VCT 2022

Virtual Conference on Thermoelectrics

An online event to highlight the work of early-career researchers in the thermoelectrics community

July, 20-22, 2022

Book of Abstracts

International Thermoelectric Society

vct2022.mines.edu

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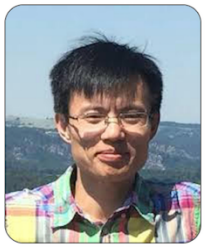

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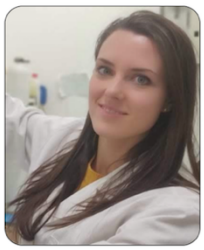

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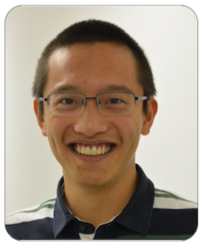

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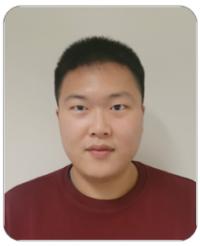

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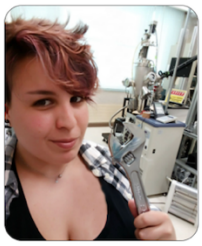

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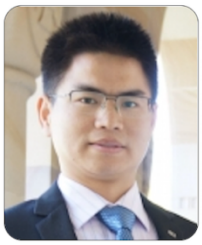

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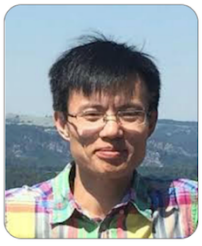

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Foreword

The cancellation of the International Conference on Thermoelectrics (ICT) for a third year in a row and sustained interest from the thermoelectrics community has motivated the organization of the third edition of the Virtual Conference on Thermoelectrics (VCT 2022, July 20-22, 2022). When we first organized VCT 2020, our vision was to provide early-career researchers in the thermoelectrics community with an online platform to highlight and share their work. That vision has guided the organization of VCT 2021, and now, VCT 2022. In this spirit, the call for oral contributions was restricted to students and postdocs.

VCT 2022 is a free event, with no registration fee. In response to the call for abstracts, we received almost 200 oral contributions and dozens of abstracts for poster presentations. Given the broad interest in VCT, we continue to organize three regional chapters – US, Europe, and Asia, each with a dedicated organization team. Oral presentations are scheduled across 12 time zones to accommodate the global scale of this event. Registered participants can attend talks in all regional chapters. Plenary talks by world-renowned thermoelectric scientists are planned for the purpose of motivating the next-generation of thermoelectric scientists.

VCT 2022 is endorsed by the International Thermoelectrics Society (ITS). The organization of VCT 2022 is made possible by a dedicated team of faculty members, senior researchers, postdocs, and graduate students from across the world.

We hope you will enjoy and actively participate in the conference.

VCT 2022 Organizers

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US Program

Abstract number: US-A1.01 (PLENARY TALK)

Defects and Dopants in Thermoelectric Materials

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All thermoelectric materials to date have required careful control of intrinsic and extrinsic defects to achieve their success. Defects and dopants in semiconductors contribute to (i) carrier concentration, (ii) scattering and (iii) even changes in electronic and phononic band structures. Conversely, many candidate thermoelectric materials have failed due to the inability to control these defects. As such, a robust framework to identify, control, and predict the impact of defects and dopants is a crucial aspect to any effort in thermoelectric materials. In this talk, we begin by highlighting efforts to predict native defect concentrations and dopant solubility and the experimental control therein. In particular, we highlight the complementary advances in defect calculations and experimental phase boundary mapping in tricking materials into becoming dopable. Strategies for dopant selection in complex materials are discussed in terms of challenges involving competing sites and chemical potential space. Having established defects and dopants in a material, we consider how such defects alter charge carrier scattering and computational approaches that have recently emerged therein. We conclude by considering the potential for defects and dopants to positively influence the electronic and phononic band structures.

Abstract number: US-A2.01 (PLENARY TALK)

Data-Driven Discovery and Design of Thermoelectric Materials

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Thermoelectrics have potentially significant energy applications, but only if high efficiency materials can be found. However, discovery and design of novel thermoelectrics is particularly challenging, due to the complex set of materials properties that must be simultaneously optimized. Data-driven approaches to discovery and design of materials are a research area that has the potential to significantly accelerate discovery of these energy materials. Here we discuss our efforts at developing and applying data-driven computational techniques that enable an accelerated discovery of novel thermoelectrics. These techniques involve a combination of high-throughput density functional theory (DFT) calculations, inverse design approaches, and machine learning and artificial intelligence based methods. We discuss several recent examples of these methods: (i) inverse design strategies based on a materials database screening to design a solid with a desired band structure, specifically both flat and dispersive components with respect to crystal momentum, (ii) inverse design strategies to identify compounds with ultralow thermal conductivity (iii) an effective strategy of weakening interatomic interactions and therefore suppressing lattice thermal conductivity based on chemical bonding principles, and (iv) the development of crystal graph based neural network techniques to accelerate high-throughput computational screening for materials with ultralow thermal conductivity.

Abstract number: US-O1.01

Band Inversion-Driven High Valley Degeneracy

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The thermoelectric performance of a material can be improved by tuning the valley degeneracy. One way in which valley degeneracy can be increased in rock-salt IV-VI compounds is by modifying the degree to which bands are inverted through e.g. alloying. In this talk, we generalize this concept of “band inversion-driven high valley degeneracy” and derive simple rules for when inverted-band materials exhibit high thermoelectric performance. Using k.p perturbation theory, we show that electronic bands must generally be inverted to a critical degree for a material to possess high valley degeneracy. We apply this rule to discover potentially high-performing thermoelectric materials within the ABX chemical space of materials. We find that NaCaBi (space group: P63/mmc) is a promising candidate with a degeneracy of 6 for both the conduction and valence bands. Through detailed Boltzmann transport theory-based calculations, we find that the material can reach zT between 0.4 and 0.8 at 300 K. Accordingly, band inversion is a rational descriptor for identifying high-performing thermoelectric materials.

Abstract number: US-O1.02

Calculation of Thermomagnetic properties Using First-principles Density Functional Theory

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The BoltzWann code uses the first-principles density-functional theory to calculate the material's response to an electric field and temperature gradient within the constant relaxation time approximation. We extend this code to include the response of the system to a magnetic field. The carrier dynamic is described by the semi-classical Boltzmann transport equation. This equation is solved in the presence of an external magnetic field within the constant relaxation time approximation and using the Jones-Zener expansion. This is done through a Wannier interpolation of the density functional theory bands using the Boltzwann code, followed by the computation of group velocities and effective masses leading to the energy-dependent transport function. This work leads to a generalized method for the calculation of thermomagnetic properties of materials. The results are validated by comparison to the analytical solutions of the thermomagnetic properties for several simple energy dispersion types and close agreements at moderate computational costs are achieved. This method can pave the path for the discovery of materials with potentially high thermomagnetic power factor.

Abstract number: US-O1.03

Doping Response of Thermopower and Magnetic Anisotropy in MnTe

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This work was supported by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division. A portion of this research used resources at the High Flux Isotope Reactor and Spallation Neutron Source, supported by DOE, BES, Scientific User Facilities Division.

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Developing simple ways to control spin states in spintronic devices is a crucial step towards increasing their functionality. Local thermal magnetization fluctuations in Li-doped MnTe are found to increase its thermopower strongly at temperatures up to 900 K. MnTe is a room-temperature antiferromagnet with promising spintronic properties, including for thermospintronics and magnon-based devices. Below T_N, there is a significant magnon-drag contribution to the thermopower. This effect persists up to 900 K as paramagnon drag. This contribution leads to a $zT > 1$ at $T > \sim 900$ K with optimal doping. Additionally, we show that as little as 0.3% Li in MnTe is sufficient to produce a dramatic spin reorientation of the Mn spins from planar in the pure material to almost completely axial, as observed by neutron diffraction. The temperature dependence of the magnetic peaks in Li-doped samples indicates that axial spins shift back to planar suddenly upon approaching the Néel temperature (T_N = 307 K). Density functional theory calculations support the idea that a shift in the Fermi level caused by doping is responsible for switching the material between two competing magnetic ground states. This takes an essential step towards further development of the easy switching of spin orientations in spintronic material and devices such as spin valves and promises to open new avenues of spintronics and transport research in antiferromagnetic semiconductors.

Abstract number: US-O1.04

Role of phase-transition and topology in $Mo_{1-x}W_xTe_2$ for thermal to electrical energy conversion

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The 1T'-$MoTe_2$ to T_d-$MoTe_2$ (type-II Weyl) phase transition induced hysteresis is studied using temperature-dependent X-ray diffraction, resistivity, and Seebeck coefficient measurement. The Seebeck coefficient demonstrates better sensitivity in studying semimetal-semimetal phase transition in $MoTe_2$ compared to commonly used resistivity measurements. The phase change is found to induce a large enhancement in the Thompson coefficient. Nernst coefficient exhibits a topologically induced peak at lower temperatures. A detailed analysis of the thermoelectric and thermomagnetic transport parameters of the $Mo_{1-x}W_xTe_2$ ($0<x<0.08$) alloy is also provided. The Seebeck measurement highlights the competing contribution of electrons and holes in this material. This study provides a comprehensive analysis of a promising material system for applications in thermoelectric and thermomagnetic devices.

Abstract number: US-O1.05

Influence of composition and crystal structure on the thermal properties of GeSe-$AgBiSe_2$ alloys

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Recently, alloys of IV-VI and I-V-VI2 semiconductors (with IV=Ge,Sn; VI=Se,Te; I=Ag; V=Bi,Sb) have been the object of intense investigations in thermoelectrics. Indeed, they possess very low thermal conductivity attributed to a spontaneous formation of nanostructures, lone-pair anharmonicity, and ferroelectric instabilities. An interesting case is that of GeSe-$AgBiSe_2$ alloys. In fact, within a narrow alloying region (0-40% of $AgBiSe_2$), the crystal structure progressively transitions from an orthorhombic Pnma, to a rhombohedral R3m, to a cubic Fm-3m arrangement, with marked consequences on the lattice thermal conductivity (κ_L). With temperature, all the compositions eventually evolve to the rock-salt phase. In this work, we investigate the elastic behavior of the GeSe-$AgBiSe_2$ system to shed light on the respective contributions of chemistry and crystal structure to thermal transport. Within the same structure, alloying progressively reduces κ_L due to point-defect phonon scattering. An anomalous increase in κ_L is noticed upon increasing temperature with the transition from the rhombohedral to the cubic phase, and correlated with a significant increase in elastic moduli. This is connected with a reduction in the average bond length, likely related to an increase in the ionic character, leading to lattice stiffening. The improved understanding of the intrinsic properties of this system can guide the design of chalcogenide thermoelectrics with tailored thermal properties.

Abstract number: US-O1.06

Mapping the structural phase transition and transport measurements in polycrystalline GeTe-SnTe solid solutions

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GeTe and SnTe have long been studied as base materials for thermoelectric applications. Forming a complete solid solution, $Ge_{1-x}Sn_xTe$ alloys undergo a reversible structural phase transition from rhombohedral to face-centered-cubic as a function of Sn content as well as temperature. GeTe makes this transition at ~700K and increasing Sn content lowers this transition temperature until it reaches the SnTe transition at 97K. This study of polycrystalline samples reveals this phase transition via X-ray diffraction, electrical transport measurements and thermal conductivity. X-ray diffraction data is presented to quantify the phase purity of the material as well as the temperature of the phase transition. A discontinuity in the thermal conductivity by Laser Flash Analysis is observed near the expected phase transition temperature. Resonant Ultrasound Spectroscopy analysis of elastic constants is also presented.

Abstract number: US-O1.07

Origin of suppressed phonon transport in BiSb alloys

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Bismuth-antimony alloys are among the best performing thermoelectric materials at low temperatures. Their lattice thermal conductivity is known to be suppressed despite relatively simple crystal structure, with values below 1 W/mK at 300 K. The current study is aimed at identifying origin of this important property by combination of theoretical and experimental tools. Low thermal conductivity is found to stem from: (i) exceptionally soft bonding, (ii) sizable anharmonicity, and (iii) efficient point-defect scattering of phonons due to strain field. Soft character of bonding is indicated in pure Bi by the lowest speed of sound among known thermoelectrics (v_s = 1284 m/s), and small values of the calculated elastic moduli. Large anharmonicity origins from resonant character of the atomic interactions in Bi. We confirm it by experimental Gruneisen parameter of γG = 2.04. Lastly, it is shown, that BiSb alloys exhibit strong scattering of phonons on strain fields related to point defects. Efficiency of this scattering mechanisms stems from disparity of elastic properties (bulk, shear, and Young's moduli as well as Poisson ratio) between the Bi and Sb. The presented conceptual framework can be useful for analysis of thermal properties in novel compounds and alloys.

Abstract number: US-O1.08

Control Over Thermal Conductivity via Host Sublattice Disorder in Single Crystals of $Ba_8Cu_{16}P_{30}$ Clathrate

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The $Ba_8Cu_{16}P_{30}$ clathrate-I material has been subject to various substitutions in the field of thermoelectricity, resulting in improved thermoelectric performance in bulk polycrystalline state. In this study, we explored the growth of large single crystals (~3 mm x 3 mm x 2 mm) of both undoped and Sr-doped $Ba_8Cu_{16}P_{30}$ clathrate phases. Thermoelectric properties were measured on selected single crystals in the 10-300 K range. A 40% reduction in thermal conductivity was noticed for the crystals with 7.5% Sr-content compared to the undoped crystals. Heat capacity measurement indicated no significant modifications of the electronic structure of parent and Sr-containing compounds. As a result, it was hypothesized that Sr-doping can lead to additional phonon scattering, originating from the changing nature of rattling, i.e. Cu-P cages are oversized for Sr cations. As a result, overall thermoelectric figure of merit of the single crystals at room temperature improved by ~60% with Sr-doping.

Abstract number: US-O1.09

Synthesis and Temperature Dependent Structural Properties of Phase Pure Clathrate-II $Rb_{12.9}Si_{136}$

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Clathrates have continued to evoke interest over the last two decades due to the promise they hold for useful applications, including thermoelectrics. The host framework occupied by the guest atoms present numerous opportunities to achieve diverse physical properties by manipulation of type of the guest atom and their occupancy, and the constituents that form the framework. We report on the synthesis of phase pure clathrate-II $Rb_{12.9}Si_{136}$ by kinetically controlled thermal decomposition (KCTD). The selective synthesis of clathrate-II $Rb_{12.9}Si_{136}$ and clathrate-I $Rb_{6.7}Si_{46}$ was successfully achieved by KCTD by varying the processing temperature. Temperature dependent lattice parameters and estimated coefficient of linear thermal expansion of $Rb_{12.9}Si_{136}$ revealed the existence of lattice anharmonicity. Our results are compared to that of other clathrate-II compositions. This work will assist in the synthesis of new clathrate compositions as well as developing targeted synthetic methods for other open framework materials.

Abstract number: US-O1.10

Concluding Maximum Solubility Using Impurity Phase Stoichiometry

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Solubility of dopant species is an important materials property which determines its potential for optimizing its thermoelectric figure of merit. Experimental reports often conclude reaching the solubility limit upon observation of any impurity phase. However, this approach does not necessarily ensure reaching the actual maximum solubility in compounds. As a result, solubility limit in many thermoelectric materials were mistakenly underestimated in the past, thereby unknowingly discouraging further attempts to realize better thermoelectric performance. Here, we summarize in simple graphical guidelines --- rooted in thermodynamics --- how the maximum dopant solubility can be concluded with certainity using the stoichiometry of the impurity phase observed.

Abstract number: US-O1.11

Effect of grain boundary oxidation on thermal transport in SnSe

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SnSe is deemed one of the most promising thermoelectric materials so far, especially due to the intrinsic low lattice thermal conductivity. Surprisingly, in several reports, polycrystalline samples present a higher thermal conductivity (κ) than single crystals. This has been attributed to nano segregations of Sn oxides with high thermal conductivity at the grain boundaries. It was hypothesized that these impurity phases, though in minimal amount not detectable by X-rays, could significantly increase the overall sample κ. Buttressing this hypothesis was the recent finding that Sn purification steps, intended to remove the oxides, could reduce κ by nearly 50%. Motivated by these findings, we wanted to explore the impact on thermal transport of the following changes: (i) tuning the type of oxide by exploiting thermodynamic stability regions; indeed, Sn-rich compositions favour the formation of SnO, with κ ~ 2 W/mK, while the most stable oxide for Sn-poor SnSe is SnO_2, with κ in the order of 30-100 W/mK; (ii) varying the quantity of oxide, testing samples with quantifiable amounts. Despite the current literature opinion, we do not observe significant variations of κ for samples with tailored SnO or SnO_2 impurities, nor in samples containing ~15% SnO_2. These results call for a more complex picture, beyond the law of mixture, to explain recently published results.

Abstract number: US-O1.12

Investigating the oxidation of $Yb_{14}MSb_{11}$ (M = Mn, Mg, Zn)

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$Yb_{14}MSb_{11}$ (M = Mg, Mn, Zn) are p-type Zintl phases with high thermoelectric efficiencies at 1000˚C and melting points above 1200˚C under vacuum and/or inert atmosphere. In a thermoelectric generator, even within an evacuated jacket, small amounts of oxygen may be present and therefore elucidating chemical reactions in the presence of air or oxygen provide a framework for engineering design. The oxidation of $Yb_{14}MSb_{11}$ (M = Mg, Mn, Zn) was investigated from room temperature to 1000˚C in dry air with thermogravimetry/differential scanning calorimetry (TG/DSC) on small pellets and visually after heat treatment to 1000˚C under ambient conditions on large pellets. Scanning electron microscopy/ energy dispersive spectroscopy (SEM/EDS), and powder X-ray diffraction provide identification of the oxidation products. In the presence of dry air, $Yb_{14}MSb_{11}$ initially oxidizes initially slowly at room temperature with a sweeping exotherm and weight gain with rapid oxidation at 400˚C, after which the exotherm signal plateaus at about 600˚C, with M = Zn showing the smallest overall exothermic curve. All samples showed a paired endo-/exotherm at 785–803°C indicating the melting/solidification of $YbSb_2$ which in the case of M = Mg, Mn extrudes from the sample. In the case of M = Mn, there is also evidence for $YbMnSb_2$. The various sections of the samples, outer layer, inner layer, and core are analyzed, and oxidation reactions proposed.

Abstract number: US-O1.13

Mechanical behavior of thermoelectric materials, another perspective

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Although the mechanical behavior of thermoelectric materials has been gaining more interest in the community, little has been done to understand its real impact on the thermoelectric transport properties. Since thermoelectric materials are meant for long-term applications, creep deformation could be one of the design limitations, not just because of the dimensional instability that it introduces, but also due to the impact it leaves on the electronic transport. Our previous work has shown that the electrical conductivity shows a drop post creep deformation, possibly due to the increase in the dislocations and point defects density. In this talk, we will report the in-situ high temperature creep-electrical conductivity measurement for I-doped PbTe. There, the drop in electrical conductivity was shown to scale linearly with the strain. Since the designed deformation lies in a dislocation-controlled regime, minimal direct influence of point defects is expected, and such conductivity drop is attributed mainly to the increased dislocation density. TEM examination of the deformed samples revealed the formation of sub-grain boundaries that are considered stable against climb annihilation at the testing temperature. This, in fact, opens a door to introduce stable dislocations structures via creep deformation with minimal impact on the electrical conductivity, but significant enough to reduce the thermal counterpart.

Abstract number: US-O2.01

Predicting the Free Energy of Mixing and Local Structure of Alloys Below the High-temperature Limit

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We have developed a first-principles method for simulating the configurational free energy of mixing and structural distortions in alloys as a function of synthesis temperature. This is particularly useful for studying the effects of short-range order on local structure. The method approximates disordered alloys as an ensemble of ordered configurations, each simulated individually. Statistical mechanics is applied post hoc to derive the configurational free energy and structure of the alloy from the ensemble of ordered configurations. This method is constructed to provide a computationally tractable route to modeling the mixing thermodynamics of alloys with many components and/or alloys with large structural distortions. The PbTe-PbSe-PbS pseudoternary system will be studied as a case example, and predictions for the thermodynamics of mixing are corroborated with experiment.

Abstract number: US-O2.02

Increased zT and Investigations of Defect Behavior in (Ag/Cu)(In/Ga)Te_2 Alloys

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Alloys of thermoelectric materials have been studied for over 100 years as a means to increase the figure of merit (zT). Typically, increases in alloys' zT are attributed to a lowered lattice thermal conductivity or optimized carrier concentration that increases thermoelectric performance. Often neglected, though, is the effect of defects in alloyed thermoelectric materials. Many alloy studies fail to pin alloy endmembers to specific points of chemical potential space, resulting in small datasets with indecipherable trends in electronic properties due to changing defect conditions. In this work, we present electronic data on bulk samples of spanning the $AgInTe_2$-$CuInTe_2$-$AgGaTe_2$-$CuGaTe_2$ alloy space, which show an increased zT due to the lowered thermal conductivity of the alloy. Our previous studies have shown Group I site (Ag/Cu) vacancies are the dominant defects in the In containing compounds. Despite having similar defects, the vacancy concentration in the system varies, which translates to exponential changes in electronic and thermal properties. By investigating the changes in electronic data as a function of alloy composition, we can begin to understand and control trends in the defect behavior of thermoelectric alloys.

Abstract number: US-O2.03

Investigating the role of vacancies on the structure, bonding, and thermoelectric properties of $EuCu_{1-x}Zn_xSb$

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The ZrBeSi structure type, consisting of planar hexagonal nets intercalated by a cation layer, can accommodate the removal of greater than 50% of its metal species. The structure's tolerance for disorder and varying structural complexity provides routes to amorphous-like lattice thermal conductivity making this family of materials exciting for thermoelectrics. Here, we investigate the impact of vacancies on the structural, thermal, and electronic properties of $EuM_{1+x}M'_{0.5x}Sb_2$ (M = Cu, M'= Zn), members of the ZrBeSi family of materials. The transition from a fully occupied hexagonal net to one with a quarter of the atoms missing has wide ranging consequences particularly. With increasing vacancy concentration, we observe a non-linear expansion along the hexagonal net and simultaneous contraction in the perpendicular direction. While EuCuSb is a stiff material with moderate thermal conductivity, $EuZn_{0.5}Sb$ exhibits soft bonding which corresponds to the decrease in sound velocity. This, combined with increased scattering, leads to a precipitous drop in lattice thermal conductivity in $EuZn_{0.5}Sb$, which exhibits ultralow thermal conductivity. Models incorporating different electron scattering mechanisms paint varied understanding of the compositional trends in electronic properties, particularly the mobility. These differing explanations warrant further investigation to understand how the stability of the planar hexagonal nets influences the electronic properties.

Abstract number: US-O2.04

Uncovering the Remarkable Thermoelectric Properties of Na-doped $Eu_{11}Zn_4Sn_2As_{12}$: A Novel Layered Zintl Phase

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Layered Zintl phases are a promising class of thermoelectric materials with diverse chemistry. The quaternary phase $Eu_{11}Zn_4Sn_2As_{12}$ is one example of a potential thermoelectric material, given its large unit cell, high density of states near the Fermi level, and honeycomb-like Zn-As sheets with delocalized bonding. Here we report the synthesis and thermoelectric properties of Na-doped $Eu_{11-x}Na_xZn_4Sn_2As_{12}$ (x = 0, 0.05, 0.075, 0.1). Given synthetic challenges associated with Eu due to high reactivity, malleability and vapor pressure, a binary route was employed to synthesize phase pure samples from EuAs and elemental Zn, Sn, and As via ball-milling and annealing. Thermal conductivity is low (~0.5 W/mK at 675 K) for all samples in the series and electrical resistivity decreases substantially with Na incorporation. The Seebeck coefficient is high, reaching a maximum value of 431 μV/K at 675 K for x = 0.1 and, anomalously, increases with Na content. The band structure indicates the presence of three additional bands just below the Fermi level, which may be the reason for the simultaneous increase in Seebeck coefficient and decrease in electrical resistivity with Na doping. These unusual property trends make $Eu_{11-x}Na_xZn_4Sn_2As_{12}$ a promising thermoelectric material and a good candidate for further optimization.

Abstract number: US-O2.05

Thermoelectric Properties of Semimetal $ZrTiSe_4$ with a Layered van der Waals Structure

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Semiconductors have been studied as the most promising thermoelectric materials for the past decades due to their high Seebeck coefficient. Semimetals usually have a small Seebeck coefficient due to a small difference in the density of states between electrons and holes , compensating each other in the longitudinal direction. However, recent studies suggested that semimetals with large asymmetry between electrons and holes could be good thermoelectric candidates. High thermoelectric performance has also been experimentally realized in semimetals with topological bandstructures. Here, we report the synthesis and thermoelectric properties of semimetal $ZrTiSe_4$ with a layered van der Waals crystal structure. Polycrystalline $ZrTiSe_4$ samples consolidated by cold pressing show a metallic type of resistivity in the temperature range of 2–400 K and an n-type conducting behavior. The samples exhibit an unusually large Seebeck coefficient of -202 ± 11 μV K^{-1} at 300 K, notably higher than other semimetals. Furthermore, owing to a low sound velocity and strong phonon scattering by boundaries and defects, the thermal conductivity exhibits a weak temperature dependence and a low value of 2.2 ± 0.4 W $m^{-1}K^{-1}$ at 300 K. Theoretical calculations are carried out to better understand these transport properties. This work provides useful insights into the development of novel semimetals with unique electronic properties for thermoelectric applications.

Abstract number: US-O2.06

A New Quaternary Chalcogenide Material System: Sphalerites

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Recent studies have shown that quaternary chalcogenides are promising for thermoelectric applications as certain materials, such as the kesterites, exhibit high power factor and intrinsically low thermal conductivity. The discovery of new quaternary chalcogenides and an understanding of their structure-properties relationships are paramount and have a major role to play in the development of future high-performance chalcogenide thermoelectric materials. We report on our ongoing investigation on a new class of quaternary chalcogenide. Sphalerites (I-II2-III-VI4, where I = Cu or Ag; II = Zn, Cd, or Mn; III = Al, Ga, or In; VI = S, Se or Te) primarily consist of low-cost, earth-abundant, and non-toxic constituent elements. Temperature-dependent electrical and thermal properties were investigated on varying compositions. An insulator-to semiconductor transition with stoichiometric variation was observed for these p-type materials. Furthermore, analysis of specific heat capacity and thermal expansion provide valuable information on lattice anharmonicity, which contributes to an understanding of the low thermal conductivity these materials possess. This work advances the fundamental investigation of multinary chalcogenides by adding a new material system to the exploration of multinary chalcogenides.

Abstract number: US-O2.07

Accelerated Discovery and Design of Ultralow Lattice Thermal Conductivity Materials Using Chemical Bonding Principles

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Semiconductors with very low lattice thermal conductivities are highly desired for applications relevant to thermal energy conversion and management, such as thermoelectrics and thermal barrier coatings. Although the crystal structure and chemical bonding are known to play vital roles in shaping heat transfer behavior, material design approaches of lowering lattice thermal conductivity using chemical bonding principles are uncommon. In this work, an effective strategy of weakening interatomic interactions and therefore suppressing lat-tice thermal conductivity based on chemical bonding principles is presented and a high-efficiency approach of discovering low κ_L materials by screening the local coordination environments of crystalline compounds is developed. The resulting first-principles calculations uncover 30 hitherto unexplored com-pounds with (ultra)low lattice thermal conductivities from 13 prototype crystal structures contained in the Inorganic Crystal Structure Database. Further-more, an approach of rationally designing high-performance thermoelectrics is demonstrated by additionally incorporating cations with stereochemically active lone-pair electrons. These results not only provide atomic-level insights into the physical origin of the low lattice thermal conductivity in a large family of copper/silver-based compounds but also offer an efficient approach to dis-cover and design materials with targeted thermal transport properties.

Abstract number: US-O2.08

Monte Carlo simulation of power generation using non-equilibrium electron gas thermodynamic cycle

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We present a Monte Carlo simulation of power generation by non-equilibrium electron gas undergoing an analogous Otto thermodynamic cycle. 'Hot electrons' which are out-of-equilibrium with the Fermi electrons and the lattice are generated by electron gas compression using electrostatic gating and heating using an external local heat source. Upon removal of heat and pressure (gating confinement), these hot electrons retain their energy for a short time of the order of picoseconds before they reach equilibrium with other electrons and release their energy to the lattice. Power can be generated if these non-equilibrium hot electrons are allowed to reach contacts within this very short period of time. We propose a nanoscale device of GaAs semiconductor with a gating mechanism that confines electrons locally and use an external heat source like a laser to heat the confined non-equilibrium electron gas. The cycle is then completed when electrons are released and they release their energy via long-range Coulomb interactions in the load region, delivering power to the load region. Hence the device can generate power by converting the heat energy into electrical current upon repeating this Otto-like cycle. The simulation results show that the solid-state device is not limited by the Carnot efficiency due to its transient nature and can have very high energy conversion efficiency.

Abstract number: US-O2.09

Globally Optimal Band Structure for Thermoelectrics in Realistic Systems

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One of the ultimate questions in the field of thermoelectrics is the optimal band structure for the figure of merit. The observation made here is that a linear band dispersion, of any dimension, under acoustic-phonon-deformation-potential scattering comprises the theoretical regimen for delivering boxcar transport distribution, which has been mathematically proven to deliver optimum figure of merit. This is guaranteed in theory by the interplay of the energy-dependencies of group velocity and density of states of linear dispersion as well as the deformation-potential scattering rates. It is thus proposed that linear dispersion with as high a Fermi velocity as possible and capped with optimized bandwidth is the globally optimal band structure for thermoelectricity.

Abstract number: US-O2.10

Optimization of Segmented Thermoelectric Generators with Section-Search Methods

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To increase thermal conversion efficiency of thermoelectric generators (TEGs), segmented designs can be used to leverage temperature-dependent properties of each constitutive material. The addition of segments can introduce additional temperature constraints that should be considered in making reliable designs. As a result, the analysis and optimization of segmented TEGs can be more complex than that of unsegmented designs. Given a fast solver for estimating TEG performance, it is possible to perform a linear grid sweep over various segment heights to find the configuration that maximizes performance while satisfying constraints. This parametric method is effective, but as more dimensions are added to the design space (load resistance, n- and ¬p-type areas, etc.), the number of solver calls increases exponentially. As such, large studies that attempt to maximize specific-power for radioisotope thermoelectric generators can become computationally intractable. The present work uses a sample study with realistic material properties and constraints as a basis for comparing various novel optimization methods. These novel approaches feature section-search approaches, which can find output maxima much faster than using a grid sweep, and gradient-based optimization methods. The results from a linear, parametric grid sweep are compared to the novel methods to determine their relative speed in reaching the known optimum.

Abstract number: US-O2.11

Laser Additive Manufacturing of Bismuth Telluride (Bi_2Te_3)

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Traditional thermoelectric manufacturing methods are complex, limited to planar shapes, require use of expensive equipment and result in a substantial loss of material. Additive manufacturing has effectively been used to address these limitations lately. In this research, an in-depth investigation of the process-structure-property relationship of laser additive manufactured bismuth telluride was conducted. The effect of process parameters such as laser scan speed, laser power, number of scans and scan pattern on microstructural and thermoelectric properties are reported. Our findings reveal that scan pattern and number of scans can be optimized to enhance the relative density and electrical conductivity. On the other hand, excessive rescanning was observed to change the primary charge carriers, resulting in a negative Seebeck coefficient.

Abstract number: US-O2.12

Design of High Thermoelectric Performance through Compositing 2D Sb_2Te_3 and Bi_2Te_3 Nanoplates

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Thermoelectrics are an important class of materials with great potential in alternative energy applications. In this study, two-dimensional nanoplates of the layered chalcogenides, Sb_2Te_3 and Bi_2Te_3, are investigated for their thermoelectric properties. These materials exhibit high thermoelectric performance due to their intrinsically low thermal conductivity, high electrical conductivity and high Seebeck coefficients. The thermal conductivity of these materials is lowered even further by creating nanoplate composites that effectively scatter low and mid-frequency phonons. The two materials, Sb_2Te_3 and Bi_2Te_3, were synthesized as hexagonal, two-dimensional nanoplates via a colloidal route and were characterized by a variety of methods including X-ray diffraction, electron microscopy, and energy dispersive X-ray spectroscopy. The nanoplates were consolidated in the form of a nanostructured pellet via spark plasma sintering. Thermal conductivity in the parallel and perpendicular directions has been measured, revealing strong anisotropy with a significant reduction in the perpendicular direction due to nanostructuring. The Seebeck coefficient is also increased dramatically in the nanocomposite, which is an effect we attribute to energy carrier filtering at the nanoplate boundaries. Overall, these enhanced thermoelectric properties lead to a drastic increase in the thermoelectric performance of the two-dimensional Sb_2Te_3 / Bi_2Te_3 nanocomposite near 425 K.

Abstract number: US-P.01

The ExB Thermoelectric Effect

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The ExB drift can operate as an efficient thermoelectric effect. When two fields, electric and magnetic are perpendicular, and mobility of the medium infinite, particles drift along cycloids perpendicularly to both fields. In contrast to the Seebeck and Nersnt effects, particles drift because of a field configuration, not because of drag by heat flow. With infinite mobility, a return path has the same properties as a forward path and no energy can be extracted because the fields are conservative. However, with finite mobility, the drift becomes a function of dissipative properties such as mobility and concentration. High mobility and low concentration turn the drift on; conversely, low mobility and high concentration turn it off without altering the material's conductivity. Therefore, a system with the drift enabled in a forward path and disabled in a return path can overcome the limitation of the conservative fields, thereby converting heat in the semiconductor to electrical energy. Microscopic asymmetry operating at the thermodynamic limit in the cycloidal thermal motion of carriers biases their velocity distribution in the drift's direction. Unlike other thermoelectric effects which are time-symmetric and rely on unbiased distributions, the ExB effect is CPT-symmetric, and not bound by limitations of the H-Theorem.

Abstract number: US-P.02

High carrier mobility and ultralow thermal conductivity in the synthetic layered superlattice $Sn_4Bi_{10}Se_{19}$

Lu R, Olvera A, Bailey T P, Fu J, Su X, Veremchuk I, Yin Z, Buchanan B, Uher C, Tang Z, Grin Y, Poudeu P. High carrier mobility and ultralow thermal conductivity in the synthetic layered superlattice Sn 4 Bi 10 Se 19[J]. Materials Advances, 2021, 2(7): 2382-2390.

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Among ternary metal chalcogenides, $(SnSe)_w(Bi_2Se_3)_t$ achieves ultra-low thermal conductivity and high carrier mobility through its ingenious crystal structure. In this work, we successfully synthesize $Sn_4Bi_{10}Se_{19}$ bulk samples in both poorly crystallized (S1) and well-crystallized (S2). $Sn_4Bi_{10}Se_{19}$ adopts a complex monoclinic structure consisting of a Bi_2Se_3-like layer and a SnSe-like layer parallel to the (001) plane that are stacked alternatively along [001] to form a / Bi_2Se_3/ SnSe / Bi_2Se_3/ superlattice structure. S1 and S2 have similar atomic structures, carrier density, and carrier mobility above 300K. However, the interesting point is, against common sense, S2 has 30% lower lattice thermal conductivity than S1, which derives from the decrease in (1) the inhomogeneity and anisotropy of chemical bonding and (2) the density of interfaces between building blocks in the S1 sample due to their poor arrangement. Therefore, a more efficient phonon scattering at the ordered atomic-scale interfaces between the building blocks in the crystalline sample, whereas the random orientation of building blocks in the poorly crystallized sample inhibits such effect. What's more, the well-crystallized sample S2 displays larger electrical conductivity, carrier density, and carrier mobility than the S1 sample in the temperature range from 2 K to 300 K, which is attributed to the decrease in the density of carrier trapping and scattering defects in the S2 sample.

Abstract number: US-P.03

Temperature gradient and transport of heat and charge in a semiconductor structure

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A detailed analysis of the influence of thermal nonequilibrium on transport in semiconductors was carried out. It is shown that the transport of heat and electricity in bipolar semiconductors are interdependent and self- consistent. In a general case, the distribution of the temperature in homogeneous semiconductors cannot be constant or a linear function with respect to the coordinate even in a linear approximation. The roles of nonequilibrium charge carriers and the recombination in the heat transport are established.

Abstract number: US-P.04

Effect of carrier diffusion on thermoelectric energy conversion

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This work presents a thermoelectricity model to investigate the effect of carrier diffusion on the energy conversion efficiency of semiconducting thermoelectric (TE) materials. Carrier diffusion plays a significant role in many semiconductor applications but its influence on the energy conversion efficiency of TE materials has basically not been explored. In the newly developed model, the current density depends not only on the electric field intensity and the temperature gradient, but also explicitly on the carrier concentration gradient. The energy efficiency model for the n-type TE materials indicates that the efficiency increases with an increase in the difference between the electron concentrations at the hot and cold ends of the TE leg. The numerical results for a Bi_2Te_3 material show that the efficiency is enhanced by the diffusion current when the carrier concentration at the hot end is higher than that at the cold end. The efficiency increase becomes more pronounced for short TE legs in micro- and nano-electronics applications.

Abstract number: US-P.05

Dual Role of Fe in Electrical Properties of Slater-Pauling Heusler Thermoelectric $TiFe_{1.5}Sb$

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Semiconducting properties in Heusler phases are of great interest for thermoelectric applications. The semiconducting defective Heusler phase $TiFe_{1.5}Sb$ --- a prototype for emerging low thermal conductivity (κ_L) compounds such as $MRu_{1.5+x}Sb$ and $MCo_{1.5}Sn$ (M = Ti, Zr, and Hf) --- stablizes with a stoichiometry and electron count unusual for Heusler compounds. Although $TiFe_{1.5}Sb$ is identified as a non-magnetic semiconductor using the Slater-Pauling rule, this rule offers little structural understanding of its semiconducting properties. Using first-principles based electronic structure analysis, we show that Fe --- unlike in traditional Heusler stoichiometries --- acts both as a Fe^{2+} cation as well as a covalently bonded Fe^{2-} species in $TiFe_{1.5}Sb$. In structures where these two types of Fe atoms are indistinguishable by symmetry (attainable at higher temperatures) the electronic properties are metallic. Therefore, a Slater-Pauling electron count alone does not guarantee semiconducting properties and structural understanding of electrical properties is critical for engineering desirable thermoelectric properties.

EU Program

Abstract number: EU-KN (PLENARY TALK)

Developments in computational methods for complex bandstructure and nanostructured thermoelectric materials

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Over the last two decades a plethora of new thermoelectric materials, their alloys, and their nanostructures were synthesized, while their performance more than doubled. The *ZT* figure of merit, which quantifies the thermoelectric efficiency of these materials increased from values of unity to values consistently beyond two across material families [1]. At the same time, the need to understand their electronic transport properties, and the ability to identify and optimize such materials, has stressed the need for advanced numerical tools for computing electronic transport in materials with arbitrary bandstructure complexity, multiple scattering mechanisms, and a large degree of nanostructuring. The convenient and arbitrary use of the constant relaxation time approximation offers limited predictive capabilities in this case, because the scattering processes are energy, momentum, and band dependent, $\tau(E,k,n)$. Fully *ab initio* electron-phonon scattering methods exist, but they are computationally prohibitive and rarely used. In a similar manner, simple series resistance models for nanostructures fail to predict and explain data.

In this talk I will describe the development of our recently deployed advanced electronic transport simulator ElecTra [2], which considers arbitrary DFT electronic structures of materials and allows for their full $\tau(E,k,n)$ dependence, providing accurate and reliable extraction of thermoelectric properties of materials. The electron-phonon scattering times considered are based on deformation potential scattering, for which however, deformation potentials are in general unavailable. For this, I will describe a novel method that we have developed to extract the necessary deformation potentials from first principles [3]. The new methods described, allow for the calculation of the thermoelectric properties of materials at the same accuracy as fully *ab initio* methods, but at a fraction of the computational cost, typically at less than 10%. A few examples of material performance evaluation studies are discussed [4, 5]. Finally, I explain our main findings for the design of nanostructured materials with optimized power factors, which can provide benefits to *ZT* beyond those that are provided by thermal conductivity reductions [6, 7].

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Abstract number: EU-O.1.1

Investigation of the discrepancies in the effective band structure parameters obtained from transport modelling of Mg_2Si

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Electrical and thermal transport properties in thermoelectric (TE) materials are governed by the electronic and the phonon band structures and the scattering mechanism associated with the energy carriers. Within the framework of the Boltzmann transport equation, the transport properties are described by a set of microscopic, material specific parameters, e.g. scattering potentials, effective masses. Compiling data from different literature sources for Mg_2Si, an attractive TE material with a simple band and crystal structure, we attempt to identify a unified set of microscopic parameters using the Single Parabolic Band model as a starting point. While the scattering mechanism can differ for samples from different sources e.g. due to different microstructures, the majority carrier effective mass would be expected to remain similar. However, our analysis shows a large scatter in the effective mass, m^*, among different samples, with m^* ranging from $0.6m_e$ to $1.4m_e$ (m_e is the electron rest mass). Due to a relatively large amount of available data for Mg_2Si, it has been possible to test different hypotheses including non-parabolicity, measurement uncertainties and energy filtering effects. For instance, our analysis shows there is no systematic dependence of m^* on the carrier concentration, thus there is no strong indication of non-parabolicity. This work will help to identify the so far hidden parameters that are necessary to describe the material transport more consistently.

Abstract number: EU-O.1.2

A novel Monte Carlo ray-tracing electron transport method for nanostructured thermoelectric materials

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Carrier transport phenomena in a bulk thermoelectric (TE) material is modeled semi-classically by the Boltzmann transport equation (BTE). Solution to the BTE can be evaluated either analytically or numerically. Specifically for nanostructured materials, Monte Carlo (MC) computational algorithms, which use statistical sampling approach to solve the BTE numerically, are frequently used for the an accurate solution, which takes into account the details of the nano-features in the real space domain. Vast existing literature describes a the typical MC process, however, specifically for nanostructured materials, many difficulties are encountered, which make simulations computationally very expensive and logistically cumbersome, such as the large number of backscattering events and the limited statistics gathered under low field transport. In order to address these issues, we have developed an efficient and hybrid MC algorithm by combining the analytical BTE plus the numerically extracted flux from ray-tracing to compute the TE transport coefficients. Our method provides the same accuracy as existing methods, but with a significantly reduced computational cost.

Abstract number: EU-O.1.3

Thermoelectric performance of $CuInTe_2$ from first principles using hybrid-DFT and lattice dynamics

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Thermoelectric (TE) materials can convert heat into electricity through the Seebeck effect allowing them to increase the overall efficiency of existing processes, as well as serve as a clean source of electricity. Materials in use today are composed of toxic elements like lead or are plagued by low efficiencies. To measure efficiency, we use the figure of merit, *ZT* and for comparison, a well-known TE PbTe, has an average value of 1.4.

In this work, we explore a chalcopyrite semiconductor, $CuInTe_2$ (CIT) with an experimental *ZT* of 1.18 at 850 K which has been predicted to increase up to 1.72 (10^{18} carriers/cm^3). Here, we combine density functional theory (DFT) with lattice dynamics to determine the transport and thermal properties of CIT. The hybrid-DFT functional (HSE06) with spin-orbit coupling (SOC) is used to accurately predict the band structure and the AMSET code is used to calculate its transport properties beyond the constant relaxation time approximation. We use the supercell approach employed by Phono3py to calculate third order phonon-phonon interactions and determine the lattice thermal conductivity.

These results allow us to calculate the ZT of CIT from first principles where previous theoretical studies have used a semi-empirical approach. A study of the intrinsic and extrinsic defects is also underway to provide a crucial understanding of the material for effective doping to unlock the thermoelectric potential of $CuInTe_2$.

Abstract number: EU-O.1.4

Nanoscale thermal transport at Bi_2Te_3 interfaces

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Nanostructured thermoelectric materials are generally highly polycrystalline, meaning defects such as interfaces are prevalent. Advancing beyond state-of-the-art nanostructured thermoelectric materials requires a detailed understanding of the impact of interfaces on their thermal properties. It is also desirable to achieve high efficiency at room temperature. Bi_2Te_3 is the best performing thermoelectric material at room temperature. To achieve highly efficient thermoelectrics at room temperature it is of critical importance to understand the impact of interfaces on thermal transport in materials such as Bi_2Te_3 at an atomistic level.

In this work, we utilise reverse non-equilibrium molecular dynamics simulations (rNEMD) with a classic interatomic potential [1], to examine the effect of specific interfacial structures on thermal transport in Bi_2Te_3. The interfacial thermal resistance and lattice thermal conductivities are calculated and compared for a number of twin boundaries. In addition, we will also discuss finite-length effects in rNEMD simulations of interfaces as they are often overlooked in these cases. We find that interfacial thermal resistance increases with decreasing stability of the interface. This analysis enables us to identify which specific interfaces may be most effective in suppressing lattice thermal conductivity at room temperature.

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Abstract number: EU-O.2.1

Experimental performance study of multistage thermoelectic heat pumps used for thermal energy storage

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The need to carry out an energy transition towards a 100% renewable horizon places the energy storage as the key, since it is capable of solving the natural intermittency of renewable energies. Thermal energy storage has the potential to be an optimal technology presenting low costs. Electrical resistances are the current technology used to transform the exceeding electricity into thermal energy by heating an air flux that obtains a COP of 1.

In this work, a multistage thermoelectric heat pump (TEHP) is proposed to improve the COP of the transformation of energy. Two multistage configurations have been designed using efficient heat exchangers (HXs), specifically two types of intermediate HX have been developed in order to optimize thermal transfer between stages. One is based on a conventional aluminium block, while other is based on phase change. Experimental characterization has concluded that the novel HX outperforms the aluminium block, obtaining a 50% reduction in its thermal resistance.

Two multistage TEHP prototypes have been built and experimentally studied. It is demonstrated how the use of efficient HX improve multistage thermoelectric heat pump performance, where the use of phase change internal HXs improves the heating COP of the system by a 20%, compared to the conventional technology, obtaining COP values between 2 and 5. These values show the great potential of thermoelectric technology in order to improve the performance of thermally storing energy.

Abstract number: EU-O.2.2

Power enhanced micro-thermoelectric generators (μTEGs) by heat sink integration

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Internet of Things (IoT) is raising as a keystone of our society. One of the main needs of the IoT is the self-sustainable supply of energy to the sensors, and among the available environmental sources, heat can be harvested by means of thermoelectric devices. Earlier, the group developed all-Si based μTEGs with planar architecture based on Si (or SiGe) nanowires acting as the thermoelectric material. This approach benefits from Si and MEMS technologies for the downsizing and scalability, and from the fact that Si is abundant and environmentally sound. Unfortunately, the thermal resistance from the suspended platform, acting as the cold side, to the ambient has limited the power generated by the μTEG. This work presents a procedure to reliably place a heat sink on top of the μTEGs, and on the improvement of its output characteristics. The integration of the heat sink on top of the fragile suspended platforms has only been possible by means of an adapter, together with the development of a custom pick and place system. With the integrated heat sink the ΔT across the NWs is kept higher and the power generated increases. The μTEGs generate an average of 22 μW/cm^2 under natural convection, and 195 μW/cm^2 under an airflow of 1.3 m/s (equivalent to a natural breeze), when in contact with a 200 °C heat source. This power output is in the range of the requirements for IoT applications at the microscale.

Abstract number: EU-O.2.3

A robust thermoelectric module based on MgAgSb/$Mg_3(Sb,Bi)_2$ with a conversion efficiency of 8.5% and a maximum cooling of 72 K

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The applications of thermoelectric (TE) technology around room temperature are monopolized by bismuth telluride (Bi_2Te_3). However, due to the toxicity and scarcity of tellurium (Te), it is vital to develop a next-generation technology to mitigate the potential bottleneck in raw material supply for a sustainable future. Hereby, we develop a Te-free *n*-type compound $Mg_3Sb_{0.6}Bi_{1.4}$ for near-room-temperature applications. A higher sintering temperature of up to 1073 K is found to be beneficial for reducing the electrical resistivity, but only if Mg is heavily overcompensated in the initial stoichiometry. The optimizations of processing and doping yield a high average *zT* of 1.1 in between 300 K and 573 K. Together with the *p*-type MgAgSb, we demonstrate module-level conversion efficiencies of 3% and 8.5% under temperature differences of 75 K and 260 K, respectively, and concomitantly a maximum cooling of 72 K when the module is used as a cooler. Besides, the module displays exceptional thermal robustness with a < 10% loss of the output power after thermal cycling for ~32000 times between 323 K and 500 K. These proof-of-principle demonstrations will pave the way for robust, high-performance, and sustainable solid-state power generation and cooling to substitute highly scarce and toxic Bi_2Te_3.

Abstract number: EU-O.2.4

Thermoelectric recovery of the waste heat produced by a wood dryer

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Due to the growing push for a greener and sustainable economy, a great effort is being made to cut energy consumption and greenhouse gas emissions in industrial processes. One way to do this is recovering some of the heat wasted in these processes and convert it to electricity.

Organic Rankine Cycle (ORC) and Thermoelectric (TE) Generators (TEGs) are two notable alternative ways to produce electricity from waste heat. TEGs tend to have lower efficiency than ORC but are able to convert directly heat into electricity with no moving parts, are easier to implement due to their geometric simplicity and modularity and, if carefully designed, have little to no maintenance needs, contrary to mechanically complex ORC. Until recently, their cost per unit power was high, but new affordable TE materials will soon be commercially available, opening a window of opportunity for large scale affordable TEG industrial waste heat recovery applications.

In previous VCT editions the potential of TEGs using geometries adapted for large-scale applications and promising affordable TE materials such as those developed by the group were assessed. The present study explores experimentally a small size TEG absorbing the heat of a hot air flow produced by a wood dryer. This serves to validate previous TEG models and test solutions for large-scale such as low cost long fin heat sink assemblies. After careful design and construction, tests were performed for several air flow rates and temperatures.

Abstract number: EU-O.2.5

Thermoelectric generator with thermal control applied to Heavy Duty Vehicle

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Heavy duty vehicle (HDVs) account for an important portion of fossil fuel consumption and greenhouse Gas (GHG) emissions worldwide. The transition of long haul HDVs to full powertrain electrification will occur much later than with light vehicles. Nevertheless, increasing degrees of electrification and high onboard electricity demand makes the conversion of a portion of their exhaust heat especially attractive for improved medium term HDV sustainability.

The heat recovery potential for long haul HDV trips is high, since they are normally made under high average engine loads. Thermoelectric generators (TEGs) convert heat into electricity with no moving parts and thus, with little to no maintenance needs. The authors have been exploring a concept allowing to maximize heat absorption under highly variable engine load.

The present study assesses an Exhaust TEG with thermal control installed on an HDV performing long haul trips. A wavy fin heat exchanger was installed at the gas side and variable conductance vapour chambers embedded for thermal control. Simulations were made with AVL Cruise and a custom TEG model developed by the authors. Results indicate that the conjunction of high exhaust heat absorption fraction and optimal hot face temperature allows to overcome previous poor performance of these systems. This, along with a new generation of affordable and performing thermoelectric materials might finally render HDV TEGs a viable option for onboard electricity production.

Abstract number: EU-O.2.6

The smart thermoelectricity Safety System with Soil-Air Generator

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In this study, the thermoelectricity Safety System with Soil-Air Generator that works with soil temperature is being analyzed and examined. To achieve this goal, a special electronic safety device was built, and the parameters of the output of the device were investigated. To investigate the way the Thermoelectricity "Soil-Air" generator operates, the soil depth that equals the generator in terms of the length and the temperature of the soil surface is calculated throughout four seasons, and the outcome is modeled. With the special test assembly that was set up, the physical parameters such as the power P(W) that the generator created based on ΔT, the voltage (V), and the flow I(A) were observed with the help of all of this scientific data. According to the results, the fact that the Smart Thermoelectricity Safety System with Earth-Air Generator (ATES) can produce its own electricity by using the temperature of the soil, without requiring any kind of electric cable, and it can inform the security units in case of an area breach, are determined results. Also, as an environmentally friendly and innovative product, the ATES system is envisaged as a part of various areas of work, especially in military applications.

Abstract number: EU-O.3.1

The $Sm_y(Fe_xNi_{1-x})_4Sb_{12-\delta}Sn_\delta$ skutterudite system: synthesis and characterization in view of thermoelectric applications

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Systems of filled skutterudites are an extremely interesting class of intermetallic materials with general formula $RE_yM_4Sb_{12}$ (*RE* = rare earth, *M* = transition metal). As their composition changes, they can reveal important thermoelectric properties that can be modulated through the insertion of *RE* atoms that fill available voids within the structure.

Starting from the already characterized structure of $Sm_y(Fe_xNi_{1-x})_4Sb_{12}$, Sb was partially replaced by Sn and the new skutterudite under investigation has the following stoichiometry: $Sm_y(Fe_xNi_{1-x})_4Sb_{11.5}Sn_{0.5}$. This partial substitution is intended to introduce new scattering centers and therefore, further reduce the phonon thermal conductivity.

A previous study was performed to determine the amount of Sm actually entering the structure. Eleven compositions belonging to the $Sm_y(Fe_xNi_{1-x})_4Sb_{11.5}Sn_{0.5}$ system ($0.35 \leq x \leq 1.00$; $0.15 \leq y \leq 0.55$) were prepared. The Skutterudite was synthesized by the melting-quenching-annealing technique starting from the metal elements and the precursor $Sm_{0.15}Sb_{0.85}$.

Composition and structure of the obtained materials were studied by light optical microscopy (LOM), scanning electron microscopy (SEM), X-ray powder diffraction (XRPD). Structural models were optimized using the Rietveld technique. Differential thermal analyses (DSC) were also performed, and the results were compared to the ones obtained from the Sn-free system.

Abstract number: EU-O.3.2

Stress/pressure-stabilized cubic polymorph of Li_3Sb with improved thermoelectric performance

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Li_3Sb has two polymorphs crystallizing in a face-centered cubic cell (BiF_3 structure type; space group *Fm3m*) and in a hexagonal unit cell (Na_3As structure type; space group *P6₃/mmc*). *c*-Li_3Sb was predicted to be a promising thermoelectric material based on recent first-principles studies; however, the experimental transport characteristics have remained unknown so far. Herein, successful preparation of *c*-Li_3Sb is reported by stress-induced mechanochemical synthesis along with its high-temperature TE properties. *h*-Li_3Sb was revealed to be the stable phase at ambient conditions, while it starts unexpectedly transforming to *c*-Li_3Sb by ball milling or under 60 MPa at RT. The transport properties measurements performed on two polycrystalline specimens evidence that *c*-Li_3Sb behaves as a *p*-type degenerate semiconductor due to the formation of Li vacancies. In agreement with lattice dynamics calculations, *c*-Li_3Sb exhibits very low lattice thermal conductivity despite the lightweight of Li. A *zT* value of around 0.3 was obtained at 550 K. Modelling suggests that the hole concentration should be reduced through aliovalent substitutions or under Li-rich conditions for further optimization. Although the strong air sensitivity of Li_3Sb makes its use in TE applications challenging, this simple superionic binary provides an attractive experimental platform to elucidate the effect of stress/pressure on phase transitions as well as that of Fermi surface complexity on TE properties.

Abstract number: EU-O.3.3

Thermoelectric properties of high quality, epitaxial (Si)GeSn/Ge layers with various Sn content

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Several thermoelectric (TE) materials efficient in a wide temperature range are either unfriendly to the environment or not suitable for mass production. On the contrary, Silicon-based alloys are low-cost and CMOS compatible. Here, we propose to combine Sn with SiGe a breakthrough step towards an efficient TE group IV material. SiGeSn alloys provide lower thermal conductivity (k) than Ge or SiGe because of higher phonon scattering due to alloy disorder, higher atomic mass and, anharmonicity, while simultaneously keeping high electrical conductivity. We aim to examine the thermal conductivity of high-quality epitaxial SiGeSn layers deposited by industry-grade Chemical Vapor Deposition technique with Sn content between 5 at.% – 14 at.% and Si content of 5 at.%. To measure k, we use Raman thermometry. In this method, the phonon energy is measured *via* Raman spectroscopy and is correlated to the heating induced by a laser beam. Subsequently, the thermal conductivity of the material was determined by a semi-analytical model. The result is that k decreases from 56 W/m·K for pure Ge to 4 W/m·K for a $Ge_{0.86}Sn_{0.14}$ alloy. We also investigated samples with 12 at.% Sn and strain from −1.5% to −0.3%, finding that tetragonal deformation has little effect on k. Measurements on SiGeSn show an even larger reduction of k down to 2 W/m·K. Combined with estimation for electrical conductivity and Seebeck coefficient, these results are extremely promising for TE applications.

Abstract number: EU-O.3.4

Thermoelectric properties of $NbCoNi_xSn$ (x = 0 – 1)

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The half-Heusler (HH) compound NbCoSn with 18 valence electrons is a promising thermoelectric (TE) material due to its appropriate electrical properties as well as its suitable thermal and chemical stability. Doping/substitution and tailoring of microstructures are general approaches to enhance the TE performance of HH compounds. In this work, Ni was introduced into NbCoSn to form $NbCoNi_xSn$ compounds/composites, and the effects of Ni content on the microstructure and TE properties of $NbCoNi_xSn$ compounds/composites were investigated. Adding Ni into NbCoSn first forms $NbCoNi_xSn$ compounds with interstitials and then $NbCoNi_xSn$ with full-Heusler composites when $x > 0.05$. Co/Ni interstitials were able to enhance TE properties by forming in-gap states and introducing point defect scattering of phonons. Moreover, the formation of a NbCoNiSn full-Heusler (FH) phase is energetically preferred over the formation of a $NbCo_2Sn$ phase, making it able to tailor the amount of FH phase by varying Ni concentration. The crystal structure transition from HH phase to FH phase and their effects on TE properties are discussed. A maximum figure of merit ZT of ~0.56 at 875 K was found in a nominal $NbCoNi_{0.05}Sn$ compound, which is comparable to the highest reported ZT values.

Abstract number: EU-O.3.5

Identifying the role of interstitial Cu in ZrNiSn half-Heusler thermoelectric

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Both the first-principles theory calculations and experiments have confirmed that *ABC* type half-Heusler compounds with 3*d* elements in the *B* position are naturally 3*d* rich. The naturally 3*d*-off-stoichiometry is thermodynamically stable and able to synergistically optimize the electrical and thermal transport properties of half-Heusler compounds. In this work, Cu ($3d^{10}4s^{1}$) is introduced into the ZrNiSn compound to form Cu interstitial defects intentionally. The correlations between the phase structure, microstructure, and thermoelectric properties of $ZrNiCu_xSn$ (x = 0 – 0.15) are systematically investigated by means of X-ray and neutron diffraction, transmission electron microscopy, atom probe tomography, band structures and phonon spectrum calculations. The diffraction results reveal that Ni/Cu atoms partially occupy the 4*d* (¾, ¾, ¾) position of the half-Heusler crystal structure, forming interstitial defects. The interstitial Cu defects gradually move the conduction band minimum close to the valence band maximum and reduce the bandgap, rather than induce in-gap states as Ni interstitials. Besides the interstitial defects, the full-Heusler phase is also formed in the half-Heusler matrix with increasing Cu content. Due to the interstitial defects and interfaces, the thermal conductivity is suppressed. As a result, a higher *ZT* value is achieved (~1.1 at 950 K) in the $ZrNiCu_{0.05}Sn$ sample.

Abstract number: EU-O.4.1

Synthesis and transport properties of the tetradymite $Bi_{2-y}Pb_yTe_2Se$

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Bi_2Te_2Se, a ternary derivative of the state-of-the-art thermoelectric compound Bi_2Te_3, exhibits topologically-protected surface states and bulk insulating properties below room temperature, characteristic of the recently discovered topological insulating behavior. Density functional theory calculations highlighted the opportunity to create a resonant level in this compound upon Sn doping, thereby possibly inducing enhanced thermoelectric properties near room temperature. However, no detailed study of the influence of various dopants has been undertaken so far.

In this communication, we will present an experimental study on polycrystalline samples of $Bi_{2-y}Pb_yTe_2Se$, $0 \leq y \leq 0.03$. The samples were synthetized by using a conventional powder metallurgy route in sealed silica tubes followed by spark plasma sintering. Structural and chemical analyses were performed to assess the phase purity and chemical homogeneity. A special attention was devoted to the study of the ternary compound phase diagram. The transport properties were measured over a wide range of temperatures (2 – 700 K), both parallel and perpendicular to the pressing direction, in order to assess the influence of lead. A *n*- to *p*-type crossover was observed when slightly increasing lead concentration in the samples. This was additionally confirmed by electronic structure calculations. A favorable combination of thermoelectric properties leads to high *ZT* values of up to 0.7 near room temperature.

Abstract number: EU-O.4.2

Effects of grain size on the thermoelectric properties of Cu_2SnS_3: An experimental and first-principles study

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A new synthesis method was investigated to produce high-density Cu_2SnS_3 (CTS) samples using a two-step method, in which high energy ball-milling was followed by spark plasma sintering (SPS). This method adds a distinct advantage by maintaining the nanostructure while reaching the required high density. Rietveld refinement on the XRD patterns revealed average domain sizes below 50 nm for all the samples. The experimental results show that the Seebeck coefficient (S) and electrical resistivity (ρ) decrease with decreasing domain sizes, while the thermal conductivity (κ) increases. A smaller domain size correlates with a lower resistivity and a degenerate semiconductor-like behavior due to higher carrier concentration. At the same time, our synthesis method leads to materials with very low lattice thermal conductivity, thanks to the nanometric size of grains and structural disorder. As a result, the sample with the smallest grain size exhibits the highest zT of ~0.4 at 650 K. First-principles density functional theory (DFT) simulations on various CTS crystallite surfaces revealed localized states near the Fermi level and the absence of band gap, indicating the metallic nature of the surfaces. This synthesis method also provides an interesting route for many materials to synergistically tune their electrical and thermal properties.

Abstract number: EU-O.4.3

Impact of local structural distortion on the thermal conductivity of Ge substituted $CuFeS_2$

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Chalcopyrite ($CuFeS_2$) offers a rare example of a promising *n*-type thermoelectric sulfide. It possesses a moderate power factor (S^2/ρ) but a high lattice thermal conductivity (κ_L). Substitution with Ge in $CuFe_{1-x}Ge_xS_2$ ($0.02 \leq x \leq 0.1$) results in reductions of up to 60% in lattice thermal conductivity, κ_L, compared to that of the parent $CuFeS_2$ phase. The maximum figure-of-merit, zT ~0.35 achieved at 673 K represents a more than 3-fold increase over that of $CuFeS_2$. Preliminary structural studies using X-ray diffraction and scanning electron microscopy indicate the retention of the chalcopyrite structure on Ge substitution, with no evidence for secondary phase(s) or precipitates. Mass fluctuation scattering of phonons alone is not enough to explain the substantial reduction of κ_L in the substituted samples. Pair-distribution function analysis using X-ray synchrotron radiation indicate displacement of the Ge atoms within the GeS_4 tetrahedra, which induces a local structural distortion and introduces asymmetry into the chemical environment, thereby affecting the phonon modes and phonon transport. This leads to lattice softening and enhanced strain-field fluctuation scattering, also evidenced by a significant reduction in the measured sound velocities, Debye temperature and elastic moduli. Our results provide new insights into the dynamical properties of these materials and further our understanding of the behaviour of lattice thermal conductivity in substituted chalcopyrite phases.

Abstract number: EU-O.4.4

Investigation of thermoelectric properties of composites based on polycrystalline chalcogenide $Sn_{0.9}Mn_{0.1}Te$ with multilayered carbon nanotubes.

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From the point of view of thermoelectric conversion efficiency, thermoelectric materials are characterized by power factor parameter $PF = \sigma S^2$ and thermoelectric figure of merit $ZT = \sigma S^2 T/k$ where σ is electrical conductivity, S is Seebeck coefficient, k is thermal conductivity, T is temperature. An important task is to search for new promising thermoelectric materials that optimally combine this set of parameters.

$Sn_{0.9}Mn_{0.1}Te$ chalcogenides are promising materials for thermoelectric applications and addition of multilayer carbon nanotubes (CNT) to their composition will optimize the thermal conductivity of a polycrystalline sample.

In this work, low-temperature measurements of the temperature dependences of electrical conductivity and Seebeck coefficient were carried out to identify a sample with the maximum power factor (*PF*) among a series of $Sn_{0.9}Mn_{0.1}Te$ samples, with the addition of multilayer carbon nanotubes in an amount of 0, 0.05, 0.1, 0.15, 0.2, 0.25 wt.%.

As a result, the thermal conductivity of a sample containing 0.25 wt.% CNT, measured at room temperature, showed a decrease of about 20% relative to a sample without the addition of CNT and Seebeck coefficient and electrical conductivity in measured temperature range remain unchanged.

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Abstract number: EU-O.4.5

Thermoelectric optimization of tetrahedrite – co-doping with nickel and selenium

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Costly and potentially hazardous thermoelectric materials (TMs), often composed of rare or toxic elements such as Bi, Pb and Te, hinder the wide range application of thermoelectric generators. A potential, cheap and less toxic alternative is a naturally abundant mineral, tetrahedrite ($Cu_{12}Sb_4S_{13}$), that has good thermoelectric properties as a *p*-type semiconductor ($zT \approx 0.6$ at 700 K). While less efficient than most commercial grade TMs ($zT \approx 1.0$), recent studies indicate that single isovalent doping can improve thermoelectric performance and reach zTs near unity. With the scope to further improve the thermoelectric performance of tetrahedrite, this work studies the thermoelectric properties after co-doping with Ni and Se, following the formula $Cu_{12-x}Ni_xSb_4S_{13-y}Se_y$.

Simulations carried out with Wien2K and BoltzTrap softwares, place the optimum stoichiometric content for Ni and Se at $x = 0.5$ and $y = 0.5$.

Samples were produced and characterized with Powder X-Ray Diffraction, Raman Spectroscopy and SEM-EDS, after undergoing annealing at 723 K for 7 days and sintering at 848 K with 56.2 MPa for 1 h 30 m.

Seebeck coefficient and electrical resistivity measurements suggest that co-doping improves the power factor and in accordance with simulations, indicate that at 300 K, the $Cu_{11.5}Ni_{0.5}Sb_4S_{12.5}Se_{0.5}$ sample achieved the highest power factor (1277.73 μW/m K^2) and a $zT = 0.32$, by estimating thermal conductivity with the Wiedemann-Franz law.

Abstract number: EU-O.4.6

Defect engineering boosted ultrahigh thermoelectric power conversion efficiency in polycrystalline SnSe

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Two-dimensional (2D)-layered atomic arrangement with ultralow lattice thermal conductivity and ultrahigh figure of merit in single-crystalline SnSe drew significant attention among all thermoelectric materials. However, the processing of polycrystalline SnSe with equivalent thermoelectric performance as single-crystal SnSe will have great technological significance. Herein, we demonstrate a high zT of 2.4 at 800 K through the optimization of intrinsic defects in polycrystalline SnSe *via* controlled alpha irradiation. Through a detailed theoretical calculation of defect formation energies and lattice dynamic phonon dispersion studies, we demonstrate that the presence of intrinsically charged Sn vacancies can enhance the power factor and distort the lattice thermal conductivity by phonon-defect scattering. Supporting our theoretical calculations, the experimental enhancement in the electrical conductivity leads to a massive power factor of 0.9 mW/m K^2 and an ultralow lattice thermal conductivity of 0.22 W/m K through the vacancy-phonon scattering effect on polycrystalline SnSe. The strategy of intrinsic defect engineering of polycrystalline thermoelectric materials can increase the practical implementation of low-cost and high-performance thermoelectric generators.

Abstract number: EU-O.5.1

Strained and unstrained $Ge_2Sb_2Te_5$: Effects on the electronic and thermoelectric properties investigated by DFT

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Chalcogenide phase-change materials, such as $GeSb_2Te_4$, $Ge_2Sb_2Te_5$, show strikingly contrasting optical and electrical properties, leading to promising extensive implementation in both memory devices and thermoelectric (TE) applications. For 2(GeTe)·(Sb_2Te_3), namely $Ge_2Sb_2Te_5$, two different sequences have been reported. In this paper, we performed a series of first principles calculations using density functional theory (DFT) to determine electronic and TE properties of $Ge_2Sb_2Te_5$ with these 2 sequences. The compounds GeTe and Sb_2Te_3 were also investigated. Different exchange-correlation functionals (LDA, PBE, WC and HSE potentials) were tested, w/o spin-orbit coupling, which has been found to have important effects. The electronic bands indicate that S1 is a direct band gap semiconductor, whereas S2 shows metallic characters. We also calculated elastic moduli, dielectric constants, Born effective charges, and phonon dispersion within the quasi-harmonic approximation. Based on the above-mentioned calculations results, thermal conductivity has been obtained by solving the Boltzmann transport equation. The most interesting compound for thermoelectric applications was found to be $Ge_2Sb_2Te_5$ with the S1 sequence. Furthermore, S1 shows robust bandgap under slight biaxial strains (−1.6% to 2%) and a sensitive semiconductor-to-metal transition (−1.6% to −1.8% and 2.1% to 3%). Additionally, the QTAIM theory was employed to explain the differences in the properties of the 2 stackings.

Abstract number: EU-O.5.2

Impact of biaxial/uniaxial strain on the electronic, and thermoelectric properties of the rhombohedral halide perovskite $CsGeBr_3$: First-principles investigation

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The impact of biaxial/uniaxial strain ($-0.15 < \varepsilon < 0.15\%$) on the electronic and thermoelectric properties of the rhombohedral halide perovskite $CsGeBr_3$ was investigated using an *ab initio* calculation. The bandgap is shown to increase in the presence of tensile and compressive strain. The sign of the strain determines the proportionate increase in the bandgap. The effect of biaxial/uniaxial strain on the transport properties of the rhombohedral halide perovskite $CsGeBr_3$ was also investigated. It is also found that both strains modify the dispersion of bands around the Fermi level, significantly increasing the thermoelectric performance of the material.

Abstract number: EU-O.5.3

Structural, topological and transport DFT calculations of Mg-doped tetrahedrite thermoelectrics

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Tetrahedrite-based ($Cu_{12}Sb_4S_{13}$) materials are of interest to thermoelectric community due to their very low, intrinsic thermal conductivity and high power factor. Tetrahedrite's lattice conductivity is linked to their complex structure and rattling Cu atoms, which disrupts heat-carrying phonons. In this study, DFT calculations are carried out to thoroughly investigate structure of Mg-doped tetrahedrite. Various dopant concentrations and structural modifications are considered for their energy of formation, energetically favorable site occupation and disruption of their local environment – especially rattling Cu atom. Topological analysis of electron density provides insight into bonding character and strength. More global, statistical parameters based on Bond Valence Model reveals that tetrahedrite's structure becomes gradually unstable for Mg concentration $x > 1.0$. Finally, electronic band structure calculations predict transition from *p*-type to *n*-type conductivity for $x > 1.0$. However, in light of other results, experimentally obtaining *n*-type tetrahedrite with Mg doping seems dubious due to expected limit of solubility.

Abstract number: EU-O.5.4

Exploring the role of chemical composition in the lattice thermal conductivity of oxychalcogenides assisted by machine learning

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Oxychalcogenides represent a large chemical space with potential application as thermoelectric materials due to their low thermal conductivity and low-cost. However, the nature of this behavior is still under debate. Understanding the origin of the anharmonicity of these materials is key to developing new materials improving their thermoelectric efficiency. In this work [1], we combine machine learning with first principles calculations to explore oxychalcogenides materials. To afford accurate predictions across this large family of compounds, we solve the Boltzmann transport equation with force constants derived from density functional theory calculations and machine learning-based regression algorithms, reducing by between 1 and 2 orders of magnitude the computational cost with respect to conventional approaches of the same accuracy. Machine learning not only accelerates the prediction of the lattice thermal conductivity for large chemical spaces with high accuracy, but also catalyzes the development of design principles to discover new thermoelectric materials. Using this approach, lattice thermal conductivity has been directly connected to the effect of each species in the material, using atomic projections of the scattering rates.

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Abstract number: EU-O.5.5

The first-principle study of the electronic, and thermoelectric properties of Ba_2MnMoO_6

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Perovskite such as materials which include magnetic elements have relevance due to the technological perspectives in the spintronics industry. In this work, the FP LAPW method is utilized to investigate the optoelectronic and thermoelectric properties of Ba_2MnMoO_6 material with the density functional theory. The interchange correlation potential was included through the generalized gradient approximation. Our structural calculations are in agreement with the experimental results which show that the material crystallizes in the 225 space group ($Fm\bar{3}m$). The density of states study was carried out by considering the up and down spin orientations. Results show that the present oxide–doubles perovskite compounds Ba_2MnMoO_6 has a conductor behavior due to dominant Mn spin-up and Mo spin-down contributions. The transport properties are applied as a function of the variable temperatures or carrier concentration. It is found that the compounds under study are classified as a *p*-type semiconductor. The majority charge carriers responsible for conduction in these calculated compounds are holes rather than electrons.

Abstract number: EU-O.6.1

Computational study of geothermal thermoelectric generators with phase change heat exchangers

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Geothermal traditional systems have high initial investment costs and large environmental impact. Thermoelectric generators (TEGs) with phase change heat exchangers have demonstrated to be an interesting alternative to enhanced geothermal systems (EGS) in shallow hot dray rock fields (HDR).

This work studies the possibilities of TEWs in Timanfaya National Park (Canary Islands, Spain), one of the greatest shallow HDR fields, presenting temperatures up to 500 °C at only 2 m deep. A computational model was developed to study the potential of geothermal electric generation applying TEGs and analyzing the influence of several parameters on their performance. This kind of TEG is robust, reliable and can operate with no auxiliary consumption.

The model, based on the thermal-electrical analogy, was validated thanks to a real prototype, leading to an error of less than 8%. The considered phenomena are heat transfer based on phase-change for the hot and cold side of the TEG, heat transfer through the modules and heat dissipation to the environment thanks to forced or natural convection.

As a result, this tool allows the behavior analysis of such devices under different conditions obtaining valuable information related to the temperature distribution inside the system, the performance of the heat exchangers and heat flow through the generator. The potential of the solution is demonstrated, leading to a electricity generation of 681.53 MWh/year thanks to the scalability of the TEGs.

Abstract number: EU-O.6.2

Computer simulations of tetrahedrite-based thermoelectric generators

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Thermoelectric Generators (TEGs) are devices capable of converting heat into electricity and *vice versa* through the thermoelectric (TE) effects. These solid-state devices are based on arrays of semiconductor legs that are electrically connected in series, usually using copper electrodes. To insulate them thermally and electrically, the TE legs and contacts are normally covered by alumina. Due to the potential for waste heat harvesting, absence of moving parts and low maintenance needs, TEGs are considered eco-friendly. However, most of the commercial TEGs are based on rare and toxic elements such as Te, Bi, and Pb, and present low efficiencies (< 15%). The low performance and high costs allied to a reduced supply of raw materials, make current TE devices limited to small scale applications, being used mostly in niche markets. With the growing energy needs and the efforts from industries to become greener, the TEGs market is boosting the search for more efficient and cheaper materials such as the Tetrahedrites and the Magnesium silicides being explored by the authors. In this work, a tetrahedrite and MgSi-based TEG was simulated using a finite elements software (COMSOL). Several models were developed and validated based on data acquired on a custom-made test bench working with a Bi-Te commercial device. Simulations to study the influence of the thermal and electrical contacts on the performance of commercial and new TEG (working on the same set-up and conditions) are presented.

Abstract number: EU-O.6.3

Additive manufacturing of silicon germanium alloys for thermoelectric applications

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Nowadays, Additive Manufacturing (AM) has revolutionized current production methods in many areas like aeronautics, defence or medicine. Among these methods, Laser Powder Bed Fusion (L-PBF) is prevalent to printing complex metal parts in small and medium series. Recent studies in L-PBF processing develop the manufacturing of new materials, including thermoelectric (TE) materials. The AM approach brings several advantages over usual TE manufacturing techniques: the huge geometry variety allows designing TE modules of all kinds of shapes. As legs of TE modules can directly be printed, dicing step is no longer necessary, which allows reducing material losses caused by this step. Finally, L-PBF processing unlocks new microstructures that could lead to enhance TE materials performances.

This study presents the manufacturing of silicon-germanium alloy by L-PBF, a TE material intended for high temperature applications. It is the first time that this semiconductor material is developed by AM technology. Several dense samples were produced, and a first process window was identified. Structural analyses have been performed, highlighting very good densification but revealing mechanical cracking. Dopant repartition was also studied, by chemical analysis and Energy Dispersive X-Ray Spectroscopy (EDS). Finally, TE properties were also investigated, with a peak ZT = 0.11 at 600 °C.

Abstract number: EU-O.6.4

Contact systems for thermoelements obtained by the methods of chemical and electrochemical deposition of Ni and Co

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Creation of efficient generator thermoelements operating in a wide temperature range is a complex technological task. One of the main problems is creating quality contacts. Used contact systems should provide: diffusion barrier functions; low-resistance ohmic contact to thermoelectric materials; high adhesive strength and commutation properties. The methods of chemical and electrochemical deposition of contact systems are of interest in terms of the simplicity of the technological process and the possibility of obtaining thick layers.

The formation of nickel and cobalt contact layers by chemical deposition using hypophosphite and borohydride as a reducing agent, as well as electrochemical deposition from sulfate electrolytes, was carried out. Contact systems were formed with and without a sublayer obtained by magnetron sputtering.

According to the results of properties studies, nickel contact systems formed by chemical reduction in a boron hydride solution and deposited on a Ni sublayer have the best parameters. They have the highest adhesion strength, not less than 14.5 MPa; low specific $10.24 \cdot 10^{-8}$ Ohm·m and contact $1.70 \cdot 10^{-9}$ Ohm·m^2 resistances. At the same time, good results have also been obtained using cobalt-based contact systems. They have a lower adhesion strength 11.0 MPa; but surpassed nickel contacts in specific $7.08 \cdot 10^{-8}$ Ohm·m and contact $1.59 \cdot 10^{-9}$ Ohm·m^2 resistances.

This work was supported by the Russian Science Foundation (grant number 20-19-00494).

Abstract number: EU-O.6.5

Thermal stability studies on Cu-contacted Mg_2X-based solid solutions (X = Si, Sn) in high temperature region

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For practically working TEGs contact development is as important as material optimization. Mg_2(Si,Sn)-based solid solutions are a promising class of materials for mid-to-high temperature waste heat recovery. Cu was identified as possibly suitable electrode due to its high electrical conductivity, similar coefficient of thermal expansion and good adhesion to Mg_2(Si,Sn). But, it has also been observed that *n*-type Cu-contacted Mg_2(Si,Sn) samples show a degradation of their performance upon annealing, caused by a reduction of the carrier concentration. Two mechanisms are plausible: first, a loss of Mg by evaporation, potentially causing a reduction in Mg interstitials and/or an increase in Mg vacancies. The second option is interdiffusion of Cu and Mg, changing carrier concentration also by a change in intrinsic and extrinsic charged point defect concentrations.

We have coated *n*-type Mg_2(Si,Sn) samples with Al_2O_3 by ALD to identify the underlying degradation mechanism. Integral measurements of electrical conductivity and Seebeck coefficient at 450 °C show an enhanced stability of coated samples compared to uncoated samples for samples without a Cu electrode, while integral measurements and spatially resolved mappings of the Seebeck coefficient indicated similar degradation for coated and uncoated samples with Cu electrode. This identifies Mg-Cu interdiffusion as main degradation mechanism and illuminates the road for further technological development for Mg_2(Si,Sn)-based TEGs.

Abstract number: EU-O.7.1

Flexible thermoelectric thin films based on layered nanoporous $Ca_3Co_4O_9$

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Flexible thermoelectrics is an emerging area of research, in particular for wearable applications. One strategy used for the flexible thermoelectrics is to combine an inorganic and organic material as composite/hybrid material. The electronic, thermal, and mechanical properties of thin films can be altered by porosity but is controllable by engineering of the nanoporosity in layered crystalline inorganic materials such as $Ca_3Co_4O_9$ remains a challenge. The nanoporisity of the $Ca_3Co_4O_9$ layer was synthesized in a controlled fashion way. The porosity and average pore size of $Ca_3Co_4O_9$ films can be tuned by adjusting individual layer thickness in the multilayers ($Ca(OH)/Co_3O_4$). The oriented nanopores formation in textured $Ca_3Co_4O_9$ is driven by local epitaxy and strain relaxation between $Ca(OH)_2$ and Co_3O_4 during annealing. The nanoporous $Ca_3Co_4O_9$ films not only exhibit a high electrical conductivity of ~90 S cm^{-1} and a high Seebeck coefficient of ~135 μV K^{-1}, but also a thermal conductivity as low as ~1 W m^{-1} K^{-1}. Moreover, the nanoporous $Ca_3Co_4O_9$ films exhibit a greater mechanical compliance and resilience to bending than the bulk. The nanoporous $Ca_3Co_4O_9$ films incorporating organic PEDOT:PSS fillers can form hybrid films and show high mechanical flexibility maintaining the initial thermoelectric properties, with potential use in mechanically flexible energy-harvesting applications.

Abstract number: EU-O.7.2

Optimizing the thermoelectric performance of nanocrystalline Si thin films by à la carte B doping using sputtering co-deposition.

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The thermoelectric performance of semiconductors is strongly dependent on the charge carrier concentration. High boron doping levels produce a simultaneous increase in electrical conductivity and Seebeck coefficient in nanocrystalline Si films [1]. This way, exceptional power factors have been obtained in nanocrystalline Si films highly doped with B using ion implantation [2]. However, this doping technique is expensive, time-consuming and may cause structural damage when large doses are required.

Sputter deposition is a well-established, inexpensive, and versatile technique for the fabrication of films with different composition, which can be controlled by the simultaneous use of several magnetrons. Here, we achieve a high control of B doping and of the carrier concentration on Si nanocrystalline films grown by sputtering co-deposition. Starting from an B-doped Si target, we adjust the doping by simply changing the B magnetron power.

We observe a continuous increase in carrier concentration from 10^{19} to 10^{21} cm^{-3} and in the electrical conductivity for B power between 10 and 60 W. Along with this, there is a steady decrease in the Seebeck coefficient from 500 to 100 μV/K. These values result in power factors that present a marked maximum of around 5 mW/K^2m for a carrier concentration around 10^{21} cm^{-3}.

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Abstract number: EU-O.7.3

Screen-printed fabrication of thermoelectric thin-films from PbSe colloidal nanocrystals

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Thin-film thermoelectrics (TEs) with small thickness of below 10 µm present an increasing opportunity for powering wearable electronics and internet of things. Here, we propose screen-printing as an easy to scale-up and industry-relevant technology to fabricate TE thin-films from colloidal nanocrystal (NC) building blocks.

Monodisperse colloidal PbSe NCs with cubic morphology and size of 13 nm were synthesized by heating-up method. Next, PbSe ink was formulated and screen printed to fabricate the TE thin-films. After, heat treatment at 600 °C was performed to remove organic matter from the thin-films, since carbon residues can reduce film electron mobility. Electrical properties measured at room temperature by Hall effect revealed that PbSe screen printed thin-films have a bulk carrier concentration of $3.8 \cdot 10^{18}$ cm^{-3}, electron mobility of $7.9 \cdot 10^{-1}$ cm^2 V^{-1} s^{-1} and electrical conductivity of 50 S m^{-1}. A maximum Seebeck coefficient of 561 µV K^{-1} was obtained at 143 °C and a highest electrical conductivity of 123 S m^{-1} was reached at 197 °C. Positive Seebeck coefficient indicates that as-fabricated PbSe thin-films behave like a *p*-type material. Power factor calculations resulted in maximum of $2.47 \cdot 10^{-5}$ W m^{-1} K^{-2} at 143 °C. Since TE characterization of thin-films with thickness of few microns is yet a very challenging task, different methods for measuring electrical conductivity and Seebeck coefficient were assessed and will be discussed.

Abstract number: EU-O.7.4

Improvement of thermoelectric properties of PEDOT:PSS based flexible thin film composites for generator applications

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The thermoelectric effect is known as the conversion of thermal energy into electrical energy or *vice versa*. When the temperature difference occurs between the ends of the semiconductor material, the hot side generates more free electrons. These free electrons move from the hot side to the cold side. Electron movement and heat conduction are directly related to its thermoelectric property. Low thermal conductivity is required to achieve a high figure of merit. Polymers; provide advantages to such studies due to its low thermal conductivity, ease of processing, and flexible distribution. This work aimed to develop thermoelectric and flexible PEDOT: PSS-based films. Firstly, PEDOT: PSS-based films were made. While producing PEDOT: PSS film, there are some important points such as substrate selection, drying process, and flexibility. Experiments in different drying conditions with various substrates were performed for these steps. These trials prevented overdrying and both facilitated substrate selection and eliminated the flexibility problem. Later, carbon-structured materials such as graphene and MWCNT were added to improve their thermoelectric properties. Dispersion difficulties and a tendency to coagulation are frequently observed in carbon-based materials. To prevent this, the solution and then the films were prepared using a magnetic stirrer and sonication together. The synthesized films were characterized.

Abstract number: EU-O.8.1

Electron-phonon scattering and thermoelectric transport in *n*-type monolayer MoS_2: Multiscale deformation potential approach

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Transition-metal dichalcogenides, such as two dimensional (2D) MoS_2 have drawn the attention of the thermoelectric community since the 2D crystal structure leads to a high Seebeck coefficient and inherently low lattice thermal conductivity in comparison to other 2D materials. Here we present multiscale first-principles and machine learning techniques to calculate electron-phonon scattering rates and thermoelectric transport coefficients in single layer MoS_2. Our models can obtain the scattering rates due to each of the phonon modes at reduced computational time. These models are in good agreement with brute force first principle techniques. Our results suggest that the most dominant scattering mechanism can be ascribed to the longitudinal acoustic phonon mode. The thermoelectric transport coefficients are in excellent agreement with available experimental data [1,2].

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Abstract number: EU-O.8.2

A thermoelectric figure of merit-based performance analysis of a concentrated photovoltaic-thermoelectric system

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A concentrated photovoltaic-thermoelectric (CPV-TE) system has potential of exploiting a full solar spectrum to generate electrical energy. To understand the effect of the transport properties of the TE materials on the performance of a CPV-TE system, a figure of merit-based analysis is conducted. Each transport property that is Seebeck coefficient, thermal conductivity, and electrical conductivity is set to either a high or a low value, and the corresponding performance of the hybrid system is computed. When a transport property is set to a high value, the other two properties are set to low and *vice versa*. This is done in order to maintain the overall value of the *ZT* to either 1 or 2. The results revealed that the output performance of the TE module is enhanced by almost 100% when the value of the dimensionless figure of merit increases from 1 to 2. At a high concentration ratio when the dimensionless figure of merit is 2, the contribution of the TE module can be higher than that of the PV. Moreover, it is found that the best way to improve the performance of the CPV-TE system is to use TE materials with very low thermal conductivities. This approach is more effective in comparison to maintaining a very high value of either Seebeck coefficient or electrical conductivity. It is also concluded that a TE material with a low value of either Seebeck coefficient or electrical conductivity can be used in place of a TE material with a high value of thermal conductivity

Abstract number: EU-O.8.3

Transport properties of solid solutions of Co(Fe)Si with nontrivial topology of the band structure

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The discovery of topological phases of matter caused a great interest in the field of condensed matter physics. Topological semimetals are especially attractive. Their band structure possesses topological points or lines called Weyl nodes and nodal lines, respectively. Linear energy dispersion near such nodes affects the density of states and transport properties. Besides that, such materials have unique properties, such as the presence of spin-dependent surface states (Fermi arcs), potentially non-dissipative transport, and may also exhibit unusual transport properties in a magnetic field, for example, negative magnetoresistance. Materials based on CoSi belong to this family of topological semimetals.

In this work, the band structure, topological and transport properties of solid solutions of Co(Fe)Si are considered. These materials belong to the non-centrosymmetric space group No.198 and have Weyl nodes with topological charges of ±4 at the G and R points of the Brillouin zone. With the change of Fe content, a smooth change in the band structure and the position of the Fermi level relative to these Weyl nodes is possible while maintaining a topologically non-trivial band structure. Their topological and transport properties depending on the composition were investigated, taking into account modification of the band structure, variation of concentration and using energy dependent relaxation time.

Abstract number: EU-O.8.4

Development of transient measurement principles to characterize thermoelectric materials

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In studying the figure of merit ($zT = S^2\sigma/\kappa$) of a thermoelectric material, the characterization of the individual transport properties Seebeck coefficient (S), electric conductivity (σ) and thermal conductivity (κ) can be time-consuming and the properties are often measured separately. Here, we report on the Combined ThermoElectric Measurement (CTEM) apparatus which provides a simultaneous characterization of a thermoelectric sample in a temperature range between room temperature and 600 °C and has the opportunity to perform transient measurement procedures while the temperature of the sample is changing continuously.

Currently, several error-sources disturb the experimental principles, while the measurements of the thermal conductivity are particularly affected. Consequently, it is impossible to improve the actual steady-state measurement principles in the real CTEM experiment. As a method of resolution, a numerical model of the CTEM was developed on the base of a network simulation using ModelicaTM environment, in which possible approaches of the aforementioned transient measurement procedures can be implemented. The continuous change of the sample temperature can be achieved by direct heating, Joule heating or heating due to radiation by increasing the sample's background temperature. During the talk, we compare the three mentioned transient procedures and present the effects of the results of the thermoelectric transport properties.

Abstract number: EU-O.8.5

Grading studies for efficient thermoelectric devices

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The efficiency of thermoelectric generators (TEG) is governed by the properties of the employed materials. Functional material grading involves tuning the properties along the TE leg to obtain gain in performance such as efficiency. Such changes can be done by adjusting e.g. the carrier concentration *n*. Typically, chemically homogeneous materials with a constant *n* along the leg are employed in a TEG. However, for most TE materials the optimum *n* has a pronounced temperature (*T*) dependence and the *T* varies from the hot (T_h) to cold (T_c) side of a TEG according to a certain *T* profile *T*(*x*), giving us room to tune *n* according to *T*(*x*). Predictions on efficiency gain in such cases are challenging and an adequate physical model is required here. To address this challenge, we have combined a two-band model (to describe the material properties) with a device model based on the solution of the one-dimensional heat equation. Using Mg_2Sn as an example, we have adjusted the *n* profile along the leg to maximize the thermoelectric figure of merit *zT* locally. We show that this would result in an increase in conversion efficiency of more than 7% for T_h = 700 K and T_c = 300 K, respectively. Using the thermoelectric compatibility criterion, we verify that the chosen *n* profile is indeed close to the best possible one. The presented methodology can be transferred to other material systems and can also be used to calculate the effect of segmentation and other, practically more feasible *n* profiles.

Abstract number: EU-O.9.1

Screen-printed bismuth telluride nanostructured composites for flexible thermoelectric applications

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We herein report the results of a facile two-step surfactant assisted reflux synthesis of bismuth telluride (Bi_2Te_3) nanowires (NWs). The as-synthesised NWs had diameters ranging from 70 to 110 nm with a length varying between 0.4 and 3 µm and a preferential lattice orientation of (015) as determined by grazing incidence X-ray diffraction. We demonstrate for the first time that a solvent/binder paste formulation of N-methyl-2-pyrrolidone/polyvinylidene fluoride (PVDF) is suitable for screen-printing the Bi_2Te_3 NWs with the potential for the fabrication of flexible thermoelectric (TE) materials. The wt.% of PVDF in the composite films was varied between 10% and 20% to identify the optimal composition with a view to achieving maximum film flexibility whilst retaining the best TE performance. The films were screen-printed onto Kapton substrates and subjected to a post-printing annealing process to improve TE performance. The annealed and screen printed Bi_2Te_3/PVDF NW composites yielded a maximum Seebeck coefficient −192 µV K^{-1} with a power factor of 36 µW m^{-1} K^{-2} at 225 K. The flexible screen-printed composite films were flexible and found to be intact even after 2000 bending cycles.

Abstract number: EU-O.9.2

Enhanced power factor by dehydrogenation of heavily doped nanocrystalline silicon films

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We reported how boron heavily doped nanocrystalline silicon (nc-Si) shows an increase of the thermoelectric power factor (*PF*) after a thermal treatment (TT) at 1000 °C for 2 hours in Ar as a result of the concurrent increase of the Seebeck coefficient and of the electrical conductivity. This enhancement is due to energy filtering (EF) occurring at the grains boundaries (GBs) upon precipitation of SiB_x. Quite unexpectedly, *PF* increase was found to depend on the size of the samples. We stipulated that the presence of hydrogen dissolved in nc-Si during the CVD process, could complex boron, interfering with its precipitation and thus hampering the formation of potential barriers needed to enable EF. Removal of hydrogen during the TT was found to depend on sample size and Ar flux, as the eventual formation of a stagnating H_2 layer at film surface prevents hydrogen outdiffusion. To verify this hypothesis, large samples were submitted to a TT at 1000 °C for 2 hours under a tripled Ar flux. We found that *PF*s of the small and large sample aligned to each other removing the size effect. Without hydrogen more B is available for the formation of SiB_x precipitates with a consequent enhancement of the *PF*s, reaching values up to 31 mW/K^2 m.

Abstract number: EU-O.9.3

Precision interface engineering by ALD in CuNi alloys towards high thermoelectric performance

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Phase boundaries play a critical role in the carrier/phonon transport in thermoelectric materials. Herein, a novel technique for surface engineering of thermoelectric materials based on powder atomic layer deposition (pALD) of single/multi-layers of second phase on CuNi powders is presented. Ultrathin layers of various oxides (10–100 cycles of ZnO and Al_2O_3) are uniformly formed on the surface of CuNi alloy particles. The formation of energy barriers and hierarchical interface modifications emerge from the deposition of ZnO/Al_2O_3 layers, leading in a considerable increase in the Seebeck coefficient. Although there is a slight decrease in electrical conductivity after 50 ALD cycles of ZnO, the increased Seebeck coefficients compensate for the loss and result in a 45% increase in power factor when compared to the pristine sample. In addition, the ZnO/Al_2O_3/ZnO multilayer structure was designed to improve electrical resistance at phase boundaries. In coatings with a high cycle number of samples (> 25 cycles ZnO/5 cycles Al_2O_3/25 cycles ZnO cycles), the multi-layer structure retained an enhanced power factor while dramatically reducing heat conductivity. At 673 K, a maximum figure of merit (zT) of 0.22 was attained in 44 cycles ZnO/11 cycles Al_2O_3/44 cycles ZnO cycles multi-layer samples. When compared to pure CuNi, the zT value increased 144% due to pALD decoupling of thermoelectric parameters, which is comparable to the highest value ever recorded.

Abstract number: EU-O.10.1

$Y_2Ti_2O_5S_2$ — A quasi-layered oxysulphide for thermoelectric energy generation

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$Y_2Ti_2O_5S_2$ has been studied as a potential battery anode, with both experimental and computational studies agreeing on the presence of fast Li-ion diffusion through the material [1, 2]. The unique cation deficient Ruddlesden-Poppler structure opening type I Wadsley-Roth intercalation windows in the distorted perovskite-like TiO_5S layer was found to govern the diffusion of species. The relative stability to Li, Na, K and Mg intercalation also signposts the dopability of the material, which is important for thermoelectric purposes.

Using hybrid density functional theory, we calculated the electronic and transport properties of $Y_2Ti_2O_5S_2$, going beyond the constant time relaxation approximation using AMSET. With experimentally determined high thermal stability [3] and calculated favourable band alignment, $Y_2Ti_2O_5S_2$ has the potential to be a promising high-temperature *n*-type thermoelectric. Using nanostructuring to lower the phonon mean free path, the material could achieve $ZT \sim 1$, provided it can sustain a charge carrier concentration of $10^{19} - 10^{20}$ cm^{-3} [4]. To that effect, we are investigating the intrinsic defect chemistry of $Y_2Ti_2O_5S_2$ to determine the doping potential and stability with respect to competing phases.

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Abstract number: EU-O.10.2

Synergistic effects of Eu and Nb dual substitution on improving the thermoelectric performance of the natural perovskite $CaTiO_3$

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Driven by the development of sustainable and regenerable energy conversion materials, the mineral perovskite ($CaTiO_3$) is considered to be a potential candidate for large-scale high-temperature applications owing to its abundance, light-weight, non-toxicity, and low cost. A series of compounds with the nominal composition $Ca_{1-x}Eu_xTi_{0.9}Nb_{0.1}O_3$ ($0 \le x \le 0.4$) has been synthesized and studied in this paper. The phase purities and crystal structures were evaluated by powder X-ray diffraction (XRD) and subsequent Rietveld analysis. Through X-ray photoelectron spectroscopy (XPS) characterization, the by far dominating valence states of Ti and Nb are confirmed to be +4 and +5 in $Ca_{1-x}Eu_xTi_{0.9}Nb_{0.1}O_3$ compounds, respectively. Dual substitution by Nb and Eu yields a synergistic effect of improving electrical transport properties and simultaneously suppressing thermal conductivity. The former is mainly attributed to the *d*–*f* electron exchange induced by the strong hybridization of Eu 4*f*, Nb 4*d*, and Ti 3*d* orbitals. The latter is mostly attributed to the dominant phonon scattering by the mass fluctuation originating from the large mass contrast of Eu and Ca. The results demonstrate the evolution of insulating $CaTiO_3$ to metallic-like conduction performance with increasing Eu content. Due to the largest power factor and lowest thermal conductivity, the sample $Ca_{0.8}Eu_{0.2}Ti_{0.9}Nb_{0.1}O_3$ exhibits the maximum *ZT* of up to 0.3 at around 1173 K.

Abstract number: EU-O.10.3

(paper withdrawn)

Abstract number: EU-O.10.4

Study of the effect of carbon nanotubes on the thermoelectric properties of $Ca_3Co_4O_9$ composites

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In recent years, the thermoelectric oxide material $Ca_3Co_4O_9$ has attracted a lot of attention, due to its good stability, convenient preparation, environmental friendliness and low cost.

We synthesized composites based on $Ca_3Co_4O_9$ oxide with the addition of multilayer carbon nanotubes and subsequent sintering by the SPS method at temperatures of 600 and 700 °C. The complex characterization of the obtained composites (scanning electron microscopy, XRD analysis and other methods) demonstrated that during the heat treatment of the obtained composites in vacuum by the SPS method, at a temperature of 600 °C, carbon nanotubes are preserved.

From the obtained data, it was concluded that the material consists of well-conducting crystallites separated by poorly conducting contacts at the grain boundaries. According to the literature, it was assumed that the addition of nanotubes would lead to a decrease only in thermal conductivity. However, in this material, nanotubes significantly reduce the thermoelectric parameters. This is due to the appearance of cobalt carbides in the sample and, although classical structural analysis methods did not detect the appearance of other phases, analysis of magnetic properties clearly indicates the presence of cobalt carbides in the material.

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Abstract number: EU-O.10.5

Split-anion approach: a novel path to increase the electrical conductivity in Bi-based perovskite-derivates with a significant Seebeck coefficient

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Heat is an inexhaustible source of energy and *stimuli*. Thermoelectric generators and thermal sensors can produce power or an electrical signal, harvesting the waste heat. The search for a material that could be low cost, guarantee high efficiencies and be directly scalable has drawn attention to the family of halide perovskites. Here, we report bismuth-based perovskite-derivates to be used in thermal harvesting applications and suggest a path to increase the electrical conductivity by applying the split-anion approach, where the halide was partially substituted with sulphur to reduce the electrical resistivity. The layers were produced by drop-casting or spin coating in a nitrogen-filled glovebox; bismuth tri-ethylxanthate has been successfully used as a sulphur source. The delivered thermopower was measured higher than 40 mV K^{-1} in doped and undoped bismuth-based perovskite-derivates. The significant Seebeck coefficient and the micrometre-sized sample dimensions make these compounds highly attractive for heat-flow sensing applications and, above all, for those technologies requiring miniaturised and flexible devices.

Abstract number: EU-O.10.6

Computational and experimental studies on improving the performance of *n*-type thermoelectric strontium titanate

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We first used density functional theory to calculate the thermoelectric (TE) performance of strontium titanate doped with group V and VI elements *via* a 2 × 2 × 2 supercell. From this we selected niobium as the primary doping element for its highest predicted performance/price ratio. Experimentally, we sought to improve the electrical performance of polycrystalline 15 at.% niobium-doped strontium titanate (Nb-$SrTiO_3$) by incorporating 0.2 – 1 wt.% electrochemically produced graphene oxide (eGO). Pseudo-single-crystal carrier transport behaviour was achieved after sintering at 1700 K for 24 hrs in a reduced (5% H_2/Ar) atmosphere. Electrical conductivity reached ~2750 S/cm at ~300 K after incorporating with eGO, an increase of one order of magnitude compared to the standard Nb-$SrTiO_3$ samples (200 – 300 S/cm). It is believed that the eGO reduced the grain boundary double Schottky barriers in polycrystalline strontium titanate, resulting in an enhancement of the carrier mobility. Consequently, a vastly increased electrical conductivity, a moderate Seebeck coefficient and a similar lattice thermal conductivity value leads to a high power factor value up to ~1700 μW/m K^2 at ~330 K and a TE figure-of-merit *zT* value of 0.25 at ~873 K. This provides a wider temperature operation window for strontium titanate as the power factor is directly link to the maximum output power of the device, and provides another method to potentially create 'phonon-glass-electron-crystal' oxide TE materials.

Abstract number: EU-P.1

Thermoelectric properties of potassium-doped strontium manganite

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The studies on the thermoelectric effect in $Pr_{0.6}Sr_{0.4-x}K_xMnO_3$ (where $x = 0.05$ or $x = 0.1$) provide important information about the electronic nature of charge carriers in this system. Seebeck coefficient S [μV/K] and thermal conductivity κ [W/mK] were studied by the thermal transport option of the Physical Properties Measurement System from Quantum Design® in a temperature range 2 K – 250 K, with additional measurements near the paramagnetic-ferromagnetic phase transition in an external magnetic field up to 2 T. In all investigated samples one can observe a change in the slope of the Seebeck coefficient in the vicinity of PM-FM phase transition. A subtle, but noticeable influence of the magnetic field is also present. In the whole investigated temperature range the Seebeck coefficient is of negative sign suggesting that *n*-type conduction dominates the thermoelectric transport in these materials. The value changes from large negative at high temperatures, to minimally negative, approaching zero at lowest temperatures corresponding to the changing nature from insulating to metallic, respectively. The Seebeck coefficient is described by the polaron model (insulating regime), while at low temperatures electron-magnon scattering prevails. The analysis is supported by the thermal conductivity data. The effect of increased doping is reflected with a very smeared low-temperature phonon peak of $\kappa(T)$. Lower values of κ are attributed to the presence of the JT distortion in those manganites.

Abstract number: EU-P.2

Glass forming ability of Nb-Co-Sn alloys as an amorphous Heusler phases precursors for thermoelectric applications

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NbCoSn is a well-known thermoelectric material belonging to the Heusler phases with *zT* reaching up to ~0.6. Recently, it has been shown that the thermoelectric parameters of this material can be improved through the formation of a nanocomposite [1]. The structure of this nanocomposite consists of a matrix of the NbCoSn phase (MgAgAs-type structure) in which the nanoinclusions of the $NbCo_2Sn$ phase (Cu_2MnAl-type structure) are immersed. Such a composite was obtained from an amorphous precursor with the composition $NbCo_{1.1}Sn$ in a short-time annealing process. Inspired by this work, we decided to investigate the glass-forming ability of the Nb-Co-Sn system in a wider range of compositions. Using computational methods (based on Miedema's model), the values of enthalpies of formation of the amorphous phase and crystalline counterpart were determined. Additionally, the calculations were verified experimentally for selected compositions. Our study extends the range of compositions in the Nb-Co-Sn system for which an amorphous phase can be obtained, what opens the possibility of creating new nanocomposites with enhanced thermoelectric properties.

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Abstract number: EU-P.3

Thermoelectric properties of ScPtSb half-Hausler compound

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ScPtSb belongs to a broad group of rare-earth-bearing half-Heusler phases (MgAgAs-type crystal structure, space group *F-43m*, no. 216), which exhibit various interesting physical properties and high application potential, e.g. in energy conversion. In this work, we focus on thermoelectric performance of this compound, which we studied as a follow-up of our research on the Ni-based counterpart ScNiSb. *Ab-initio* calculations predict a three times larger energy gap for semiconducting ScPtSb than in ScNiSb, which should result in an enhancement in the thermoelectric power factor. As-cast polycrystalline sample of ScPtSb was obtained by induction melting and characterized by means of X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and nanoindentation. The thermoelectric properties were characterized from 2 to 900 K by Seebeck effect, electrical resistivity, and thermal conductivity measurements. In addition, heat capacity and Hall coefficient were measured at temperatures below 300 K. The compound was found a *p*-type semiconductor. At room temperature, the power factor equals $9.2(3)\cdot10^{-4}$ W m^{-1} K^{-2}, and the thermoelectric figure of merit amounts to 0.04(1).

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Abstract number: EU-P.4

Oxidation behavior of Se/Te-doped skutterudite materials

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The $CoSb_3$-based thermoelectric materials belong to the skutterudites group widely studied for thermoelectric applications. In the last decade, valuable research concerning this group allowed the fabrication of high-quality *n*- and *p*-type thermoelectric materials characterized by high figure-of-merit *ZT*. One of the examples is Se/Te-doped skutterudites with $ZT > 1$. Se and Te are very effective in enhancing thermoelectric properties, but the corresponding impact on the oxidation behavior of the alloy is barely explored. In the present study, we concentrated on the oxidation resistance of Se/Te-doped skutterudites in an air atmosphere at 773 K for 10, 30, 100, and 500 h. To evaluate the impact of Se and Te, the oxidation behavior of the doped $CoSb_3$ was compared to pure $CoSb_3$ oxidized in the same experimental conditions. Microstructure examinations with chemical composition analysis and X-ray diffraction were conducted to identify the oxide layers formed at the surface of the materials. The results show that the Se and Te dopants promote oxidation reactions and influence the morphology of the oxide layers.

Abstract number: EU-P.5

Microstructure and thermoelectric properties of Ni/Bi_2Te_3 cermet composites

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Starting Bi_2Te_3 and Ni powders were spark-plasma-sintered (SPS) to prepare thermoelectric cermet composites consisting of thermoelectric Bi_2Te_3 matrix with different content, *x*, of ferromagnetic Ni filler (*x* = 0.00, 0.50, 0.85, 1.25 and 1.50 at.%). Grained Bi_2Te_3 matrix of composites is texturing under sintering. Texturing degree is *x*-dependent that is attributed to ability of Ni particles act as lubricant. New trigonal $NiTe_2$ phase is formed under SPS-process. The Ni and $NiTe_2$ phases correspond to filler Ni@$NiTe_2$ ("core"-"shell") inclusions. Forming these inclusions is originated from chemical interaction between Bi_2Te_3 and Ni during SPS-process. A Ni → $NiTe_2$ reaction is accelerated with increasing *x* that results in growing Ni@$NiTe_2$ inclusions and increasing fraction of shell. Thermoelectric properties of composites are *x*-dependent that is due to non-monotonic changes in texturing degree, size of the inclusions and concentration of majority carriers with increasing *x*. Thermoelectric figure-of-merit of composites is remarkably enhancing as compared to that of Bi_2Te_3 matrix.

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Abstract number: EU-P.6

Effects of the current and temperature distribution on a synthesis of functional materials

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One of possible ways to create a phase diagram is by a set of experiments conducted *via* the reaction crucible method. A profound comprehension of thermal and electrical processes within the reaction zone may simplify an adjustment of the synthesis.

This study investigates the distribution of thermal, mechanical and electrical gradients during the process and how they may influence the diffusion development. Deeper understanding of all factors, affecting the synthesis process, could help to adapt a technology for the manufacturing of effective functional materials, including thermoelectrics.

The study was based on a real setup with a tin sample in an iron crucible at the temperature around 1000 K. Finite element modelling of the process *via* Comsol Multiphysics was conducted in order to deepen an understanding of a process and reveal main ways to obtain desired material phases. A thermal, mechanical, electrical and chemical modules were used in order to accurately simulate the process. As a result, distribution of all gradients at any time point was acquired. An influence of a current flow magnitude on a diffusion process was examined. Collected results were compared to a real experiment outcome in order to investigate an array of arrangements needed to create a desired phase. An impact provided by a range of factors was displayed.

Abstract number: EU-P.7

Mechanocheminal synthesis of TiNiSn-based Half-Heusler alloys

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Half-Heusler (HH) alloys are one of the most promising materials for thermoelectric generators in the middle-temperature range due to their chemical stability, good mechanical properties, and relatively high thermoelectric performance, mostly associated with the exceptional electrical properties. Up to date, the highest zT_{max} = 1.5 at 825 K has been reported by Rogl for *n*-type $Ti_{0.5}Zr_{0.25}Hf_{0.25}NiSn$ HH alloy.

In the case of industrial application, specific *zT* values are not as crucial as the development of an up-scaled fabrication route. We demonstrate that a polycrystalline single phase $Ti_{0.5}Zr_{0.25}Hf_{0.25}NiSn$ with a fine microstructure can be obtained *via* mechanochemical synthesis within 30 minutes. Optimal synthesis parameters during high-energy ball milling were empirically identified with respect to phase composition evolution upon the milling process.

Furthermore, this methodology allows preparation of materials in a large amount at ambient temperature and is potentially scalable for large-scale industrial production of thermoelectrics based on the half-Heusler alloys. Moreover, a considerable reduction in the particle size leads to reduced lattice thermal conductivity values *via* additional grain boundary phonon scattering as well as additional point defect scattering.

This work was carried out with the support of the Ministry of Science and Higher Education of the Russian Federation in the framework of the State Task (project code 0718-2020-0037).

Abstract number: EU-P.8

Computer simulation of a flexible film TEG with a vertical legs based on $Ge_2Sb_2Te_5$ and Bi_2Te_3 thin films

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In the present work, computer simulation of a flexible film TEG with a vertical arrangement of leg was carried out in order to predict the optimal thickness of *n*- and *p*-type leg, the size of the gap between the leg, and the influence of the substrate.

The properties of $Ge_2Sb_2Te_5$ *p*-type and Bi_2Te_3 *n*-type thin films obtained by DC magnetron sputtering of polycrystalline targets were used in the simulation. Temperature dependences of conductivity and Seebeck coefficient were measured simultaneously on the developed setup. Correlation dependences of the generated power on the substrate thickness, the thickness of the current-carrying electrodes, and the magnitude of the external load were obtained.

The simulation results showed that despite the decrease in the temperature drop on the thermoelectric legs with an increase in the thickness of the current-carrying electrodes, the generated power increases. The maximum value of the generated power is achieved with an electrode thickness of 10 μm, a substrate thickness of 20 μm and an external load of 0.5 Ohm and is $8.18 \cdot 10^{-9}$ W for one pair of legs.

Thus, in the course of computer simulation, the optimal geometrical parameters of a TEG film based on $Ge_2Sb_2Te_5$ and Bi_2Te_3 materials were obtained. The main correlation dependencies were revealed, which will allow developing of an optimized design of a flexible film TEG.

This work was supported by the Russian Science Foundation (project number № 18-79-10231).

Abstract number: EU-P.9

Interconnected effects of Sm-doping on grain structure and transport properties of the textured $Bi_{2-x}Sm_xTe_{2.7}Se_{0.3}$ compounds

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Textured $Bi_{2-x}Sm_xTe_{2.7}Se_{0.3}$ compounds with x = 0; 0.005; 0.01; 0.02; 0.05; 0.1; 0.2 and 0.3 were prepared by using solvothermal synthesis and spark plasma sintering of starting powders. Sm-doping results in several interconnected effects. First of them is reducing in size of particles in starting powders with increasing x. This effect is attributed to increasing in ionic bonding fraction in polar covalent Bi(Sm)-Te bonds, which occurs at increasing Sm content due to difference in electronegativity of Bi and Sm. With increasing x, grain size in bulk samples is also reducing, which is governed by relevant changing in the size of particles. This effect also results in enhancing in texturing degree in samples at gradual increasing x. Finally, grain size effects on the specific electrical resistivity and the thermal conductivity are observed in bulk samples with different grain size. With increasing the grain size, the resistivity increases, whereas the total thermal conductivity decreases. These features are due to electron scattering by grain boundaries.

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Abstract number: EU-P.10

Solvothermal synthesis of submicron particles $Bi_2Te_{2.7}Se_{0.3}$ with controlled morphology

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The thermoelectric properties of materials based on bismuth telluride are highly anisotropic. The maximum anisotropy of properties is observed in single crystals; it can also be partially restored in polycrystalline samples during their texturing, which leads to ordering of crystal grains. The development of texture depends, among other things, on the morphology of particles in the initial powder used to obtain textured materials. Initial powders consisting of one-dimensional (nanosized whiskers, submicron rods) or two-dimensional (thin plates) particles are the most suitable for obtaining textured materials. The purpose of this work is the synthesis of initial $Bi_2Te_{2.7}Se_{0.3}$ powders with particle morphology (1D submicron rods or 2D hexagonal plates) and certification of powders and bulk materials. The powders are intended for further preparation of samples of textured materials using spark plasma sintering and a comparative analysis of the grain structure and thermoelectric properties of the samples. The starting powders with various particle morphologies were synthesized by a high-throughput solvothermal method at a low temperature (180 °C) using ethylene glycol as a reducing agent and solvent. To characterize the powders, X-ray phase analysis, scanning electron microscopy, transmission electron microscopy, and electron diffraction in a selected area were used.

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Abstract number: EU-P.11

Thermoelectric properties of the $CeFeGe_3$ compound

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The cerium-based compounds belong to a group of strongly correlated systems, in which it is expected to observe a wide variety of anomalous physical properties and phenomena, such as the Kondo effect, heavy fermion state, or complicated magnetic structures. The occurrence of exotic phenomena may influence the application possibilities of the studied material, for example, by an enhancement of the magnetocaloric or thermoelectric properties. In this work, we investigate the thermoelectric properties of the $CeFeGe_3$ compound, which belongs to the vast $RTGe_3$ group (R – rare earth, T – transition metal) of materials. $CeFeGe_3$ crystallizes in a noncentrosymmetric $BaNiSn_3$-type tetragonal structure (space group $I4mm$, No. 107) and shows a metallic behavior. At the same time, the value of the Seebeck coefficient is positive in the entire tested temperature range (2 – 300 K) and it has a relatively high value, reaching 65 μV K^{-1} at 89 K. The maximum values of the thermoelectric power factor is $1.9 \cdot 10^{-3}$ W m^{-1} K^{-2} at 62 K, while the thermoelectric figure of merit ZT slightly exceeds 0.03 at 89 K.

Abstract number: EU-P.12

Synthesis by reactive spark plasma sintering, microstructure and thermoelectric properties of medium-entropy $BiSbTe_{1.5}Se_{1.5}$ and PbSnTeSe

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Reactive spark plasma sintering (RSPS) is used to obtain single-phase samples of medium-entropy $BiSbTe_{1.5}Se_{1.5}$ compounds (low-temperature thermoelectric electronic type of conductivity) and PbSnTeSe (medium temperature hole-type thermoelectric conductor) from a mixture of powders of the corresponding elemental metals. The obtained samples are polycrystalline with lamellar grains with the average size of ~3.3 μm in $BiSbTe_{1.5}Se_{1.5}$ and with irregularly shaped grains with the average size of ~18.9 μm in PbSnTeSe. The maximum thermoelectric figure-of-merit of the samples is ~0.43 (at 500 K for $BiSbTe_{1.5}Se_{1.5}$) and ~0.35 (at 725 K for PbSnTeSe).

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Abstract number: EU-P.13

Control of thermoelectric properties of TiO_2 ceramics by niobium doping through defect engineering

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Donor-doped TiO_2 ceramics are very promising *n*-type oxide thermoelectric materials. $(1-x)TiO_2$–xNb_2O_5 ($0.005 < x < 0.06$) ceramics were prepared by a single step, mixed oxide route under reducing conditions. All samples contained polygonal-shaped grains with uniform grain size distributions. Intragranular defect structures were formed in samples with lower Nb contents by the mixing of rutile and higher Magnéli phases, revealing the high-density crystallographic shear planes and oxygen vacancies. Samples prepared with higher Nb content showed a high concentration of linear and planar defects, whilst lower contents of oxygen vacancies. Through optimizing the concentration of point, linear and planar defects, the carrier concentration and electrical conductivity were effectively improved, promoting a much-enhanced power factor of $5.3 \cdot 10^{-4}$ W m^{-1} K^{-2} at 823 K; lattice thermal conductivity was significantly reduced by phonon scattering. A low, temperature-stable thermal conductivity of 2.6 W m^{-1} K^{-1} was achieved, leading to a *ZT* value of 0.17 at 873 K for compositions with $x = 0.06$; the highest *ZT* value reported for single Nb-doped TiO_2 ceramics without the use of SPS. This investigation demonstrate the control of thermoelectric properties of Nb-doped TiO_2 ceramics through engineering defect structures, which could guide the development of future oxide thermoelectric materials.

Abstract number: EU-P.14

Enhancing the thermoelectric performance by reduced phonon life time by solid state solution of $SnSe_{1-x}Cu_xSe_{0.75}S_{0.25}$

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Abstract

Thermoelectric materials consider as an alternative energy resource to tackle the energy crisis and solve the environmental problem by enabling the direct conversion of waste into electricity. Earth abundant IV-VI semiconductor tin selenide (SnSe) regarded as suitable candidate due to their thermal conductivity and high electrical transport performance. Herein, solid state solution $SnSe_{1-x}Cu_xSe_{0.75}S_{0.25}$ samples are synthesized by ball milling and followed by hot press method. The effects of Cu into solid state solution of SnSe on the phase composition, microstructure, and thermoelectric properties of the composites are investigated. The formation of orthorhombic crystal structure is confirmed by X-ray diffraction pattern. HRTEM micrographs highlight the samples' highly crystalline structure, as well as the formation of defects, distinguishable grains, and grain boundaries, all of which aid in lowering heat conductivity. These formation of solid-state solution leads to enhance the phonon scattering and reduced the thermal conductivity.

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Abstract number: EU-P.15

Thermoelectric properties of iron intercalated TiS_2 with sulfur deficiency

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Iron intercalated TiS_2 with sulfur deficiency ($Fe_xTiS_{2-\delta}$) with x varying from 0 to 0.05 were prepared using solid-liquid-vapor reaction and spark plasma sintering. The preferred grain orientation along the applied pressure direction leads to different transport properties for the in-plane and cross-plane directions. The iron intercalation donates extra *n*-type charge carriers, resulting in decreased electrical resistivity in both in-plane and cross-plane directions. The electrical conductivity and the absolute value of the Seebeck coefficient with different iron contents are consistently higher in-plane than cross-plane, leading to higher in-plane power factors. Along the cross-plane direction, a significant decrease in the lattice thermal conductivity was found due to the structural disorders induced by iron intercalation. Both sulfur deficiency and iron intercalation contribute to the enhanced figure of merit (ZT), reaching 0.4 – 0.6 at 700 K.

Abstract number: EU-P.16

Structural and thermoelectric properties of *p*-type SiGe/MnTe composites

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SiGe based alloys used in deep-space missions is benchmark among the high-temperature thermoelectric material. Nevertheless, further enhancement of the thermoelectric figure-of-merit (*zT*) is necessary for their practical applications. One of the approaches for *zT* enhancement is obtaining composites. In this work, we report on high-temperature SiGe/MnTe bulk composites. MnTe is an antiferromagnet with a clearly observed effect of entrainment of charge carriers by paramagnons at a temperature above the Neel temperature, also known as the paramagnon-drag effect. Therefore, it is expected that due to additional contribution from magnonic thermopower, the total electronic transport properties of the composites should increase.

The composites were obtained *via* spark plasma sintering of mixed powders consisted of boron (B)-doped SiGe and MnTe. The addition of MnTe powder in the SiGe matrix increased the electrical conductivity and decreased the lattice thermal conductivity of the composites. However, an increase in the carrier concentration led to a decrease in the Seebeck coefficient of the composites. Therefore, the addition of MnTe in a concentration range from 2 to 6 wt.% insignificantly affected in thermoelectric figure-of-merit, which reaches 0.94 – 0.99 at 1000 K.

The study was carried out with financial support from the Russian Science Foundation (project no. 21-12-00405).

Abstract number: EU-P.17

Thermoelectric power of ultrathin bismuth and bismuth-antimony solid solutions films

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In the work were investigated the thermoelectric, electrical, and galvanomagnetic properties of pure bismuth and solid solutions bismuth-antimony with 3, 5, and 12 at.% Sb thin films 10 – 50 nm thick on a mica substrate. An increase in the conductivity of all samples with a decrease in the film thickness was found, which may be due to the presence of topologically protected surface states. The high surface electrical conductivity of film materials, combined with the thermal conductivity, which is determined by its bulk properties, can make it possible to achieve an increase in the thermoelectric figure of merit. However, despite the observed increase in the conductivity of the samples, the thermopower coefficient decreases with decreasing thickness. The thermoelectric power factor of the studied samples decreases with respect to films of the same composition with a 0.3 – 1 μm thick. It was found that of pure bismuth and bismuth-antimony 12 at.% Sb films are characterized by the transition of the resistance temperature dependence from the semiconductor type to the metals form at a thickness of less than 18 nm. In addition, it was found that in films of this thickness with 12 at.% Sb there is a change in the sign of the thermopower coefficient, which may be of interest for the development of thin-film thermoelectric converters.

Abstract number: EU-P.18

Interstitial engineering of ZrNiSn

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Half-Heusler (HH) compounds, bearing a cubic structure, hold immense potential for high-temperature thermoelectric applications. A grave challenge with their synthesis is the co-existence of residual phases, particularly a Heusler phase, that degrade the thermoelectric properties. Interstitial engineering is an approach to getting better control over the fraction of post-synthesis phases. Ni content variation may influence the interstitial occupation – which also is the primary difference between HH (ZrNiSn) and Heusler ($ZrNi_2Sn$) compounds. This work studies the phases formed and interstitial occupation with Ni content reduction to elucidate the aforementioned concept. Ni has been systematically reduced up to 10% (atomic) with a step-size of 2% in ZrNiSn HH. Arc-melting was used to synthesize HH compounds since they are generally processed by a melting-solidification route. While the residual phases (non-Heusler ones) enhanced significantly after 4% Ni reduction because of the formation of thermodynamically stable binary phases owing to a distorted starting ternary (HH) phase stoichiometry, a reduction in lattice parameter was also observed, which may indicate an absence of Ni in the interstitials. This study may lead to the fundamental establishment of interstitial engineering in the ZrNiSn material system. In the future, it will help researchers further work on methods to enhance *ZT* by optimizing carrier concentration, etc after engineering their interstitial occupation.

Abstract number: EU-P.19

Phase transformation in *p*-type skutterudites during mechanochemical synthesis and spark plasma sintering

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We presented a fast and up-scaled fabrication route for the filled *p*-type skutterudites $LaFe_{3.5}Co_{0.5}Sb_{12}$, using mechanochemical (MC) synthesis followed by spark plasma sintering (SPS), which is much faster than traditional route. As part of the refinement of the process of obtaining skutterudite phase, we carried out high-energy ball milling (HEBM) of a mixture of initial components in the form of elemental powders of La, Fe, Co, and Sb for 15, 30, and 60 minutes. The empirically identified parameters for MC synthesis were used for the obtaining of double-filled skutterudites.

A skutterudite phase is formed in a sample of nominal composition $La_{0.75}Ce_{0.25}Fe_{3.5}Co_{0.5}Sb_{12}$ after 15 min HEBM, after 30 min secondary phases were not identified. However, in the series $Yb_{0.75}Ce_{0.25}Fe_{3.5}Co_{0.5}Sb_{12}$, phase stabilization is energetically less favorable, so after 15 min HEBM the sample contains two more phases, antimony and ytterbium antimonide, in addition to the main one and after 30 min $FeSb_2$ is formed.

All the obtained powders were consolidated by SPS at 823 K. The skutterudite phase completely decomposes after SPS of the powders obtained in 30 min. On the contrary, in the samples after 15 min HEBM, the process of phase formation continues in mechanically activated powders. According to the XRD data, the samples had ~90 wt.% skutterudite phase. The Seebeck coefficient was increased by three times using the reaction sintering method for the powders obtained in 15 min.

Abstract number: EU-P.20

Sustainable thermoelectrics: from fast production to close to room temperature applications

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The thorough search for suitable energetic alternatives is an endless and much needed effort that has been acquiring a new emergent strength as societies evolve and gain environmental conscience. In that sense, thermoelectric materials emerge not as a revolutionary all-solving problem, but as a part of the solution to promote a greener world and mitigate the current energy crisis.

Despite the increased use, most widely employed thermoelectric materials still rely on rare and/or toxic elements. Thus, researches are searching novel sustainable thermoelectric alternatives.

Magnesium-based materials are sustainable and have been explored before as promising thermoelectrics with high figures of merit ($zT > 1$) up to ~500 °C. Nevertheless, magnesium entails some problems, such as its high reactivity and low vapour pressure.

In this work an unusual fast technique (through induction heating) is used to synthesise both *p*- and *n*-type magnesium-based materials, followed by hot-pressing. The samples were characterized by XRD, SEM, coupled with EDS, and thermoelectric measurements (Seebeck coefficient and electrical resistivity) from 25 to 300 K. Even though the optimization of the whole production process is still undergoing, MgAgSb and Mg_2X (X = Si, Sn)-based materials with interesting thermoelectric properties were successfully produced, being good starting points for close to room temperature applications.

Abstract number: EU-P.21

Thermoelectric and magnetic properties of Co_2ZrSn and Co_2HfSn Heusler alloys

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Half-metallic ferromagnetic alloys are attracting considerable interest for their potential applications in spintronic devices. Co-based Heusler alloys are considered to be among the most promising classes of half-metallic compounds as they combine suitable magnetic, electronic and transport properties with compositional versatility and high thermal stability. In this work, Co_2ZrSn and Co_2HfSn Heusler alloys were studied by combining experimental and *ab-initio* investigations in order to accurately estimate their electronic density of states in proximity of the Fermi level and to measure their transport properties over a wide range of temperatures. The effect of secondary phases which are typically present in this type of alloy was also taken in account. The thermoelectric properties were determined both for compounds in which the amount of such impurities is negligible and for samples with secondary phases content up to 20% in weight. The effect of these on the transport properties is discussed in detail.

Abstract number: EU-P.22

Nano thermal engineering of bismuth antimony telluride (BiSbTe)

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Nanoengineering of thermoelectric materials is an effective approach to decouple their electronic and thermal transport properties, hence enhancing their thermoelectric efficiency. Nanoengineering strategies can significantly reduce the thermal conductivity through the corporation of different phonon scattering mechanisms, while the electrical conductivity may not be affected considerably. Here, we compare the effect of three nanoengineering approaches on the structural and thermal properties of a $Bi_{0.5}Sb_{1.5}Te_3$ alloy: (a) nano-hybridization of the alloy by adding Sb_2O_3 nanoparticles, (b) severe plastic deformation via high-pressure torsion, and (c) grain refinement by sonication of $Bi_{0.5}Sb_{1.5}Te_3$ powders before sintering. It is shown that among these methods, severe plastic deformation induces ultrafine grains and a high density of dislocations, resulting in a large reduction of the total thermal conductivity (> 30%) at 300 K. A notable decrease in the lattice thermal conductivity (> 50% at 300 K) was attributed to midfrequency phonon scattering by the dislocations together with low and high frequency scatterings through grain boundaries and point defects, respectively. The present work opens a new pathway for designing highly efficient thermoelectric materials through nanoengineering approaches, particularly severe plastic deformation.

Asia Program

Abstract number: AS-O.1.00 (PLENARY TALK)

Utilizing novel enhancement principles to develop high performance thermoelectric materials & devices

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Development of thermoelectric (TE) materials is important, as in addition to energy saving via waste heat power generation [1], they can also serve as dynamic power sources for innumerable IoT sensors and devices [2]. To achieve enhanced thermoelectric performance, it is necessary to find ways to overcome the traditional tradeoffs between the key properties, namely, between the Seebeck coefficient *S* and electrical conductivity *s*, and between the electrical and thermal conducivity *k*. Find ways to enhance *S*, and also selectively lower *k* [3]. I would like to systematically present several principles we have been developing, most which can be widely applied to different materials.

For the first tradeoff overcoming, we have found that magnetism can be utilized to to enhance the Seebeck coefficent and overall power factor. Strong coupling of the electrical carriers with magnetic moments, can lead to effective magnon drag [4], e.g. like for $CuFeS_2$ chalcopyrite and the recently indicated origin of the huge power factor in metastable Fe_2VAl-based thin films, and furthermore paramagnon drag, where magnetic ion doping into nonmagnetic materials could enhance *S* [5]. Spin fluctuation and spin entropy has also been demonstrated to enhance the Seebeck coefficient [6].

For the second aspect, in addition to various nanostructurings, intrinsic low *k* mechanisms have been demonstrated. Materials informatics approach led to identification of a material catalogue with low *k* [7]. Particular doping into SnTe was shown to lead to softening of the lattice and a dramatic reduction of thermal conductivity largely exceeding the contribution from phonon scattering [8]. Finally, the heterogeneous bonding in mixed anion compounds was shown to result in exceptional low thermal conductivity [9].

Defect engineering has also been shown to be a powerful method. Cr doping in GeTe serendipitously lowered the formation energy of Ge defects leading to homogenously distributed Ge precipitations and vacancies, coupled with typical band convergence doping to obtain ZT~2 [10]. A high entropy approach of $AgInTe_2$ alloying into GeTe, stabilized the cubic phase, thereby enabling enhanced doping of Bi, leading to the first stable n-type conduction in GeTe [10]. The hidden role of rhombohedral distortion degree on the Ge-vacancy formation energy was revealed and utilized leading to high power factor and ZT_{av} [10]. Incidentally, a combined theoretical and experimental screening of some unusual dopants of GeTe revealed Zr to be an effective dopant [10].

Recently an interesting dual effect of small amounts of Cu doping in Mg_3Sb_2 was revealed. Interstitial Cu doping was indicated to lower the phonon group velocity, while Cu doping into the grain boundaries promoted grain growth and unusual optimum chemical composition leading to very high mobilities similar to single crystals, while being a polycrystalline material with low thermal conductivity. An initial realistic 8 pair module composed of Cu doped Mg_3Sb_2-type and MgAgSb exhibited an efficiency of 7.3% @hot temperature side of 320°C, with an estimated efficiency from the actual performance of materials actually reaching close to 11% [11]. Tuning toward room temperature yielded an initial realistic 8 pair module with an efficiency of 2.8% with temperature difference of 95 K from RT and cooling of 56.5 K. Once again, the performance of materials are much higher, so further improvements are expected as the module technology becomes developed [12].

I will also present an overview on different thermoelectric power generation devices which can be utilized for energy harvesting for possible IoT applications. We have also recently fabricated a miniaturized in-plane □-type thermoelectric device utilizing the microfabrication techniques of photolithography and dry etching which are industrial compatible [13].

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Abstract number: AS-O.1-01

Special techniques for precisely estimating the power generation in Ag_2S simultaneously possessing large Seebeck coefficient and moderately small electrical resistivity

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Recent investigation of colossal Seebeck effect in Cu_2Se under unusual temperature gradient by D. Byeon et al. has triggered search of similar effects in other compounds. High values of thermopower generation was also observed in Ag_2S when measured with this unusual temperature gradient. A high Seebeck coefficient of approx. −650 μVK^{-1} was observed along with a relatively low electrical resistivity (~ 2 mΩcm). The special measurement setup consists of two heaters. One usual heater and the other is used to generate a temperature gradient in a direction perpendicular to the usual temperature gradient. This heater induces coexistence of insulating low temperature phase at top and metallic high temperature phase at bottom. This coexisting phase may be fueling the power factors to higher values.

We realized that a straight forward measurement of power generation from Ag_2S is challenging due to the non-trivial Peltier effect and Joule heating at the junctions of the sample and the contact leads. Palladium paste was used to attach the contact point of lead wires to avoid the convergence of electrical current. We confirmed that the pad size at the contacts possesses a significant effect on the heating/cooling of the tip of thermocouples during the power measurements. Different probe arrangements were also employed to understand more on measurements of power from Ag_2S by significantly reducing the local heating/cooling in association with the electrical current convergence.

Abstract number: AS-O.1-02

Low temperature co-sintering of monolithic thermoelectric devices using chalcogenide thermoelectric materials

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Generation of electricity from waste heat using thermoelectric (TE) materials is one of the cleanest forms of renewable energy. Typical commercial TE generators (TEG) use a *π*-type structure, where the *p*- and *n*-type TE legs are bridged by a metal interconnect and the empty spaces between the legs and between each *pn*-pair are filled with insulting materials.

In this work, we fabricate TEGs for near *RT* waste heat applications using a novel device architecture and high performance TE materials. Using a monolithic multilayer, robust and dense devices can be fabricated using an easy and low energy cost method without metal interconnects and less space between each *pn*-pair. Thin layers of *p*- and *n*-type TE materials are stacked alternatingly, with a thin insulating layer partially inserted between each layer. The assembled layers are then co-sintered together to form a robust and dense TE device.

Our TEG structure was designed and optimized using calculations (finite element method using COMSOL Multiphysics). The actual devices were fabricated by assembling thin layers of $Ag_2S_{1-x}Se_x$, Ag_2S and Cu_2Se, and co-sintering at 373 K with an applied pressure of 100 MPa. The prototype single pair device had a maximum output power density of 0.2 mW/cm^2 at a ΔT = 50K. With further improvements to the contact resistance, and fabricating multilayer devices, our results show that this device can be used as a power source for low power consumption wireless devices and sensors.

Abstract number: AS-O.1-03

Analysis and Experimental Confirmation on Inter-conversion Energy between Heat and Electricity in Thermoelectric Cooling and Thermoelectric Power Generation using Peltier Device

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Peltier devices used for both thermoelectric cooling and thermoelectric power generation produce the Peltier effect and Seebeck effect, when an electric current is flowing. We analyzed the amount of heat generated by each effect based on the basic equations for thermoelectric cooling and thermoelectric power generation, and proposed a thermal equivalent circuit that shows the flow of thermal energy clearly. And we clarified the mutual conversion process between thermal energy and electrical energy by using the electrical equivalent circuit when the Peltier element is driven as a thermoelectric cooling element or as a thermoelectric power source. From the analysis results of the thermal and electrical equivalent circuits, it was confirmed in the thermal equivalent circuit during thermoelectric cooling, there was an increase in heat dissipation due to the Seebeck effect and the accompanying increase in back-flow heat and power consumption. In the thermal equivalent circuit during thermoelectric power generation, It was found half of the generated power is lost due to power loss from self-heating of the Peltier element, resulting in a power generation efficiency of less than 50%. This paper, we also report the results of experimental measurements to confirm the accuracy of these analyses and to quantitatively demonstrate the effects of the simultaneous occurrence of the Peltier effect and the Seebeck effect and the conversion relationship between thermal and electrical energy.

Abstract number: AS-O.1-04

Experimental verification of band convergence in Sr, Na doped PbTe

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PbTe has been known for its high-performance thermoelectric properties. Recently, its figure of merit records ZT=2.5 in Sr, Na doped PbTe. However, the physical origin of the unusually high ZT is still elusive experimentally. Although typical studies on thermoelectric materials conduct transport measurements at high temperature on polycrystalline samples, multi-band effects such as band convergence are hardly accessible in such measurements. In our study, we investigate the electronic structure of Sr, Na doped PbTe by the analyses of quantum oscillation and angular dependence of magnetoresistance in single crystals. We found that electrical conduction is dominated by the carriers at the L point in the Brillouin zone at low temperature (T < 150 K). In contrast, the effect of the carriers at the sigma point is observed at high temperature (T >150 K). Temperature induced band convergence of the L point and the sigma point is considered to enhance the thermoelectric properties at high temperature.

Abstract number: AS-O.1-05

Effect of Stereochemically Inactive Lone-pair Electrons on Thermal Conductivity in Muntinary Cubic Chalcogenides

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Lone-pair electrons account for an extremely low lattice thermal conductivity in several multinary cubic chalcogenides, which is typically beneficial for obtaining high thermoelectric performance. Those materials containing lone-pair electrons also show an unconventional variation of lattice thermal conductivity upon doping, especially when cation sites are substituted with dopants. However, a systematic study on the underlying mechanism of those peculiar behavior has not been conducted. Here, we present an experimental evidence showing a monotonic increase of the lattice thermal conductivity upon doping. DFT calculations reveal that these compounds originally contain an off-centered cations from a centrosymmetric positions because of a stereochemically active lone-pair electrons, which makes the lattice more anharmonic and reduce the lattice thermal conductivity. However, upon doping, these lone-pair electrons become stereochemically inactive (or disappear), resulting in a highly symmetric lattice, eventually reducing zT values for entire operating temperatures. These results suggest that the lone-pair electrons should remain stereochemically active, and some dopants which disturb them should be avoided.

Abstract number: AS-O.1-06

High thermoelectric potential of copper-based low-dimensional metal halides

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Thermoelectric materials can directly convert waste heat into electricity where their performance can be evaluated by the dimensionless figure of merit, *ZT*. Recent studies have suggested the possibility of metal halides for thermoelectric applications because of their intrinsic ultra-low lattice thermal conductivity and efficient electrical conductivity. However, studies were mainly conducted on conventional halide perovskites, while emerging low-dimensional metal halides have yet to be explored. Following our previous prediction of high *ZT* in 0D copper halide $Cs_3Cu_2I_5$, we assess the thermoelectric potential of 1D copper halide $CsCu_2I_3$ by performing first-principles calculations. Due to the anisotropic nature of phonon and electron transport of the 1D chain structure, $CsCu_2I_3$ is predicted to exhibit maximum *ZT* of 2.2 at 600 K under *n*-type doping along the *b*-axis. We also find that the reported centrosymmetric Cmcm crystal structure of $CsCu_2I_3$ is an average over non-centrosymmetric *Amm2* structures from our phonon analysis. Our work will deepen the understanding of instabilities in low-dimensional metal halides and trigger more attention towards their application for thermoelectrics.

Abstract number: AS-O.1-07

Improvement of thermoelectric properties of β-$FeSi_2$ by Ni substitution

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As a semiconducting material having an orthorhombic crystal structure with Cmce space group, β-$FeSi_2$ is considered as promising candidate for high temperature thermoelectric application owing its ability of strong oxidation resistance, good thermal stability, and low cost. However, due to the negative impact of its narrow band gap of about 0.73 eV, the absolute value of Seebeck coefficient ($|S|$) significantly decreases at high temperature because of bipolar effect. This issue can be effectively solved by increasing carrier concentration (n_H) with impurities doping. In this study, we attempt to eliminate the bipolar effect by doping Ni into Fe site with activation rate (2 electrons per Ni) in order to increase n_H of β-$Fe_{1-x}Ni_xSi_2$. The samples were fabricated by using arc-melting in Ar atmosphere and the powder XRD data were measured using SmartLab. The S and electrical resistivity (ρ) were measured by ResiTest8300 and homemade apparatus, and thermal conductivity (κ) was measured using PEM-2. As a result, the addition of Ni significantly reduces the bipolar due to the increase in n_H and the S of β-$Fe_{1-x}Ni_xSi_2$ is remarkably more stable than that of β-$FeSi_2$ above 400 K. We observed that both $|S|$ and ρ remarkably decreases with increasing x, while κ is not significantly varied with x. Therefore, the highest ZT = 0.01 is obtained at 760 K for β-$Fe_{0.99}Ni_{0.01}Si_2$ with $n_H = 2.3(9) \times 10^{17}$ cm^{-3} due to the stability in $|S|$, the significant reduction in ρ, and no remarkable effect in κ.

Abstract number: AS-O.1-08

Thermoelectric properties in composites of germanium and silicon-based clathrate by planetary ball milling

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Si clathrate with type-*I* clathrate structure is composed of abundant and environmentally friendly elements and is attracting attention as a material with high Seebeck coefficient at high temperatures. However, if Si clathrates are to be put to practical use as thermoelectric materials, new attempts at material design are needed to improve their thermoelectric performance. In this study, we investigated the thermoelectric properties of composites of *n*-type Ge and Si clathrate with different volume fractions of Ge. Mixtures of *n*-type Ge and Si clathrate with different volume fractions of Ge were milled by planetary ball milling, and the milled powders were sintered by spark plasma sintering. The samples were characterized by X-ray diffraction (XRD) and SEM observations with an electron probe microanalysis (EPMA). The Seebeck coefficient, electrical conductivity, and thermal conductivity were measured. XRD and SEM with EPMA confirmed that there was little decomposition of Si clathrate and no obvious reaction between Si clathrate and Ge. The Seebeck coefficient of the composites was found to be greater than that of bulk Si clathrate in the temperature range of 300 K–500 K. The thermal conductivity of composites was lower than that of bulk Si clathrate, but it increased monotonically with increasing volume fraction of Ge due to the higher thermal conductivity of Ge.

Abstract number: AS-O.1-09

High power factor and Peltier conductivity in Yb_3Si_5 single crystal at low temperatures

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Valence fluctuating materials are reported to show high power factors such as 22 mW/m K at 120 K in $YbAl_3$ and 14.5 mW/m K at 200 K in α-$YbAlB_4$. Here, in the valence fluctuating state of Ce or Yb based materials, the valence is fluctuating both temporally and spatially due to the hybridization between the localized *4f* electron and the conduction electron. In this situation, a sharp and large density of state of *4f* electron exists near the Fermi level, leading to the high power factor. Recently, we succeeded in synthesizing the valence fluctuating material Yb3Si5 and found a very tiny electrical resistivity at low temperatures ($\rho_{(2\,K)}$ = 0.13 μΩ cm) in a high-quality single crystal. In spite of the tiny electrical resistivity, Seebeck coefficient is not small ($S_{(150\,K)}$ = -78 μV/K and $S_{(10\,K)}$ = -15 μV/K) due to the valence fluctuation. These results lead to a high power factor (S^2/ρ) of 45 mW/m K at 12 K which value is the largest among valence fluctuating materials. Furthermore, Peltier conductivity (S/ρ) is very huge with 35 A/K cm at 8 K which is the second best among the reported materials and is nearly two order of magnitude higher than that of the third best material. Our result suggests the possible application to the electrical current source for the superconducting magnet.

Abstract number: AS-O.1-10

Stretchable molybdenum disulfide/carbon fabric-based wearable thermoelectric generator for energy harvesting from the human body

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The design and construction of a state-of-the-art wearable thermoelectric material are very important for the development of self-powered wearable thermoelectric generators (WTEGs). MoS_2 has been reported as a noteworthy thermoelectric (TE) material due to its large intrinsic bandgap and high carrier mobility. In this work, MoS_2 and Zn-doped MoS_2 were effectively grown on C fabric (CC) by a simple hydrothermal method. The uniform growth of pristine MoS_2 and Zn-doped MoS_2 on CC was confirmed by structural and morphological analysis. The compositional analysis confirmed the interactions between the MoS_2 and C fabric. The sample with 2 at% of Zn sample demonstrated an increase in electrical conductivity of 14378.97 S/m at 303 K and 16902.59 S/m at 373 K, which was higher than the pristine MoS_2/CC, 2 at% of Zn-doped MoS_2 and 6 at% of Zn-doped MoS_2. The enhancement in electrical conductivity was due to an increase in carrier concentration by the addition of Zn in the MoS_2 matrix. The optimal electrical conductivity and Seebeck coefficient have led to enhancing the power factor of the Zn0 sample and it was around 666.86 nW/mK^2 at 303 K and1340.15 nW/mK^2 at 373 K.

Abstract number: AS-O.1-11

Fe,Ni-based skutterudites thin films and on-chip device characterization

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After a deep characterization of skutterudite thin films, we fabricated on-chip thermoelectric thin film module containing five n-type and five p-type legs on a fused silica substrate. Thin film and the module were prepared by pulsed laser deposition (PLD) using a Nd:YAG (266 nm, 10 Hz) laser at room *T*. To prepare the device, the substrate was covered with a custom-made Nickel mask to deposit only one of the desired sets of legs at time.

Following the results of the characterization of the material, in order to improve the thermoelectric properties, the device underwent to an annealing process in Ar at 200°C for 3 h before depositing the Au contacts with a gold sputter. The performance of the module was measured using ad custom-made apparatus, following the procedure previously reported [1]: the device was heated up and the voltage was measured together with the ΔT. This thermoelectric voltage is acquired by using a variable resistance (in the range of 10 Ω to 10^6 Ω), called load resistance R_L, and power was estimated at different temperatures (100, 200 and 300 °C) for each value of external resistance. The peak value of the polynomial bell-shape fitting the experimental points (Power *vs* Voltage) is considered as the maximum power output of the device, which in this case is ≈ 0.16 μW, 3 to 4 magnitude orders bigger than what previously measured for oxide thin films by S. Saini et al.[1].

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Abstract number: AS-O.1-12

Effect of heat treatment on thermoelectric properties of carbon nanotube thin films by spin coating method

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Carbon nanotubes (CNTs) are attracting attention as thermoelectric materials capable of forming flexible thin films. However, in the case of thin film formation using CNT dispersion using surfactants and solvents, it is difficult to measure the original performance of CNTs due to the influence of additives. In this study, we investigated the improvement of thermoelectric properties by heat treatment of CNT thin film prepared by a spin coating method. CNTs dispersed in water using a surfactant were spin-coated on a quartz glass substrate. After drying, the thin films were heat-treated at 300 °C under vacuum. Thermoelectric properties were measured using the ZEM3-HR apparatus. Comparing CNT thin films before and after heat treatment, the Seebeck coefficient increased from 20 μV/K to 40 μV/K. The electrical conductivity increased from 5 S/cm to 35 S/cm. Since the melting point of the surfactant is 300 °C, it is presumed that the surfactant is removed from the CNT thin film by heat treatment. The increase in electrical conductivity and Seebeck coefficient can be explained by improved electrical connections between CNTs due to the removal of residual surfactant in the thin films. Thus, the results confirm that heat treatment is an effective method for improving the thermoelectric properties of CNT thin films.

Abstract number: AS-O.1-13

Thermoelectric properties of two-dimensional titanium disulfide nanosheets studied by density functional theory

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In recent years, titanium disulfide has attracted attention as one of n-type thermoelectric materials. Titanium disulfide consists of covalently bonded layers connected by weak van der Waals forces. The single layer of titanium disulfide is called a “sulphene” [1]. A previous study based on density functional theory (DFT) calculations [1] reported that the Seebeck coefficient of two-dimensional titanium sulphene is higher than that of bulk titanium disulfide. In this study, we calculated the thermoelectric properties of 1-, 2-, and 3-layer titanium sulphenes by DFT and the non-equilibrium Green’s function (NEGF) method. The thermoelectric properties vary with the number of layers. The magnitude of the Seebeck coefficient at the Fermi level increases from −21 μV/K for bulk titanium disulfide to −72 μV/K for one layer. The increase in Seebeck coefficient can be attributed to the increase in density of states. Both the electrical conductivity and the electron thermal conductivity decrease as the number of layers decreases. For a single layer, the electrical and electron thermal conductivities at the Fermi level are 48 kS/m and 0.50 W/(mK), respectively. The electron thermal conductivity is considered to decrease according to the Wiedemann-Franz law as the electrical conductivity decreases. The phonon properties have not yet been calculated and further studies are needed.

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Abstract number: AS-O.1-14

Reduction of lattice thermal conductivity for unfilled skutterudite compounds MSb_3 (M = Co, Rh) by pressure-induced structural change.

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The unfilled skutterudite compounds MSb_3 (M = Co, Rh and Ir) or $\square M_4Sb_{12}$ ($\square$ = void) have a body-centered cubic structure. Although the compounds exhibit excellent thermoelectric performance, they have the disadvantage of higher thermal conductivity κ compared to conventional thermoelectric (TE) materials. However, it is known that κ can be significantly reduced by filling the void of the icosahedral cage formed by Sb atoms with guest ions R ($R_xCo_4Sb_{12}$) [1,2]. Kraemer et al. and Matsui et al. reported pressure-induced structural changes in MSb_3 (M = Co, Rh and Ir) in which Sb enters into the void of the cage [3,4]. Although κ is expected to be reduced by the entry of Sb into the cage ($Sb_xM_4Sb_{12-x}$), the TE properties of the samples after the self-insertion reaction have not been reported so far. Therefore, we attempted to synthesize $Sb_xM_4Sb_{12-x}$ (M = Co, Rh) using a high-pressure synthesis method and succeeded in obtaining samples of a size that are suitable for TE properties measurements. The lattice thermal conductivity of $Sb_xM_4Sb_{12-x}$ (M = Co, Rh) was reduced from 6.48 W/mK (Co_4Sb_{12}) to 4.12 W/mK and from 7.38 W/mK (Rh_4Sb_{12}) to 1.32 W/mK at 300 K, respectively. Other TE properties and bulk modulus will be discussed.

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Abstract number: AS-O.1-15

An extraordinary thermoelectric figure of merit observed in Ag_2S with a spatially separate composite effect

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We report observation of a huge figure of merit (ZT~20) using polycrystalline Ag_2S composed of spatially separated low- and high-temperature phases realized with our developed setup: “bottom heating and top measurement (BHTM)”. This high value of ZT is originated from the simultaneous observations of the large magnitude of the Seebeck coefficient (−0.65 mVK^{-1}) and low electrical resistivity (2 mΩ cm) at 390 K − 440 K. The large value of the Seebeck coefficient is obtained from the insulating low-temperature phase at the top surface of the sample, while the low electrical resistivity is from the metallic high-temperature phase lying below the low-temperature phase. The low lattice thermal conductivity of ~0.5 $Wm^{-1}K^{-1}$ also contributes to the large magnitude of ZT. The large ZT value is confirmed by the power generation measurements showing 0.03 mW cm^{-2} in the power density of single sample under ΔT = 5 K at around 420 K. These results strongly suggest that the Ag_2S with the BHTM setup could be one of the best component materials in the thermoelectric generators working near room temperature.

Abstract number: AS-O.1-16

Improved high-temperature stability in thermoelectric legs made of nanostructured Na and Ge substituted *p*-type PbTe

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Thermoelectric modules fabricated from high-performance *p*- and *n*-type PbTe materials in recent years achieved high conversion efficiencies. However, the experimentally measured module efficiencies are still significantly below the theoretical values which is attributed to issues of the material stability and compatibility with contact layers. In this work, we successfully improved the high-temperature stability of nanostructured *p*-type PbTe with Na and Ge substitution by adjusting the Na content of the material. High Na content has been found to improve the thermoelectric properties of *p*-type PbTe but negatively impacts the material stability. By lowering the Na content, the formation of Na-rich precipitates was suppressed. The material stability was significantly improved which is shown by increased flexural strength at 773 K and by increased temperature for plastic deformation under constant force. At the same time, the high thermoelectric performance of the nanostructured *p*-type PbTe with Na and Ge substitution was maintained. Single leg thermoelectric elements with metal contact layers were fabricated from this material. The power generation characteristics of the single legs were measured and compared with finite-element method simulation results.

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Abstract number: AS-O.1-17

The influence of Ag doping on thermoelectric properties of *n*-type Mg_3Sb_2-based material

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Thermoelectric material can directly convert heat energy into electric energy by using Seebeck effect, which has become a promising approach for developing clean and sustainable energy-conversion

Recently, Mg_3Sb_2-based compounds have become promising thermoelectric materials because they consist of low cost and environmentally friendly elements as well as high thermoelectric performance near room temperature. In this study, the influence of Ag doping on thermoelectric properties of Mg_3Sb_2-based material is investigated. We found that the doped samples show a higher electrical conductivity than pristine sample, which contributed to the carrier concentration gaining. Also, decrease of thermal conductivity on doped samples also were observed, this phenomenon may arise by sliver enhanced acoustic phonon scattering, leading a reduce on mean free path and resulting thermal conductivity decrease. In this work, the highest value of *ZT* obtained is 1.54 at 400 °C.

Abstract number: AS-O.2-01

Electronic Topological Transition as a Route to Improve Thermoelectric Performance in $Bi_{0.5}Sb_{1.5}Te_3$

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The electronic structure near the Fermi surface determines the electrical properties of the materials, which can be effectively tuned by external pressure. $Bi_{0.5}Sb_{1.5}Te_3$ is a *p*-type thermoelectric material which holds the record high figure of merit at room temperature. Here it is examined whether the figure of merit of this model system can be further enhanced through some external parameter. With the application of pressure, it is surprisingly found that the power factor of this material exhibits λ behavior with a high value of 4.8 $mWm^{-1}K^{-2}$ at pressure of 1.8 GPa. Such an enhancement is found to be driven by pressure-induced electronic topological transition, which is revealed by multiple techniques. Together with a low thermal conductivity of about 0.89 Wm^{-1} K^{-1} at the same pressure, a figure of merit of 1.6 is achieved at room temperature. The results and findings highlight the electronic topological transition as a new route for improving the thermoelectric properties.

Abstract number: AS-O.2-02

Broadening temperature plateau of high *zT*s in PbTe doped $Bi_{0.3}Sb_{1.7}Te_3$ through defect carrier regulation and multi-scale phonon scattering

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$(Bi,Sb)_2Te_3$ alloys are a promising class of thermoelectrics family for ambient temperature application, which has been widely concerned by the community. However, due to the narrow bandgap, the bipolar excitation limits thermoelectric the figure of merit (zT) improvement as temperature rises. We herein combinate extrinsic impurities with intrinsic defects to regulate carrier concentration and enable multi-scale phonon scattering simultaneously. Multiple types of defect interaction are triggered by PbTe doping to tune hole concentrations, as well as the band gap is further expanded to suppress the bipolar excitation at high temperatures. This result leads to the overall enhancement of electrical transport properties. With PbTe addition, the homologous multi-scale defects (including point defects, Te nanoprecipitates, and high-density grain boundaries) are produced to strengthen phonon scattering effectively in BST matrix, resulting in a decline in lattice thermal conductivity. Finally, a high zT of ~1.25 at 425 K and a superior average zT (zT_{avg}) of ~1.21 (350-500 K) are obtained in BST samples, projecting a maximum conversion efficiency (η_{max}) of ~7.8% at ΔT = 200 K. Importantly, this enhancement of high ranged zTs achieved by rational defect design in BST provides a new insight for promoting high-efficiency thermoelectrics in real applications.

Abstract number: AS-O.2-03

Isotropic Thermoelectric Performance of Layer-Structured *n*-Type $Bi_2Te_{2.7}Se_{0.3}$ by Cu Doping

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The lamellar structure of $(Bi,Sb)_2(Te,Se)_3$ alloys makes it difficult to achieve isotropic thermoelectric properties in the directions along and perpendicular to the *c*-axis, especially for *n*-type samples. In this report, by introducing Cu in polycrystalline *n*-type $Cu_xBi_2Te_{2.7}Se_{0.3}$ and applying the traditional synthesis process of high-energy ball milling and hot pressing, substantial enhancement of the thermoelectric figure of merit zT is obtained in both in-plane and out-of-plane directions. The intercalated Cu not only provides electron transport media for mobility improvement but also reduces the lattice thermal conductivity owing to the strain fluctuation. Typically, the van der Waals gap in the out-of-plane direction leads to relatively slower mobility and lower lattice thermal conductivity. Taking into account the same average density-of-state effective mass ($m_{avg}^* \sim 1.5m_e$) predicted based on a single parabolic model, the obtained quality factor β is comparable in both directions. As a result, a peak $zT \sim 1.05$ at 420 K and the average zT approaching to 1.0 in the temperature range 300-500 K are obtained in both directions for the $Cu_{0.02}Bi_2Te_{2.7}Se_{0.3}$ sample. The simple synthesis process and isotropic thermoelectric properties in this report make *n*-type Bi_2Te_3 more convenient for potential production and application.

Abstract number: AS-O.2-04

Development and industrialization of "stuck neck" high-performance and high-strength bismuth telluride-based thermoelectric materials

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Most optical modules and devices in 5G optical communication systems are very sensitive to the temperature, and traditional mechanical compression refrigeration devices are difficult to meet the requirements of miniaturization, high efficiency, light weight, and high reliability for temperature control, while thermoelectric microdevices have high power density, high cooling temperature, accurate, fast temperature control and small size, which makes it the most ideal temperature control solutions for 5G optical modules. At present, commercial thermoelectric refrigeration devices are still prepared with zone-melting Bi_2Te_3-based materials, but the machinability of zone-melting samples is relatively poor, which makes it difficult to meet the requirements for the preparation of microscale devices. Although the polycrystalline Bi_2Te_3 prepared by hot pressing or plasma sintering process has relatively high mechanical properties, the special crystal structure of Bi_2Te_3 makes the samples prepared by the above process not capable of large-scale industrial application. In order to solve the above problems, we designed the first domestic Bi_2Te_3- shrinkage hot extrusion device, through which the Bi_2Te_3 bar with a diameter of 25.4 mm can be hot extruded, which has both high thermoelectric performance and high mechanical strength. A single thermoelectric arm can reach below 200 μm, which can fully meet the current needs in industry, and is expected to realize the industrial upgrading of Bi_2Te_3-based thermoelectric materials in our country.

Abstract number: AS-O.2-05

Large Transverse and Longitudinal Magneto-Thermoelectric Effect in Polycrystalline Nodal-Line Semimetal Mg_3Bi_2

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Topological semimetals provide new opportunities for exploring novel thermoelectric phenomena, owing to their exotic and nontrivial electronic structure topology around the Fermi surface. Herein, we report on the discovery of large transverse and longitudinal magneto-thermoelectric (MTE) effects in Mg_3Bi_2, which is predicted to be a type-II nodal-line semimetal in the absence of spin-orbit coupling (SOC). The maximum transverse power factor is 2182 $\mu Wm^{-1}K^{-2}$ at 13.5 K and 6 Tesla. The longitudinal power factor reaches up to 3043 $\mu Wm^{-1}K^{-2}$, which is 20 times higher than that in a zero-strength magnetic field and is also comparable to state-of-the-art MTE materials. By compensating the Mg loss in Mg-rich conditions for tuning the carrier concentration close to intrinsic state, the sample fabricated in this study exhibits a large linear non-saturating magnetoresistance (MR) of 940% under a field of 14 Tesla. Using density functional calculations, we attribute the underlying mechanism to the parent linear-dispersed nodal-line electronic structure without SOC and the anisotropic Fermi surface shape with SOC, highlighting the essential role of high carrier mobility and open electron orbits in the moment space. Our work offers a new avenue toward highly efficient MTE materials through defect engineering in polycrystalline topological semimetals.

Abstract number: AS-O.2-06

N-type transport properties in single-crystalline Mg_3Sb_2

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As a top candidate for competing with the conventional *n*-Bi_2Te_3 thermoelectrics, Mg_3Sb_2-based materials have attracted increasing attentions for low-grade (< 300 °C) waste heat recovery applications, due to the high thermoelectric performance, low cost, abundance and nontoxicity. Because of its anisotropic crystal structure as that of Bi_2Te_3, possible property anisotropy and the resultant similar requirement of texturing for preferential performance remain not entirely clear Mg_3Sb_2-thermoelectrics at working temperatures. This motivates the current work to focus on the transport-property anisotropy of *n*-type Mg_3Sb_2, centimeter-sized single crystals of which are successfully grown by a flux-assisted vertical Bridgman technique with a post-annealing under a Mg vapor pressure. This enables a revelation of nearly isotropic transport properties in this anisotropically structured material, guaranteeing reasonably high performances in polycrystalline materials achievable by cheap and scalable processing approaches such as powder-metallurgy.

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Abstract number: AS-O.2-07

Efficient lanthanide Gd Doping Promoting Thermoelectric Performance of Mg_3Sb_2-based Materials

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N-type Mg_3Sb_2-based thermoelectric materials have recently received heightened attentions due to its diverse merits of high band degeneracy, ultralow lattice thermal conductivity and high carrier mobility. However, the inherently low carrier concentration in pristine Mg_3Sb_2 seriously hinders the improvement of thermoelectric performance. Therefore, searching for proper dopants to optimize carrier concentration is one of the primary avenues to realize superior TE performance in Mg_3Sb_2-based materials. Herein, by considering the electronegativity difference $\Delta\chi$ and mass difference ΔM between dopant and host elements, we theoretically and experimentally demonstrate the lanthanide Gd as an effective dopant to tune the carrier concentration of $Mg_3Sb_{1.3}Bi_{0.7}$ alloys. Owing to its high doping efficiency, a large carrier concentration up to 8.9×10^{19} cm^{-3} is realized through Gd doping, which is close to the optimal value. Moreover, the coarse grain size commendably mitigates the grain boundary effects and thus ensure high carrier mobility. Combining the greatly suppressed lattice thermal conductivity by point defect scattering, a maximum zT of 1.55 is achieved at 700 K in $Mg_{3.065}Sb_{1.3}Bi_{0.7}Gd_{0.015}$.

Abstract number: AS-O.2-08

Enhanced thermoelectric performance of p-type narrow band-gap semiconductor $Bi_2Si_2Te_6$

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$Bi_2Si_2Te_6$, a *p*-type narrow band-gap semiconductor, is synthesized via high-energy ball milling followed by annealing. The thermoelectric performance of pristine $Bi_2Si_2Te_6$ is drastically restricted by the detrimental effect of bipolar charge transport on the Seebeck coefficient. We demonstrate that Mn doping at the Bi site and Ge alloying at the Si site are effective strategies to suppress the bipolar effect, enhancing the thermoelectric performance of $Bi_2Si_2Te_6$. The peak zT is enhanced from 0.39 for pristine $Bi_2Si_2Te_6$ to 0.53 for $Bi_{1.99}Mn_{0.01}Si_2Te_6$, while a higher zT of 0.68 is achieved in $Bi_2Si_{1.9}Ge_{0.1}Te_6$.

Abstract number: AS-O.2-09

Topological Insulator $V_xBi_{1.08-x}Sn_{0.02}Sb_{0.9}Te_2S$ as a Promising *n*-type Thermoelectric Material

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As one of the most important *n*-type thermoelectric (TE) materials, Bi_2Te_3 has been studied for decades, with efforts to enhance the thermoelectric performance based on element doping, band engineering, etc. In this study, we report a novel bulk-insulating topological material system as a replacement for *n*-type Bi_2Te_3 materials: V-doped $Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$ (V:BSSTS) . The V:BSSTS is a bulk insulator with robust metallic topological surface states. Furthermore, the bulk band gap can be tuned by the doping level of V, which is verified by magnetotransport measurements. Large linear magnetoresistance is observed in all samples. Excellent thermoelectric performance is obtained in the V:BSSTS samples, e.g., the highest figure of merit *ZT* of ~ 0.8 is achieved in the 2% V-doped sample (denoted as $V_{0.02}$) at 530 K. The high thermoelectric performance of V:BSSTS can be attributed to two synergistic effects: (1) the low conductive secondary phases Sb_2S_3, and V_2S_3 are believed to be important scattering centers for phonons, leading to lower lattice thermal conductivity; and (2) the electrical conductivity is increased due to the high-mobility topological surface states at the boundaries. In addition, by replacing one third of costly tellurium with abundant, low-cost, and less-toxic sulfur element, the newly produced BSSTS material is inexpensive but still has comparable TE performance to the traditional Bi_2Te_3-based materials, which offers a cheaper plan for the electronics and thermoelectric industries. Our results demonstrate that topological materials with unique band structures can provide a new platform in the search for new high performance TE materials.

Abstract number: AS-O.2-10

The unique eletronic and vibrational properties of thermoelectric material $RuSb_2$

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Phonon is essential for thermoeletric materials, which not only carries heat directly but also can affect the electronic transport properties. A colossal Seebeck coefficient for an intermetallic compounnd, $FeSb_2$, (about 45mV/K) has been reported [1,2], and the quasi-ballistic phonons dragging d electrons with large effective mass is demonstrate as the origin [3]. Although $FeSb_2$ is a strongly correlated semiconductor and has attarcted a lot of attention in the past years [4,5], the electronic and lattice properties of the iso-structural $RuSb_2$ is seldom reported. In this work, we measured the lattice structure, electric conductivity, specific heat, magnetic susceptibility and Hall effect of $RuSb_2$. Not only the electron activation process is analyzed, but also the low frequency Debye vibrational modes and relatively high Einstein vibration modes are considered with the combination of DFT calculation.

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Abstract number: AS-O.2-11

The atomic vibration distribution and soft anharmonic phonons in Zintl compounds SrB(Cu,Ag,$Zn_{0.5}$)Sb

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Zintl compounds are considered to be potential thermoelectric materials due to their “phonon glass electron crystal” (PGEC) structure. Here, we report a comprehensive analysis of phonons in the series of Zintl phase 1-1-1 type SrB(Cu,Ag,$Zn_{0.5}$)Sb (P63/mmc) [1,2] based on neutron scattering and density functional theory(DFT) calculations and show that the anomalously low κ_l of $SrZn_{0.5}Sb$ has inherent phononic origins. The neutron diffraction data presents that the 50% vacancies of the $SrZn_{0.5}Sb$ would lead to tighter bonding between layers, which makes similar atomic vibrational temperature stability with SrAgSb, meanwhile, $SrZn_{0.5}Sb$ exhibits most of the atomic vibration distribution of SrCuSb due to close electronic environment and ion mass to monovalent Cu^+. In the analysis of inelastic neutron scattering density-of-state (DOS) data, we find that only the optical branch of these three materials changes significantly with temperature, and the acoustic energy of $SrZn_{0.5}Sb$ and SrAgSb are very low. Combined with DFT calculations, it is found that the acoustic branch and the optical branch overlap seriously, which suggests the acoustic-optic interaction and induces anharmonicity. Combined with the estimated large Grüneisen parameter of $SrZn_{0.5}Sb$ and the deviation of the specific heat of the three materials deduced from the DOS data and the experimental data at high temperature, it is proved that there exists a strong anharmonicity. Hence, these results provide key insights into manipulating phonon scattering without relying on traditional equivalence doping.

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Abstract number: AS-O.2-12

The coexistence of Brittleness and Plasticity in $Ag_2Te_{1-x}S_x$ inorganic Thermoelectric Semiconductors

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The $Ag_2Te_{1-x}S_x$ semiconductors with an amorphous main phase have recently been reported to exhibit plastic deformation with a compressive strain reaching 25% [1-4]. However, we found both brittleness and superior plasticity can exist in $Ag_2Te_{1-x}S_x$ and they can reversibly transform if tuning the phase structure. Here, we investigated the transformation between brittleness and plasticity in $Ag_2Te_{1-x}S_x$. We found that the as-prepared $Ag_2Te_{1-x}S_x$ ingots can exhibit a brittle behavior, while exceptional plasticity with a giant compressive strain is observed if a different phase dominates. In addition, a brittleness-to-plasticity transformation in $Ag_2Te_{1-x}S_x$ can be realized. This study uncovers the influence of phase structure on mechanical properties and proposes an efficient method to ensure the exceptional plasticity of $Ag_2Te_{1-x}S_x$, facilitating its prospect application in flexible/wearable electronics.

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Abstract number: AS-O.2-13

Constructing Ag_2Se/CNTs Nanocomposites with Enhanced Thermoelectric and Mechanical Performance

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Silver selenide (Ag_2Se) is emerging as an intriguing material for thermoelectric refrigeration and energy harvesting at near room temperature. However, the syntheses of Ag_2Se commonly require energy-intensive, high-temperature melting-annealing processes. Herein, we have developed a general surfactant-free and scalable solution synthesis strategy to nano/micro-particles of Ag_2Se, which requires neither high temperature nor long reaction duration. By modifying the Ag^+/Se^{2-} molar ratios in the solution precursors, the thermoelectric properties of Ag_2Se have been effectively optimized, leading to a maximum zT value of 0.84 at 380 K. Furthermore, to promote the practical applications of Ag_2Se, it is imperative to further depress its lattice thermal conductivity (κ_L) and enhance its mechanical properties. Therefore, through in situ solution synthesis combined with fast sintering, a series of Ag_2Se/carbon nanotubes (CNTs) nanocomposites are controllably constructed. Tuning the concentration of CNTs effectively optimizes the transport and mechanical properties simultaneously. Finally, Ag_2Se/CNTs nanocomposite with 0.5 wt% CNTs obtains an exceptional peak zT of 0.97 at 375 K and a compressive strength of 99.5 MPa. This study provides a general surfactant-free solution approach to silver selenide nano/micro-materials and develops an effective strategy to construct Ag_2Se/CNTs nanocomposites, which advances both thermoelectric and mechanical performance.

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Abstract number: AS-O.2-14

Thermoelectric and Mechanical Properties of Ag_2Se-based alloys

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Silver chalcogenides and their alloys exhibit tunable transport properties and decent mechanical properties, which can be used in next-generation flexible electronics. Among them, Ag_2S and its alloys demonstrate excellent thermoelectric (TE) performance and high plasticity, $Ag_2S_{0.5}Se_{0.5}$ and $Ag_{20}S_7Te_3$ to name a few; Ag_2Se shows the highest TE property but little plasticity compared to Ag_2S. Alloying S and Te into Ag_2Se is a promising way to simultaneously optimize TE properties and mechanical performance. Detailed composition-related performance of Ag_2X pseudo-ternary materials remains unclear. In this research, a serious of $Ag_2Se_{1-x}Te_x$ and $Ag_2Se_{1-x}(S_{0.5}Te_{0.5})_x$ (x = 0-1) polycrystalline materials are synthesized by melting and SPS mentioned. The phase structure, TE properties and mechanical properties are investigated to illustrate the influence of alloying. The TE and mechanical performance show a strong correlation with phase structure. The Ag_2Se orthorhombic phase exhibits good TE properties but with brittle mechanical behavior. Ag_2S cubic phase, on the other hand, performs excellent plasticity and decent TE properties with a wild temperature range. Our research enriches the pseudo-ternary phase diagram of the Ag_2S-Ag_2Se-Ag_2Te system. The results show that the pseudo-ternary cubic phase exhibits tunable TE performance and excellent mechanical properties, which provides a serious material composition for further performance optimization.

Abstract number: AS-O.2-15

High-Performance Ag_2Se-based Flexible Thermoelectric Film for Wearable Electronics Power Supply

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Flexible thermoelectric generators (TEGs) are attractive for their ability to power wearable electronics continuously by utilizing the temperature difference between the human body and the environment. Herein, we present a flexible TEG assembled with high-performance Ag_2Se films. A room-temperature power factor as high as 20.8 μW cm^{-1} K^{-2} was obtained after optimizing the carrier concentration and effective mass via isoelectronic doping of Cu. The relative change in the resistance of the film is less than 5% of the initial value after 1000 times of bending. The 6-leg flexible thermoelectric generator demonstrates a maximum output power of 1.1 μW and a maximum power density of 80 W m^{-2} at a temperature difference of 50 K, surpassing all the other reported Ag_2Se-based TEGs. The output voltage of 1.5-2.8 mV can be achieved as dressed on the arm in different motion states. These results demonstrate the promising application of Ag_2Se-based flexible thermoelectric generators in wearable electronics.

Abstract number: AS-O.2-16

Thermal conductivity reduction and thermoelectric performance improvement in Cu-Ni alloy

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It has been a long-time challenge for Cu-Ni based alloys to achieve satisfactory thermoelectric performance, due to their high thermal conductivity. Herein, in order to reduce the thermal conductivity in $Cu_{70}Ni_{30}$, rolling bulks at room temperature and spark plasma sintering (SPS) melt-spun ribbons are used respectively. The rolling process introduces refined grains and twin boundaries. Those increased interface decreases the thermal conductivity by 15.1 % when the rolling reduction ratio is 94%. Since the power factor is 8.0 mW $m^{-1}K^{-2}$ attributed to the slightly improved Seebeck coefficient, an increase of 30% in zT is achieved, with the value reaching 0.14 at 573 K. Meanwhile, a multi-interface structure is constructed in the SPS samples. A 76.1% reduced thermal conductivity (~ 7.7 W $m^{-1}K^{-1}$) is obtained, which is 71.8 % lower than the rolling process. It is attributed that a variety of formed micron-scale interfaces scatter phonons in the broadband frequency range. The power factor is 4.1 mW $m^{-1}K^{-2}$ but the Seebeck coefficients of the as-sintered bulks are maintained, due to the simultaneously decreased charge effective mass and carrier concentration. A zT ~0.24 at 573 K is obtained, which is 130.3% higher than the pristine counterpart. Our work demonstrates that improved thermoelectric performance in Cu-Ni based alloys can be obtained by creating various interfacial defects even at micron scales, which paves the way to suppress thermal conductivity largely in metallic thermoelectric materials via sintering melt-spun ribbons directly or largely deforming the bulks at room temperature [1].

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Abstract number: AS-O.2-17

Thermoelectric Transport Properties of $TmAg_xCu_{1-x}Te_2$ solid solutions

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Ternary rare-earth copper-containing tellurides usually show semiconducting behavior and come with a richness in both composition and crystal structure, suggesting the possibility for potential thermoelectric applications [1-4]. Among these ternary compounds, $TmCuTe_2$, crystallized in a *P-3m1* (164) structure, is particularly interesting because of its intrinsic partial occupation at the Cu sites for an extremely low lattice thermal conductivity, which leads this material to be a promising candidate for thermoelectric applications [5]. This work focus on the electronic and phononic transport properties of $TmCuTe_2$ with Ag-alloying on the Cu site. Such a Ag/Cu substitution is found to enable a decrease in Hall carrier concentration from 14×10^{19} to 8×10^{19} cm^{-3} for an evaluation of the charge transport based on a single parabolic band (SPB) model with acoustic scattering. In addition, Ag-substitution simultaneously introduces Cu/Ag point defects for extra phonon scattering, leading the lattice thermal conductivity to be as low as ~0.25 W/m-K in a broad temperature. The optimization in carrier concentration and the reduction in lattice thermal conductivity contribute to a ~40% improvement in average thermoelectric figure of merit (zT). The determination of band parameters enables a guidance for further advancements in this promising thermoelectric material.

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Abstract number: AS-O.2-18

Synergic enhanced thermoelectric power factor and phase stability of tin-based perovskites by A-site cation engineering

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Tin-based halide perovskites are promising room-temperature thermoelectric materials due to their ultra-low thermal conductivity and propensity for doping. However, poor phase stability and inferior electrical transport properties are obstacles in their practical application. Herein, we found A-site formamidine (FA) doping, which is not possible by high-temperature processing, could simultaneously enhance the stability and electrical conductivity of $CsSnI_3$ films through simple solution process. The carrier concentration of 3×10^{19} cm^{-3} was obtained in FA doped films, which leads to 8-times enhancement in electrical conductivity to 26.5 Scm^{-1} but maintains a Seebeck coefficient as high as 131 μVK^{-1}, resulting in a power factor of 45.53 $\mu Wm^{-1}K^{-2}$. Further theoretical calculation shows that the enhanced carrier concentration originates from the lower transition energy of tin vacancies in the doped film. More importantly, remarkable phase stabilization of FA doped films is achieved under ambient atmosphere, which stems from entropic gains by FA doping. This work suggests A-site doping by facile solution processing is an avenue for synergic improving thermoelectric power factor and phase stability of tin-based halide perovskites, and appliable for flexible and wearable thermoelectric generators to harvest energy from low-grade heat sources.

Abstract number: AS-O.3-01

Advances in the design and assembly of flexible thermoelectric device

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Owing to their capabilities of solid-state conversion between heat and electricity, zero-emission, and high flexibility, flexible thermoelectric devices (F-TEDs) have exhibited great application possibilities for both portable power generation and localized refrigeration. However, with the rapid development of thermoelectric science and technology, there is still a lack of comprehensive review on the rational design of F-TEDs from the fundamentals to structures, which critically determines the performance and conformality of F-TEDs. To address this issue, here, we timely overview the latest progress on the up-to-the-date F-TEDs with their unique designs. We carefully summarize the structure-related principles and factors that determine the performance of F-TEDs and the advanced strategies for improving their utilities. Besides, we focus on the timeliest designs for the inorganic-based devices, organic-based devices, and hybrid-based devices targeting both power generation and refrigeration. In the end, we point out the current challenges, controversies, and prospects of F-TEDs.

Abstract number: AS-O.3-02

Thermoelectrics for medical applications: progress, challenges, and perspectives

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Thermoelectrics, enabling the direct conversion between heat and electrical energy, exhibit great potentials for employing to localized power generation and refrigeration. Their unique characteristics, such as tunable dimension, noiselessness, stability, and portability, make thermoelectrics suitable for medication-related applications. Thermoelectric applications in medicine have received increasing attention in recent years, but the research is extensive and therefore a review is needed for a systematic summary. Here, we report a timely and comprehensive review on the field of thermoelectric-assisted related materials and their medical devices, including thermoelectric power generators and thermoelectric coolers. Different medication-related thermoelectric devices are illustrated in detail, and their underlying mechanisms are discussed. In the end, we point out the challenges and future directions on medication-related thermoelectrics. This review can act as a useful tool for guiding the design of thermoelectrics with various medical applications.

Abstract number: AS-O.3-03

Understanding of Thermoelectric Coolers for Micro-chip Application

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Compared with traditional active cooling methods, thermoelectric coolers are more accessible to be integrated with electronics as an effective thermal management solution due to their reliability, silence, compatibility, and controllability. Considering the rapid development of processors and chips in electronics, this work comprehensively reviews the progress of state-of-the-art on-chip thermoelectric coolers and summarizes the related fundamentals, materials, designs, and system logic. Particularly, we highlight on-chip thermoelectric coolers with self-cooling design and on-demand requirement. In the end, we point out current challenges and opportunities for future improvement of designs, performance, and applications of on-chip thermoelectric coolers.

Abstract number: AS-O.3-04

A solvothermal synthetic environmental design for high-performance SnSe

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SnSe is challenging for employing in thermoelectric devices due to difficulties in simultaneously optimizing its thermoelectric and mechanical properties. Here we show a unique solvothermal synthetic environmental design to fabricate super-large and micro/nanoporous $Sn_{0.965}Se$ microplates by using $CrCl_3$. Cl- ions trigger the Sn-vacancy formation and optimize the hole concentration to ~3×10^{19} cm^{-3}, while the as-formed $Cr(OH)_3$ colloidal precipitations act as "templates" to achieve micro/nanoporous features, leading to low lattice thermal conductivity of ~0.2 $W\,m^{-1}K^{-1}$ in the as-sintered polycrystal, contributing to a high *ZT* of ~2.4 at 823 K and an average *ZT* of ~1.1. Particularly, the polycrystal exhibits high hardness (~2.26 GPa) and compression strength (~109 MPa), indicating great potential for applying to practical thermoelectric devices.

Abstract number: AS-O.3-05

Synergistic Texturing and Bi/Sb-Te Anti-site Doping Induce High Thermoelectric Performance in $Bi_{0.5}Sb_{1.5}Te_3$-based Thin Films

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Bi_2Te_3-based thin films are attracting increasing attention due to their considerable wearability and flexibility feature. However, the relatively low performance compared to their bulk counterparts limits their development and wider application. In this work, we use synergistic texturing and Bi/Sb-Te anti-site doping to achieve a high room-temperature *ZT* of ~1.5 in *p*-type $Bi_{0.5}Sb_{1.5}Te_3$ thin film by a magnetron sputtering method. Structural characterization confirms that carefully tuning the deposition temperature can strengthen the texture of as-prepared polycrystalline $Bi_{0.5}Sb_{1.5}Te_3$ thin films, leading to significantly enhanced carrier mobility and electrical conductivity. Simultaneously, rational engineering of the deposition temperature can induce anti-site doping between Bi/Sb and Te, which can reduce the carrier concentration and make it closer to the optimized level. In turn, a high power factor of 45.3 μW $cm^{-1}K^{-2}$ and a maximized *ZT* of ~1.5 at room temperature are obtained. These high power factor and *ZT* are highly competitive to other state-of-the-art *p*-type thin-film-based thermoelectric materials, showing great potentials for practical applications.

Abstract number: AS-O.3-06

Thermoelectric energy harvesting as a means to power IoT sensors for safer manufacturing environements

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The ever-growing demand for innovative manufacturing has led to the development of Industry 4.0 (i4.0), which includes IoT sensor networks able to monitor manufacturing environments, such as conditions within modern factories. . Battery power is the one drawback when a network of multiple i4.0 IoT sensors is deployed, as it restricts these sensors from achieving true fit-and-forget connectivity, while also placing significant replacement/re-charging burdens on a factory.

The talk will discuss the feasibility of a new thermoelectric generator (TEG) system that will be implemented in a research Nano-brewery at UTS to power a CO_2 sensor by harvesting the waste heat from the brewery kettle's stainless steel outlet pipe, which reaches 90°C. The physical system was designed based on temperature difference across hot- and cold-side faces derived from computational modelling as 16°C. Peakpower generation is approximately 1200 mW. The system will utilize the CO_2 sensor to monitor concentrations within the brewery. A discussion of the TEG power with respect to temperature and force (of application on the pipe) will be presented to validate the system's feasibility.

Abstract number: AS-O.4-01

Structural and spectroscopic studies of Se doped SnTe for thermoelectric applications

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SnTe is an efficient thermoelectric material in mid temperature range (500-900 K). However its high carrier concentration and small band gap limits the overall performance of the thermoelectric device. Pristine and Se doped SnTe were synthesized using solvothermal method to improve its thermoelectric properties. Pristine SnTe has FCC crystal structure with space group *Fm-3m*. Secondary phase of SnSe was observed in 3% Se doped SnTe material. Increase in lattice strains and lattice defects were observed in Se doped SnTe. Nanoparticle formation is confirmed using FESEM micrographs. Heat carrying Phonons scatter at the interfaces of nanoparticles, secondary phase and lattice defects. The scattering of phonons reduces lattice thermal conductivity. Raman shift is observed towards higher wavenumber in Se doped SnTe. Band gap increases after Se doping in SnTe. Increase in band gap may enhance power factor ($S^2\sigma$). Hence Se doping can enhance figure of merit (ZT) of SnTe with widening of band gap and reduction of lattice thermal conductivity. Therefore, Se doped SnTe can be a potential material for thermoelectric applications.

Abstract number: AS-O.4-02

High power factor of layered Ag_2Se via tuning the carrier concentration by induced cation vacancies for thermoelectric applications

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Non-stoichiometric $Ag_{2-x}Se$ is a promising thermoelectric (TE) candidate for room-temperature applications due to its intrinsically high performance in 300-423 K. For this study, we report the TE properties of nanostructured Ag deficient Ag_2Se synthesized by using hydrothermal method followed by hot press densification method. The effect of Ag deficiency and their TE properties by the variation in carrier concentration is scientifically investigated. The scope of this work is to increase the carrier concentration (*n*) resulting in increased TE performance at room temperature (*RT*). Additionally, we calculate the density of states effective mass increases with decreasing Ag content, which should enhance the experimentally maximum *zT* 0.43 at 393 K for $Ag_{1.99}Se$. Meanwhile, complex nanostructures including nanograins, dislocations, grain boundaries, and lattice distortions have been observed in binary $Ag_{2-x}Se$. These nanostructures strengthen phonon scattering and in turn lead to low thermal conductivity (κ) in the range of 0.9–1.1 W $m^{-1}K^{-1}$ in $Ag_{2-x}Se$ at 303 K. This study indicates that Ag deficient $Ag_{2-x}Se$ is a promising candidate for *RT* thermoelectric applications.

Abstract number: AS-O.4-03

Effect of nano-structuring on the thermoelectric performance in polycrystalline Bi_2Se_3

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Bi_2Se_3 is an important semiconducting material with excellent thermoelectric properties from room temperature to intermediate temperature region. Herein, we report the effect of nanostructuring on the thermoelectric properties of Bi_2Se_3 compound, synthesized through vacuum melting method followed by hot-press densification technique. The low lattice thermal conductivity and improved electrical properties synergistically boost the thermoelectric performance of Bi_2Se_3. The HR-TEM and IFFT pattern exposes the presence of dense stacking faults. These highly dense stacking faults contributes as a phonon scattering centers, which effectively scattered the heat carriers, results in extremely low lattice thermal conductivity of 0.2 W/mK at 543 K. On the other hand, the contribution of phonon-phonon scattering primarily reduced the lattice thermal conductivity at elevated temperatures. Moreover, the enhancement of Seebeck coefficient plays an vibrant role in improving the power factor of 388 $\mu W/mK^2$ at 543 K. The synergistic combination of low thermal conductivity and the maximum power factor helps to achieve the high peak zT of 0.32 at 543 K.

Abstract number: AS-O.4-04

Enhanced Thermoelectric Performance of Polycrystalline SnSe Via Double Doping of Al/Te

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SnSe-based thermoelectric materials are being investigated since they have potential high thermoelectric figure of merit. Herein, we report the synthesis of $Sn_{1-x}Al_xSe$ (x = 0.01, 0.02, 0.03 and 0.04) solid solutions prepared by one-step ball-milling. To investigate the influence of Al doping on their TE performance, as-prepared powder samples were hot-pressed at 773 K. The effect of XRD and HRTEM analyses confirmed the size reduction and the presence of amorphous regions with polycrystalline behavior of the samples can effectively adjust the band structure of SnSe by introducing intermediate band. Our study shows that the introduction of Al has a mild effect in increasing the resonance level owing to increase the power factor and large effective mass. In addition, Al dopant can adjust the anisotropy of polycrystalline SnSe. In high temperature region (498 K < T < 823 K), the electronic transport properties significantly enhance with thermal excitation. The high Seebeck coefficient with optimum carrier concentration and low thermal conductivity was achieved due to wide range of phonon scattering . The results suggested that $Sn_{1-x}Al_xSe$ is a promising candidate for highly efficient thermoelectric material.

Abstract number: AS-O.4-05

A thorough descriptor search to machine learn the lattice thermal conductivity of half-Heusler compounds

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Predicting the lattice thermal conductivity (κ_L) of compounds prior synthesis is an extremely challenging task because of complexity associated with determining the phonon scattering lifetimes for underlying normal and Umklapp processes. An accurate ab-initio prediction is computationally very expensive, and hence one seeks for data-driven alternatives. We perform machine learning (ML) on theoretically computed κ_L of half-Heusler (HH) compounds. An exhaustive descriptor list comprising of elemental and compound descriptors is used to build several ML models. We find that ML models built with compound descriptors can reach high accuracy with fewer number of descriptors, while a set of large number of elemental descriptors may be used to tune the performance of the model as accurately. Thereby, using only the elemental descriptors, we build a model with exceptionally high accuracy (with R^2 score of ~0.98/0.97 for train/test set) using one of the compressed sensing techniques. This work, while unfolding the complex interplay of the descriptors in different dimensions, reveals the competence of the readily available descriptors elemental descriptors in building a robust model for predicting the κ_L.

Abstract number: AS-O.4-06

Probing Chalcogen atom based Half Heusler Alloys for Thermoelectric Application - from First-principles calculations

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In this work, our main motivation is to study the thermoelectric properties (TEP), namely, Seebeck coefficient (*S*) and power factor (*PF*) of a host of chalcogen atom based Half Heusler alloys (HHAs), predicted to be energetically and lattice-dynamically stable for the first time. We have carried out first principles calculations based on density functional theory (DFT). In order to be a good TE material, higher values of *S* and *PF* are required, which in turn requires high valley degeneracy, i.e a number of bands in the proximity of VBM and CBM. Band structure and constant energy surface reveal that most of these chalcogen based HHAs have a higher value of valley degeneracy, compared to the well known HHAs, for example, TiNiSn. A high band-convergence without any external doping gives them an edge for thermoelectric applications. Further, we have calculated the transport properties based on semi-classical Boltzmann transport equation. We have observed 50%-100% enhancement in the value of PF compared to TiNiSn. In addition to the electronic properties, a lower value of thermal conductivity is also required to enhance the performance of a thermoelectric device. Phonon-dispersion curves of these materials reveal intermixing of acoustic and optical phonons, which typically leads to a lower value of thermal conductivity. All these properties make these chalcogen based HHAs promising candidates to be extensively probed for thermoelectric applications.

Abstract number: AS-O.4-07

Spin-driven Thermoelectrics: Short-Range Magnetic Order in Self Consistent Spin-Wave Theory

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The thermopower of some antiferromagnetic materials significantly increases near the Neel temperature (*TN*) due to the magnon-electron drag. The remarkable observation happens when the temperature exceeds *TN*, and the long-range magnetic order is lost. For example, the experimental data of manganese telluride (MnTe), with *TN* ≈ 305 K, shows that the thermopower keeps its high magnitude at temperature up to 900 K, indicating that the drag thermopower has persevered into the paramagnetic phase. It has been hypothesized that short-range magnetic order (SRO) above TN creates a carrier drag similar to the magnon-drag thermopower, namely a paramagnon drag thermopower. Here, a version of the self-consistent spin-wave theory quantifies the SRO and the correlation for layered antiferromagnetic materials in the Heisenberg model. This approach diagonalizes the Hamiltonian by considering the Baryakhtar-Krivoruchko-Jablonsky (BKJ) representation of spin operators via bosons and pseudofermions and using a mean-field approximation for decoupling of the quartic terms in the transformed Hamiltonian, applicable to both the ordered and the disordered phases. We prove the existence of a robust SRO above TN that extends deep into the paramagnetic domain. Comparing these theoretical results, the thermopower experimental data, and the paramagnon lifetimes from Inelastic Neutron Scattering indicates that the SRO correlates with the MnTe thermopower enhancement above *TN*.

Abstract number: AS-O.4-08

Sb-Bi_2Te_3 Based Flexible Thermoelectric Generator with High Power Density for Wearable Energy Harvesting Applications

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The ability of flexible thermoelectric (TE) generators to convert waste heat into electricity, which can then be used to power wearable gadgets, has garnered a significant deal of attention in recent years. Although organic thin-film TE materials are a common option when it comes to the preparation of flexible TE generators, these materials suffer from low TE performance since their figures of merit (zT) are so low. As part of this research, a flexible TE generator was fabricated using elemental thin films of Sb (p-type) and Bi_2Te_3 (n-type) on a plastic substrate. With a temperature gradient of 50 K, this generator demonstrated both a high-power factor and a high-power density. This research contributes to the design paradigm of TE generators for wearable devices by serving as a guide.

Abstract number: AS-O.4-09

Solid-liquid Based Hybrid Thermoelectric Systems

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The performance of thermoelectric (TE) materials has been improved in recent years by a significant reduction of the thermal conductivity. This parameter has now reached its amorphous limit, which makes the enlargement of the power factor (*PF*) critical. In this work, we fabricated a hybrid system on a paper substrate using Bi_2Te_3 thin film that is permeated by an electrolyte. The significant improvement in *PF* is attributed to the alteration of the electrostatic environment of the porous film that occurs as a result of the presence of ions in the electrolyte at the solid–liquid interface. These findings establish a new approach for the major improvement of the *PF*.

Abstract number: AS-O.4-10

Thermoelectric application of tungsten Disulfide (WS_2) thin-film grown in Chemical Vapor Deposition

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The advancement in technology is growing faster irrespective of the available energy resources. The next-generation needs a sustainable resource which is inevitable. Thermoelectrics, an energy transformation technique, recently attracted the researchers by showing continuous growth in its efficiency, tungsten disulfide (WS_2), a two-dimensional transition metal dichalcogenide, is identified as an auspicious thermoelectric material for its low thermal conductivity (κ) and better Seebeck coefficient (S) and also for its environmental stability. Atomically thin sheets of WS_2 shows high in-plane carrier mobility and transition of indirect to direct bandgap. In this work, we have deposited WS_2 thin films on SiO_2/Si wafer by atmospheric pressure chemical vapor deposition technique in a single-step process. The optical microscopy analysis shows as-grown triangular shaped WS_2. The Raman spectra shows first-order modes: LA(M) at 175 cm^{-1}, E^1_{2g} at 355 cm^{-1} and A_{1g} at 420 cm^{-1}. The thermoelectric measurements show the better thermoelectric performance and further the results will be discussed in detail.

Abstract number: AS-O.4-11

Chemical Vapor Transport Fabrication of MoS_2 via Double-Step Sulphurization for Thermoelectric Applications

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Thermoelectricity, in nanoscale dimension has gained attention as a potential platform for micro-chip energy harvesting technologies. An atomically thin layer, two-dimensional (2D) transition metal dichalcogenides (TMDCs), in particular molybdenum disulphide (MoS_2) can be considered as a promising materials over decades due to its superior electrical and phonon transport properties. Moreover, confining materials to quantum size will increase the sharp density of states near the Fermi level and it will enhance the Seebeck coefficient (S) and electrical conductivity (σ) simultaneously which is a major interdependent problem in thermoelectricity (Power factor $PF = S^2\sigma$). In this work, we deposited the molybdenum disulfide (MoS_2) thin films on SiO_2/Si substrate by single step and double sulfurization process through vapor phase transport. From the vibrational analysis, the deposited films were confirmed as MoS_2 by the presence characteristic peaks at 384.9 cm^{-1} (E^1_{2g}) and 411.8 cm^{-1} (A_{1g}) with frequency difference of $\Delta\omega$ = 26 cm^{-1}. The morphology analysis revealed that the single-step sulfurization process has the triangle and a six edge star shape, whereas the double-step sulfurization process has vertical nanosheets along with rods are obtained. The thermoelectric characterizations showed the better performance of deposited MoS_2. Further, the results will be discussed in detail.

Abstract number: AS-O.4-12

Incorporation of MXene in Perovskite oxide for thermoelectric power generation

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The energy conversion efficiency of thermoelectric materials has been enormously improved by making their nanocomposites. In our work, we have used 2D material MXene as reinforcement to enhance the composite material's figure of merit (*ZT*). We have synthesized $Ti_3C_2T_x$ MXene by selectively etching out the Al layer from the Ti_3AlC_2 MAX phase by a one-pot synthesis route. Nano-layered sheets of MXene have been incorporated into the matrix of perovskite oxide $SrTi_{0.85}Nb_{0.15}O_3$ by Spark Plasma Sintering (SPS) route. Thermoelectric properties such as electrical conductivity, Seebeck coefficient, and thermal conductivity have been measured in the temperature range from 323 K to 921 K. MXene incorporation has shown significant improvement in the power factor and thermoelectric figure of merit of these nanocomposites. Transport properties of these composites have been analyzed in correlation with XRD, XPS, SEM, TEM, and Raman spectra.

Abstract number: AS-O.4-13

Environment Friendly $Sr_{2-x}Bi_xCoRuO_6$ ($0 \leq x \leq 0.8$) Double Perovskite Oxide Materials for High-Temperature Thermoelectric Application

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A series of $Sr_{2-x}Bi_xCoRuO_6$ ($0 \leq x \leq 0.8$) double perovskites have been synthesized in air by a traditional solid state chemistry method at 1200 ºC. Powder X-ray diffraction data (x = 0.0, 0.2, 0.4, 0.6 and 0.8) show that all the samples are phase pure and adopt monclinic crystal structure with space group I2/c. Scanning electron micrographs (SEM) show uniform distribution of micron size particles in all samples. Energy dispersive spectroscopy microanalysis (EDS) confirms the chemical homogeneity and elemental compositions of all samples. Thermogravimetric analysis (TGA) suggests the formation of oxygen vacancies in all the $Sr_{2-x}Bi_xCoRuO_6$ materials. Magnetic measurements on vibrating sample magnetometer (VSM) indicate an antiferromagnetic ordering below Neel temperature *TN* = 70 K in most of the oxide samples. However, the x = 0.2 sample shows ferromagnetic domains characterized by a Curie temperature of *TC* = 280 K.

Abstract number: AS-O.5-01

Thermoelectric properties enhancement in *n*-type NbFeSb via defect resonant state engineering

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The *p*-type NbFeSb Half-Heusler compound has been proved to be promising for high-temperature thermoelectric applications. However, its corresponding *n*-type alloys harbor a fairly low *ZT*, which extremely hamper its realistic applications due to the asymmetrical thermoelectric performance. In this work, using first-principles calculations, we systematically investigate the defect effect on enhancing its thermoelectric performance and in theory pave the way to narrow the gap between both the *n*- and *p*-type. For its intrinsic defects, donor-like FeNb antistites and Fei interstitials have low formation energies with the energy-favorable for the *n*-type conductivity. As for the extrinsic defects, with high-throughput screening in the Periodic Table, we identify optimal dopants with low formation energy, which will benefit future experiments. We find by the CoNb dopant the power factor can be boosted to 3 times of pure NbFeSb at room temperature due to the strong resonant effect. Additionally, the doping of F/Cl/P/S at Sb sites with low formation energies have large disorder scattering parameters that can decrease at least half of lattice thermal conductivity by mass and stress fluctuations. Our work reinforces motivation for the exploration of *n*-type NbFeSb materials and especially in tandem with high-throughput defect calculations advance effective dopants in this system

Abstract number: AS-O.5-02

Thermoelectric properties and phonon transport mechanism of ZrCoSb-based triple half-Heusler alloys

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Inspired by double half-Heusler (HH) compounds [1] and entropy enginering [2], this study proposes a new concept to realize a low thermal conductivity in HH compounds and develop triple HH compounds via entropy engineering. The n-type medium-entropy $M_{1-x}N_xCoSb$ (M = Zr, Ti, Hf; N = V, Ta, equimolar) triple HH compounds are prepared via levitation melting and spark plasma sintering. Entropy engineering induced Zr-site disorder is characterized via the Raman spectroscopy. Subsequently, the thermal conductivity of the n-type $M_{0.9}N_{0.1}CoSb$ triple HH compound (4.1 $Wm^{-1}K^{-1}$) at 323 K is less than ~67.5% that of the ZrCoSb HH compound (12.6 $Wm^{-1}K^{-1}$). Furthermore, the Zr-site donor doping considerably improved the power factor, affording a peak figure of merit of ~0.18 for the $M_{0.9}N_{0.1}CoSb$ HH compound at 923 K. This approach proposes a new pathway to lower the thermal conductivity of HH compounds, establishing a high standard for developing high-performance HH compounds.

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Abstract number: AS-O.5-03

Simplification of Slater-Pauling Rule in the Heusler System

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The Slater-Pauling (S-P) rule is used to conveniently describe the regularity of the magnetic moment with the number of valence electrons. According to the S-P rule, the half-Heusler (HH) and full-Heusler (FH) alloys exhibit semiconductor behavior when they have 18 electrons and 24 electrons, respectively. Based on the well-studied *18-e* HH compound NbFeSb, we mix the corresponding *17-e* and *19-e* systems to construct the novel 18-e compounds. Owing to the merging valence band maximum in *17*-e NbMnSb and *19-e* NbCoSb, the $Nb_4Mn_2Co_2Sb_4$ mixture possesses high band degeneracy (*NL* = 16) and significantly boosts the Seebeck coefficient and the power factor, much higher than those of NbFeSb. In the Heusler system, in addition to the HH and FH with integer stoichiometric of 1:1:1 and 1:2:1, there is a class of “S-P semiconductors” with stoichiometric between HH and FH, the valence electron number does not meet “the rule of 18 or 24”, which still exhibit semiconductor behavior. We further investigate two Heusler systems, Ti-Fe-Sb and M-Co-Sn (M = Ti, Zr, Hf), by cluster expansion method, and discovered a new class of “S-P semiconductor”. We have discussed the origin of the bandgap in “S-P semiconductor” by molecular orbital theory, and simplified the S-P rule to be suitable for the Heusler system. Our work not only provides guidance for the experimental discovery of new stable systems, but also enriches the application of Heusler systems in the field of thermoelectricity.

Abstract number: AS-O.5-04

Computational study on the thermoelectric properties of single ZnO nanowire

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In this paper, four different diameters of Wurtzite-ZnO ⟨0001⟩ nanowires have been conducted a comprehensive study of their geometrical configuration, thermal transport properties, carrier transport capacity, and thermoelectric properties at T = 300 - 700 K.

We find that the difference in the energy band properties between the CBM and VBM of ZnO nanowires leads to 3.2-13 times higher *p*-type thermoelectric values than *n*-type. This is due to the multiple energy band structure at the VBM, energy bands of similar energy will all be involved in carrier transport, which is degeneracy effect. Degeneracy effect effectively enhances carrier transport, and the enhancement effect is more pronounced at elevated temperatures. Moreover, a turning point of diameter at 1.27 nm is found in the carrier transport and thermoelectric properties with increasing diameter. After the turning point, the carrier transport and thermoelectric properties monotonically rise with increasing diameter. It is suggested that this phenomenon is due to the enhanced phonon-electron scattering caused by the axial overlapping charge density distribution and the difference in symmetry due to the two configurations of ZnO nanowires.

Abstract number: AS-O.5-05

Ultra-low lattice thermal conductivity and promising thermoelectric figure of merit in borophene via chlorination

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Monolayer boron-based materials are of current interests due to its polymorphism. Herein, motivated by the recent experimental synthesis of semiconducting hydrogenated *α′*-borophene and the regulation of the physical properties in layered materials by surface functionalization, we study the thermal and electronic properties of α′-borophene with three different types of gas functional groups (H, F and Cl) based on first-principles and Boltzmann transport theory. It is found that α′-borophene can be well stabilized by fluorination and chlorination and maintain the semiconductor nature. More interestingly, when hydrogen is replaced with fluorine or chlorine, the lattice thermal conductivity changes from 24.3 $Wm^{-1}K^{-1}$ to 5.2 $Wm^{-1}K^{-1}$ or 0.73 $Wm^{-1}K^{-1}$ along armchair direction at 300 K, exhibiting a huge reduction by two orders of magnitude. The main reason is the decrease of both phonon group velocities and acoustic phonon relaxation time resulting from the strong phonon mode softening due to the weaken *B-B* bond strength and heavier atomic mass of fluorine and chlorine. Consequently, the chlorinated *α′*-borophene exhibits a high thermoelectric figure of merit ~2 at 300 K along armchair direction. Our study illustrates the importance of the modulation of transport properties by gas functional groups, which may promote the thermoelectric application of boron-based materials.

Abstract number: AS-O.5-06

Tunable Thermal Conductivity and Enhanced Thermoelectric Performance in Janus Transition-Metal Dichalcogenides Monolayers: The Role of Tensile Strain and Finite Size

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Janus transition-metal dichalcogenides (TMDCs) monolayer is a kind of promising 2D thermoelectric material, which contains different atoms on each side of its unit cell, and thus breaks the mirror symmetry. In this work, first-principles calculations combined with the phonon Boltzmann transport theory are used to investigate the thermal conductivity and thermoelectric properties of six different Janus TMDCs monolayers by considering the effects of tensile strain and finite size. First, the thermal conductivities of all six Janus monolayers are evaluated, in which PtSSe exhibits the highest lattice thermal conductivity (K_{ph}) of 104 W/m·K, and WTeSe shows the lowest K_{ph} of 18 W/m·K. It can be observed that the K_{ph} of MTeSe (M = Pt, W, and Mo) is significantly lower than that of MSSe, which is mainly due to the reduction of phonon lifetime. Moreover, the K_{ph} with different tensile strains is investigated. The results show that the K_{ph} of MSSe decreases monotonously with the increase of tensile strain. However, the K_{ph} for MTeSe exhibits unexpectedly nonmonotonic dependence on the tensile strain. By evaluating the relative contributions of the main factors affecting K_{ph}, we find that the different responses of K_{ph} to tensile strain are attributed to the phonon lifetime. Afterwards, shrinking the system size significantly limits the K_{ph} by excluding the contribution of long mean free path phonons. When the sample size is reduced to 0.1 μm, the K_{ph} of all systems decreases significantly. Finally, we evaluated the thermoelectric performance of all systems at room temperature. The maximum calculated room-temperature ZT value reaches 1.04 under the tensile strain of 10% and system size of 0.1 μm in the p-type PtSSe monolayer, which is 4 times higher than that of unstrained PtSSe monolayer with infinite length. Our findings show that the Janus TMDCs monolayer is a competitive candidate for thermoelectric applications, especially under tensile strain and finite size. This work was supported by the National Natural Science Foundation of China under Grant Nos. 51825604 and 52130604.

Abstract number: AS-O.5-07

The study of phonon-point-defect scattering using the spectrum energy density method

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Point defects exist widely in thermoelectric materials and are known to scatter phonons, result in reducing thermal conductivity. Based on the perturbation theory, Klemens calculated the scattering rate of phonons from point defects, including mass fluctuation scattering caused by atomic mass difference, force constant fluctuation scattering caused by interatomic force change, and strain fluctuation scattering caused by atomic radius difference. The intensity of these scattering processes is proportional to the fourth-order of the phonon frequency. Although the above scattering processes are independent, in experiments, it is necessary to adjust the relative scattering rate between them by a fitting parameter ϵ to obtain an excellent fitting result. Usually, this parameter varies widely (for example, 1~500). The spectrum energy density method based on molecular dynamics can obtain the phonon scattering rate in the crystal. Using the solid Argon as model material, we calculate the phonon scattering rate of models with different atomic mass changes and vacancy concentrations. We show the rate of the scattering processes changing with mass difference and defect concentration, and give the estimated value of the fitting parameter ϵ. The related results help to understand the phonon-point-defect scattering process and have important guiding significance for tuning the thermal conductivity of materials through alloying.

Abstract number: AS-O.5-08

Enhancing thermoelectric performance of *n*-type Cr or Nb-doped PbTe by compensating resonant level

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Introducing resonant levels is a potent strategy to improve the thermoelectric properties of the thermoelectric systems. However, the beneficial effect of resonant levels tends to be weakened with rising temperature for the PbTe system. This motivates us to introduce dynamic doping of Cu into Nb or Cr-doped *n*-type PbTe to achieve the fully optimized carrier transport over a wide temperature range. As a consequence, an extraordinary average *ZT* of ~ 1.02 and 1.01 in the range of 323 to 823 K are obtained in the n-type $Pb_{0.975}Cr_{0.025}Te$-0.2%Cu and $Pb_{0.975}Nb_{0.02}Sb_{0.005}Te-0.004Cu_2Te$. Meanwhile, to determine the underlying mechanism for the dramatic reduction in lattice thermal conductance, we employ comprehensive electron microscopy to reveal the underlying mechanism for the dramatic reduction in lattice thermal conductance. This work clarifies the fundamental Cr and Nb-doping mechanism in PbTe and demonstrates that dynamic Cu-doping engineering is an effective approach to boosting thermoelectric performance, which should be applied in other thermoelectric materials.

Abstract number: AS-O.5-09

Extraordinary Role of Elements with Temperature-Dependent Solubility for Improving Thermoelectrics in Valley-Modified *n*-PbTe Alloys

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The optimization of electronic performance for *n*-type PbTe with a single band transporting requires a nearly constant reduced Fermi level, which inspires the doping of elements with temperature-dependent solubility such as Cu/Ag in matrix *n*-type PbTe to achieve a carrier concentration strongly dependent on $\sim(m_d^*T)^{1.5}$. However, such role in carrier transport property is still under investigation. In this report, we focus on the effect of Cu/Ag on carrier transport in *n*-PbTe alloys with small bandwidth and distorted band. Based on the fact that Cu/Ag does not affect the band structure, Cu doping can alleviate the compromises among thermoelectric parameters through carrier mobility enhancement and self-optimization of carrier concentration, thereby significantly optimizing the thermoelectric performance of *n*-type PbTe-MnTe alloys near room temperature. In addition, Ag forms a nanostructure to establish a potential barrier with the matrix, and enhances energy-dependent carrier scattering through the energy filtering effect to further improve the Seebeck coefficient in *n*-type $Pb_{0.975}Cr_{0.025}Te$ with distorted band, while establishing a coherent interface to maintain relatively high carrier mobility, thereby achieving a substantial increase in peak figure of merit. Strategies discussed here are expected to provide a reference for designing high-peak or high-average performance thermoelectric materials.

Abstract number: AS-O.5-10

One-step fabrication of bulk SnTe thermoelectric material through self-propagating high-temperature synthesis in high-gravity field

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The conventional fabrication process of bulk thermoelectric materials involves multi-step processes, which is time and energy consumption, and restricts its large-scale application. Here, the bulk SnTe were prepared by a fast and one-step self-propagating high-temperature synthesis combing with high-gravity field (SHS-HG) and produces single-phase structures, which shortens the synthesis time from several days to a few seconds. The zT of the undoped SnTe sample reached 0.51 at 873 K, which are almost on par with other methods. Compared with the conventional synthesis methods, the SHS under high-gravity field technique shortens the synthesis time from several days to dozens of seconds and offers a fast, one-step way for producing bulk SnTe-based thermoelectric materials, which is more time-saving and more energy efficient.

Abstract number: AS-O.5-11

Boosting Thermoelectric Performance of SnTe by Band Manipulation and Mechanical Alloying

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SnTe-based materials have become attractive thermoelectric candidates in recent years due to the lead-free properties. However, it's a challenge to optimize the thermoelectric performance because of its large energy separation between light and heavy valence bands and high intrinsic lattice thermal conductivity. Herein, we deeply studied its electron-phonon transport relationship through band engineering, vacancy engineering and mechanical alloying, and have successfully produced a series of excellent SnTe-based materials.

(1) Trivalent Sb is introduced into SnTe-CdTe alloys, benefiting from band structure optimization caused by band flattening and convergence, the power factor has been significantly reinforced in the whole temperature range. In addition, abundant vacancy defects, substitution defects and impurity phases significantly reduce its lattice thermal conductivity (κ_L). An enhanced zT of ~1.1 has been achieved for $Sn_{0.83}Cd_{0.05}Sb_{0.12}Te$ at 823 K.

(2) With the aid of mechanical alloying, the composition and structure of SnTe-15%MnTe-2%Bi alloys have been significantly changed. The remarkable reduction of grain size as well as the formation of dense dislocations and nanoprecipitates effectively decrease κ_L. Adding the energy filtering effect at the precipitate-substrate interface, the figure of merit of SnTe-15%MnTe-2%Bi is dramatically increased to ~1.5 at 850 K.

(3) Based on Mn-doped SnTe-based materials, its lattice complexity is characterized. The results indicate that Mn precipitates prior to reaching solubility, and then splits into MnSn substitution and γ-MnTe hetero-phases via mechanical alloying. This unique crystallographic evolution of Mn as a "dynamic" dopant further quantitatively predicts its lower lattice thermal conductivity. These strategies provide the efficient routes to improve the thermoelectric performance, and establish mechanical alloying as a controllable synthesis method for high-performance thermoelectric materials.

Abstract number: AS-O.5-12

Achieving Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance in GeTe Alloys via Introducing Cu2Te Nanocrystals and Resonance Level Doping

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The binary compound of GeTe emerging as a potential medium-temperature thermoelectric material has drawn a great deal of attention. Here, we achieve ultralow lattice thermal conductivity and high thermoelectric performance in In and Cu codoped GeTe thermoelectics. In dopants improve the density of state near the surface of Fermi of GeTe by introducing resonance levels, producing remarkably enhancement of Seebeck coefficient. In and Cu codoping not only optimize carrier concentration but also substantially increases carrier mobility to a high value of 87 cm^2V^{-1} s^{-1} due to the diminution of Ge vacancies. The enhanced Seebeck coefficient and increase of carrier mobility help to achieve significant enhancement of *PF* in $Ge_{1.04-x-y}In_xCu_yTe$ series. Meanwhile, Cu_2Te nanocrystals and high density of dislocations cause strong phonon scattering, significantly diminishing lattice thermal conductivity. The lattice thermal conductivity reduced as low as 0.31 W $m^{-1}K^{-1}$ at 823 K, which is not only lower than the amorphous limit of GeTe but also competitive with those of thermoelectric materials with strong lattice anharmonicity or complex crystal structures. Consequently, a high *ZT* of 2.0 was achieved for $Ge_{0.9}In_{0.015}Cu_{0.125}Te$ by decoupling electron and phonon transport of GeTe. This work highlights the important of phonon engineering in advancing high performance GeTe thermoelectrics.

Abstract number: AS-O.5-13

Quasi-commercial production of SnS-based nanosheets with enhanced thermoelectric performance via a wet chemical synthesis

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Tin sulfide (SnS) is a low-cost, earth-abundant, and eco-friendly thermoelectric (TE) material whose layered orthorhombic structure is similar to that of SnSe; however, current studies on SnS are limited because of its difficult synthesis due to the use of volatile sulfur, and its thermoelectric figure of merit (zT) is also low because of its intrinsically low electrical conductivity. Herein, we present a facile wet chemical synthesis to prepare uniform and well-dispersed SnS nanosheet crystals. Low-rate initial production with 3.5 L solvent was performed to obtain high-quality crystals, and also to adapt the process to commercial preparation. The carrier concentrations were enhanced from 3.2×10^{18} cm^{-3} to 4.8×10^{19} cm^{-3} (at 873 K) step-by-step via increasing Sn vacancies, adding SnSe, and embedding Ag atoms. The maximum power factor (PF) at 873 K of 0.48×10^{-3} $W\cdot m^{-1}K^{-2}$ was achieved in the selenium-silver co-doped sample, which presented a state-of-the-art value for the polycrystalline SnS. Correspondingly, the lattice thermal conductivities (κ_L) decreased from 0.8 $W\cdot m^{-1}K^{-1}$ to 0.47 $W\cdot m^{-1}K^{-1}$ (at 873 K) due to enhanced phonon scattering. The highest zT was 0.80 at 873 K, which is about 5 or 6 times higher than those of the pristine SnS(1:1) or SnS(1:0.8) samples. These findings provide a novel method to prepare high-quality and high-performance TE semiconductors via a wet chemical synthesis.

Abstract number: AS-O.5-14

Realizing enhanced thermoelectric properties in Cu_2S-alloyed SnSe based composites produced via solution synthesis and sintering

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SnSe emerges as one of the most promising Te-free thermoelectric materials due to its strong anharmonicity and multiple valence band structure. Compositing has been proven effective in optimizing thermoelectric performance of various metal chalcogenides. We will present our results of thermoelectric performance of Cu_2S-alloyed polycrystalline SnSe-based composites fabricated *via* solution synthesis and sintering. The materials after the incorporation of Cu_2S become SnSe-based composites with Cu doping, S substitution and Cu_2SnSe_3 secondary phase. The power factor of SnSe can be tuned and enhanced at varied temperature ranges through adjusting the addition amount of Cu_2S. Meanwhile, the composites achieve suppressed lattice thermal conductivity, because the introduced point defects and SnSe/Cu_2SnSe_3 interfaces intensify phonon scattering. Consequently, SnSe-0.5%Cu_2S and SnSe-3%Cu_2S achieve a peak zT of 0.70 at 830 K (intermediate temperature range) and a highly increased zT of 0.28 at 473 K (low temperature range), respectively, which are ~130% and 200% of values reached by SnSe at the corresponding temperatures [1]. These results prove effective for thermoelectric performance optimization of SnSe at varied temperature ranges by the approach that combines compositing with elemental doping and substitution.

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Abstract number: AS-O.5-15

MXene as charge reservoir promotes the thermoelectric performance of metal dichalcogenide $SnSe_2$

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Metal dichalcogenides have attracted widespread attention in the field of energy related materials due to their unique layered structure [1]. However, as potential thermoelectric materials, their thermoelectric performance suffers from low electrical conductivity especially along out-of-plane direction [2]. Herein, two-dimensional MXene with metallic conductivity is introduced into $SnSe_2$ matrix as a carrier reservoir to alleviate the carrier shortage. Br-doped $SnSe_2/Ti_3C_2T_x$ composites are successfully fabricated by a hydrothermal method combined with solid-state synthesis. Compared with that of pristine $SnSe_2$, the carrier concentration of $SnSe_{1.97}Br_{0.03}$/0.40 wt% $Ti_3C_2T_x$ is enlarged by three orders of magnitude from 10^{17} cm^{-3} to 10^{20} cm^{-3}. Meanwhile, it is revealed that electrons transfer from the MXene layers into the $SnSe_2$ matrix facilitated by elevated temperature based on the first-principles calculations. Moreover, the addition of MXene introduces affluent phase interface, which effectively hinders the phonon transport and results in an ultralow lattice thermal conductivity of 0.33 W m^{-1} K^{-1}. Finally, a peak zT up to 0.9 is achieved along out-of-plane direction at 818 K in $SnSe_{1.97}Br_{0.03}$/0.40 wt% $Ti_3C_2T_x$ sample. These findings offer an available strategy to efficiently increase the carrier concentration of wide-gap layered compounds.

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Abstract number: AS-O.5-16

Thermoelectric optimization of *n*-type $AgBiSe_2$ via selenium vacancy and metal doping

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Silver bismuth selenide ($AgBiSe_2$) has drawn attention as a lead-free material with potential high thermoelectric efficiency, due to its intrinsically low thermal conductivity. Pristine $AgBiSe_2$ shows an *n*-type property, but it is also reported as a weak *p*-type material, as the carrier type and concentration are very sensitive to selenium vacancies. Here we report the enhancement of thermoelectric performance of $AgBiSe_2$ by introducing selenium vacancies and aliovalent transition metal doping on the silver site, which significantly increase the *n*-type carrier concentration and electrical conductivity. The highest dimensionless figure of merit (zT_{max}) reaches a value of ~0.65 at ~773 K for the $Ag_{0.97}Cd_{0.03}BiSe_{1.995}$ sample.

Abstract number: AS-O.5-17

Achieving High Thermoelectric Properties of Cu_2Se via Lattice Softening and Phonon Scattering Mechanism

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Co-alloying solid solution was regarded as a convenient approach to optimize the thermoelectric properties. In this study, the densified $Cu_{2-x}(MnFeNi)_xSe_{1-y}Te_y$ (x = 0–0.09; y = 0–0.03) designed by entropy engineering was prepared *via* microwave melting and hot-pressing sintering. The scattering mechanism and thermoelectric performance of Cu_2Se were evaluated. Due to the regulation of the carrier concentration and structural stabilization of the β-phase, the electrical performance was significantly enhanced. Moreover, the infrared spectroscopy analysis and the decrease in sound velocity unambiguously demonstrated the existence of a lattice softening effect of bulk Cu_2Se. By manipulating the lattice conductivity using entropy engineering, the thermal transport property gradually decreased (~0.4 $Wm^{-1}K^{-1}$ at 300 K) due to the lattice softening effect and phonon scattering mechanism. The obtained zT_{max} was 1.37 at 750 K in the $Cu_{2.91}(MnFeNi)_{0.09}Se_{0.99}Te_{0.01}$ sample.

Abstract number: AS-O.5-18

Unconventional Doping in $Cu_3Sb(Se,S)_4$ Composites

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Thermoelectric materials are typically highly degenerate semiconductors, which require high carrier concentration. However, the efficiency of conventional doping by replacing host atoms with alien ones is restricted by solubility limit, and, more unfavorably, such a doping method is likely to cause strong charge-carrier scattering at ambient temperature, leading to deteriorated electrical performance. Here, an unconventional doping strategy is proposed, where a small trace of alien atoms is used to stabilize cation vacancies in $Cu_3Sb(Se,S)_4$ by compositing with $CuAl(Se,S)_2$, in which the cation vacancies rather than the alien atoms provide a high density of holes. Consequently, the hole concentration enlarges but the carrier mobility is well maintained. As a result, in the Cu_3SbSe_4-$CuAlSe_2$ composites, a record-high average power factor of 19 μW cm^{-1} K^{-2} in the temperature range of 300~723 K as well as a peak *zT* value of 1.4 at 723 K are achieved. In the Cu_3SbS_4-$CuAlS_2$ composites, the average power factor reaches 15.8 μW cm^{-1} K^{-2} in the temperature range of 300~773 K as well as a peak *zT* value of 1.3 is attained at 773 K. This new doping strategy not only can be applied for boosting the average power factor for thermoelectrics, but more generally can be used to maintain carrier mobility for a variety of semiconductors that need high carrier concentration.

Abstract number: AS-O.5-19

Defect engineering synergistically modulates power factor and thermal conductivity of $CuGaTe_2$ for ultra-high thermoelectric performance

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The ternary chalcopyrite $CuGaTe_2$ has emerged as a promising *p*-type thermoelectric material with its advantages of low cost, good stability, non-toxic elements. However, its thermoelectric performance is limited by the intrinsic low electrical conductivity and high lattice thermal conductivity. In this work, a deficiency of Cu in $Cu_{1-x}GaTe_2$ semiconductors can be used to optimize the electrical properties by improving the carrier concentration, and to reduce thermal conductivity through multi-scale phonon scattering, which is predicted and guided by the First-principles density functional theory calculations. The carrier concentration is increased to 10^{20}, which compensates for the low electrical performance caused by the intrinsic low n_H of $CuGaTe_2$. The average power factor of $Cu_{0.96}GaTe_2$ reaches 106.3% higher than that of the original $CuGaTe_2$. In addition, the lattice thermal conductivity of the defective samples is greatly reduced at high temperature, which is mainly due to the reduction of sound speed and phonon scattering. All the above factors contribute to the highest *ZT* value of 1.23 at 823 K in $Cu_{0.96}GaTe_2$, which is 114% higher than the pristine $CuGaTe_2$, and the average *ZT* is 171.4% higher.

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Abstract number: AS-O.5-20

The deviation of T^{-1} in lattice thermal conductivity of $CuInX_2$ (X=Se, Te)

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The lattice thermal conductivity κ_L of crystals usually follow $\kappa_L \sim T^{-1}$ when is T is higher than the Debye temperature. Interestingly, κ_L of diamond-like materials $CuInX_2$ (X=Se,Te) shows the obvious deviation of T^{-1}. By combining the first-principle molecular dynamics with the Boltzmann transport equation calculations, the phonon renormalization effect is found to be crucial to understand the phenomenon due to the strong temperature dependence of the 2nd interatomic force constants (IFCs). The temperature sensitive IFCs brings the unusual softening phonon dispersion of $CuInX_2$ at high temperature, which leads to the higher scattering rate and unexpected lower thermal conductivity. By further analysis, we find the strong temperature-dependence thermal conductivity is closely related to the vibration of Cu atoms, which shows much larger mean square displacement and stronger anharmonicity at high temperature than those at 300K. This work reveals the origin of anomalous temperature dependence of κ_L in thermoelectric candidates $CuInX_2$ (X=Se,Te).

Abstract number: AS-O.6-01

Effect of Bismuth doping on the Electronic Band Structure of Mg_2Sn

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Mg_2Si-Mg_2Sn solid solutions are attractive candidates for thermoelectric energy harvesting in the medium temperature range (500- 800 K). In this study nominal compositions of $Mg_{2.2}Sn_{1-x}Bi_x$ (x = 0, 0.005, 0.01, 0.0125, 0.015 and 0.02) were prepared by induction melting followed by hot-pressing. Seebeck coefficient, electrical conductivity and Hall coefficient were measured in the temperature range of 300 K – 673 K. High power factor values were observed in the doped compositions indicating a single parabolic band mass which is much higher than that expected for the lowest conduction band in Mg_2Sn. To probe the origin of this anomaly, a MultiBand Fitting Technique (MBFT) based on multivariable minimization technique has been carried out. Our results indicate doping induced convergence of conduction bands to be the likely origin of the observed high thermoelectric power factor values. In this presentation, details of the MBFT along with the obtained results and likely causes will be discussed.

Abstract number: AS-O.6-02

Enhanced thermoelectric efficiency over wider temperature range in multiphase $Mg_{3.2}Sb_{1.5-\delta}Bi_{0.5-\delta}Te_{2\delta}$

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$Mg_{3.2}Sb_{1.5}Bi_{0.5}$ is a proven thermoelectric material in middle temperature range due to high degeneracy of conduction band and low thermal conductivity. Tellurium is used as a dopant in $Mg_{3.2}Sb_{1.5}Bi_{0.5}$. Excess amount of tellurium doping has result in thermoelectric performance in dual temperature range in $Mg_{3.2}Sb_{1.5-\delta}Bi_{0.5-\delta}Te_{2\delta}$. This makes the material very useful for practical applications due to enhanced figure of merit over wider temperature range. The FESEM-EDS and EBSD studies have been done to visualize phase distributions. We anticipate formation of two compatible phases due to addition of excess tellurium. The compatibility of the phases might be responsible for retention of electrical conductivity. This enhancement is attributed to higher Seebeck coefficient at room temperature as well as middle temperature range. The enhanced Seebeck coefficient at low temperature is peculiar in the present cases, even for significantly lower amount of the possible corresponding phase. The utility of this low cost thermoelectric material has been enhanced by this dual temperature range.

Abstract number: AS-O.6-03

A Highly Efficient Quasi-2D Thermoelectric Material: KMgBi

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Half Heusler alloys have emerged as promising candidates for thermoelectric (TE) applications due to their various interesting properties. Here, we present a first principles study of KMgBi which is a promising candidate for thermoelectric (TE) applications. This compound has been experimentally synthesized in the past [1], but has never been studied from TE perspective. The presence of flat bands near valence band edge and strong spin-orbit coupling provide a fertile ground to explore the potential of this material. We show that KMgBi exhibits low values of lattice thermal conductivity. The energy and temperature dependent relaxation time was calculated carefully taking into account different scattering mechanisms. The system shows a high TE figure of merit $ZT \sim 2.21$ (for *p*-type) at ~ 600 K temperature. We have further discussed enhancing the TE performance of KMgBi via alloy engineering. With proposed alloy engineering, we expect atleast a 10-11% enhancement in ZT.

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Abstract number: AS-O.6-04

Unravelling the effect of rGO on the thermoelectric properties of Sr-doped $LaCoO_3$ ceramic

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As promising thermoelectric material with high stability at extreme temperature and repeated thermal cycling, $LaCoO_3$ based ceramics have gained much attention, eventhough the thermoelectric performance remains very low for the application. In this work, a series of $La_{0.95}Sr_{0.05}CoO_3$/rGO (x = 0.3, 0.5, 0.7 and 1.0 wt%) composites are synthesised by solid-state reaction method, where rGO sheets are incorporated into LSCO matrix. The composites performs two major roles: (i) significantly reduces the thermal conductivity of the material, which can be attributed to the enhanced scattering of phonons at the high density LSCO/rGO interface, and (ii) increasing the power factor of the samples over the low temperature range by enhancing the charge carrier density and weighted mobility. The thermoelectric properties of LSCO has been optimized by varying the rGO concentration, with LSCO/rGO-0.5wt% achieving low thermal conductivity value of 1.24 W/mK and high power factor value of 100 $\mu W/mK^2$ at room temperature. This work provides a new avenue of improving the thermoelectric performance of oxide based ceramics at room temperature by the way of engineering metal oxide/rGO composites.

Abstract number: AS-O.6-05

Enhancing Thermoelectric Performance of $Cu_{12}Sb_4S_{13}$ Tetrahedrite through Substitution of Ag

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Among Pb/Te free thermoelectric materials, tetrahedrite $Cu_{12}Sb_4S_{13}$ has drawn worldwide attention because of its low cost, earth-abundant and less toxic constituents. The tetrahedrite has relatively high electrical conductivity originating form dispersive bands near the Fermi level and intrinsically low thermal conductivity originating from the complex crystal structure but the thermoelectric performance this compound is limited because of its moderate Seebeck coefficient. In this study, the +1 oxidation state of Ag was confirmed by X-ray photoelectron (XPS) study. The solubility of Ag at the copper site was verified using the Reitveld refinement of powder X-ray diffraction data. Reitveld refinement also showed the presence of a minor weight percentage of the secondary phase of Cu_3SbS_4 and $Cu_{12-x}Ag_xSb_4S_{13}$ as a major phase. This was also confirmed by Electron Probe Microanalysis (EPMA) study. In this work, a 14% enhancement of Seebeck coefficient was achieved through substitutions of Ag^{+1} at Cu(I) site. Consequently, a relatively high power factor of 1.3 mW/m K^2 was obtained for the composition $Cu_{11.975}Ag_{0.025}Sb_4S_{13}$. Owing to a lowest thermal conductivity ~ 1.1 W/m K the sample with composition $Cu_{11.975}Ag_{0.025}Sb_4S_{13}$ showed a highest thermoelectric figure of merit ~ 0.87.

Abstract number: AS-O.6-06

Nanostructured *n*-type $CuFeS_2$ Chalcopyrite: Towards high thermoelectric performance

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Thermoelectric (TE) technology has received great attention in renewable energy conversion technologies as they directly convert untapped waste heat into usable electricity. The heat-to-electricity conversion efficiency is determined by the dimensionless constant, figure of merit, $zT = S^2\sigma T/\kappa$, where σ is the electrical conductivity, S is the Seebeck coefficient, κ is the thermal conductivity, and T is the absolute temperature. However, due to the interdependent nature of σ, S, and κ, obtaining the large zT and thereby high conversion efficiency remains challenging in TE research. In this regard, a new class of materials has been investigated to achieve high zT. Here, we report the low-cost and eco-friendly bulk and nanostructured *n*-type $CuFeS_2$ chalcopyrites, proposed as promising TE material, prepared via vacuum-sealed tube melting reaction and conventional hydrothermal process. Powder XRD analysis confirmed the phase purity, and the average crystallite size of $CuFeS_2$ nanoparticles is calculated as ~30 nm. Interestingly, quantum confinement-driven bandgap widening is observed in the nano-$CuFeS_2$, which results in an enhanced Seebeck coefficient (S) and ultra-low thermal conductivity (κ). Notably, a huge reduction in total thermal conductivity of ~0.69 W/mK is observed in nano-$CuFeS_2$ as compared to bulk sample (~4.18 W/mK) at 300 K, leading to the enhanced figure of merit, zT of ~0.28 at 623 K, which suitable dopants can further improve.

Abstract number: AS-O.6-07

Metavalent Bonding in GeSe Leads to High Thermoelectric Performance

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Orthorhombic GeSe is a promising thermoelectric material. However, large band gap and strong covalent bonding result in a low thermoelectric figure of merit, $zT \approx 0.2$. Here, we demonstrate a maximum $zT \approx 1.35$ at 627 K in *p*-type polycrystalline rhombohedral $(GeSe)_{0.9}(AgBiTe_2)_{0.1}$, which is the highest value reported among GeSe based materials. The rhombohedral phase is stable in ambient conditions for x = 0.8–0.29 in $(GeSe)_{1-x}(AgBiTe_2)_x$. The structural transformation accompanies change from covalent bonding in orthorhombic GeSe to metavalent bonding in rhombohedral $(GeSe)_{1-x}(AgBiTe_2)_x$. $(GeSe)_{0.9}(AgBiTe_2)_{0.1}$ has closely lying primary and secondary valence bands (within 0.25–0.30 eV), which results in high power factor 12.8 μW $cm^{-1}K^{-2}$ at 627 K. It also exhibits intrinsically low lattice thermal conductivity (0.38 $Wm^{-1}K^{-1}$ at 578 K). Theoretical phonon dispersion calculations reveal vicinity of a ferroelectric instability, with large anomalous Born effective charges and high optical dielectric constant, which, in concurrence with high effective coordination number, low band gap and moderate electrical conductivity, corroborate metavalent bonding in $(GeSe)_{0.9}(AgBiTe_2)_{0.1}$. We confirmed the presence of low energy phonon modes and local ferroelectric domains using heat capacity measurement (3–30 K) and switching spectroscopy in piezoresponse force microscopy, respectively.

Abstract number: AS-O.6-08

High thermoelectric performance in $Zn_{1-x}Cd_xSb$ (x = 0 – 0.375) solid solutions by dynamic optimization of carrier concentration

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Zinc Antimonide (ZnSb) and its solid solution with CdSb are well-known *p*-type thermoelectric (TE) materials. Our previous work showed that the charge carrier concentration in this system has a strong temperature dependence due to the formation of acceptor type Zn-site vacancy, whose concentration depends on temperature. The objective of this work was to optimize temperature-dependent carrier concentration and lower lattice thermal conductivity by forming ZnSb-CdSb solid solutions. Different $Zn_{1-x}Cd_xSb$ (x = 0, 0.0625, 0.125, 0.25 and 0.375) compositions doped/co-doped with Ag and Sn were prepared by melting – rapid compaction – annealing process. TE properties have been measured between room temperature and 673 K and analyzed using the single parabolic band model. It has been observed that the doping/co-doping technique (simultaneous doping with Ag and Sn) can be used to precisely tune the charge carrier concentration. The Sn co-doping with Ag restrict the formation of Zn-site vacancy and help in optimizing the dynamic charge carrier concentration. Thus a record high TE figure-of-merit (zT) of 1.22 at 645 K and TE efficiency (η_{max} = 10% at ΔT = 375 K) has been attained in the co-doped ZnSb. Moreover, TE performance was further increased with Cd substitution, which preferentially scatters the phonons and lowers the lattice thermal conductivity. This resulted in a zT value of 1.41 and η_{max} value of 12.2% at ΔT = 375 K for the 37.5 at% Cd substitution.

Abstract number: AS-O.6-09

3D Printing of Thermoelectric Materials and Devices: An Upcoming Outbreak

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In recent years, there has been a tremendous advancement in 3D printing technology due to the versatility of the method in creating complicated and intricate shapes. In very recent times, it has also been making inroads into the realm of materials that are functional and energy-related. In general, thermoelectrics field has a solid foundation in terms of both understanding and design. In this specific review, we focused on the various techniques of 3D printing, as well as the thermoelectric (TE) properties of 3D printed TE materials, the performance of 3D printed TE devices, and relationships between 3D technique and property. The most essential thing that we discussed about was the challenges and future prospects that lie ahead for the 3D printing of TE materials and devices.

Abstract number: AS-O.6-10

Enhancing thermoelectric properties in TiNiSi structure-type semimetal by doping

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At Fermi energy, TiNiSi structure-type compounds, also known as distorted-Heuslers, have an electronic structure with a pseudo-gap in the density of states and many small electron and hole pockets. We looked at doping electrons in ZrNiSi in this study; and discovered an intriguingly synchronous increase in S and σ. To explain, we used first-principles density functional theory-based band structure calculations. The doped samples' peak value of σ as compared to ZrNiSi, increases from 1000 S cm^{-1} to as high as 2500 S cm^{-1} at 300 K; at the same time, the peak value of S, which is 20 V K^{-1} in ZrNiSi, increases by more than a factor of two. Phase segregation is observed in the as-cast (unannealed) $ZrNiSi_{1-x}Sb_x$ samples due to a spinodal-type breakdown with two co-existing TiNiSi structure-type phases with distinct Sb/Si ratios. At 300 K, the thermal conductivity (κ) of the doped samples falls from 12 $Wm^{-1}K^{-1}$ (x = 0) to approximately 2 $Wm^{-1}K^{-1}$ (x = 0.2). The peak thermoelectric figure of merit (zT) rises from 0.005 (x = 0) to 0.023 (x = 0.2). At 300 K, the doped materials' thermal conductivity (κ) drops from 12 $Wm^{-1}K^{-1}$ (x = 0) to around 2 $Wm^{-1}K^{-1}$ (x = 0.2). As a result, the maximum thermoelectric figure of merit (zT) increases from 0.005 (x = 0) to 0.023 (x = 0.2). Co-doping of Hf (Zr site) and Sb (Si site) enhances phase stability and chemical homogeneity while maintaining thermal conductivity low due to Zr-Hf point mass fluctuation, resulting in a peak zT value of 0.055.

Abstract number: AS-O.6-11

Improved thermoelectric properties of Fe doped Si-rich higher manganese silicide

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Thermoelectric (TE) technology is an environmentally beneficial energy conversion method as it has the advantages of high reliability, emitting no pollutants, and operating over a wide temperature range. Material with low thermal conductivity, high electrical conductivity, and a large Seebeck coefficient could be regarded as an ideal TE material. Though alloys of Bi_2Te_3, PbTe, and SiGe are known for their superior TE performance, they are not attracted much because of the presence of toxic and expensive elements. In this regard, higher manganese silicide (HMS) is viewed to be a good candidate for mid-temperature thermoelectric application due to its high abundance, structural/thermal stability and cost-effectiveness.

In this work, we report the enhancement of thermoelectric properties of Si-rich HMS by doping Fe at Mn site. Pure and Fe doped $MnSi_{1.8}$ samples have been synthesized by induction melting followed by induction hot-pressing. The phase purity of Fe in $MnSi_{1.8}$ was validated using powder XRD. Furthermore, the presence of excess Si in the matrix of HMS and the elemental homogeneity of $MnSi_{1.8}$ were examined by FE-SEM and EDS, respectively. Fe doping and presence of Si in $MnSi_{1.8}$ scatter low- and mid-wavelength phonons and reduce the lattice thermal conductivity to 1.7 W/mK at 773 K, resulting to a maximum zT of 0.50 at 773 K for the composition $Mn_{0.9}Fe_{0.1}Si_{1.8}$. Additionally, $Mn_{0.9}Fe_{0.1}Si_{1.8}$ shows a large hardness of 11.57 GPa as compared to pure $MnSi_{1.8}$ (5.81 GPa).

Abstract number: AS-O.7-01

Next-generation thermoelectric cooling modules based on high-performance $Mg_3(Bi,Sb)_2$ material

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As the core component of any real thermoelectric cooling system, the Bi2Te3-based modules have been used for decades. Recently, *n*-type $Mg_3(Bi,Sb)_2$ material was proposed as a promising substitute for Bi2Te3. The cooling performance of $Mg_3(Bi,Sb)_2/Bi_2Te_3$ unicouple prototype has been demonstrated by Mao et al [1]. However, the fabrication of commercially viable modules with such new materials is challenging. Herein, full-scale cooling modules based on the optimized *n*-type $Mg_{3.2}Bi_{1.4975}Sb_{0.5}Te_{0.0025}$ and *p*-type $(Sb_{0.75}Bi_{0.25})_2(Te_{0.97}Se_{0.03})_3$ were successfully fabricated [2]. A maximum ΔT of 76 K with the hot-side temperature of 350 K, a COP of 8 with a temperature difference of 5 K, and a serving time > 6 months were achieved. These were attributed to the enhanced stability and well-secured *n*-type transport of the $Mg_{3.2}Bi_{1.4975}Sb_{0.5}Te_{0.0025}$, a highly reliable Mg_2Cu barrier layer, and other key techniques involved in the module assembling. The most striking benefit of our modules lies in its 23% higher performance-cost ratio over commercial Bi_2Te_3 system, which paves its way for next-generation thermoelectric cooling applications.

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Abstract number: AS-O.7-02

Optimizing the hH/Bi_2Te_3 segmented thermoelectric module for its highest efficiency

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Thermoelectric module(TEM) has potential applications in many fields including waste heat recovery (vehicles [1], industries [2] et al) and power supply (self-powered sensors [3], flexible electronics [4] et al) for its compactness, quiet and reliable performance. The reasonable design of TEM structure is an important prerequisite for its high-performance output. For segmented TEM(STEM), there are many interrelated and coupled structural parameters affecting its output performance including the sectional area A_{pleg} and A_{nleg} of p-type and n-type thermoelectric leg (TEL) respectively, the total height L_{leg} of TEL, the height ratio Lr_p of p-type TEL's hH section to Bi_2Te_3-based section and Lr_n of n-type TEL's hH section to Bi_2Te_3 section. Therefore, it is difficult to select the structural parameters that can achieve the optimal output performance of the STEM. This paper presents an optimal design method of STEM. Firstly, the one-dimensional(1-D) mathematical model of STEM is established, and its accuracy is verified by comparing with the experimental results in a reference with error less than 2%. The 1-D model is programmed mixed with MATLAB and C language, and the calculation time is reduced to 2% of that programmed by MATLAB alone, which greatly improves the calculation efficiency. Taken the 1-D model as objective function and combined with intelligent algorithm, the structure of STEM is optimized to obtain the structural parameters to achieve the maximum efficiency. The applicability of differential evolution(DE), genetic algorithm(GA),particle swarm optimization (PSO), ant colony optimization (ACO) and taboo search (TS) is compared in five aspects of computation speed, computation efficiency, stability, robustness, and simplicity [5-6]. Results show that DE has more advantages of stability and robustness in dealing with the optimization of STEM than other algorithms and the maximum theoretical efficiency of the STEM can reach 12.21%. This method can provide guidance for the design of STEM and even shows the great potential to contribute to the development of TEM technologies to some extent.

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Abstract number: AS-O.7-03

Thermoelectric Materials Research and the Applications in Micro TEC

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Bi_2Te_3-based compounds are the most mature and widely used thermoelectric materials. The further improvement of their performance is of great significance. Besides, the industrialization promotion of related devices and the wide development of application scenarios are becoming more and more important developing directions in thermoelectric field. In addition, with the rapid development of 5G communication, temperature control of 5G optical modules is becoming an increasingly important issue. To use Micro TEC fabricated by Bi_2Te_3 materials is the best solution for this issue. In this report, we will introduce the R&D results of Bi_2Te_3 materials in Jianju Technology Co., LTD. The micro-processing methods and the requirements for materials in Micro TEC will also be involved. This report focuses on the practical application, considers the developing direction of thermoelectricity from the perspective of industrialization, and injects the power into the wide application of thermoelectric devices.

Abstract number: AS-O.7-04

Rapid Selective Ablation and High-precision Patterning for Micro Thermoelectric Device Using Femtosecond Laser Direct Writing

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Highly integrated miniature thermoelectric devices are desirable for applications of chip thermal management and self-powered energy harvesting. Currently, further performance improvement of the micro thermoelectric device is largely limited by the micro-nano patterned processing, which exists the incompatibility with high-performance thermoelectric material fabrication or contradiction between machining accuracy and efficiency. This work presents a useful method to flexibly achieve high-precision array patterning for the micro thermoelectric device through the femtosecond laser direct writing technique. By experimentally examining the material ablation process and numerically analyzing the electron-lattice temperature, the laser energy threshold for different materials is determined to obtain the selective removal between thermoelectric materials and metallic electrodes. Furthermore, the evaluation criteria are established between the formation quality of microgroove in array structure and the laser pulse energy distribution, and the shape-control and property-control pattern processing can be realized through reasonable control of the laser energy. Consequently, the Bi_2Te_3-based thermoelectric pattern with competitive leg density (496 pairs/cm^2) and high filling factor (55%) is successfully constructed.

Abstract number: AS-O.7-05

Individualization of optimal operation currents for promoting multi-stage thermoelectric cooling

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Cascading multiple thermoelectric coolers offers a promising approach to promote the cooling capability for a broad scale of applications at low temperatures. Theoretically, multi-stage coolers offer an extreme cooling capability by increasing the number of stages [1]. However, the existence of electrical, thermal contact resistances [2,3] and compatibility issues leads a commercial Bi_2Te_3-based 6-stage thermoelectric cooler to show a maximal temperature reduction of ~130 K [4] at a heat sink temperature near room temperature. It is still a great challenge for multi-stage thermoelectric cooling for lower-temperature applications. In this work, it is revealed in a commercial 3-stage thermoelectric cooler that, a further 10% temperature reduction can be realized by individualizing the optimal operating currents for each stage. As compared to the lowest achievable temperature of ~191 K in a 3-stage cooler from FerroTec operating at an identical optimal current for all stages, this individualization approach enables extra cooling capability to ~181 K. The high residual cooling power at 191 K further leads to a ~100% increase in cooling rate to this temperature. The optimal currents for each stage actually reside in the vicinity of those operated as single-stage coolers, offering an easily-accessible guidance. The optimal operating currents for each stage are revealed to be very close to those operated as single-stage devices, thus, enabling a convenient guidance and strategy for promoting the cooling capability of multiple-stage thermoelectric coolers targeting at lower-temperature applications.

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Abstract number: AS-O.7-06

Highly efficient thermoelectric air conditioner with kilo-Watt capacity realized by ground source heat exchanging system for Zero-Global-Warming Potential

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The enormous need for refrigeration of modern human life has inevitably aggravated the environmental crisis worldwide. To date, there are very few refrigeration technologies available beholding both harmless refrigerant and high efficiency. We herein proposed a geothermal-thermoelectric air conditioning system (GeoTEAC) with refrigerant-free and high energy efficiency through synergistically combining the merits of thermoelectric effect and ground source heat exchanging system. The system showed competitive cooling and heating COPs of 5.83 and 2.92, respectively with kilo-Watt capacity, which are 3 - 4 times higher than that of previously reported thermoelectric air-conditioning setups. For a conceptual scenario, we demonstrated the lowest TEWI values for GeoTEAC system among different air-conditioning types. Our work provides sustainable and climate-friendly solution to realize worldwide emission peak and carbon neutralization [1].

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Abstract number: AS-O.7-07

Design of Wireless Temperature Sensor Using Thermoelectric Generator

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With the rapid development of industrial society and its urgent need to build smart IoT and Industry 4.0, wireless sensors have received extensive research [1,2]. However, due to the limited battery capacity and the complexity of the industrial environment, energy supply technology has become a key issue limiting the application of wireless sensors [3,4]. Therefore, the use of ambient temperature to obtain energy to supply power to wireless sensors has become a key technology to solve the problem [5]. At present, the ambient temperature energy extraction technology has problems such as low output power and inability to cope with different working conditions [6]. Therefore, the focus of this paper is to improve the output power of the thermoelectric generator, reduce the power consumption of the sensor, and reduce the volume of the sensor. This paper proposes a scheme to use a thermoelectric generator to power the sensor. On the one hand, a wireless temperature measurement sensor circuit with extremely low power consumption based on ambient temperature and power supply is built. This circuit module can still ensure the normal operation of the sensor through the internal boost and control circuit under the condition of extremely low output power of the thermoelectric module. On the other hand, the optimal number of thermocouples pairs and cross-section area in the thermoelectric generator were determined by iterative simulation calculation, and the radiator structure was designed according to the thermal resistance, which improved the open-circuit voltage and load voltage of the thermoelectric generator, and made the power supply performance of the sensor to achieve the best. Finally, a wireless temperature sensor based on ambient temperature and power supply is designed. The size of the sensor is 25×25×16mm. The experimental results show that the sensor can realize the temperature measurement wireless node function under the condition of lower ambient temperature. When the temperature difference between the heat source temperature and the ambient temperature is 30 ℃, the temperature wireless signal is transmitted every 10 minutes. The sensor self-powering technology presented in this paper can provide new ideas for the design and application of wireless sensors powered by thermoelectric generator in industrial intelligence.

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Abstract number: AS-O.7-08

Simultaneous realization of flexibility and ultra-high power density in heatsink–free thermoelectric generator via fine thermal regulation

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Wearable thermoelectric generators (w-TEGs) can incessantly convert body heat into electricity to power electronics. However, the low efficiency of thermoelectric materials, tiny terminal temperature difference, rigidity, and negligence of lateral heat transfer preclude w-TEGs from broad utilization [1,2]. In this report, we employ finite element simulation to find the key factors for simultaneous realization of flexibility and ultra-high normalized power density. Using melamine foam (MF) with ultra-low thermal conductivity (0.03 W/mK) as the encapsulation material, a novel lightweight π-type w-TEG with no heatsink, excellent stretchability, comfortability, processability, and cost-efficiency has been fabricated. At an ambient temperature of 24°C, the maximum power density of the w-TEG reached 7 μW/cm^2 (Sitting) and 29 μW/cm^2 (Walking). Under suitable heat exchange condition (heat sink with 1m/s air velocity), 32 pairs of w-TEGs can generate a 66 mV voltage and 60 μW/cm^2 power density. The output performance of our TEG is remarkably superior to previously reported w-TEGs.

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Abstract number: AS-O.7-09

Ultra-High Electrical Conductivity in Filler-Free Polymeric Hydrogels Toward Thermoelectrics and Electromagnetic Interference Shielding

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Conducting hydrogels have attracted much attention for the emerging field of hydrogel bioelectronics, especially poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) based hydrogels, because of their great biocompatibility and stability. However, the electrical conductivities of hydrogels are often lower than 1 S cm^{-1} which are not suitable for digital circuits or applications in bioelectronics. Introducing conductive inorganic fillers into the hydrogels can improve their electrical conductivities. However, it may lead to compromises in compliance, biocompatibility, deformability, biodegradability, etc. Herein, a series of highly conductive ionic liquid (IL) doped PEDOT:PSS hydrogels without any conductive fillers is reported. These hydrogels exhibit high conductivities up to ≈ 305 S cm^{-1}, which is ≈ 8 times higher than the record of polymeric hydrogels without conductive fillers in literature. The high electrical conductivity results in enhanced areal thermoelectric output power for hydrogel-based thermoelectric devices, and high specific electromagnetic interference (EMI) shielding efficiency which is about an order in magnitude higher than that of state-of-the-art conductive hydrogels in literature. Furthermore, these stretchable (strain > 30 %) hydrogels exhibit fast self-healing, and shape/size-tunable properties, which are desirable for hydrogel bioelectronics and wearable organic devices. The results indicate that these highly conductive hydrogels are promising in applications such as sensing, thermoelectrics, EMI shielding. etc.

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Abstract number: AS-O.7-10

Carbonized polyvinyl alcohol / poly (3,4-ethylene dioxythiophene): polystyrene sulfonic acid composites and their thermoelectric properties

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PEDOT: PSS is one of the most widely studied organic thermoelectric materials systems due to its excellent photoelectric performance, good thermal stability and adhesion and easy film formation. The thermoelectric properties of PEDOT: PSS system can be effectively improved by combining PEDOT: PSS with carbon materials containing large number of π electrons. Pyrolysis polyvinyl alcohol (PVA) has been used to prepare PEDOT:PSS/PVA composite hydrogel. PVA aerogel treated at 300 °C under N_2 atmosphere has a long conjugate structure. In PEDOT:PSS/PVA composite hydrogel, the porous structures of PVA can act as bridge among PEDOT conductive sheets, and the π-π interaction and intermolecular hydrogen bond between PVA and PEDOT: PSS enhanced the carrier mobility, thus improving the conductivity of the composites. When the content of PEDOT: PSS was 75 wt%, the power factor of PEDOT:PSS/PVA composite reached to 259.56 μ W m^{-1} K^{-2} at room temperature.

Abstract number: AS-O.7-11

Seeking New Layered Oxyselenides with Promising Thermoelectric Performance

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Layered oxyselenides have been widely investigated as promising thermoelectric materials due to their unique merits such as super-lattice structural features, intrinsic complexity and so on, which contributes to low thermal conductivity and easily controllable electrical properties. Newly developed $Bi_2LnO_4Cu_2Se_2$ (Ln stands for lanthanide) oxyselenides are found as potential thermoelectric systems since they have excellent electrical conductivity over 10^3 S cm^{-1}. In this work, an unique energy and time-saving method combined self-propagating high temperature synthesis (SHS) with spark plasma sintering (SPS) is adopted to successfully prepare highly pure $Bi_2LnO_4Cu_2Se_2$ instead of traditional solid-state reaction. To explore the most suitable lanthanide for $Bi_2LnO_4Cu_2Se_2$, thermoelectric performance in a wide temperature range (300 K to 923 K) of $Bi_2LnO_4Cu_2Se_2$ (Ln = Nd, Sm, Eu, Gd, Tb, Dy, Ho and Er) is deeply evaluated and studied. Ultimately, with a relatively high electrical conductivity, moderate Seebeck coefficient and extremely low thermal conductivity, a maximum *ZT* value of ~0.27 at 923K is achieved in $Bi_2DyO_4Cu_2Se_2$, which is 4 times larger than that of the ever-reported $Bi_2YO_4Cu_2Se_2$ and proves a potential thermoelectric system for further investigation. This work may provide some enlightenment and broaden the horizon in finding new thermoelectric materials, especially for complex layered compounds [1].

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Abstract number: AS-O.7-12

Kirigami-Based Stretchable, Deformable, Ultralight Thin-film Thermoelectric Generator for BodyNET Application

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Thermoelectric generators (TEGs) as potential power supply have great prospects for wearable application. Nevertheless, how to realize deformability, ultralight weight and high power density of TEGs at the same time has strongly frustrated their commercial application to date. Herein, inspired by the art of kirigami, we proposed an innovative design to construct stretchable, deformable, ultralight 3D thin-film TEG from 2D structure by introducing rational kirigami cuts. Meanwhile, high-performance inorganic thermoelectric films are compatibly introduced to the TEG without properties degradation. Besides, the vertical heat flow is easily realized in the planar thin-film TEG, which is beneficial to the establishment of large temperature difference. The fabricated ultralight kirigami-based TEG (only 29 mg in weight) without additional heat sink acquires the highest open voltage density of 6.712 V g^{-1} with a maximum power density of 255.395 μW g^{-1} at T_{hot} = 60 ℃. Moreover, the TEG exhibits excellent compliance to extreme mechanical deformation and adaptivity to variety surfaces. This work provides a new design concept for deformable TEGs with promising application in a broader set of BodyNET technology [1].

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Abstract number: AS-O.7-13

Durable, Stretchable and Washable Inorganic-based Woven Thermoelectric Textiles for Power Generation and Solid-state Cooling

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Wearable inorganic semiconductor (ISC) based thermoelectric (TE) devices, especially fiber-based thermoelectric textiles (TETs), show promise in electrical power generation and solid-state cooling compared with bulk ISC-based TE generators (TEGs). However, it is challenging to use the ISCs, with brittleness and mechanical instability, to produce thermoelectric fibers for weaving TETs. Here, we report a strategy to produce ISC-based segmented hierarchically ternary coaxial TE strings at large scale for semi-automatically manufacturing a highly mechanically stable, stretchable, breathable and washable woven TET by a textile machine. The TET demonstrates good stretchability (100% elongation), flexibility (bending radius of 2 mm), washability (> 20 washing cycles) and output power density of 0.58 W m^{-2} at a temperature difference of 25 K (predicted power density of 6.06 W m^{-2} at ΔT = 80 K). With the assistance of finite element analysis, the significance of the fabric's structure on the excellent mechanical and TE performance of the TET has been clarified, which reaches an output voltage of ~0.28 V at an ambient temperature of ~8°C. For practical applications, it can continuously power on-body electronics for monitoring the environment and the human body's vital signals and activities by wearing it on the arm with a self-built temperature gradient of ~16 K. Furthermore, the TET can stably generate solid-state cooling of 3.1 K in quiescent air ($T_{ambient}$ ~ 26°C, relative humidity ~60%). This work paves a new way for designing durable, stretchable and washable ISC-based TETs toward real on-body applications.

Abstract number: AS-O.7-14

Bi_2Te_3-based flexible thermoelectric generator for wearable electronics

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The rapid development of the IoT increases the demand for wearable devices. Flexible thermoelectric technology provides a special solution for solving the power supply of wearable electronics. Bi_2Te_3-based films with high performance around room temperature show the great potential.

Here, *n*-type Bi_2Te_3 and *p*-type $Bi_{0.5}Sb_{1.5}Te_3$ flexible thermoelectric films have been fabricated by magnetron sputtering method. We found that the films deposited by the RF power supply showed the (*001*)-preferred orientation, which is different from that of films prepared by the DC power supply. The carrier concentration and mobility are optimized by adjusting the deposition temperature, eventually improving the thermoelectric performance and achieving the room-temperature power factors of 3.2 and 6.1 μW cm^{-1} K^{-2} for Bi_2Te_3 and $Bi_{0.5}Sb_{1.5}Te_3$ films, respectively. After being bent 900 times with a radius of 5 mm, the resistance of these films barely increases. In order to further evaluate the practicability, these films are used to design a flexible thermoelectric generator. The power density is up to ~218.8 μW cm^{-2} at temperature differences of ΔT = 41 K. In addition, we continuously measured the 10-hours output performance of the thermoelectric device, in which the output voltage is almost unchanged at the ΔT of 35 K, indicating the good stability.

Abstract number: AS-O.7-15

Joint-free single-piece flexible thermoelectric devices with ultra-high resolution *p-n* patterns toward energy harvesting and solid-state cooling

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Joints widely exist in traditional organic electronic devices that are composed of *p-n* modules, including organic thermoelectric (TE) devices. They often harm the performance of the devices by increasing their electrical resistance and thermal resistance. Recently, a few joint-free approaches have been reported to fabricate TE devices with a single carbon nanotube (CNT) composite film. However, the resolution of *p-n* patterns is low, e.g. > 100 μm with conventional printing/drop-casting method. Herein, a plasma treatment method was reported to fabricate joint-free TE devices with a single-piece flexible CNT composite film whose performance was higher than traditional devices in energy harvesting and solid-state cooling. In addition, this method provided *p-n* patterns with a high resolution of ~1-2 μm which is promising for making future high integration level TE devices. This method can be extended to fabricate a broad range of high integration level organic electronic devices composed of *p-n* modules.

Abstract number: AS-O.7-16

Understanding the solvent effects on polarity switching and thermoelectric properties changing of solution-processable *n*-type single-walled carbon nanotube films

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Developing high-performance solution-processable *n*-type thermoelectric materials is challenging. In this work, we report that single-walled carbon nanotubes (SWCNTs) prepared in dimethyl sulfoxide (DMSO) (SWCNTs/DMSO) exhibit a high *n*-type electrical conductivity of 2298 S/cm at room temperature, which is superior to that of previously reported *n*-type solution-processable SWCNTs. The maximum *n*-type electrical conductivity was 3490 S/cm at 373 K. The great electrical conductivity results in a high *n*-type power factor of 195 μW/m K^2 for SWCNTs/DMSO films at 373 K which is larger than most of the *n*-type solution-processable SWCNTs. The theoretical calculation indicates that the wrapping morphology of the surfactant on SWCNTs is strongly affected by different solvent polarities which lead to different packing densities of the SWCNT films as demonstrated in the scanning electron microscope images, subsequently affecting the *n*-type doping efficiency and the *n*-type electrical conductivity. The electrical conductivity affected by the mixed *p*- and *n*-type carriers in the film were discussed. A full SWCNT thermoelectric generator has been fabricated to show the heat-to-electricity conversion ability of the materials. This work reveals a potential method to prepare highly conductive *n*-type SWCNTs by choosing the proper solvent for optimized thermoelectric performance.

Abstract number: AS-O.7-17

Anisotropic electrical conductivity and isotropic Seebeck coefficient feature induced high thermoelectric power factor >1800 μW/m K^2 in MWCNT films

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Light-weight and low cost flexible thermoelectric (TE) materials will improve the heat-to-electricity conversion efficiency compared to rigid materials by minimizing the heat loss between TE devices and heat sources in waste heat recovery. Multi-walled carbon nanotube (MWCNT) has excellent mechanical and electrical properties. However, the thermoelectric power factor (*PF*) of MWCNTs is much lower than single/double-walled carbon nanotube (S/DWCNT), which is often lower than 40 μW/m K^2. Herein we reported an effective way to achieve high *PFs* of ~1800 μW/m-K^2 for p-type and ~1000 μW/m-K^2 for *n*-type in flexible MWCNT films. The high power factor was achieved by taking advantage of the anisotropic electrical conductivity and isotropic Seebeck coefficient feature of one-dimensional CNTs as well as the following doping and cold-pressing to improve the electrical conductivity of MWCNT films. The *PF* values are comparable to that of state-of-the-art S/DWCNT films and most inorganic TE materials. A Lego-like thermoelectric generators (TEGs) with an assembling structure was fabricated to show the heat-to-electricity ability of the materials, which exhibited the highest areal output power of ~27 W/m^2 among CNT based flexible TEGs. This method might be extended to other one-dimensional-material based composites to boost the development of high *PF* flexible TE materials.

Abstract number: AS-O.7-18

N-type Flexible Free-standing Thermoelectric Composite Film Based on Bi_2Se_3-PVDF Hybrid Nanostructure

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In this work, *n*-type flexible free-standing thermoelectric films composed of Bi_2Se_3 nanosheets and PVDF were synthesized. In order to prepare high-quality Bi_2Se_3 nanosheets, the influence of heating method, heating time, and heating temperature on the morphology, crystallinity, and thermoelectric performance of Bi_2Se_3 nanosheets were systematically studied. It is found that Bi_2Se_3 nanosheets with uniform morphology, excellent crystallinity, and optimized thermoelectric performance can be obtained by heating at 275 ℃ for 20 h in a heating and stirring integrated device. The Seebeck coefficient of the Bi_2Se_3/PVDF composite film reached −128 μV/K at room temperature, with a comparable electrical conductivity of 618 S/m, which eventually provides a power factor of 10.23 $\mu W/mK^2$. This work developed a facile strategy to fabricate *n*-type, flexible, free-standing, non-toxic, and low-cost thermoelectric composite film. We expect this strategy can be extended to the preparation of other *n*-type flexible free-standing thermoelectric films.

Abstract number: AS-O.7-19

Enhancing Thermoelectric Properties of Snse Film by Vacancy Effect

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Nanostructured thermoelectric materials have attracted extensive attention due to the broad application prospects in the fields of micro sensors, electronic thermal management, and wearable devices. In this work, SnSe nanofilms with different thicknesses were prepared by single-target magnetron sputtering technology, annealed in argon atmosphere at 673 K for 30 minutes. The geometric structure, composition and thermoelectric properties were systematically measured. The electrical properties of thin films were measured by the four-point probe method, and the thermal properties of the thin films were measured by the time-domain thermal reflectometry method. The calculation based on the first principle theory was also conducted to understand the carrier transport mechanism in SnSe films. Se vacancies were formed in the 130 nm-thick ultrathin film since Sn atoms were preferentially deposited on the substrate. The theoretical results confirmed that the unbonded Sn^{2+} can form an intermediate band near the valance band, which reduces the indirect band gap while maintains a relatively large direct band gap over 0.48 eV, achieving band engineering strategy. Additionally, Se vacancies can improve the electrical conductivity significantly by reducing electron-phonon scattering effect. Meanwhile, the thermal conductivity of the vacancy structure has an average reduction of 33.8% compared to the pristine SnSe films due to the vacancy scattering effect. As a result, a high *ZT* value of 0.61 were achieved at 700 K in the 130 nm-thick film sample, mainly originating from the vacancies formed during the synthesis process, rather than the reduced film thickness. The work reveals the mechanism of vacancies on energy transfer in thin films, which may promote the further optimization and application of nanoscale thermoelectric. This work was supported by the National Natural Science Foundation of China under Grants 51825604 and 52130604.

Abstract number: AS-O.7-20

A sketch for super-thermoelectric materials

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Improving the dimensionless figure of merit (*zT*) is the everlasting goal for thermoelectrics. With the discovery of super-thermoelectric materials, which exhibit much higher *zT*s (arbitrarily say, *zT* > 5) than that of the traditional materials, it is possible to dramatically alter the landscape of the thermoelectric applications. Identifying super-thermoelectric materials is extremely challenging based on the current understanding of electron and phonon transport. It is interesting to wonder if it is possible to predict how the super-thermoelectric material might look like before it has been discovered. Herein, band modeling on the thermoelectric properties is conducted. It is concluded that super-thermoelectric materials should have a much lower optimal carrier concentration than the "golden carrier concentration" (in the range between 10^{19} and 10^{20} cm^{-3}). In addition, the super-thermoelectric materials should also have a much larger optimal Seebeck coefficient than that of the existing materials (~200 ⌈V K^{-1}). Based on these predictions, potential issues *i.e.*, on the development of super-thermoelectric materials are discussed. Finally, predictions on the super-thermoelectrics beyond the band modeling are also briefly discussed.

Abstract number: AS-O.7-21

Lifetime Simulation and Influence Analysis of Thermoelectric Cooler Under Thermal Cycling

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Thermoelectric cooler (TEC) is widely used in local refrigeration, chip thermal management, biomedical, deep-space exploration and other fields due to small size, no moving parts and adjustable. However, thermoelectric devices will be subjected to cyclic thermal stress under thermal cycling, which will lead to creep fatigue damage, resulting in accelerative degradation of cooling performance, lifetime and reliability reducation [1]. In this study, a strain-based thermoelectric element simulation model was established to evaluate the fatigue life and creep-fatigue life, which was verified by experimental results.And the creep lifetime was calculated by combining the linear damage accumulative law.In addition, the influence of hot side temperature range ΔT_h and minimum hot side temperature $T_{h,min}$ on the lifetime of thermoelectric element was analyzed, which were closely related to thermal stress The result shows:Compared with oscillating between 20 °C and 60 °C (ΔT_h = 40 K, $T_{h,min}$ = 20 °C), the lifetime decreased by 78% while oscillating between 20 °C and 120 °C (ΔT_h = 100 K, $T_{h,min}$ = 20 °C). Compared with oscillating between 20 °C and 80 °C (ΔT_h = 60 K, $T_{h,min}$ = 20 °C), the lifetime decreased by 84.26% while oscillating between 80 °C and 140 °C (ΔT_h = 60 K, $T_{h,min}$ = 80 °C). The higher the temperature of the hot end, the lower the rate of change of lifetime with the temperature of the hot end. This study has positive significance for improving the reliability of thermoelectric devices.

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Abstract number: AS-O.7-22

Designing a high-precision instrumentation to characterize the medium- and high-temperature thermoelectric generator modules

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Thermoelectric modules (TEMs) have been applied to many fields for its advantages of compactness, free-emission and reliable performance [1,2]. Their accurate characterization contributes to the optimum design of thermoelectric power system as well as the guidance of its application. Medium- and high-temperature TEMs have strict requirements on the characterization instrumentation regarding the accurate control of heat source's temperature, vacuum degree and isolating heat radiation. Herein an instrumentation is designed to characterize high-temperature thermoelectric couple. The main part of the instrumentation is a vacuum tank in which the TEM was placed. This instrumentation can regulate the temperature of the TEM's hot side up to 700 °C to meet the test requirement with different temperature application ranges. It can characterize lab-made high- temperature TEM up to 3*7 mm^2 in size and low temperature TEMs whose size are lower than 50*50 mm^2. It uses a molecular pump to make the vacuum degree in the tank reach 10^{-3} Pa level. It's also specially designed to satisfy the demand of clamping pressure imposed on the TEMs with different sizes. It uses springs to provide the pressure of 0-4 kg for lab-made single TEM couple and cylinder to provide the pressure of 20 kg-100 kg for common size TEMs. In order to realize the measurement of the electrical parameters of a single TE couple with small internal resistance, a current source is used as an external load, and a voltmeter is used to monitor the voltage of the TEM. By adjusting the current of the TE couple, we can change its working condition from open circuit to short circuit. For the thermal parameters, a high precision heat flux meter is designed and calibrated then to determine the heat flux of at TEM's cold side with the measurement range from 0.05W to 6W. Besides, there is an infrared imager used to obtain the temperature distribution of the TEM. We can calculate the output power, hot side heat flux and TE conversion efficiency. A lab-made hH-type TE couple is characterized at 300 °C-600 °C to verify the precision of the instrumentation. According to the simulation results, the error of the device's characterization of the TEM's output parameters and thermoelectric conversion efficiency is less than 4% . The good precision and consistency of the results demonstrate that effectiveness and reliability of the test device in this study. This instrumentation has high precision on characterizing medium- and high-temperature TEM, which is helpful for optimal design of TEMs.

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Abstract number: AS-O.7-23

Quantitative nano-scale thermal measurement of thermoelectric materials based on scanning thermal microscopy

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With the emerging demand for high-density, high-reliability, and miniaturization of electronic components, the size of thermoelectric devices with fast cooling as well as power generation at ambient temperature differences continues to shrink, and thus quantitative thermal property measurement and thermal management at the micro- and nano-scale is critical. Scanning thermal microscopy (SThM) is a high spatial resolution thermal measurement technique developed on the scanning tunneling microscopy, which can accurately reflect the changes in local thermal signals. However, because of the unpredictable contact thermal resistance at the tip-sample interface, the quantitative assessment of the thermal properties is still very limited. In this paper, combined with the thermal resistance heat transfer model, finite element thermal simulation and SThM experiment, we accurately predict the contact thermal resistance and heat transfer characteristics between the tip and sample, and obtain a quantitative function of probe temperature and sample thermal conductivity. Then we have validated the model in the $Bi_2Te_{2.7}Se_{0.3}$ and Si systems, the results of which are basically consistent with LFA, both within ±5% error. In addition, some related test work on metal-thermoelectric-metal system is also studied. In conclusion, this work offers the possibility of achieving quantitative characterization of thermal conductivity at the micro-nano scale and promises to map the local thermal conductivity to microstructures of thermoelectric materials, which can guide the design and optimization of thermoelectric materials.

Abstract number: AS-P.1-01

Preparation and High-Temperature Thermoelectric Properties of Textured Cobaltate Ceramics

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Misfit-layered cobaltate $[Ca_2CoO_3]_{0.62}CoO_2$ (Co-121) prepared by the standard solid-state reaction has relatively high electrical resistivity and/or high Seebeck coefficient *S*. It was reported that grain-alignment of Co-121 shows higher theoretical density, lower electrical resistivity and higher power factor *PF* [1]. In this work, we have prepared cobaltate ceramics with controlled density and grain-alignment, using Sr and/or Bi substituted samples for further improvement of electrical resistivity.

At first, $[(Ca_{1-x}M_x)_2(Co_{1-y}Bi_y)O_3]_pCoO_2$ (M =Bi, (*x, y*) = (0.06, 0); M =Sr, (*x, y*) = (0.50, 0); and M =Sr, (*x, y*) = (0.20, 0.05)) were prepared by the solid-state reaction (Polycrystalline samples), the Spark plasma sintering (SPS) technique was used to consolidate the obtained powders (SPS samples). For the next step, we made single-crystal flakes by means of the flux growth technique. Textured cobaltate ceramics were prepared by the SPS procedure using single-crystal flakes. Thermoelectric properties of all samples were measured to evaluate *PF*.

While the highest thermoelectric properties, *PF* = 1.5×10^{-4} W $m^{-1}K^{-2}$ at 947 K, was accomplished with the polycrystalline sample with M =Sr, (*x, y*) = (0.20, 0.05), textured cobaltate ceramics with the same chemical composition showed comparable *S* and much lower electrical resistivity, resulted in the substantial increase in *PF* = 5.5×10^{-4} W $m^{-1}K^{-2}$ at 946 K.

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Abstract number: AS-P.1-02

Pr-doped $SrTiO_3/TiO_3$ thermoelectric crystal with eutectic morphology

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Eutectic morphology composed of a phase-separated structure including two (or three) phases can be fabricated directly from the melt with the chemical composition at an eutectic point by a unidirectional solidification. In our previous report [1], we developed a eutectic material, $SrTiO_3/TiO_2$ [STO/TO], composed of the TO and STO phases as a thermoelectric material to improve the thermoelectric properties by the phase-separated structure. Nb-doped STO/TO eutectic material fabricated by the unidirectional solidification using a micro-pulling-down method showed lower thermal conductivity than half of Nb-doped STO single crystal because of the phonon-scattering at boundaries between the TO and STO phases. In addition, the eutectic morphology could be controlled by the growth rate for the La-doped STO/TO eutectic material and further improvement was achieved [2]. In this study, we focused on another dopant, Pr, for the STO and tried to grow Pr-doped STO/TO eutectic material to evaluate the thermoelectric properties.

Square-columnar Pr-doped STO/TO eutectic material with a 10 x 10 mm^2 cross section could be grown from the melt by the unidirectional solidification. Pr-doped STO/TO eutectic material was composed of the uniformly dispersed TO rod phase in the STO matrix phase. Details of the growth and the thermoelectric properties will be reported.

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Abstract number: AS-P.1-03

Investigation on Sb incorporated Metal phase assisted MoS2 with enhanced electrical conductivity for self-powered wearable thermoelectric generator

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In wearable thermoelectric devices, many numbers of modules will be used to increase the power generation. 2D transition metal dichalcogenide (TMDC) has achieved great attention in wearable thermoelectric generators over past few years. Since the physical properties of the material closely related to their *in-plane* configuration and lattice structure, electronic transport and bandgap of 2D TMDCs can be tuned by the transition of 2H to 1T phase. In this work, we focused to prepare metal phase assisted antimony doped MoS_2 grown on carbon fabric and analyzed structural, compositional, morphological characteristics along with the thermoelectric properties.

From XRD and Raman analysis, existence of 2H and 1T phase has been confirmed. Positive value of *S* for all the samples implies *p*-type behaviour of the samples. At 308 K, FMSb-0 exhibits *S* of around 9.34 μV/K, which is the maximum *S* compared to all the samples at RT. 4 wt% doping of antimony resulted in increment in electrical conductivity which reaches around 5000 S/m at 340 K. Further increase in Sb concentration leads to the increase in electrical conductivity of around 11800 S/m at RT for $FMSb_6$. Power factor of all the samples has been calculated using Seebeck coefficient and electrical conductivity. The maximum *PF* obtained for $FMSb_6$, which is around 0.60 $\mu W/mK^2$ at 315 K. The obtained *PF* is 3 times higher than pristine MoS_2 grown on CF.

Abstract number: AS-P.1-04

An Energy-Free Evaporative Cooling Technique for Improve the Output Performance of Thermoelectric Generator

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Air cooling or water cooling has been used to improve the output performance of thermoelectric generator (TEG) due to efficient cooling capacity. However, above cooling methods require additional energy consumption, which will reduces the overall output performance of the TEG system. Therefore, it urgent to develop an cooling technique without energy consumption to improve the output performance of TEG. In this study, we have developed a novel passive evaporative cooling (NPEC) technology to improve the output performance of TEG. The NPEC heat sink is constructed by super-hydrophilic porous film material and an aluminum heat sink. Based on the inherent porous structure and super-hydrophilicity of film material, energy-free water transport can be realized by capillary suction. Uninterrupted evaporative cooling will greatly improve the output performance of TEG. And both theoretical modeling and experimental verification have been carried out. The result show that the output voltage nearly 2 times higher than the control group (without evaporative cooling).

Abstract number: AS-P.1-05

Thermoelectric properties of Bi_2Te_3-$CoFe_2O_4$ nanocomposite

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Nanostructures and nanocomposites are of great interest for thermoelectric application as presence of the large phonon scattering and high Seebeck coefficient would result in the enhancement of figure of merit (*ZT*) [1]. Bismuth telluride (Bi_2Te_3) is best suited material for the thermoelectric applications due to large carrier effective mass, good electrical performance and low value of thermal conductivity and has superior heat to electrical energy conversion efficiency at room temperature [2].

In present report, we investigated the effect of magnetic $CoFe_2O_4$ (CFO) nanofillers on the thermoelectric properties of Bi_2Te_3 nanosheets and their role in the enhancement of thermoelectric power factor (*PF*) is demonstrated. A ~54% enhancement in the *PF* is obtained due to an increase in the electrical conductivity and Seebeck coefficient, simultaneously. In the presence of small magnetic field, the enhancement in the electrical conductivity and Seebeck coefficient is due to the interpenetrating network of magnetically induced reorientation of magnetic moments of CFO nanoparticles in the Bi_2Te_3 matrix which facilitate the electrical transport of charge carriers. Thus, the simultaneous enhancement in the electrical conductivity and Seebeck coefficient significantly enhanced the thermoelectric power factor.

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Abstract number: AS-P.1-06

Electronic and Thermal Transport Properties of Mg_3Sb_2

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Thermoelectric (TE) devices are used for waste heat recovery, which requires non-toxic, low-cost, and highly efficient materials. The Zintl compound Magnesium Antimonide (Mg_3Sb_2) is one of the promising materials that has a high Seebeck co-efficient, low thermal conductivity, with eco-friendly, inexpensive, and abundant in nature. We studied the structural, morphological, electronic, and thermal transport properties of the size symmetry and size asymmetric Magnesium (Mg) and Antimony (Sb) based Mg_3Sb_2. The Mg (particle size 37 µm), bulk Sb (particle size 37 µm), and Wet Chemically Synthesized Sb (WCS Sb, particle size 800 nm) were used to synthesize *p*-type Mg_3Sb_2 by solid-state reaction. The sample exhibited trigonal crystal structure with the space group of *P-3m1* (164). From the electrical transport property, the Mg_3Sb_2 synthesized using WCS Sb exhibits the low resistivity of 174 mohm-cm at 700 K, which is 75% higher than bulk Sb based Mg_3Sb_2 because, the relaxation time plays the major role in the electrical resistivity. The total thermal conductivity of the WCS Sb used Mg_3Sb_2 is lower than the bulk Sb used Mg_3Sb_2, which is 0.47 W/m-K at 700 K due to the scattering of acoustic phonon at the grain boundary.

Abstract number: AS-P.1-07

Significant improvement in Thermoelectric performance of SnS via Hydrothermal Synthesis

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Carrier concentration optimization plays a significant role in enhancing thermoelectric performance. Here we are enhancing the hole concentration of SnS by doping Cu at Sn site by hydrothermal method. Further the crystallographic and morphological studies are carried out. The X-ray diffraction data confirms the formation single phase with orthorhombic structure for pure sample and examined secondary phases for higher concentration of Cu doped samples and the homogeneity of the sample was confirmed by FE-SEM mapping. The hall measurement studies confirmed the p-type semiconductor nature of the sample. It shows that there is improvement of carrier concentration from 3.77 10^{15} cm^{-3} to 6.91 10^{17} cm^{-3} results the significant enhancement of electrical conductivity and power factor. Ultra-low lattice thermal conductivity is achieved for Cu doped SnS sample which is 0.440 W/mK at 663 K and high value of seebeck coefficient were obtained is 804.21 μV/K at room temperature. This work proves that SnS is an economical and easily fabricated and successful material for thermoelectric application.

Abstract number: AS-P.1-08

Enhancement of Thermoelectric Properties in β-$FeSi_2$ Employing Process Sequencing and Formation Kinetics

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β-$FeSi_2$ has great potential in mid-temperature range waste heat recovery applications, due to its thermal stability and non-toxic nature. However, the low figure-of-merit values and manufacturing process complexity curtails its application in thermoelectric power conversion devices. Moreover, the various phases involved in the Fe-Si phase diagram are principally affecting the thermoelectric performance and their reaction kinetics slow down the required β-$FeSi_2$ formation. In the present study, the β-$FeSi_2$ phase formation was realised with the aid of a plasma-activated in-situ reactive sintering process. The formation kinetics was investigated by applying the different process sequencing such as arc-melting, ball milling and sintering techniques followed by an annealing process. The X-ray diffraction and scanning electron microscopic techniques were used to confirm the structural and phase purity of the synthesized material. Our study experiments with the optimized processing maps which realise the high thermoelectric performance in β-$FeSi_2$ materials.

Abstract number: AS-P.1-09

Effect of Sintering temperature on phase formation and electronic properties of Chromium disilicide based thermoelectric material

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Chromium disilicide is attracting *p*-type mid-temperature range thermoelectric material owing to its large power factor. Chromium disilicide is synthesized using a reactive spark plasma sintering process at three different sintering temperatures. The electronic properties are investigated along with the phase formation at three different processing temperature conditions. The phase structure of the synthesized materials was characterized using X-ray diffraction. The material synthesized at 1150 K exhibits a single phase $CrSi_2$ and it is observed that the sintering temperature plays a main role in the phase formation. The material synthesized at 1100 K has elemental Si while the material processed at 1050 K has elemental Si, CrSi and Cr_3Si phase. The significant power factor value of ≃ 2.47 × 10-3 W/mK^2 is achieved and is mainly due to the formation of the $CrSi_2$ phase employing the reactive SPS process.

Abstract number: AS-P.1-10

Improved power factor of Higher manganese silicide by introducing ZnO prepared by spark plasma sintering

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The introducing the secondary phase on the host materials give another advantage to increase the grain boundary with change the lattice thermal conductivity of the two boundary which is improve the power factor. Higher manganese silicide (HMS) is a promising *p*-type mid-temperature range thermoelectric material with 0.77 eV band gap. HMS are the best suitable candidate for mid temperature range application due to their good mechanical and thermal stability. HMS are low cost and non toxic materials however low thermoelectric properties restrict their applications. We report the enhanced power factor by ZnO addition on the HMS via spark plasma sintering (SPS). The phase structure of the synthesized materials was characterized using X-ray diffraction. The sample sintered at 1150 K has single HMS phase. An improved power factor 2.47×10^{-3} W/mK^2 was observed by ZnO addition which is 24% higher than pristine HMS.

Abstract number: AS-P.1-11

Thermoelectric Generator for Hybrid Electric Vehicle

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The well-to-wheel efficiency of passenger vehicles is less than 40%. The remaining 60% is waste energy. There is an opportunity to use this waste of heat energy and improve the efficiency of the power train. About 25-30% of heat energy is lost in exhaust gases for an automotive vehicle. This waste heat can be trapped and converted to electrical energy directly without moving parts using the thermoelectric generator. A thermoelectric generator is a solid-state device of semiconductors connected by metal electrodes sandwiched between ceramic substrates. A thermoelectric generator is suitable for the automotive exhaust system as it is reliable and has no moving parts.

The present work is to design and fabricate a thermoelectric generator for hybrid electric vehicle. A hybrid electric vehicle is simulated in MATLAB and exhaust gas properties are extracted. Based on energy available in exhaust gases a heat exchanger for TEG is designed and fabricated. Performance of TEG is evaluated on test bench using hot gas producer that produce trainsent state hot gases. Similar to the simulated exhaust gas properties. Energy recovered from TEG is projected back on to the vehicle through simulation platform. Simulation of hybrid electric vehicle with TEG will be done and assessmentof fuel saving and emission is done. The efficiency is increased by 2%.

Abstract number: AS-P.1-12

From Indian Galena Ore to Thermoelectric Generator produce electricity for unique applications .

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Indian Galena Ore is second largest mines in world. It has good semiconducting properties which we had used for making Thermoelectric Generator. Indian Galena Ore is available in two forms; one as chunk galena ore and another one as beneficiated galena ore. We had used both types of ore for making *n*-type and *p*-type arms of thermoelectric generator by doping with different mole percent of Na_2S, Pb, In etc. at inert atmosphere heating at different temperatures and duration. After doping we had made the arms of *n*-type and *p*-type in the form of pellet by inert atmosphere sintering at different temperatures and durations or by vacuum hot pressing technique at different temperatures, durations and pressures. We had achieved optimum thermoelectric properties like electrical resistivity in the range of 20 to 30 μΩ cm level, thermoelectric power in the range of 190 to 200 μV, *k* and thermal conductivity, *K* in the range of $6.6x10^{-3}$ cal,seccmk, We had also coated both the arms by galena adhesive coating for prevention from oxidation and corrosion etc. Galena thermoelectric generator was made by making couples by hot pressing nickel contacts. A Series of 127 couples was used for one galena thermoelectric generator to produce current by maintain temperature difference of 773 K, giving the output of 5 W. This type of thermoelectric generator is very useful for cathodic protection, operations of mini electronic chips, some of specific medical purposes.

Abstract number: AS-P.1-13

Study of grain size effect on thermoelectric properties of Manganese doped MoS_2

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Molybdenum disulfide (MoS_2) as a chalcogenide with semiconducting properties might found practical applications in thermoelectric power generation if its properties being engineered properly. As an indirect gap semiconductor (E_g = 1.3 eV) in bulk morphology, it is challenging to be processed due to high melting point of MoS_2. In this research, Spark Plasma Sintering technique implemented to prepare Corbino shape geometry sample of Mn doped MoS_2. Fabricated sample is polycrystalline as PXRD structural analysis confirms with average grain size of 500 nm obtained through SEM analysis. It is *n*-type doped with the carrier density of 1.7×10^{17} cm^{-3}.

Abstract number: AS-P.1-14

Phase stability study of MoS_2+MoO_3 matrix-alloy for possible thermoelectric applications

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Fabricating novel compounds with desirable thermoelectric properties (high *zT*) is an intriguing topic within the field of thermoelectricity. Molybdenite (MoS_2) as a member of chalcogenide family benefits semiconducting properties while MoO_3 is a nonconductive oxide. In this research we tried to calculate Gibbs free energy and thermodynamical phase diagram for (MoS_2/MoO_3) Matrix-alloy for possible fabrication through sintering process. The previous sample made through sintering technique using bare MoS_2 lacks the control over the electrical conductivity due to intrinsic impurities. Through mixing these two Molybdenum based compounds, possibility of optimizing both thermal and electrical conductivity being checked to get the best *zT* for such a mixture-alloy.

Abstract number: AS-P.1-15

Enhanced electronic transport properties of $InSb_{1-x}Bi_x$ by partial substitution of Bi on the Sb site

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Thermoelectric materials can be used for converting waste heat to DC power and reduce environmental pollution. InSb has superior electronic transport properties because of its narrow bandgap and high charge carrier mobility, but its high lattice thermal conductivity makes it less pertinent for thermoelectric applications. We present an effective approach for simultaneously boosting power factor and reducing total thermal conductivity by partial substitution of isoelectronic Bi on the Sb site. A series of $InSb_{1-x}Bi_x$ (x = 0, 0.03, and 0.06) polycrystalline materials were prepared using solid-state reaction followed by hot-press sintering at 773 K with an applied pressure of 70 MPa for 2 h. The enhanced power factor is attributed to the increase of carrier concentration by charge transfer from the Bi *d*-orbital states to the In *4d*-orbital states, which is inferred from both the Bi and In L3-edge XANES spectra of $InSb_{1-x}Bi_x$. Due to the point defect, the lattice thermal conductivity of the $InSb_{1-x}Bi_x$ decreases. The blue shift in Raman spectra of $InSb_{1-x}Bi_x$ indicates the strain field fluctuations. As a result, zT of $InSb_{0.94}Bi_{0.06}$ is 0.56 at 700 K, which is 16% higher than the pristine InSb.

Abstract number: AS-P.1-16

Enhanced Power Factor of *p*- Bi_2Te_3 & *n*- Sb_2Te_3

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The power factor is an indicator of the performance of thermoelectric materials. Many researchers have attempted, to improve the thermoelectric conversion efficiency of materials by various techniques, for example doping. We present *n*-Bi_2Te_3 and *p*-Sb_2Te_3 materials prepared by hot pressing method at 673 K for 2 h in Ar atmosphere. Bulk samples were investigated for their crystalline structure, hardness, and power factor by XRD, micro-Vickers hardness and four probes method, respectively. The electrical resistivity, Seebeck coefficient, and power factor values of *n*-Bi_2Te_3 and *p*-Sb_2Te_3 bulk samples were higher than literature data in the same temperature range (325 - 475 K). The higher power factor value of Bi_2Te_3 and Sb_2Te_3 bulk samples of this study are resulted from their high density and high micro-Vickers hardness of the samples.

Abstract number: AS-P.1-17

Theoretical Prediction and Thermal Transport Properties of Novel Monolayer $TlPt_2Se_3$

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The theoretical prediction, electronic properties, and thermal transport properties of novel monolayer $TlPt_2Se_3$ are investigated using the first-principles calculations and semi-classical Boltzmann transport theory. The calculated phonon band structure and exfoliation energy confirm that monolayer $TlPt_2Se_3$ is a stable material and can be exfoliated from its bulk counterpart. The exfoliation energy of the monolayer turns out to be 37 meV $Å^{-2}$, comparable with the exfoliation energy of monolayer $PdSe_2$. The HSE06 indirect bandgap of monolayer (bulk) $TlPt_2Se_3$ amounts to 1.18 eV (0.63 eV). The relaxation time is calculated considering three types of scattering mechanisms. The monolayer outperforms the bulk counterpart in the Seebeck coefficient and power factor for both *p*-type and *n*-type dopings. Monolayer $TlPt_2Se_3$ shows a high *p*-type Seebeck coefficient of 211 μV K^{-1} compared to the *n*-type Seebeck coefficient of 103 μV K^{-1} at maximum considered temperature (600 K) and a carrier concentration ($10^{20}cm^{-3}$). The calculated lattice thermal conductivity of monolayer $TlPt_2Se_3$ is 1.92 W $m^{-1}K^{-1}$ at 600 K which is lower than the monolayer $PtSe_2$ and $MoSe_2$. The *p*-type figure of merit of 0.64 (at 600 K) affirms that the monolayer $TlPt_2Se_3$ is an excellent thermoelectric material.

Abstract number: AS-P.1-18

A dataset of semiconductor charge carrier scattering and transport properties

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The charge carrier scattering and transport processes are fundamental to semiconductors for electronics, thermoelectrics, and many other applications. However, detailed scattering and transport characterizations are limited to a small number of materials. In this work, we profile the charge transport properties of over 1700 experimentally known semiconductors by incorporating electron-phonon and electron-impurity scatterings from density functional (perturbation) theory calculations. Origin of some unexpected temperature- and doping-dependence of the transport properties are investigated in details. We demonstrate that electron-optical-phonon interaction is unambiguously the dominant scattering mechanism for the majority of these semiconductors, and remains significant even with substantial doping and impurity scattering. By combining the knowledge with machine learning models, we further predicted the carrier mobilities of over 19000 semiconductors with substantially reduced cost. High-performance semiconductors and their key structural and electronic features are also identified to assist materials discovery and optimization.

Abstract number: AS-P.1-19

Significantly enhanced thermoelectric figure of merit of *n*-type Mg_3Sb_2-based Zintl phase compounds via co-doping of Mg and Sb site

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N-type Mg_3Sb_2 thermoelectric material has a complex crystal structure and electronic structure,which is a new thermoelectric material with excellent application prospects. The state density and band structure of $Mg_{24}Sb_{16}$ and Bi/Se/Pr-Se/Nd-Se doped $Mg_{24}Sb_{16}$ are first-principles calculated. Se/Pr-Se/Nd-Se doped increases the density of states around the Fermi level. Bi-doped does not impact the band structure because the electronic structure between Sb and Bi are similar. The band gap of Pr-Se/Nd-Se doped becomes narrower, which is more conducive to carrier transport and increases carrier concentration than that of single-doped Se. The experimental results show that Pr and Nd replace Mg to provide more electrons for the system. The carrier concentration of the co-doped sample increases significantly, thus improving the power factor and optimizing the samples' electrical properties. The highest *ZT* value of the $Mg_{3.2}Sb_{1.5}Bi_{0.49}Se_{0.01}$ sample is 1.21. Pr-Se/Nd-Se co-doped *ZT* values are 1.67 and 1.74, respectively, 38% and 43% higher than the $Mg_{3.2}Sb_{1.5}Bi_{0.49}Se_{0.01}$ sample. Multi-element doped is an effective strategy to improve the thermoelectric properties of materials.

Abstract number: AS-P.1-20

Achieving high thermoelectric performance through carrier concentration optimization and energy filtering in Cu_3SbSe_4-based materials

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The previous works commonly adjust the carrier concentration through acceptor doping, but at the same time, the decrease of the Seebeck coefficient limits the further improvement of electrical properties in Cu_3SbSe_4-based materials. In this work, a microwave-assisted hydrothermal synthesis method was used to synthesize Cu_3SbSe_4/TiO_2 hollow microspheres. Part of TiO_2 participates in the reaction, replaces the Sb site of Cu_3SbSe_4 to form holes, and the rest is dispersed in the matrix in the form of the second phase. The first-principles calculations reveal that the doping of Ti significantly changes the band structure and phonon spectrum, thereby regulating carrier concentration while increasing phonon scattering. In addition, experimental results show that the energy filtering effect generated by the extra-mixed TiO_2 nano particles, which suppresses the decrease of Seebeck coefficient by acceptor doping. Consequently, the highest average power factor 897.5 μW $m^{-1}K^{-2}$ and the zT peak value of 0.70 can obtained in $Cu_3SbSe_4/6\%TiO_2$ sample of 298-623 K. This work provides a new sight to improve the thermoelectric properties in Cu_3SbSe_4 through carrier concentration regulation and nano-phase composition.

Abstract number: AS-P.1-21

Dual Post-treatments Boost Thermoelectric Performance of PEDOT:PSS Films and Their Devices

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Owing to intrinsically high electrical conductivity and low thermoelectric conductivity, poly(3,4-ethylenedioxithiophene):poly(styrenesulfonate) (PEDOT:PSS) shows promising thermoelectric properties. However, its relatively low power factor limits the practical applications of PEDOT:PSS. Here, we use unique dual post-treatments by sodium sulfite (Na_2SO_3) and formamide (CH_3NO) to boost the thermoelectric performance of flexible PEDOT:PSS films with an optimized power factor of 74.09 μW $m^{-1}K^{-2}$. Comprehensive characterizations confirm that CH_3NO reduces the excessive insulating PSS and thereby increases the electrical conductivity, while Na_2SO_3 lowers the reduction of the doping level of PEDOT, leading to an increased Seebeck coefficient. Furthermore, the rationally post-treated PEDOT:PSS films are assembled into a flexible thermoelectric device that exhibits an output voltage of 2.8 mV using the heat from the human arm, indicating great potential for practical applications on sustainably charging low-grade wearable electronics.

Abstract number: AS-P.1-22

Defect engineering synergistically modulates power factor and thermal conductivity of $CuGaTe_2$ for ultra-high thermoelectric performance

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The ternary chalcopyrite $CuGaTe_2$ has emerged as a promising p-type thermoelectric material with its advantages of low cost, good stability, non-toxic elements. However, its thermoelectric performance is limited by the intrinsic low electrical conductivity and high lattice thermal conductivity. In this work, A deficiency of Cu in $Cu_{1-x}GaTe_2$ semiconductors can be used to optimize the electrical properties by improving the carrier concentration, and to reduce thermal conductivity through multi-scale phonon scattering, which is predicted and guided by the First-principles density functional theory calculations. The carrier concentration is increased to 10^{20}, which compensates for the low electrical performance caused by the intrinsic low n_H of $CuGaTe_2$. The average power factor of $Cu_{0.96}GaTe_2$ reaches 106.3% higher than that of the original $CuGaTe_2$. In addition, the lattice thermal conductivity of the defective samples is greatly reduced at high temperature, which is mainly due to the reduction of sound speed and phonon scattering. All the above factors contribute to the highest ZT value of 1.23 at 823 K in $Cu_{0.96}GaTe_2$, which is 114% higher than the pristine $CuGaTe_2$, and the average ZT is 171.4% higher.

Abstract number: AS-P.1-23

Enhancing the thermoelectric performance by reduced phonon life time by solid state solution of $SnSe_{1-X}$ $Cu_XSe_{0.75}S_{0.25}$

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Thermoelectric materials consider as an alternative energy resource to tackle the energy crisis and solve the environmental problem by enabling the direct conversion of waste into electricity. Earth abundant IV-VI semiconductor Tin selenide (SnSe) regarded as suitable candidate due to their thermal conductivity and high electrical transport performance. Herein, solid state solution $SnSe_{1-X}$ $Cu_XSe_{0.75}S_{0.25}$ samples are synthesized by ball milling and followed by hot press method. The effects of Cu into solid state solution of SnSe on the phase composition, microstructure, and thermoelectric properties of the composites are investigated. The formation of orthorhombic crystal structure is confirmed by X-ray diffraction pattern. HRTEM micrographs highlight the samples' highly crystalline structure, as well as the formation of defects, distinguishable grains, and grain boundaries, all of which aid in lowering heat conductivity. These formation of solid-state solution leads to enhance the phonon scattering and reduced the thermal conductivity.

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