driven by circulating electronic currents in a magnetic field. Here, we report the first experimental observation of that theory. Fermi arcs are projections of Weyl nodal crossings in the surface Brillouin zone. This new transport phenomenon has no net charge transport, but a net heat transport that contributes to the magneto-thermal conductivity of the material. Experimental demonstration of the circulating current in a traditional WSM is difficult since the effect scales with thickness, yet the growth technology for thick, high-quality films of traditional WSMs is not well developed. $\text{Bi}_{1-x}\text{Sb}_x$ alloys with varying Sb concentrations have bands that close at $x \approx 5$ and have a Dirac dispersion with the Dirac point at the L-point of the Brillouin zone^[2]. In strong magnetic fields, this Dirac point theoretically is expected to split into two field-induced Weyl points. Here we experimentally demonstrate the new, magnetically-driven enhancement of thermal conductivity in bulk $\text{Bi}_{1-x}\text{Sb}_x$ samples. We report a strong, positive magneto-thermal conductivity at the Sb concentration and magnetic field where the Weyl points are expected to appear.

This work is supported by the OSU Center for Emergent Materials, an NSF MRSEC, Award Number DMR-1420451.

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9:15 AM TP03.07.05

Giant Anomalous Nernst Effect Observed in Single Crystal MnBi Bin He¹, Stephen Boona¹, Brian C. Sales² and Joseph P. Heremans¹; ¹The Ohio State University, Columbus, Ohio, United States; ²Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

MnBi is a high temperature ferromagnet ($T_c=630\text{K}$) and crystallizes in the HCP structure. Its thermal transport properties have remained uninvestigated. The anisotropic transport properties (including resistivity, thermal conductivity, thermopower and Nernst effect) of two MnBi single crystals are measured and presented here separately from 80K to 300K in magnetic field up to 1.4T along different crystallographic axis. We observed a giant anomalous Nernst thermopower in both α_{xyz} and α_{zyx} configurations (the first index indicates the direction of the flux, the second of the measured field, the third of the applied magnetic field, z =hexagonal axis). The anomalous Nernst thermopower in α_{zyx} configuration decays with temperature while in the α_{xyz} configuration the anomalous Nernst effect strengthens. Anomalous Hall effect is also observed. We suspect the presence of a strong magnon contribution to the anomalous Nernst effect. This can be understood as a self-Spin Seebeck effect, whereby a thermally driven magnon flux in the sample generates a spin polarization of

the conduction electrons through magnon-electron scattering. This in turn gives rise to an inverse spin-Hall effects via spin-orbit coupling in the materials itself.

Work supported by the National Science Foundation under Award Number DMR-1420451.

9:30 AM TP03.07.06

Nernst Thermopower in Bi - MnBi Composites Koen Vandaele, Bin He, Stephen Boona and [Joseph P. Heremans](#); The Ohio State University, Columbus, Ohio, United States.

Magnetic materials in which thermal transport involves the generation of spin fluxes provide new opportunities to improve the thermal-to-electric energy conversion efficiency over that of conventional, electron-based thermoelectrics. In bulk ferromagnetic (FM) metals such as Co, Fe, and Ni, magnon dynamics in the material result in a magnonic contribution to total thermopower, as shown by Watzman et al.¹ In thin-film structures composed of a normal metal (NM) film, such as Pt, deposited on an electrically insulating FM, such as yttrium iron garnet (YIG), a thermally driven spin flux injected from the FM into the NM layer gives rise to inverse spin-Hall voltage in the NM layer.² This voltage is perpendicular to the temperature gradient and the applied magnetic field.² Although these thin-film structures are not suitable for power generation applications, it was shown by Boona et al.³ that it is possible to obtain a contribution from the spin-Seebeck effect (SSE) to the Nernst thermopower in bulk nanocomposite structures composed of a NM (Pt) with strong spin-orbit interactions and a FM (Ni). In this work, Bi, which has a large spin-Hall angle and Nernst effect, will be used as a NM and MnBi as the FM. Bulk composites composed of Bi and MnBi needles will be studied specifically in a Nernst geometry to determine the SSE contribution to Nernst thermopower.

References

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9:45 AM TP03.07.07

Investigation of Electron Transport via Quantum Mechanical Estimation of Electrical Conductivity in Thermoelectric Materials [Semi Bang](#)¹, [Georgy Samsonidze](#)², [Boris Kozinsky](#)³ and [Daehyun Wee](#)¹; ¹Environmental Science and Engineering, Ewha Womans University, Seoul, Korea (the Republic of); ²Research and Technology Center, Robert Bosch LLC, Cambridge, Massachusetts, United States; ³Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts, United States.

A quantitatively accurate description of electron transport from first principles would greatly enhance our ability to design new materials or optimize existing materials via prediction of electronic transport properties. In particular, electrical conductivity is a key property determining the performance of many types of bulk materials for energy storage and conversion including thermoelectrics (TE). However, relatively little work has been done on fully ab-initio prediction of electrical conductivity for realistic TE materials. In this study, we perform the validation study of a newly developed computational prediction method of electrical conductivity, i.e., the electron-phonon-averaged (EPA) approximation, in order to verify the feasibility of first-principles screening applications for various realistic and complex TE materials. Regarding target TE materials, we study the pnictogen-substituted ternary skutterudites (PSTs), which are formed by isoelectronic replacement of pnictogen atoms with group 14 (Ge, Sn) and group 16 (S, Se, Te) elements. PSTs are considered as the attractive features to be investigated as potential thermoelectric materials. Nevertheless, the rigorous understanding of the chemical substitution effect on transport phenomena of the PSTs still remains largely unexplored. Therefore, we investigate the effect of pnictogen-substitution on electron transport via estimation of interrelated electronic transport properties in skutterudites compounds. Based on these results, certain guidance for the rational design of next-generation TE materials is also provided.

10:00 AM BREAK

SESSION TP03.08: New Directions and Perspectives in Heat Management and Conversion
Session Chairs: Howard Katz and Shannon Yee
Wednesday Morning, November 28, 2018
Sheraton, 3rd Floor, Gardner AB

10:30 AM *TP03.08.01

New and Emerging Applications of Nanoscale Thermal Science and Engineering [Ravi Prasher](#)^{1, 2} and [Akanksha Menon](#)¹; ¹Lawrence Berkeley National Laboratory, Berkeley, California, United States; ²Mechanical Engineering, University of California, Berkeley, Berkeley, California, United States.

It has been almost three decades since Nanoscale Thermal Science and Engineering became a well-established research field. Various major breakthroughs in fundamental understanding of thermal transport (phonons, photons, and electrons) at the nanoscale have been achieved in these three decades; however, the impact of these fundamental insights has been primarily targeted toward microelectronics and thermoelectrics applications. In this talk we provide examples of other applications such as Lithium ion battery thermal management, building thermal insulation, and high density thermochemical storage where molecular and nanoscale thermal science has a significant role to play.

11:00 AM TP03.08.02

Thermoelectric System Economics—Where the Laws of Thermoelectrics, Thermodynamics, Heat Transfer and Economics Intersect [Terry J. Hendricks](#); NASA Jet Propulsion Laboratory, Pasadena, California, United States.

Thermoelectric technology has key benefits and strengths in many terrestrial energy recovery applications. Thermoelectric system cost is a key factor governing final decisions on the use of thermoelectric energy recovery systems in all terrestrial applications; thus cost being just as important as power density or efficiency for the adoption of waste energy recovery (WER) thermoelectric generators (TEG). New integrated cost analysis / thermoelectric analysis approaches have now shown key relationships and interdependencies between overall TEG system costs, including TE material costs, manufacturing costs, and specifically heat exchanger costs; and the TE performance design metrics such as TE material properties, TE device design parameters, heat exchanger performance metrics such as hot-side and cold-side conductances and UA values, and hot side heat flux in achieving optimal TEG WER designs. These new approaches have led to a new thermoelectric system economics paradigm that strongly influences TEG cost and performance decisions. While work by Yee et al. and LeBlanc et al. provided foundations for the latest cost scaling analysis / TE performance analysis, this

new work takes prior work to new insights and understandings and provides the basis for new thermoelectric system economics. Optimum TEG system cost conditions can now be tied directly to the TE materials, TEG design parameters, and heat exchanger design parameters through critical non-dimensional analysis. The non-dimensional analysis and metrics show the TEG system cost and performance interdependencies and interlinks in one unifying and cohesive relationship. Prior work has shown that the system design that minimizes cost (e.g., the G [$\$/W$] value) can be close to designs that maximize power, but these design regimes are not necessarily aligned with high system conversion efficiency or high specific power. This paper will explore the key sensitivities and interrelationships between critical cost metrics and critical TE performance and design metrics in the new thermoelectric system economics paradigm, provide quantitative data showing these sensitivities, and their serious implications on TEG system design in terrestrial WER applications. Critical non-dimensional parameter mapping has shown where heat exchanger cost-dominated conditions, TE material or manufacturing cost-dominated conditions, and combinations of cost conditions control and drive the overall TEG cost and performance. This new cost-performance paradigm shows the required pathways and challenges to achieving TEG system costs of $\$1$ - $\$3/W_{elec}$.

11:15 AM TP03.08.03

Optimization of Thermoelectric Power Generators for Low-Grade Heat Recovery [Kazuaki Yazawa](#), Yee Rui Koh and Ali Shakouri; Purdue University, Minneapolis, Minnesota, United States.

The most suitable thermoelectric properties for low-grade heat recovery is very well matched to the material in Peltier devices for general cooling application. This is based on an analytical modeling and optimization with temperature dependent material properties. The analytic model is validated based on experiments with commercially available thermoelectric modules. This highlights the importance of the geometric aspect ratio of the thermoelements which is key for thermal impedance matching with the heat transfer coefficients at both hot and cold contacts. Especially, reduction of thermal conductivity has bigger impact compared to the TE power factor. At the same time, however, relative thermal conductivity of TE material compared to the gap fill material has a big impact on the performance. The latter is often neglected in high temperature applications. The talk will go over the experimental results of TE systems optimized for small temperature differences for various heat transfer conditions. The cases include (a) Heat energy harvesting from inaccessible two parallel water pipelines with 10 cm separation and 10-20 deg-C temperature difference for powering wireless sensors transmitting self-diagnostic information about heating and cooling supplies in datacenters. (b) Reversible body heat recovery and spot heating for winter sport jackets with compact heat exchanger design. In the experiments, power generation is measured at room temperature with water chiller and adjusted with temperature-dependent material properties to determine the performance in real conditions. The power output at the level of 1-100 mW with a 40 mm x 40 mm off-the-shelf module were observed depending on the heat/water flow path. At the optimum design, 1.2 V can be generated with electrical series connection of two modules each with 127 thermopairs.

11:30 AM TP03.08.04

Experimental Proof of Thermoelectric Charge Generation and Separation within p-i-n Junction TEGs [Franziska Maculewicz](#)¹, Khaled Arzi², Timo Wagner¹ and Roland Schmechel¹; ¹Institute of Technology for Nanostructure & CENIDE, University of Duisburg-Essen, Duisburg, Germany; ²Components for High Frequency Electronics, University of Duisburg-Essen, Duisburg, Germany.

Common thermoelectric generators are built from unipolar p- and n-legs and use the Seebeck-effect for power generation. In theoretical studies (Span et al.) a p-i-n structure operated parallel to the temperature gradient was proposed. A big advantage of this device concept is beside the conventional thermoelectric effect is the additional ability to harvest energy from thermal excited bipolar carriers in the space charge region (i-region) and their separation in the built-in field of the p-i-n TEG.

Here we present for the first time the experimental evidence of thermal excited bipolar carriers in the space charge region and its contribution to the electrical output power of the TEG. Silicon p-i-n TEGs were fabricated by laser sintering of highly doped boron and phosphorus nanoparticles on each side of an intrinsic silicon wafer. I - V -characteristics were measured under different temperature gradients. The hot side was heated to a temperature around 300 °C. The fundamental characteristics of this complex 2-dimension problem, could be explained by a simple lumped equivalent circuit. It is shown that an additional physical mechanism, beside the regular Seebeck-effect is needed to describe the measured behavior. This indicates the present of a second independent energy conversion process, as predicted by Span et al. This energy which is assigned to the separation of thermally excited bipolar charge carriers within the i-region can be measured by excluding the contribution from the p- and n-legs. In this experiment the Seebeck-effect which occurs mainly in the p- and n- region is canceled by electrically short circuiting the p- and n- legs of the TEG with a full metallization of the legs. The short-circuited device assures a direct access to the thermally excited bipolar charge carriers in the i-region. The output power of the short-circuited devices kept raising with the hot side temperature, which confirms the mentioned assumption. The extracted electric power from the i-region by bipolar charge separation is compared to the Seebeck-effect of the bare i-region. This comparison underlines again the different nature of both mechanism. Besides that, device simulations are carried out on same structures and achieved a good agreement to the measured data. The generated power dependency on the i-region thickness is currently investigated to maximize the contribution of thermally generated bipolar carriers in the i-region to the p-i-n TEG power output.

11:45 AM TP03.08.05

Ferroelectric Energy Conversion by First Order Phase Transformation in the Small Temperature Difference Regime [Ashley Bucsek](#)¹, William Nunn², Bharat Jalan² and Richard James¹; ¹Aerospace Engineering and Mechanics, University of Minnesota Twin Cities, Minneapolis, Minnesota, United States; ²Chemical Engineering and Materials Science, University of Minnesota Twin Cities, Minneapolis, Minnesota, United States.

Ferroc materials respond to external stimuli by undergoing spontaneous changes in macroscopic behavior via advanced deformation mechanisms such as a reversible phase transformation. This includes ferroelastics or shape memory alloys, ferromagnetics, ferroelectrics, and multiferroics. For instance, ferroelectrics that undergo a reversible phase transformation can alternate between one phase that is a strong ferroelectric and another phase that is non-ferroelectric. The transformation between one phase and the other can be induced through small changes in temperature. This material system is incredibly promising for society-improving technological advances in direct energy conversion from heat to electricity, where "direct" means that the material itself generates the electricity. Furthermore, the ferroelectric heat recovery system is ideal for operation in the "small temperature difference regime," e.g. solar-thermal sources, waste heat from air conditioners, data centers, or even hand-held electronic devices. We present a thermal energy conversion device that utilizes the first order phase transformations in ferroelectric capacitors. We demonstrate the validity of such a device, present a theoretical framework to model and optimize the circuit parameters, and discuss using phase engineering to achieve extreme cyclic repeatability.

1:30 PM *TP03.09.01/BM08.09.01**Ionic Effects in Organic Thermoelectrics** [Rachel Segalman](#); University of California, Santa Barbara, Santa Barbara, California, United States.

Thermoelectric materials for energy generation have several advantages over conventional power cycles including lack of moving parts, silent operation, miniaturizability, and CO₂-free conversion of heat to electricity. Molecular materials and hybrid organic-inorganics bring the promise of inexpensive, solution processible, mechanically durable devices potentially suitable for wearable applications. While highly conductive polymers are now commonplace, they generally demonstrate lower thermopower at a given conductivity than inorganic counterparts. Ion conducting materials have previously been demonstrated to have very large Seebeck coefficients, and a major advantage of polymers over inorganics is the high room temperature ionic conductivity. Notably, PEDOT:PSS demonstrates a significant but short-term increase in Seebeck coefficient which is attributed to a large ionic Seebeck contribution. We have recently shown that doping with protic ionic liquids and other proton conductors can be used to control the thermoelectric power factor. In this talk, I will discuss how electrochemical transistor geometries can be used to understand the scaling of thermopower with carrier concentration and to begin to untangle the intertwined ion/electron effects in mixed conductor thermoelectrics. I will also discuss how electrochemistry can be utilized to stabilize the Seebeck enhancement leading to stable improvements to power factor in mixed conductor thermoelectrics.

2:00 PM TP03.09.02/BM08.09.02**Design and Fabrication of Textile-Based Wearable Thermoelectric Devices** [Hend M. Elmoughni](#), Akanksha K. Menon, Shannon Yee and Rylan Wolfe; Georgia Tech, Atlanta, Georgia, United States.

Textile fabrics as substrates for wearable thermoelectric generators (WTEG) are attractive for body heat harvesting. Textile-based WTEGs can be integrated into clothing to convert temperature differences between the human body and ambient into electricity. One target application of the technology is powering body mounted electronics with low energy consumption that ranges from 1 μW to 10mW. Transformation of the conventionally rigid thermoelectric devices consisting of p- and n-type inorganic semiconductors into flexible fabrics offers various advantages including: better conformity to the skin which maximizes the temperature difference needed for power generation, light weight structure which does not restrict mobility or comfort, and easy integration of the technology into clothing. Development of WTEGs has been mainly focused on employing additive printing techniques such as screen printing to deposit the thermoelectric material onto the flexible substrate. While this approach has demonstrated great potential, a number of challenges have to be overcome before a fully functioning textile-based WTEG can be realized. Device-level challenges include small fill factors <0.2 requiring large areas to generate appreciable amounts of power, low fabric thickness that results in small temperature differences, and dominant interconnect and electrical contact resistances for thin-film devices that hamper the power output; these factors need to be considered when designing WTEGs in order to maintain device structure flexibility and high power density. Furthermore, a material-level challenge lies primarily in the development of p- and n-type thermoelectric ink formulations that can be compatible with a cost-effective, scalable fabrication technique without compromising thermoelectric properties. Herein, we present strategies to overcome the aforementioned challenges and fabricate a knitted-base WTEG capable of human body heat harvesting using a through-plane temperature difference. Both the proposed device design and proof-of-concept prototype are presented to demonstrate the feasibility and potential of this technology for low grade heat energy harvesting.

2:15 PM TP03.09.03/BM08.09.03**Towards a Thermoelectric Fabric—3D-Extruded Thermoelectric Threads** [Jun Peng](#)¹, Ian Witting¹, Nicholas Geisendorfer¹, Mingyi Wang¹, Mingchiang Chang¹, Ramille N. Shah^{1,2}, Jeff J. Snyder¹, Matthew Grayson¹ and Adam Jakus²; ¹Northwestern University, Evanston, Illinois, United States; ²Dimension Inx, Evanston, Illinois, United States.

Thermoelectrics (TE) have the potential for diverse applications in energy harvesting, however the rigid configuration of typical TE modules can be a limiting factor whereas flexible platforms would find much broader use. Here, we realize continuous, flexible thermoelectric threads via three-dimensional extrusion through the extrusion of 3D — paints: — self-solidifying, particle laden suspensions. Viscoelastic inks These paints were synthesized using a small volume fraction (10%) of polymer as a binder for Bi₂Te₃-based n- and p- type micrograins. The thermoelectric performance of these threads was quantified using a home-built *in-situ* conductivity/Seebeck vise for calibrated temperature gradient and voltage drop, with a pressure-control function to study the effect of lateral pressure on thread operation. The resulting threads showed electrical conductivity only 1 order of magnitude lower than the annealed sintered micrograin samples. A particle boundary model was introduced to explain the resulting energy barrier for charge transport as a consequence of charge depletion at the boundary. The threads showed a thermopower very close to that of the annealed sintered samples.

To demonstrate the potential applications of the thermoelectric threads, woven thermoelectric fabric is design to vertically harvest heat flux. Both n-type and p-type thermoelectric threads have been successfully fabricated in air ambient from 3D-inks made from thermoelectric semiconductor powders (Bi₂Te₃) embedded in a polymer matrix and extruded. A new double-sided insulating/conducting ribbon will be developed to interconnect a weave of such threads to create the thermoelectric fabric. Textile fabrication is inherently scalable, and weaving fabrics from looms of such thermoelectric threads will drive down manufacturing costs for large-scale production.

2:30 PM BREAK**3:30 PM *TP03.09.04/BM08.09.04****High Power Density Mico-Thermoelectric Generators for Powering Wireless Sensor Nodes** Jian Zhang, Wenhua Zhang and [Dongyan Xu](#); The Chinese University of Hong Kong, Shatin, Hong Kong.

Thermoelectric generators (TEGs) are promising for harvesting waste heat from the environment to power wireless sensor nodes in smart buildings. In this talk, I will share our recent research effort on developing non-flexible micro-TEGs by integrating pulsed electroplating with microfabrication processes.

We systematically studied the effects of the pulsed electroplating conditions on the composition, microstructure, and thermoelectric properties of the electroplated Bi₂Te₃ thin films. Our results show that the thermoelectric figure of merit of the electroplated Bi₂Te₃ films can be enhanced by increasing the pulse off-to-on ratio, which is mainly due to the reduced thermal conductivity and the increased Seebeck coefficient. A maximum ZT of 0.16 is obtained at the pulse off-to-on ratio of 50 at room temperature. Based on the fundamental materials research, we further developed cross-plane micro-TEGs on a SiO₂/Si substrate. The device consists of a total of 127 pairs of n-type Bi₂Te₃ and p-type Sb₂Te₃ thermoelectric pillars embedded in a SU-8 matrix. Both thermoelectric pillars and interconnectors are formed by electroplating, which is advantageous because of low parasitic electrical resistances. The micro-TEG we developed demonstrates a maximum power of 3 mW at a temperature difference of 52.5°C, corresponding to a power density as high as 9.2 mW cm⁻². The power density of our TEG is more than two times the highest value reported for the electroplated TEGs in the literature, which can be attributed to the low internal resistance and high packing density of thermoelectric pillars.

4:00 PM TP03.09.05/BM08.09.05**Compliant and Stretchable Thermoelectric Coils for Energy Harvesting in Miniature Flexible Devices** [Kewang Nan](#)¹, Stephen D. Kang^{2,3}, Kan Li⁴,

Yonggang Huang⁵, Jeffrey G. Snyder³ and John A. Rogers^{7,6,8}; ¹Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States; ²Applied Physics and Materials Science, California Institute of Technology, Pasadena, California, United States; ³Materials Science and Engineering, Northwestern University, Evanston, Illinois, United States; ⁴Mechanical Engineering, Northwestern University, Evanston, Illinois, United States; ⁵Civil and Environmental Engineering, and Mechanical Engineering, Northwestern University, Evanston, Illinois, United States; ⁶Materials Science and Engineering, Biomedical Engineering, Neurological Surgery, Chemistry, Mechanical Engineering, Electrical Engineering and Computer Science, Northwestern University, Evanston, Illinois, United States; ⁷Simpson Querrey Institute and Feinberg Medical School, Northwestern University, Chicago, Illinois, United States; ⁸Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

With expediting trends in electronic device miniaturization, thermoelectric energy harvesting becomes increasingly valuable, especially in wearable technologies and sensors for the internet-of-things. However, it has been impossible to match the device thermal impedance with the natural heat gradient using the thin-film thermoelectric materials much needed for device miniaturization. This limitation has prevented thermoelectrics from competing as a harvester at small scale. Here, we propose and demonstrate an architectural solution to this dilemma, where thin-film thermoelectric materials are mechanically assembled into three-dimensional (3D) coil architectures. This approach not only allows thermal impedance matching but also multiplies the heat flow through the harvester, thus increasing the efficiency for energy conversion. We design and fabricate thermoelectric coils with silicon as the active material that achieve flexibility, scalability, and durability. An array of such coils produces a power of 2 nW, with calculated projections showing the orders-of-magnitude improvement up to a few μ W by replacing silicon with state-of-the-art thermoelectric materials. Demonstrations of the idea open up long-awaited paths to utilize thermoelectric thin films and provides strategies to interface hard thermoelectric materials with soft harvesting environments, such as those of the human body.

4:15 PM TP03.09.06/BM08.09.06

Flexible Photo-Thermoelectric Nanogenerators Based on MoS₂ Nanocomposites for Energy Harvesting Yannan Xie^{1,2}; ¹Institute of Advanced Materials, Nanjing University of Posts and Telecommunications, Nanjing, China; ²College of Energy, Xiamen University, Xiamen, China.

With the rapid growth of economy, the fossil fuel consumption has been sharply increasing to satisfy the energy demand, which results in global warming and environmental pollution. It is crucial to develop clean and renewable energy technology for the sustainable development of human society. Targeting at scavenging thermal energy, thermoelectric effect has been utilized to develop thermal energy harvesting technology. Compared to the pyroelectric energy harvester which has little energy output, thermoelectric devices have been widely recognized as more effective and efficient technologies which has been utilized in practical applications. However, how to harvest thermal energy by using thermoelectrics when the environmental temperature is spatially uniform without any gradients is still a crucial issue and needs to be conquered. The key challenge is to create a significant temperature difference (ΔT) across the device which can act as driving force of thermoelectric generators.

In our living environment, in addition to the direct heat source, light source (such as the infrared light) can also provide thermal energy through the photothermal effect. Based on the photothermal effect and Seebeck effect, photo-thermoelectric generator has been rapidly developed for converting photo energy into electricity without a spatial temperature gradient in the environment. To generate a necessary ΔT , the conventional approach is utilizing various bulky components such as a vacuum enclosure, condenser lens, and heat sink. Nevertheless, these extra modules will not only increase the weight and size of thermoelectric generators but also are unfavorable for the flexibility of the whole devices which is of great importance for wearable electronics. Therefore, developing novel photothermal materials and device structure is essential for the photo-thermoelectric nanogenerator (PTENG).

In this work, we report on a flexible photo-thermoelectric nanogenerator (PTENG) by hybridizing MoS₂/PU photothermal layer with tellurium (Te) nanowire based thermoelectric device. The MoS₂/PU film which is flexible and transferable exhibits excellent photothermal characteristics due to exceptional surface-area-to-mass ratio of MoS₂ nanoclusters. Te nanowire is chosen for the thermoelectric nanogenerator because of its reported outstanding thermoelectric properties, such as low thermal conductivity and a wide temperature range. By integrating the photothermal layer with thermoelectric device, the PTENG can absorb infrared light to form a temperature difference across the device. With this, a potential difference between two electrodes can be established and used for electrical energy generation. Therefore, the PTENG can generate electricity without a spatial temperature gradient. Furthermore, the PTENG which is flexible and shape-adaptive can demonstrate great practical application of photo-thermoelectric energy harvesting for wearable electronics and implantable electronics.

4:30 PM TP03.09.07/BM08.09.07

Low-Cost Flexible Energy Harvesters Based on Transverse Thermoelectric Effects Radhika Prabhakar and Je-Hyeong Bahk; Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, Ohio, United States.

Considerable thermal energy is available for energy harvesting from diverse sources in our environment like industrial machines, heat engines and human bodies. This heat, otherwise wasted, can be converted to electrical energy by a thermoelectric energy generator and used to meet daily energy needs like battery charging, powering smart wearable devices or even enabling the Internet of Things. State of the art thermoelectric generators (TEGs) make use of the Bi₂Te₃ (bismuth telluride) thermoelectric alloys, which are inorganic, brittle, non-flexible, and require expensive processing. The TEGs are typically based on a longitudinal π structure, which is complex, both in terms of electrical connections and manufacturing. Moreover, such TEGs often feature a bulky heat sink to maintain high temperature differences between the hot and cold sides. These reasons limit their large scale use in ambient energy harvesting.

In this work we report a low cost, flexible TEG based on transverse thermoelectric effects. A transverse TEG consists of tilted multi-layers made of alternating metal and semiconductor materials. In such a device, a thermoelectric voltage can be generated in the direction perpendicular to the vertical temperature gradients, which makes the transverse structure suitable for planar devices. For our transverse TEG we use aluminum or nickel as the metal layers and carbon-nanotube (CNT)-polydimethylsiloxane (PDMS) composites as the semiconductor layers. Both materials are inexpensive with the TE composites being solution processable. For device fabrication the polymer composite solution is cast in between 3D-printed metal layers followed by air drying to obtain the transverse device. By filling the metal layer gaps partially with the polymer composite solution the upper portions of the metal layers are directly exposed to air at the cold side, thus acting as a fin type heat exchanger for lowering the cold side temperature by air convection. The use of flexible composites as the semiconductor material imparts flexibility to the TEG in one direction. It can therefore make good thermal contact with curved surfaces like hot water pipes, solar reflectors and even human skin, thus enabling TE energy harvesting from such surfaces. Transverse TEG architecture provides a number of degrees of freedom like the layer thickness, tilt angle, fin length, which can be varied to study the power generated. We present detailed thermoelectric properties of the CNT-PDMS polymer composites as well as its performance under bending tests. We also present a full range of experimental results of the fabricated transverse TEGs augmented with finite element simulations to optimize the device design for maximum power output.

4:45 PM TP03.09.08/BM08.09.08

Development of N-Type Single-Walled Carbon Nanotube Sheet with Excellent Air Stability Tsuyohiko Fujigaya^{1,2}; ¹Kyushu University, Fukuoka,

Japan; ²JST, Saitama, Japan.

Thermoelectric (TE) conversion is one of the most promising methods for the generation of cost-effective electricity. TE devices have applications in many fields especially microelectronics devices due to their simple device structures. TE generation using Seebeck effect requires both n-type and p-type TE materials for the efficient conversion; however, deterioration of n-type nature due to air oxidation has been the critical issue. Recently, we reported single-walled carbon nanotubes (SWCNT) sheet doped by 2-(2-methoxyphenyl)-1,3-dimethyl-2,3-dihydro-1H-benzimidazole (o-MeO-DMBI) showed n-type property and remarkable air-stability.[1] We chose o-MeO-DMBI because of the following reasons; i) o-MeO-DMBI is stable under atmospheric conditions, ii) the cationic form of o-MeO-DMBI is also stable and, iii) n-doping of the other carbon materials such as fullerene and graphene has already been reported.[2,3] Here, we study the mechanism of the air stability of o-MeO-DMBI-doped SWCNT films by changing the doping level. eDIPS (Meijo Nano Carbon, EC1.5) was used as SWCNT. SWCNT films were dipped in the 0.01, 0.1, 1.0, 10 and 50 mM ethanol solutions of o-MeO-DMBI for 10 min and dried in vacuum at room temperature for 12 h. The time course of Seebeck coefficient of the SWCNT films doped with various concentration of o-MeO-DMBI solution was studied. It is noted that the films were kept under air condition at room temperature to evaluate the air stability of the o-MeO-DMBI-doped SWCNT films. Positive value of Seebeck coefficient for 0.01 and 0.1 mM doped films indicated p-type, and negative value for 1.0, 10 and 50 mM doped films showed n-type nature of the films. Interestingly, we found that Seebeck coefficient of 1.0 mM doped film changed to positive, while 10 mM doped film showed stable negative value. From above results, we conclude that the mechanism of the air-stabilization of n-doping is the passivation effect by the formation of o-MeO-DMBI layer onto the surface of SWCNT films.

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SESSION TP03.10: Inorganic Thermoelectric Materials

Session Chair: Kedar Hippalgaonkar

Thursday Morning, November 29, 2018

Sheraton, 3rd Floor, Gardner AB

8:00 AM *TP03.10.01

Engineering Defects and for Thermoelectrics G. J. Snyder; Northwestern University, Evanston, Illinois, United States.

In thermoelectrics we often understand the physical properties of thermoelectric materials by considering the perfect crystalline material that is defect free. Yet this perfect, stoichiometric (valence balanced) crystal is an intrinsic semiconductor with equal number of electrons and holes. To make a n-type or p-type thermoelectric we typically use point defects to introduce a slight valence imbalance that leads to excess electrons or holes. Often intrinsic defects such as vacancies, interstitials or antisite defects, provide the necessary carriers to make the material a good thermoelectric (e.g. Zn_4Sb_3 , Bi_2Te_3 - Sb_2Te_3 , Yb_xCoSb_3 , etc.). Most materials, however, require extrinsic dopants to be a good thermoelectric and intrinsic defects only make it more complicated. Sometimes intrinsic defects are so prevalent they are *killer defects* that prevent any dopant from making the material n-type or p-type. By understanding that atomic chemical potentials influence defect energy and also define regions in phase diagrams we can use *phase boundary mapping* to explore all the possible thermodynamic defect states of a material to avoid killer defects. The most dramatic demonstration of this is the discovery of high zT -n-type Mg_3Sb_2 which only occurs in Mg-rich Mg_3Sb_2 where Mg-vacancies are suppressed.

Point defects can also make gradual but profound changes to the band structure compared to the defect free compound. This includes increasing band gap for higher temperature application, reducing conductivity mass for higher mobility or band convergence for dramatic increase in density of states ($Pb(Se,Te)$, $Mg_2(Si,Sn)$, Bi_2Te_3 - Sb_2Te_3). In principle all of these defects can be better controlled by engineering chemical potentials through phase boundaries. Even the Ni content $MNiSn$ ($M = Ti, Zr, Hf$) Half-Heusler thermoelectrics can be sufficiently altered to make substantial differences in electronic properties. The excess Ni produces impurity states in the band gap that changes the effective band gap and leads to additional electron and phonon scattering.

8:30 AM TP03.10.02

YbSiGe—A Promising Thermoelectric Material with High Power Factor at Room Temperature Sora-At Tanusilp¹, Yuji Ohishi¹, Hiroaki Muta¹, Akinori Nishide^{1,2}, Jun Hayakawa² and Ken Kurosaki^{1,3,4}; ¹Osaka University, Osaka, Japan; ²Hitachi, Ltd., Tokyo, Japan; ³University of Fukui, Fukui, Japan; ⁴JST, PRESTO, Saitama, Japan.

Metal silicide-based thermoelectric (TE) materials have been widely attracted attention, because they are less toxic, low production cost, and high chemical stability. Recently, it has been reported that $YbSi_{2.8}$ shows high electrical conductivity (σ) accompanied by uncommonly large Seebeck coefficient (S) probably due to intermediate valence behavior of Yb (Yb^{2+}/Yb^{3+}), leading to high-power factor ($S^2\sigma$) $2.2 \text{ mWm}^{-1}\text{K}^{-2}$ at room temperature [S. Tanusilp *et al.*, *prss-rrl*, 2018, **12**, 1700372.]. Here, we demonstrated that $Yb(Si_{1-x}Ge_x)_{2.8}$ is a more promising TE material. The substitution of Ge on the Si site changes the Yb^{2+}/Yb^{3+} ratio and transform the phase from the AIB_2 -type (random defects in the Si site) to the Th_3Pd_5 -type (ordered defects in the Si/Ge site). It is revealed that the $x = 0.5$, i.e., $YbSiGe$, is the best composition with the highest power factor $3.6 \text{ mWm}^{-1}\text{K}^{-2}$ at room temperature, which is comparable to or higher than those of conventional TE materials. Furthermore, the lattice thermal conductivity (κ_{lat}) of $Yb(Si_{1-x}Ge_x)_{2.8}$ is significantly reduced because the substituted Ge acts as scattering centers of heat carrying phonons. The enhanced $S^2\sigma$ and reduced κ_{lat} lead to 80% enhancement in the zT , the maximum value is 0.13 at room temperature.

8:45 AM TP03.10.03

Creating Zipper-Like van der Waals Gap Discontinuity in Low-Temperature-Processed Nanostructured $PbBi_{2n}Te_{1+3n}$ for Enhanced Phonon Scattering and Improved Thermoelectric Performance Yue Wu and Wei Zheng; Iowa State University, Ames, Iowa, United States.

Nanoengineered materials can embody distinct atomic structures that deviates from the bulk-grain counterpart and induce significantly modified electronic structure and physical/chemical properties. Besides, the phonon structure and thermal properties that can also be potentially modulated due to the modified atomic structure in nanostructured material, however, are seldom investigated. In this presentation, we will discuss a mild approach to fabricate nanostructured $PbBi_{2n}Te_{1+3n}$ using solution-synthesized $PbTe$ - Bi_2Te_3 nanoheterostructure as a precursor. The as-obtained monoliths have unprecedented atomic structure differing from the bulk counterpart, especially the zipper-like van der Waals gap discontinuity and the random arrangement of septuple-quantum layers. These structural motifs break the lattice periodicity and coherence of phonon transport, leading to ultra-low thermal conductivity and excellent thermoelectric zT . We anticipate that this strategy can be widely applicable to fabricate existing thermoelectric compounds into their nano forms

with unique atomic structures and good performances.

9:00 AM TP03.10.04

Thermoelectric Properties of All-Inorganic Halide Perovskite Nanowires Woochul Lee; Mechanical Engineering, University of Hawaii at Manoa, Honolulu, Hawaii, United States.

Controlling the flow of thermal energy is crucial to numerous applications ranging from microelectronic devices to energy storage and energy conversion devices. I will present experimental ultralow lattice thermal conductivities of solution-synthesized, single-crystalline all-inorganic halide perovskite nanowires composed of CsPbI₃, CsPbBr₃, and CsSnI₃. I will also discuss mechanisms behind ultralow thermal conductivity values of all-inorganic halide perovskites. Further, I will present a rare combination of ultralow thermal conductivity and high electrical conductivity of CsSnI₃, which is a promising candidate for thermoelectric applications.

9:15 AM TP03.10.05

Hyper-Doped Nanocrystalline Silicon Thin Films for Low-Temperature Thermoelectric Harvesting—Energy Filtering and the Role of Hydrogen Dario Narducci¹, Laura Zulian¹, Carlos J. Álvarez², Andrea P.C. Campos², Claude Alfonso², Marion Descoins², Dominique Mangelinck², Xanthippi Zianni³ and Ahmed Charaï²; ¹Department Materials Science, University of Milano Bicocca, Milan, Italy; ²Laboratoire IM2NP, CNRS, Aix Marseille Université, Marseille, France; ³Dept. of Aircraft Technology, Technological Educational Institution of Sterea Ellada, Psachna, Greece.

Despite its intrinsic low thermoelectric figure of merit, silicon has found applications in low-temperature thermal microharvesting due to the available know-how for planar manufacturing [1,2]. In recent years, many groups have revived the interest toward enhancing silicon ZT [3]. This can be achieved either by reducing the thermal conductivity of single-crystalline silicon [4] or increasing the power factor (PF) of polycrystalline silicon. Some of the present authors reported in 2010 [5] first evidence about the possibility of enhancing the power factor (PF) of nanocrystalline silicon by a factor 10 through the controlled precipitation of second phases at grain boundaries. Such results were extensively confirmed [6–8], and modeling showed that enhanced PF was mostly related to energy filtering by potential barriers at grain boundaries [9,10]. However, effort to move these results toward production has shown that PF enhancement is more elusive than expected, with a puzzling dependence upon sample size. This communication reports about the analysis of the dependence of PF upon sample size in hyper-doped p-type nanocrystalline Si thin films. Nanocrystalline Si thin films were deposited by PECVD on SiO₂ and then ion-implanted with B⁺. After damage recovery, samples were cut to varied sizes and submitted to annealing for 2 h at 1000 °C in Ar. Their electrical conductivity and Seebeck coefficient were found to depend on the sample size, with a standard PF of 1.3 mW/mK² in 200-mm wafers that raises to 13.6 mW/mK² in 5x50 mm² chips. Analyses by transmission electron microscopy, high-resolution scanning electron microscopy, and atomic probe tomography could prove that the disappearance of PF enhancement in wafer-scale samples was due to the combined effect of B-H complexation and incomplete implantation damage recovery at film surface. These results indicated proper remediation measures, therefore opening the path toward full industrial exploitation of silicon as a high-performance material for heat microharvesting in the low-temperature range. Possible applications of integrated thermoelectric harvesters will be discussed.

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9:30 AM TP03.10.06

Magnon Drag and Spin Entropy Contribution to Thermopower of Li-Doped MnTe Yuanhua Zheng¹, Tianqi Lu², Morteza Rasoulianboroujeni³, Md Mobarak Hossain Polash³, Ning Liu², Huaizhou Zhao², Daryoosh Vashaee³ and Joseph P. Heremans¹; ¹The Ohio State University, Columbus, Ohio, United States; ²Institute of Physics, Beijing, China; ³North Carolina State University, Raleigh, North Carolina, United States.

In ferromagnetic and antiferromagnetic materials, magnons interact with electrons strongly, creating an advective transport process called the magnon drag effect. This effect adds an extra contribution to the thermopower. A hydrodynamic model developed recently [1] predicts that the magnon drag thermopower is proportional to the magnon specific heat and is inversely proportional to the total number of free electrons.

We present here the specific heat and thermopower data of antiferromagnetic semiconductor Li-doped MnTe. By separating the magnon contribution to the specific heat and measuring carrier concentration from Hall effect, the calculated magnon drag thermopower based on the hydrodynamic model is consistent with the measured value below the Néel temperature. This magnetic contribution, however, seems to extend to the paramagnetic regime, of which spin entropy is proposed to be the cause. The thermopower is essentially the entropy per electron. Spin works as another degree of freedom and spin degeneracy adds to the total entropy per electron. In the paramagnetic regime, a quantitative explanation is given based on a spin entropy thermopower theory [2].

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9:45 AM TP03.10.07

Ab Initio Thermal Conductivity and Thermoelectricity in Mg₃Sb₂—Dominance of Size Effects Roberta Farris, Barbara Maccioni and Vincenzo Fiorentini; University di Cagliari, Monserrato, Italy.

Lattice thermal conductivity in the candidate thermoelectric material Mg₃Sb₂ is studied from first principles, with the inclusion of anharmonic, isotope, and boundary scattering processes. Purely anharmonic conductivity is over an order of magnitude larger than observed experimentally at room temperature, the anomalously low observed value being in fact due to microstructure, i.e. to grain boundary scattering of phonons due to polycrystallinity, which we model by Casimir scattering (anisotropy and isotopic scattering affect the conductivity at the level of 10% at room temperature). We use the calculated thermal conductivity to estimate ZT for a range of different situations, also including effects of grain boundaries on electrical conductivity and Seebeck.

10:00 AM BREAK

10:30 AM TP03.10.08

Internal-Strain Softening Significantly Reduces Thermal Conductivity and Leads to High Thermoelectric Efficiency PbTe—Reconsidering Phonon Scattering [Riley C. Hanus](#)¹, Matthias T. Agne¹, Zhiwei Chen², Yanzhong Pei², Peter W. Voorhees¹ and G. J. Snyder¹; ¹Northwestern University, Chicago, Illinois, United States; ²Materials Science and Engineering, Tongji University, Shanghai, China.

The influence of micro/nanostructure on thermal conductivity is a topic of great scientific interest and of particular technological importance to thermoelectrics. The current paradigm of understanding is that structural defects primarily decrease thermal conductivity through phonon scattering where the phonon dispersion (and thus the speeds of sound) are fixed when describing the thermal transport, especially when chemical composition is unchanged. Experimental work on a PbTe model system is presented which shows that the speed of sound significantly decreases in PbTe with increasing internal-strain which completely accounts for the reduction in lattice thermal conductivity without assuming an increase in phonon scattering centers. Furthermore, we experimentally show that internal-strain is linearly related to the materials speed of sound, which provides evidence for the thermodynamic origin of this phenomena. It is also shown that this mechanism is a major part of the reduction in thermal conductivity and the resulting improvement in thermoelectric figure of merit in high efficiency PbTe ($zT > 2$). This presents new avenues to engineer thermal conductivity, beyond phonon scattering, by modifying the phonon dispersion relation (i.e. speeds of sound and lattice stiffness) with microstructural defects and internal-strain, and shines new light on studies of thermal conductivity in fields of energy materials, microelectronics, and nano-scale heat transfer.

10:45 AM TP03.10.09

Development of Low-Cost and Non-Toxic Al₂Fe₃Si₃ Thermoelectric Material—Experiment, Theoretical Calculation and Machine Learning Prediction [Yoshiki Takagiwa](#)¹, Yukihiko Isoda¹, Masahiro Goto¹, Yoshikazu Shinohara¹, Zhufeng Hou¹, Yibin Xu¹ and Koji Tsuda^{2,1}; ¹National Institute for Materials Science, Tsukuba, Japan; ²The University of Tokyo, Kashiwa, Japan.

To develop new thermoelectric materials that are low-cost and non-toxic with sufficient power output toward practical applications, in particular, at a low-temperature region below 400 K, we performed materials screening of Al-Fe-Si ternary system using band structure calculations [1,2]. We found that τ_1 -Al₂Fe₃Si₃ phase forms a narrow band gap near the Fermi level and has shown potential as a thermoelectric material. We demonstrated that fine tuning of the Al/Si ratio could control its conduction type and enhance power factor without chemical substitutions [2]. Relatively large power factors exceeding 500 $\mu\text{W}/\text{mK}^2$ were obtained for both p- and n-type materials below 400 K, which can be used in such as sensor applications. Recently, we succeeded in an enhancement of power factor at mid temperatures using machine-learning-assisted synthesis [3]. However, remaining important issue is to develop the single phase of Al₂Fe₃Si₃ and optimize the sample composition for better thermoelectric performance. In this presentation, we will review the recent progress of newly developed thermoelectric material Al₂Fe₃Si₃ and discuss how to enhance the power output toward practical usage.

[1] Y. Takagiwa, Y. Isoda, M. Goto, and Y. Shinohara, *J. Therm. Anal. Calorim.* **131** (2018) 281-287.

[2] Y. Takagiwa, Y. Isoda, M. Goto, and Y. Shinohara, *J. Phys. Chem. Solids* **118** (2018) 95-98.

[3] Z. Hou*, Y. Takagiwa*, Y. Shinohara, Y. Xu, and K. Tsuda, *submitted*. *These authors contributed equally.

11:00 AM TP03.10.10

High Sn⁻-type Thermoelectric Power Factor and Efficiency in Ba₂SbBiAu from a Highly Dispersive Band [Junsoo Park](#)^{1,2,4}, Yi Xia³ and Vidvuds Ozolins^{2,4}; ¹Materials Science and Engineering, University of California, Los Angeles, Los Angeles, California, United States; ²Applied Physics, Yale University, New Haven, Connecticut, United States; ³Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois, United States; ⁴Energy Sciences Institute, Yale University, West Haven, Connecticut, United States.

Using first-principles density-functional theory calculations, we predict the potential for unprecedented $zT \geq 5$ at 800 K in Sn⁻-type Ba₂SbBiAu full-Heusler compound. Such a high efficiency arises from intrinsically ultralow lattice thermal conductivity coupled with very high power factor reaching 7 $\text{mW m}^{-1} \text{K}^{-2}$ or more at 500 K. The high power factor originates from the highly dispersive conduction band pocket along Γ -X with sixfold multiplicity. It experiences very weak acoustic phonon scattering due to the limited phase space, leading to long electron lifetime and high conductivity. The multitude of pockets further benefits high conductivity and sustains high Seebeck coefficient. The Lorenz numbers at optimal doping are smaller than the Wiedemann-Franz value, an integral feature for zT enhancement as electrons are the majority heat carriers. Finally, using Ba₂SbBiAu and the parallel case of Fe₂TiSi, we propose that purely dispersive bands with multiple pockets are more promising for thermoelectrics than flat-and-dispersive, a.k.a., low-dimensional, bands.

11:15 AM TP03.10.11

Thin-Film Tin Selenide (SnSe) Thermoelectric Generators Exhibiting Ultra-Low Thermal Conductivity [Matthew R. Burton](#)¹, Tianjun Liu², James McGettrick¹, Shahin Mehraban¹, Jennifer Baker¹, Adam Pockett¹, Trystan Watson¹, Oliver Fenwick² and Matt Carnie¹; ¹Swansea University, Swansea, United Kingdom; ²School of Engineering and Materials Science, Queen Mary University of London, London, United Kingdom.

Tin selenide (SnSe) has attracted much attention in the field of thermoelectrics since the discovery of the record figure of merit (ZT) of 2.6 ± 0.3 along the b-axis of the material. The record ZT is attributed to an ultralow thermal conductivity that arises from anharmonicity in bonding. Whilst it is known that nanostructuring offers the prospect of enhanced thermoelectric performance, there has been minimal studies in the literature to date of the thermoelectric performance of thin films of SnSe. Tin selenide (SnSe) has attracted much attention in the field of thermoelectrics since the discovery of the record figure of merit (ZT) of 2.6 ± 0.3 along the b-axis of the material. The record ZT is attributed to an ultralow thermal conductivity that arises from anharmonicity in bonding. Whilst it is known that nanostructuring offers the prospect of enhanced thermoelectric performance, there has been minimal studies in the literature to date of the thermoelectric performance of thin films of SnSe. In this presentation, we will demonstrate the first known example of a working thin-film SnSe thermoelectric generator [1], fabricated in an extremely simple thermal evaporation method. Seebeck coefficients are comparable to that seen in bulk SnSe, whilst materials characterisation reveals that the microstructure of the SnSe material is of a preferentially orientated porous network of thin film SnSe nanosheets which exhibited an unprecedentedly low thermal conductivity of $0.08 \text{ W m}^{-1} \text{K}^{-1}$ between 375 K and 450 K which can be primarily attributed to the reduction of the lattice component.

[1] M. R. Burton, T. Liu, J. McGettrick, S. Mehraban, J. Baker, A. Pockett, T. Watson, O. Fenwick, and M. J. Carnie, *Advanced Materials*, **Accepted Proofs In Press**, DOI: 10.1002/adma.201801357

11:30 AM TP03.10.12

Copper Iodide-Based Composite Materials for Thermoelectric Application [Shiqiang Bai](#); Institute of Materials Research and Engineering, A*STAR, Singapore, Singapore.

Novel hybrid thermoelectric materials have attracted great attentions for their potential applications for thermal energy conversion and sustainable environment. As an environment-friendly, abundant, economic and semiconducting material with broad band gap values, copper iodide has been systematically investigated in the research areas of photophysics, photochemistry and light-emitting diodes. A recent report demonstrates a promising room temperature thermoelectric performance of $ZT = 0.21$. We are exploring inorganic-organic thermoelectric composites using molecular materials. In this presentation, a series of copper iodide-based thermoelectric composites with robust pellets and low densities shall be introduced. The fabrication procedure, structures, recyclable electrical conductivities and Seebeck coefficients will be discussed.

SESSION TP03.11: High Temperature Inorganic Thermoelectric Materials
Session Chairs: Jenny Pringle, Jeff Snyder and Dongyan Xu
Thursday Afternoon, November 29, 2018
Sheraton, 3rd Floor, Gardner AB

1:30 PM TP03.11.01

Coherent Phonon Scattering in SnTe Nanocomposite Resulting in High Thermoelectric Performance Junphil Hwang^{1,2}, Jisook Hong³, Mi-Kyung Han², Ji Hoon Shim³, Sung-Jin Kim², Ying-Shi Jin², Hoon Kim¹, Jiyong Kim¹, Hwanjoo Park¹ and Woochul Kim¹; ¹School of Mechanical Engineering, Yonsei University, Seoul, Korea (the Republic of); ²Department of Chemistry and Nano Science, Ewha Womans University, Seoul, Korea (the Republic of); ³Department of Chemistry, Pohang University of Science and Technology, Pohang, Korea (the Republic of).

We are reporting that coherent phonon scattering can induce severe thermal conductivity reduction while maintaining electrical transport which is ideal for thermoelectric application. SnTe has been drawn attention for last several years to replace Pb containing thermoelectric materials especially PbTe. However, larger thermal conductivity compared with that of PbTe hinders higher thermoelectric performance. We synthesized polycrystalline SnTe where the grain boundaries were coated by nanosized CdTe, SnO₂, SnTe particles which were clarified by TEM study. The thermoelectric figure of merit (zT) for the SnTe nanocomposites is 2.18 at 923 K which is higher than that of PbTe. The main reason for such a high zT was low thermal conductivity, i.e., 1.09 W/m-K at 923 K. Our developed modeling based on dependent phonon scattering, i.e., coherent phonon scattering, adequately explain extremely low thermal conductivity of SnTe nanocomposites. We found that with same concentration of impurities which scatters phonons, coated grain nanocomposite shows lower thermal conductivity compared with that of nanoparticle nanocomposite.

1:45 PM TP03.11.02

Low Cost Scalable Printed Tin Selenide (SnSe) for Thermoelectric Generators Matthew R. Burton, Shahin Mehraban and Matt Carnie; University of Swansea, Swansea, United Kingdom.

Tin selenide (SnSe) sparked much interest in the field of thermoelectrics when Zhao et al.[1] reported an unprecedented ZT of 2.6 ± 0.3 at 923 K along the b axis. This discovery was observed in single crystals formed at high temperature (1223 K) over several hours. Whilst doping SnSe with elements such as Na[2] and Bi[3] have also shown promising thermoelectric performance, these too were shown on single crystals with expensive and lengthy fabrication techniques which are unfavorable for commercial applications. Since the discovery of the record ZT in single crystal SnSe,[1] studies on the thermoelectric performance of polycrystalline SnSe have been reported.[4]–[12] These fabrication techniques presented in the literature, however, require high temperature, lengthy fabrication times and in most cases high pressure. This makes these processes of fabrication unfavorable for commercial development.

In this work we present a cheap, facile and scalable technique, with the aim of producing a commercially viable thermoelectric device. Polycrystalline SnSe was fabricated by low-cost ball milling of the constituent elements. Films were printed in a water-based ink using carboxymethyl cellulose as a binder. The effect of variation of the binder concentrations on properties (including electrical conductivity, Seebeck coefficient and thermal conductivity) were studied. Thermoelectric characterization of the printed polycrystalline SnSe, reveals peak ZT ~ 0.14 at 760 K, which is comparable to examples in the literature for polycrystalline SnSe.

- [1] L.-D. Zhao et al., *Nature* **2014**, *508*, 373.
- [2] L.-D. Zhao et al., *Science* **2016**, *351*, 141.
- [3] A. T. Duong et al., *Nat. Commun.* **2016**, *7*, 13713.
- [4] S. Sassi et al., *Appl. Phys. Lett.* **2014**, *104*, 212105.
- [5] X. Shi et al., *Energy Storage Mater.* **2018**, *10*, 130.
- [6] T.-R. Wei et al., *J. Am. Chem. Soc.* **2016**, *138*, 8875.
- [7] Y. Li et al., *Energies* **2015**, *8*, 6275.
- [8] Y. Fu et al., *J. Mater. Chem. C* **2016**, *4*, 1201.
- [9] Y. Li et al., *J. Mater. Chem. C* **2016**, *4*, 2047.
- [10] J. O. Morales Ferreiro et al., *Appl. Therm. Eng.* **2017**, *111*, 1426.
- [11] C.-L. Chen et al., *J. Mater. Chem. A* **2014**, *2*, 11171.
- [12] E. K. Chere et al., *J. Mater. Chem. A* **2016**, *4*, 1848.

2:00 PM TP03.11.03

Defect Engineering and Controlling Dopability of PbTe Using Phase Boundary Mapping James P. Male, Matthias T. Agne and G. J. Snyder; Northwestern University, Evanston, Illinois, United States.

A lack of control over the dopability of thermoelectric materials continues to limit the efficiency of potentially good material systems. Phase boundary mapping has recently been shown to be an effective means of engineering defects in materials such as Mg₃Sb₂, where Mg-rich conditions are required to overcome “killer defects” and achieve n-type behavior. Herein, we demonstrate that defect engineering is critical for efficient doping in a PbTe model system, validating the principles of phase boundary mapping in a material system that does not have a history of difficult dopability. PbTe ingots with increasing levels of n-type iodine dopant were annealed at 700 C under Pb-rich and Te-rich partial pressures and quenched. Ingots annealed in Pb-rich conditions have degenerate, n-type thermoelectric properties typical of a good thermoelectric material, while the same materials annealed in Te-rich conditions show intrinsic, poorly performing properties and are p-type at lower doping levels. The drastic difference in performance agrees with expectations from a defect model and demonstrates the effectiveness of phase boundary mapping to engineer dopability in PbTe. Using the same experimental technique, it was possible to repeatably switch between degenerate n-type and non-degenerate p-type conduction in a single material. This behavior corresponds to the subtle change in composition associated with crossing the small phase width of the single-phase region of the phase diagram.

Lastly, the volatility of Te at relatively low temperatures is suggested as a possible explanation of the doping efficiency observed in previous studies of PbTe systems. Thus, phase boundary mapping effects are likely to be important when considering the non-equilibrium conditions associated with synthesis and experimental techniques.

2:15 PM TP03.11.04

Effect of Element Substitution on The High-Temperature Stability and Thermoelectric Properties of FeNb_{0.9}M_{0.1}Sb (M=Ti, Zr, Hf) Half-Heusler Compounds [Wanthana Silpawilawan](#)¹, Sora-At Tanusilp¹, Yuji Ohishi¹, Hiroaki Muta¹ and Ken Kurosaki^{1,2,3}; ¹Engineering, Osaka University, Suita, Japan; ²PRESTO, JST, Kawaguchi, Japan; ³Research Institute of Nuclear Engineering, University of Fukui, Fukui, Japan.

Half-Heusler (HH) compounds are prominent thermoelectric (TE) materials, however the high-temperature stability is scarcely reported. Among the *p*-type HH compounds, FeNbSb exhibits the best TE properties. Recently, our group has revealed that FeNbSb has good high-temperature stability [W. Silpawilawan *et al.*, *J. Mater. Chem. C*, 2017, **5**, 6677-6681]. However, the high-temperature stability of doped FeNbSb is unknown. Here, the effect of element substitution (Ti, Zr, Hf) at the Nb-site of FeNbSb on the TE properties as well as high-temperature stability is examined. Polycrystalline samples of FeNb_{0.9}M_{0.1}Sb (M= Ti, Zr, Hf) were prepared by arc-melting followed by spark plasma sintering. The high-temperature stability was checked by high-temperature X-ray diffraction (HT-XRD) from room temperature to 800 °C in both air and He atmosphere. It is revealed that the substitution of Ti, Zr, and Hf enhances the TE properties and does not deteriorate the high-temperature stability of FeNbSb.

2:30 PM TP03.11.05

Correlation of Crystallographic Defects in Ag_{16.7}Sb₃₀Te_{53.3} Thermoelectric Bulk Materials with Their Thermoelectric Properties [Lamya Abdellaoui](#)¹, Siyuan Zhang¹, Stefan Zaeferrer¹, Ruben Bueno Villoro¹, Cynthia Rodenkirchen³, Baptiste Gault¹, Oana Cojocaru-Mirédin¹, Yaron Amouyal², Dierk Raabe¹ and Christina Scheu¹; ¹Max Planck Institut für Eisenforschung, Düsseldorf, Germany; ²Technion–Israel Institute of Technology, Haifa, Israel; ³RWTH Aachen University, Aachen, Germany.

Research on thermoelectric (TE) materials has experienced a considerable increase in interest within the last years. The design of different microstructures and new classes of materials like complex chalcogenides is considered a promising approach for improving the efficiency of potential TE materials [1]. TE materials directly convert heat into electricity through the Seebeck effect. The conversion efficiency is determined by the dimensionless *figure of merit*, ZT, which depends on the thermal conductivity κ , electrical conductivity σ , the Seebeck coefficient S and the temperature T. Attempts to optimize ZT require reducing κ , while maintaining relatively high values of σ and S.

The AgSbTe₂ compound is a promising *p*-type semiconductor. The δ phase, which is stable between about 600 and 550° C, and exists metastable after quenching to room temperature has a rocksalt cubic crystal structure where Ag and Sb atoms are randomly distributed on the Na⁺ sites and Te occupying the Cl⁻ sites. It is suitable for thermoelectric power generation in the low-to mid-temperature range (e.g. 600-800 K).

The as-quenched (AQ) δ -phase Ag_{16.7}Sb₃₀Te_{53.3} synthesized in our study exhibits a good TE performance with a merit of figure value of ZT=0.5 at 300°C. This performance value is related to the various microstructural features, which were investigated down to the atomic scale. We used several methods such as electron backscatter diffraction (EBSD) and electron channeling contrast imaging (ECCI) (both are SEM-based techniques), Cs-probe corrected scanning transmission electron microscopy (STEM), focused ion beam (FIB) sectioning, energy dispersive X-ray spectroscopy (EDS) and atom probe tomography (APT). Notably the AQ material produced as a single crystal, shows a distinct mosaic structure with abundant low angle grain boundaries, where an array of dislocation and stacking faults networks are accumulated. We analyzed the number densities of the different types of structural defects in large scale and studied the atomic structure and chemistry of the defects. We observed a different chemical composition, specifically a change of the Ag and Sb content, within the stacking faults compared to the bulk. The presence of these stacking faults at the low angle grain boundaries seems to play a major role to achieve a low κ , [2].

The AQ bulk samples were subjected to a heat treatment for 8h and 192h at 380°C [3]. The 8h annealed sample showed similar good TE behavior as the AQ samples. Large precipitates (3 μ m in width) were found within the matrix which contain 1 to 8% Ag and possess a Sb₂Te₃ crystal structure. We will discuss the impact of this different microstructural features on the performance of our compounds [3].

[1] D. M. Rowe. Thermoelectric handbook: Macro to Nano (Taylor&Francis, New York, 2006, pp51-1)

[2] Roychowdhury, S, et.al. ACS Energy Letters 2 (2): 349-356. (2017)

[3] Cojocaru-Mirédin, O. Abdellaoui, L, et.al. ACS Appl Mater Interfaces 9 (17):14779-14790. (2017)

2:45 PM TP03.11.06

TE Thin-Film Materials from Organic Electronics [Xizu Wang](#); IMRE, Singapore, Singapore.

In the past two decades, materials and thin film structures that were well-known for their applications in organic electronic devices, such as LEDs and solar cells, had found new applications through engineering of their semiconductor properties, nanoscale structures, and designs. In our research, we have found many thin film materials in organic solar cells to be the strong candidates for novel applications in thermoelectric devices. Here we report some high performance thermoelectric thin films based on materials commonly used in organic electronics, including PEDOT:PSS, ITO, P3HT and inorganic-organic MAPbI₃ perovskite crystals. The high electrical conductivity of 2980 S/cm and correspondingly high power factor of 142 μ W/mK² are observed in anhydrous, treated PEDOT:PSS thin films. Ultra-high Seebeck coefficient and low thermal conductivity are obtained in a centimeter-sized perovskite single crystal. Furthermore, we discover some newly optimized methods for the enhancement of thermoelectric properties of ITO, P3HT and AZO thin films and devices. Our investigations show that materials discovery and development for thermoelectric applications can be accelerated by re-engineering of materials conventionally used in organic electronics.