Plenary Speakers

Durable thermoelectric devices made from sustainable magnetsium-antimony alloys

Kornelius Nielsch[2], Pingjun Ying[1], Amin Bahrami[1], Ran He[1]
[1]Institute of Materials Research, Technical University of Dresden, Germany
Plenary Talk: Kornelius Nielsch, IFW Dresden, Germany, September 16, 2026, 09:00 - 09:45

Thermoelectric technology has witnessed a resurgence in recent years due to increasing demands for sustainable energy sources and efficient cooling systems. Recently, the introduction of Te-free thermoelectric modules using non-toxic, abundant materials including p-type MgAgSb and n-type Mg3(Sb,Bi)2 marked [1-3] a significant breakthrough. Despite promising performance, questions persist regarding long-term robustness and stability, especially in harsh environments. In this study, a thorough exploration of thermoelectric modules is conducted, focusing on their performance degradation under various conditions. Through elemental mapping analysis, degradation mechanisms are identified within the modules during cycling in argon environments, where atomic migrations and the formation of complex oxides at contact regions are key factors. Furthermore, cycling tests in air reveal significant degradation, prompting the exploration of protective strategies. Surface coatings using atomic layer deposition (ALD) emerge as a promising solution, particularly by HfO2, demonstrating superior protective effects. Furthermore, re-soldering effectively restores module performance is found, highlighting the importance of developing advanced soldering techniques to promote magnesium-based thermoelectric technology as a sustainable alternative to Bi2Te3. These findings emphasize the importance of exploring novel contact materials and demonstrate the potential of ALD as a universal approach to enhancing module reliability and robustness [4].

References:
[1] P. Ying, R. He, R., J. Mao, K. Nielsch, et al., Nat Commun 12, 1121 (2021).
[2] P. Ying, H. Reith, K. Nielsch, R. He, Small 18, 2201183 (2022).
[3] P. Ying, L. Wilkens, H. Reith, N. Perez Rodriguez, X. Hong, Q. Lu, C. Hess, K. Nielsch, R. He, Energy & Environmental Science 15, 2557 (2022).
[4] P. Ying, K. Nielsch, et al., Advanced Functional Materials 34, 826 (2024).

Acknowledgements:
This work was supported by M-ERA.NET program via the funding of the THERMOS project.

Phonon transport experiments: achievements and challenges to engineer thermoelectric parameters

Porf. Dr. Clivia M. Sotomayor Torres[1]
[1]International Iberian Nanotechnology Laboratory, Portugal

Plenary Talk: Clivia M. Sotomayor Torres, International Iberian Nanotechnology Laboratory, Portugal, September 18, 2026, 09:00 - 09:45

I will review recent work on nanoscale thermal transport in 2D materials and contextualize it in the frame of both: the prospective role of 2D materials and the possible contribution of topological protection of phonon transport to enhance thermoelectric parameters.
I will consider recent progress in the community on patterned 2D materials membranes and multilayers and will discuss the potential and challenges faced to deploy them in thermoelectric applications. Recent experimental results in phonon transport in Si-based topological phonon waveguides will serve to illustrate future possible avenues of research based on concepts belonging to the realm of topological phases of matter. Two examples will be reported from recent research in my group and elsewhere to address the interplay of nanostructures, interfaces and thermal transport in the cases of silicon-based phonon-waveguides in lab-scale and selected 2D materials.

Transverse Thermoelectrics and Spin Caloritronics

Ken-ichi Uchida[1,2]
[1]National Institute for Materials Science (NIMS), Japan, [2]The University of Tokyo, Japan
Plenary Talk: Ken-ichi Uchida, National Institute for Materials Science (NIMS) & The University of Tokyo, Japan, September 17, 2026, 09:00 - 09:45

Transverse thermoelectric effects interconvert charge and heat currents in orthogonal directions due to the breaking of either time-reversal symmetry or structural symmetry, enabling simple and versatile thermal energy harvesting and solid-state cooling/heating within single materials [1,2]. The transverse thermoelectric conversion due to the time-reversal symmetry breaking appears in a conductor under a magnetic field or in a magnetic material with spontaneous magnetization, which has been actively investigated in the field of spin caloritronics [3]. The transverse thermoelectric conversion due to the structural symmetry breaking occurs in artificial anisotropic structures or single crystals with anisotropic transport properties, which does not require a magnetic field or magnetization. In comparison to the complex module structures required for the conventional Seebeck and Peltier effects, the transverse thermoelectric effects provide complete device structures, potentially resolving the fundamental issue of multi-module degradation of thermoelectric conversion performance.

In this talk, we provide an overview of currently known transverse thermoelectric conversion phenomena and principles, as well as their characteristics, and reclassifies them in a unified manner [2]. Examples of recent application research and material development in transverse thermoelectrics are also introduced [4-6], followed by a discussion of future prospects.

[1] K. Uchida and J. P. Heremans: Joule 6, 2240 (2022).
[2] H. Adachi, F. Ando, T. Hirai, R. Modak, M. Grayson, and K. Uchida: Appl. Phys. Express 18, 090101 (2025).
[3] K. Uchida: Proc. Jpn. Acad., Ser. B 97, 69 (2021).
[4] K. Uchida, T. Hirai, F. Ando, and H. Sepehri-Amin: Adv. Energy Mater. 14, 2302375 (2024).
[5] T. Hirai, F. Ando, H. Sepehri-Amin, and K. Uchida: Nat. Commun. 15, 9643 (2024).
[6] F. Ando et al.: Energy Environ. Sci. 18, 4068 (2025).

Tailoring Thermoelectrics through metavalent Bonding

Matthias Wuttig[1,2], Yuan Yu[1]
[1]RWTH Aachen University, Germany, [2]Peter-Grünberg-Institute (PGI 10), Germany

Plenary Talk: Matthias Wuttig, RWTH Aachen University, Germany,
September 15, 2026, 09:00 - 09:45

Thermoelectrics combine an interesting portfolio of properties. They possess a small thermal but a reasonably large electrical conductivity and a rather high Seebeck coefficient. This combination of properties is quite rare; but attractive for a number of applications. These properties are particularly desirable for thermoelectrics which can convert waste heat into electrical energy. Hence, different strategies have been devised to identify and tailor materials for thermoelectric applications. Recently, we have developed a design concept for thermoelectrics which is based upon an in-depth understanding of the underlying bonding mechanism. In particular, we can show that many chalcogenide- and pnictogen- based thermoelectrics employ an unconventional bonding mechanism, which differs considerably from ordinary covalent, metallic or ionic bonding. This bonding mechanism is identified by a unique property portfolio. Some of the characteristic properties are highly beneficial for thermoelectric applications including the low thermal conductivity and the modest electrical conductivity. We will unravel the origin of these unusual features and relate them to a special bonding mechanism in these chalcogenides, which has been coined metavalent bonding. This unique bonding mechanism is also characterized by an unconventional bond rupture which is quite different from covalent or metallic bonding, providing further support for the notion of a unique bonding mechanism in these chalcogenides. Subsequently, a map has been devised which quantifies chemical bonding in solids and identifies a region where (only) metavalent solids are found. This map can be utilized to locate thermoelectrics and guides the search for novel thermoelectrics as well as relevant property trends. In this presentation, a number of thermoelectrics will be presented, whose properties can be explained and designed through metavalent bonding.

Invited Speakers and Prize Speaker

Thermoelectric Subcooling Technology to Enhance Vapor Compression Systems

Patricia Aranguren[1], D. Astrain[1], A. Rodríguez[1], L. Catalán[1], A. Martínez[1], M. Araiz[1], A. Casi[1], I. Alzuguren[1]
[1]Public University of Navarre, Spain

Applications-2, September 16, 2026, 13:30 - 15:00

Refrigeration and air conditioning technologies are indispensable to modern society, yet they account for approximately 17% of global electricity consumption. In the commercial sector, refrigeration systems in supermarkets and food logistics centers represent up to 60% of total energy use, operating continuously under varying thermal loads. Similarly, vapor compression systems for cooling and heating applications account for 20% of total energy consumption in buildings. As global demand for cooling escalates, high-efficiency solutions are paramount to mitigate indirect CO2 emissions, as electricity consumption represents 80% of the total environmental impact of these systems. This talk explores the integration of thermoelectric subcooling (TESC) as a strategic modification to conventional vapor compression cycles. By implementing a solid-state TESC at the condenser or gas cooler outlet, the system achieves a significant increase in specific cooling capacity without additional compressor work, thereby enhancing overall performance with minimal added complexity. This study evaluates the thermodynamic benefits of TESC across different refrigerants and applications, demonstrating potential COP increments, increased cooling capacities, and enhanced controllability. The results highlight TESC as a compact, robust, and scalable solution for improving the sustainability of vapor compression technologies.

Keywords: Vapor compression systems, Thermoelectric subcooling, COP enhancement, Energy consumption reduction.

Anomalous Lorenz number in heavily-doped semiconductors

Christophe Candolfi[1], Bartlomiej Wiendlocha[2], Petr Levinský[3], Gwladys Steciuk[1], Sylvie Migot[1], Ilayda Terzi[1], Arthur Wieder[1], Soufiane El Oualid[1], Bertrand Lenoir[1]
[1]Université de Lorraine, France, [2]AGH University of Krakow, Poland, [3]FZU – Institute of Physics of the Czech Academy of Sciences, Czech Republic

Chalcogenides-2, September 16, 2026, 13:30 - 15:00

The Wiedemann-Franz law is an empirical relation that relates the charge and heat flows through the Lorenz number L in electrical conductors, providing a straightforward mean to disentangle the lattice and the electronic contributions to the thermal conductivity. Various physical mechanisms lead to deviations of L from the universal, constant Sommerfeld value L0 or from the temperature dependence L(T) inferred from transport models solution to the Boltzmann transport equation. While this last approach can be successfully applied to most semiconductors, it has been found to break down in several heavily-doped semiconductors, yielding unphysical lattice thermal conductivity values at high temperatures. This finding suggests that additional physical mechanisms are at play, resulting in deviations of L from the values derived from transport models. In this presentation, taking the Bi0.4Sb1.6Te3 as an example, inelastic electron-electron and electron-phonon scattering mechanisms will be discussed as a source of these deviations. A model derived for PbTe, which explicitly takes into account these two mechanisms and provides a possible framework to calculate L(T), will be further presented.

Direct Physical Modeling vs. Learned Patterns: Computation-Guided Thermoelectric Materials Discovery in the Age of Machine Learning

Elif Ertekin[1]
[1]University of Illinois at Urbana-Champaign, United States

Machine Learning, September 15, 2026, 13:30 - 15:00

The rapid adoption of machine learning methods in materials science raises several interesting questions for computational thermoelectric materials discovery [1]. Historically, computational searches for thermoelectrics have centered on direct physical modeling: we know from quantum mechanics, statistical mechanics, and transport theory what equations should be solved, and we try to solve them with sufficient fidelity to make robust and accurate predictions. Necessarily, these approaches rely on approximations and model reduction, so their predictions carry accumulated uncertainty from many sources. In contrast, many ML/AI approaches rely on learning patterns and correlations from observed data, whether computational or experimental, and may do so without explicitly invoking the underlying physical mechanisms.

Thermoelectric materials provide a particularly useful setting in which to compare these approaches. A good thermoelectric material must simultaneously satisfy many requirements, including favorable electronic transport, low lattice thermal conductivity, chemical and structural stability, and defect chemistry compatible with useful doping. As a result, thermoelectric discovery is not simply a problem of predicting one property well, but of reasoning across many coupled and uncertain materials attributes.

In this talk, I will share perspectives on computation-guided thermoelectric materials discovery from this viewpoint. First, I will discuss the level of predictive accuracy that can be expected from direct physical modeling, using Bayesian reasoning to estimate how computational uncertainty propagates into materials discovery. This analysis also asks how much computational accuracy would need to improve in order to substantially improve predictive accuracy; the lesson is that meaningful gains will require significant improvements in accuracy. I will compare this perspective with the predictive behavior observed in a simple language-model-based approach that we applied to materials search and discovery [2]. Finally, I will discuss a recent approach that combines direct physical modeling with statistical analysis to identify promising materials subspaces for thermoelectric discovery, with applications to half-Heusler compounds [3,4].

[1] Toberer et al., MRS Bulletin 50, 966 (2025).
[2] Qu et al., npj Computational Materials 10, 58 (2024).
[3] Pak et al., Journal of Materials Chemistry A 13, 19455 (2025).
[4] Pak et al., Journal of Materials Chemistry C (2026), DOI: 10.1039/d6tc01042c.

Defects and thermoelectric transport in Half-Heusler compounds

Chenguang Fu[1]
[1]Zhejiang University, China

Heusler-1, September 15, 2026, 13:30 - 15:00

Half-Heusler compounds with a valence electron count of 18 represent a class of semiconductors that hold great promise as high-performance thermoelectric materials for power generation and other functional applications. Defects play a crucial role in enhancing the thermoelectric and other functional properties of half-Heusler compounds. Therefore, defect studies had already been initiated as early as the 1990s, when half-Heusler MNiSn compounds (M = Ti, Zr, Hf) were discovered to show semiconductor behavior. This talk will review studies on the relationship between defects and thermoelectric transport properties in half-Heusler thermoelectric compounds, with a focus on n-type MNiSn—the most representative half-Heusler system to date. In addition, this talk will highlight recent advances in the typical p-type half-Heusler compound NbFeSb, emphasizing the aliovalent-doping-induced modulation of electronic and phonon structures, as well as the resulting thermoelectric transport properties. Finally, emerging research directions in half-Heusler thermoelectrics will be discussed to outline future challenges and opportunities.

Crystal and defect chemistry in thermoelectric sulfides

Emmanuel Guilmeau[1]
[1]CRISMAT, CNRS, France

Invited Talk: Emmanuel Guilmeau, CRISMAT, CNRS, France, September 17, 2026, 09:45 - 10:15

The wide diversity of crystal structures found in sulfides, ranging from synthetic compounds to natural minerals, combined with their structural complexity and chemical flexibility, offers a remarkable playground for chemists and physicists to design materials with tailored electrical and thermal properties. Using both experimental and computational approaches, our recent investigations have provided new insights into the relationship between crystal structure and thermal transport in metal sulfides. We particularly emphasize how lone-pair stereochemical activity, bonding heterogeneity, structural dimensionality, anisotropy, and cationic disorder govern their thermal and vibrational properties. These findings open new perspectives for the development of cost-effective and sustainable sulfides for thermoelectric and thermal management applications

Machine Learning for Thermoelectric Materials Discovery: From Data Curation to Validation

Philippe Jund[1]
[1]University of Montpellier, France

Materials Theory, September 17, 2026, 13:30 - 15:00

Machine learning (ML) has emerged as a powerful tool for accelerating the discovery and optimization of thermoelectric materials. However, despite an increasing number of reported predictions, only a limited fraction of ML-discovered candidates have progressed toward experimental validation. This observation raises fundamental questions about the reliability, interpretability, and practical usefulness of ML approaches for thermoelectric research.

In this presentation, I will discuss the main challenges encountered when applying machine learning to thermoelectric materials, using half-Heusler compounds as a representative case study. Particular attention will be devoted to six key questions that determine the success of an ML workflow: (i) how to construct and curate reliable databases from heterogeneous experimental data, (ii) how to design train/test strategies that genuinely assess the ability of models to generalize to new materials, (iii) the respective strengths and limitations of commonly used algorithms such as Random Forests, XGBoost, Neural Networks, and SISSO, (iv) the role of feature engineering, feature selection, and hyperparameter optimization, (v) the importance of appropriate error metrics and uncertainty quantification, and (vi) the validation of ML predictions through first-principles calculations and experiments.

Examples drawn from the curation of experimental thermoelectric databases will illustrate how data quality can have a larger impact on predictive performance than the choice of the learning algorithm itself. The presentation will further show how physically informed validation strategies, combined with interpretable machine-learning models, can provide valuable insight into the descriptors governing thermoelectric performance. Finally, the challenges associated with extrapolation beyond the training domain and with the experimental realization of predicted materials will be discussed.

More broadly, this talk aims to provide a practical guide to the development of robust and trustworthy machine-learning workflows for thermoelectric materials discovery, highlighting both the opportunities and the current limitations of data-driven approaches.

Defect engineering and triangular copper as key drivers for ultralow thermal conductivity in Cu2ZrS3 polytypes

Lucas Le Gars[1], Sakshi Verma[2], Minati Tiadi[1], Carmelo Prestipino[1], Animesh Das[2], Bin Zhang[3,4], Olivier Perez[1], Philippe Boullay[1], Bernard Raveau[1], Gaëlle Riou[1], Adèle Renaud[5], Kanishka Biswas[2], Umesh V. Waghmare[2], Xiaoyuan Zhou[3,4], Emmanuel Guilmeau[1]
[1]CRISMAT, CNRS, Normandie University, France, [2]Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), India, [3]College of Physics and Institute of Advanced Interdisciplinary Studies, Chongqing University, China, [4]Analytical and Testing Center of Chongqing University, China, [5]University Rennes, CNRS, France

Prize Talk: Lucas Le Gars, Kyushu University, Japan, September 18, 2026, 11:45 - 12:15

Among the various possibilities offered by the periodic table, copper-rich sulfides represent a highly promising class of low-cost and environmentally friendly thermoelectric materials. In these compounds, the predominance of monovalent copper enables the formation of hole carriers within extended Cu–S networks, making them particularly suitable for p-type transport. Beyond their favorable electrical properties, their structural diversity and chemical flexibility offer a unique playground to explore the relationships between crystal structure, lattice dynamics, and thermoelectric performance [1]. This PhD work focuses on understanding and tuning these structure-property relationships in copper-based sulfides through a combined experimental and theoretical approach. By investigating different structural families, including sphalerite-derived compounds and layered sulfides, this work highlights how cation distribution, local coordination environments, and structural disorder can be leveraged to control both electronic transport and lattice thermal conductivity.

In this presentation, particular attention is given to the layered compound Cu2ZrS3 [2]. The structure is built of CdI2-type edge-sharing ZrS6 octahedra layer alternating with corner-shared CuS4 tetrahedra layer. A particularity of this structure is the presence of copper in triangular coordination inside the CdI2-type layers. In the present work, based on single crystal X-ray diffraction, 3D electron diffraction, Rietveld FAULTS analyses and HR-TEM observations, we demonstrate that Cu2ZrS3 crystallizes in two new structural polytypes with different stacking schemes and structural defects, depending on the synthesis conditions. Those peculiar structural features in connection with materials processing, chemical bonds, and atomic vibration phenomena were carefully examined to establish rules and correlations between the crystal structures, nano-microstructures, electronic structures, vibrational and thermoelectric properties.

(1) P. Lemoine et al., Angewandte Chemie Int. Ed. 61 (2022) e202108686
(2) Z. Li et al., Small. 19 (2023) 2304718

Development of high performance thermoelectric materials & modules for power generation and cooling

Takao Mori[1,2]
[1]Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Japan, [2]Graduate School of Pure and Applied Sciences, University of Tsukuba , Japan

Current Modules and Beyond, September 16, 2026, 11:00 - 12:15

We have been utilizing novel routes such as magnetism, Anderson localization, etc. and also advancing defect engineering, to develop new high performance thermoelectric materials. As a result, we have succeeded in developing materials & modules that surpass the half-century champion Bi2Te3-type [1]. Electrode technologies for these new materials were also developed, with a novel concept of “active electrodes” leading to high stability and enhancement of the device performance than previously achieved. This strategy was also utilized for diffusion barrier materials [2]. Effective methodology for designing high performance thermoelectric modules (TEGs) has also been developed [3]. The accurate evaluation of performance of actual devices is critical for the industrialization of the technology, and we have also laid out the best practices for evaluation of TEGs [4], together with critical considerations for stability and also general best practices [5]. I will also present advancements made in fabrication of various formats of TEGs: bulk, thin film, flexible. Peltier devices of novel materials have also been fabricated and tested. Processes suited to industrial and mass production are important, as are development of compatible thermal management technologies, which will be presented. The progress of thermoelectric applications will also be discussed.

[1] Joule, 5, 1196 (2021), Nature Commun., 13, 1120 (2022), 15, 6800 (2024), 16, 10366 (2025).
[2] Nature Commun., 16, 1502 (2025), Adv. Mater., 37, 2508270 (2025).
[3] Nature, 652, 643 (2026), Small, 22, e08990 (2026).
[4] Joule, 8, 553 (2024).
[5] Joule, 10, 102421 (2026), Nature Sustain., (2026) doi:10.1038/s41893-026-01826-7

Enhanced Interfacial Charge Transport in Hybrid Materials for High Thermoelectric Performance

Syed Zulfiqar Hussain Shah[1,2], Weng Weei Tjiu[2], Haiwen Dai[3], Jose Recatala-Gomez[3], Pauline Kasongo-Ntumba[4], Weimin Zhang[5], Repaka Durga Venkata Maheswar[2], Iain McCullough[5], Oliver Fenwick[4], Kedar Hippalgaonkar[2,3], Zainul Aabdin[2], Pawan Kumar[2], Iris Nandhakumar[1]
[1]School of Chemistry, and Chemical Engineering, University of Southampton, United Kingdom, [2]Institute of Materials Research and Engineering, Agency for Science Technology and Research, Singapore, [3]School of Materials Science and Engineering, Nanyang Technological University, Singapore, [4]School of Engineering and Materials Science, Queen Mary University of London, United Kingdom, [5]Department of Chemistry, University of Oxford, United Kingdom

Nanomaterials, September 17, 2026, 13:30 - 15:00

Wearable technologies, including smartwatches, smart glasses, and even smart pacemakers, have revolutionized consumer electronics, significantly impacting healthcare, fashion, and entertainment. One of the main challenges for theadvancements of these devices is their reliance on batteries that require frequent replacement or periodic charging. Flexible thermoelectric (TE) materials however offer a promising solution as they can convert body heat into electricity and provide a safe, long-lasting, emission-free and continuous power source for wearables, generating up to hundreds of microwatts. Despite their potential conventional TE materials are rigid, brittle, and suffer from low efficiencies, making it challenging to integrate them into applications that require conformal geometries. Consequently, there is a clear need for developing flexible TE materials with enhanced TE performance that can be incorporated into wearable devices for harvesting body heat.

Results of recent studies [1-3] on the enhanced charge transport in hybrid inorganic-organic thermoelectric materials combining tellurium (Te) nanowires (NWs) with poly(3-hexylthiophene-2,5-diyl) (P3HT) will be presented. In particular, the effects of controlling oxidation levels within the Te NWs, the molecular weight of P3HT and the lengths of Te nanowires on the thermoelectric transport properties have been systematically investigated. The findings indicate that strict control of the oxidation the integration of longer Te nanowires (≈13 μm) with P3HT of different molecular weights (ranging from 50 to 143 kDa) enhances the thermoelectric properties of the hybrid material, resulting in a power factor of 303 ± 38 μW mK−2 for Te80-P3HT20 hybrid material with optimal doping. Thermal conductivity measurements are performed, and a value of 0.25 ± 0.03 W mK−1 is achieved for Te80-P3HT20 with a zT value of 0.36 ± 0.06 at room temperature, which represents the highest reported value for such Te-P3HT based hybrid materials to date.

References

[1] S.Z.H. Shah, D. Zhenyu, Z. Aabdin, W. W. Tjiu, J. Recatala-Gomez, H. Dai, Y. Xiaoping, R. Durga V. Maheswar, G. Wu, K. Hippalgaonkar, P. Kumar and I. Nandhakumar, Adv. Sci. 2400802 (2024).

[2] S.Z.H. Shah, D. Zhenyu, Z. Aabdin, W. W. Tjiu, J. Recatala-Gomez, H. Dai, Y. Xiaoping, R. Durga V. Maheswar, G. Wu, K. Hippalgaonkar, P. Kumar and I. Nandhakumar, ACS Applied Mat. Interfaces, 16 (35), 46191-46199 (2024).

[3] Syed Zulfiqar Hussain Shah, Weng Weei Tjiu, Haiwen Dai, Jose Recatala-Gomez, Pauline Kasongo-Ntumba, José F Serrano-Claumarchirant, Weimin Zhang, Durga Venkata Maheswar Repaka, Iain McCullough, Oliver Fenwick, Kedar Hippalgaonkar, Zainul Aabdin, Pawan Kumar and Iris Nandhakumar, Adv. Funct. Mat. doi.org/10.1002/adfm.202515055 (2025).

Thermoelectric waste heat recovery for vehicles with lean-burn spark-ignition engines

Michihiro Ohta[1]
[1]National Institute of Advanced Industrial Science and Technology (AIST), Japan

Heusler Modules, September 17, 2026, 13:30 - 15:00

This talk discusses recent progress in thermoelectric waste heat recovery for hybrid electric vehicles powered by e fuel and equipped with lean-burn spark-ignition engines. Because lean-burn operation lowers exhaust gas temperature, thermoelectric materials optimized for low-temperature operation are required. Mg3(Sb,Bi)2- and Bi2Te3-based materials were developed to enhance thermoelectric performance and mechanical properties [1]. In Bi2Te3, the zT was improved by controlling the impurity oxygen content and optimizing the crystal orientation. The impact of these materials on vehicle-level energy efficiency was evaluated using GT SUITE system simulations [1].
This work was supported by a grant project (JPNP21014) conducted by the Research Association of Automotive Internal Combustion Engines (AICE) with support from the New Energy and Industrial Technology Development Organization (NEDO).
[1] Sauerschnig, P.; Naruke, M.; Imasato, K.; Yamamoto, A.; Ishida, T.; Ohta, M., Chem. Mater., 2025, 37, 7240–7250.

Advent of the Metal Age of Thermoelectricity

Andrej Pustogow[1]
[1]Vienna University of Technology, Austria

Invited Talk: Andrej Pustogow, Vienna University of Technology, Austria, September 15, 2026, 09:45 - 10:15

Thermoelectric (TE) materials directly transform thermal into electrical energy and vice versa, making them promising for a plethora of applications. However, state-of-the-art semiconductors did not make the leap into broad applications due to low power density and poor mechanical properties. Metallic systems would be superior in this regard, but remained largely neglected so far.

Here, I introduce the novel paradigm of MEtallic THermoELectrics (METHEL) that already realized ultrahigh TE performance in metals, exceeding the benchmarks of semiconductor TE by far. To achieve a large Seebeck effect in metals, we applied the innovative enhancement principle of tuning electronic interband scattering via various mechanisms ranging from chemical pressure [1] and low dimensionality [2] towards tuning of geometrical frustration [3]. Currently, we are pushing the limits beyond the recently reached record values [1-3], utilizing a synergistic combination of synthesis, spectroscopy, microscopy and high-throughput computational materials screening.

While my ongoing endeavours in applied TE research still involve semiconductor TE – my project SPIRIT utilizes flexible TE generators for green power generation from waste heat in a thermal power plant – I will also present other promising directions where METHEL could have immediate impact on everyday technology. This way, our METHEL research truly bridges the gap all the way from solid-state theory to real-world applications.

References
[1] Sci. Adv. 9, eadj1611 (2023)
[2] Phys. Rev. X 15, 021054 (2025)
[3] Sci. Adv. 11, eadv7113 (2025)

Thermoelectric modules and applications: an industrial perspective

Aniruddha Ray[1]
[1]Thermagy, Netherlands
Invited Talk: Aniruddha Ray, Thermagy, The Netherlands, September 16, 2026, 09:45 - 10:15

Since 2014, Thermagy has specialized in silicon-germanium (SiGe) thermoelectric materials using scalable production techniques including ribbon growth, ingot casting, and ball milling. Combined with expertise in COMSOL Multiphysics simulation, thermo-mechanical and interface engineering, device ageing, and testing, this has resulted in the modular Thermagy TEG architecture. Its patented interconnection technology has undergone extensive testing, including more than 10,000 hours of continuous heat flow and thermal cycling up to 1000°C. These capabilities enable single-stage and cascaded TEG solutions tailored to different source temperatures and heat flux densities.
In industrial environments, particularly steel plants, thermoelectric technology can provide reliable local power for monitoring, wireless communication, and other distributed devices. It can also support combined heat and power (CHP) and thermal-battery systems by converting stored heat into electricity on demand. Projects with Tata Steel, Elkem, and ArcelorMittal, together with residential CHP applications, have driven Thermagy's development of high-ZT nanostructured SiGe for high temperatures and telluride-free modules for low- to mid-temperature operation.
Thermagy's SiGe materials and thermoelectric engineering expertise are also being applied to radioisotope power systems (RPS) for space, where RTGs can provide continuous, maintenance-free electrical power for long-duration lunar, planetary, and deep-space missions. These and other applications require dedicated thermoelectric architectures tailored to the mission environment, available heat flux, power requirements, and operating conditions. To address this need, Thermagy is developing THERMOS, a Thermoelectric Engineering Framework designed to fast-track the development of thermoelectric generator (TEG) components. THERMOS combines Multiphysics simulations with targeted testing, integrating thermal, electrical, and geometric modelling to optimise key design parameters. The framework has been applied in representative 15 W and 80 W RTG case studies, demonstrating its use in optimising thermoelectric performance, efficiency, and structural reliability across different power scales.
In parallel, a manufacturing and qualification framework is being developed covering thermoelectric material production, module fabrication, and multi-stage cascades targeting 10% conversion efficiency while reducing the risks associated with segmented devices. Particular emphasis is placed on thermal, mechanical, and electrical interfaces and coupling to the radioisotope heat source. Qualification toward TRL 5/6 combines material-, module-, and subsystem-level characterization with lifetime testing, thermal cycling, vacuum and high-temperature operation, vibration, and shock testing. Together, these capabilities provide an integrated pathway from thermoelectric material development and device optimization to reliable, high-efficiency power systems for terrestrial and space applications.

Development of micro-thermoelectric devices for ambient applications

Kafil M. Razeeb[1]
[1]University College Cork, Ireland

Microharvesting, September 15, 2026, 13:30 - 15:00

Thermoelectric device can convert waste heat into electricity based on Seebeck effect and also can act as a cooler based on the Peltier effect. In recent years, the development of micro-thermoelectric device on the silicon platform shows exponential growth due to their smaller size and relatively simple integration for a wide range of applications. In this talk, I will briefly discuss the development of micro-thermoelectric device on silicon platform, based on fab-compatible techniques along with the challenges of fabricating these devices. Later, the application of the micro-thermoelectric devices will be discussed as a thermoelectric cooler for thermal management of photonic integrated circuits as well as thermal management in terms of hot spot cooling for micro-electronic components.

Interplay of electronic structure, disorder and complexity to improve the performance of thermoelectric materials

Janusz Tobola[1]
[1]AGH University of Krakow, Poland

Electronic Transport Theory, September 16, 2026, 13:30 - 15:00

Some crystalline materials exhibiting specific chemical and physical properties can convert various forms of energy through thermoelectric, electrochemical, or magnetocaloric phenomena. In thermoelectric materials, the effectiveness of such effects is particularly related to specific electronic properties responsible for charge and heat transport and determining electrical conductivity, thermopower, and thermal conductivity - thus, the most important characteristics for thermoelectric conversion. To some extent, the performance of such materials can be optimized theoretically by capturing the essential quantum mechanisms responsible for the observed, interconnected electronic and thermal properties, which are moreover strongly dependent on temperature and carrier concentration. This, in turn, requires first-principles studies that incorporate more and more realistic models of the studied materials, typically exhibiting complex crystalline structures containing intentional impurities and often unintentional defects such as vacancies, interstitial imperfections, or antisites.

In this lecture, we will present our previous [1] and recent results [2,3] of electronic structure calculations, as well as some examples of modeling electron transport properties in thermoelectric materials such as magnesium-based silicides, half-Heusler alloys, and copper-based minerals with tetrahedrite and argyrodite structures. We will focus on the influence of unusual electronic structure features, such as band convergence or alignment, the interplay of nonparabolic dispersion relations and unusual anisotropy of electron transport properties, and the influence of configurational entropy on the topology of the electronic band structure.

References:
[1] K. Kutorasinski et al., Phys. Rev. B, 87 (2013) 195205; Phys. Rev. B, 89 (2014) 115205; Phys. Stat. Sol. A, 211/6 (2014) 1229.
[2] O. Cherniushok, et al., ACS Appl. Mater. Interf. 13 (2021) 39606; ACS Appl. Mater. Interf. 17 (2025) 69621.
[3] T. Parashchuk, et al., Adv. Fun. Mater. 35 (2025) 2502163.

Acknowledgments:
This work was partly funded by the National Science Centre (NCN) within the framework of the research projects “Weave-Unisono” UMO-2022/04/Y/ST5/00139.

Oral Presentations

Silicon-Based Planar µTEG Platform for the Integration and Evaluation of Thin-Film Thermoelectric Materials

Mr. Marc Aceituno[1], Mr. Xavier Vea[2], Dr. Joaquín Santander[1], Mr. Shahadev Rodríguez-Miguel[1], Prof. Luis Fonseca[1], Dr. Alex Morata[2], Dr. Llibertat Abad[1], Dr. Marc Salleras[1]
[1]Institute of Microelectronics of Barcelona (IMB-CNM, CSIC), Spain, [2]Catalonia Institute for Energy Research (IREC), Spain

Measurement and Characterisation, September 17, 2026, 15:30 - 17:00

The growing demand for autonomous and decentralized power sources to supply IoT nodes is driving increasing interest in environmental energy harvesting technologies, such as thermoelectric generators (TEGs). TEGs are capable of converting waste heat generated in several everyday processes into useful energy, offering a compact and solid-state solution, especially in harsh environments where batteries are impractical. In recent years, significant attention has been given to earth-abundant and low-toxicity materials, such as silicides [1]. While most efforts have focused on improving the material figure of merit (zT), µTEG performance is also strongly influenced by device architecture and thermal management, which are critical for maximizing the temperature gradient across the thermoelectric material [2,3]. Based on our group's previous experience in developing silicon-based micro-thermoelectric generator (µTEG) platforms integrating nanostructured materials, such as thin films [4] and nanowires [5], we present a microfabricated silicon-based planar µTEG platform designed for the integration and evaluation of novel thermoelectric materials in thin-film form within a fully operational device. This approach leverages CMOS-compatible microfabrication and provides high versatility, enabling the integration of a wide range of thermoelectric materials through different growth or deposition routes, including direct deposition and etching, as well as shadow-mask-based methods that avoid subsequent patterning. In addition, the platform allows final-stage deposition of thermoelectric materials, eliminating the need for additional lithography steps.

In order to test this, thin films of $CrSi_2$ and Mg_2Si have been integrated into the planar Si-based µTEG structure. The results demonstrate the adaptability of the fabricated µTEG platform as a reliable tool for evaluating different thermoelectric materials in fully integrated devices.

[1] O. Caballero-Calero et al., Adv. Sustain. Syst.(2021).
[2] P. Ferrando-Villalba et al., Nanomaterials(2019).
[3] C. Calaza et al., J. Electron. Mater.(2016).
[4] A.P. Perez-Marín et al. Nano Energy(2014).
[5] J.M. Sojo-Gordillo et al., Adv. Funct. Mater.(2025).

Interplay Between Vacancy Ordering and Transport Properties in Ni-base metal-rich chalcogenides Ni7−δSnSe2 and Ni7−δSnS2

Dr. Laura Agnarelli[1], Yurii Prots[2], Marcus Schmidt[2], Denis Pelloquin[1], Antoine Maignan[1], Sylvie Hébert[1]
[1]CNRS, CRISMAT Laboratory, France, [2]Max Planck Institute for Chemical Physics of Solids, Germany

Chalcogenides-2, September 16, 2026, 13:30 - 15:00

The exploration of metallic systems for thermoelectric applications has highlighted how complex electronic structures and structural disorder optimize the transport properties. [1] Studies on intermetallics (Ni_3Ge [1], Ni_3Sn [2]) and metal-rich chalcogenides (MRC) like $Ni_3Sn_2S_2$, [3] show that high carrier concentrations can coexist with notable thermoelectric responses. Building on this foundation, we investigate Ni-based MRC belonging to the $M_{7-\delta}ECh_2$ family [4] (M = Ni; E = p-block element; Ch = chalcogen), where structural complexity enable tailored lattice dynamics and electronic transport.

We studied $Ni_{5.7}SnSe_2$ [5] and $Ni_{6.34}SnS_2$ [6], both featuring $[Ni_3Sn]/[Ni_{4-\delta}Ch_2]$ intergrowth structures with Ni vacancies. $Ni_{5.7}SnSe_2$ show a reversible structural transition from tetragonal (I4/mmm) to monoclinic (C2/m) at 520 K driven by commensurate Ni vacancy ordering. This correlates with resistivity and Seebeck coefficient anomalies. $Ni_{6.34}SnS_2$ retains the tetragonal symmetry but shows weak superstructure reflections, suggesting subtle modulations or superstructures. Our data show no electronic transition in $Ni_{6.34}SnS_2$.

Both compounds are metallic n-type behavior with reduced thermal conductivities (8.4 $W{\cdot}m{-}1{\cdot}K{-}1$ for $Ni_{5.7}SnSe_2$ and 6.7 $W{\cdot}m{-}1{\cdot}K{-}1$ for $Ni_{6.34}SnS_2$) compared to those of binary Ni_3Sn (~40 $W{\cdot}m{-}1{\cdot}K{-}1$) [2]. While their κ remain high for traditional thermoelectrics, their PF are comparable to those of topological semimetals, making them promising for electronics thermal management via lateral heat spreading. [2], [7]

Current work explores transition mechanisms in $Ni_{5.7}SnSe_2$ and their absence in $Ni_{6.34}SnS_2$, examining charge-density-wave instabilities and order-disorder phenomena. We are performing E/Ch substitutions and electronic band structure calculations to optimize the properties.

[1] Garmroudi et al. Sci. Adv. 2025; [2] Garmroudi et al. Phys. Rev. X 2025; [3] Aziz et al. Phys. Rev. B 2016; [4] Kuznetsov et al. Russ. J. Inorg. Chem. 2019; [5] Agnarelli et al. Chem. Mater. 2026; [6] Agnarelli et al. Chem. Commun. 2025; [7] Mao et al. Nat. Mater. 2021

Anisotropic Scattering and Elongated Bands Lead to Ultra-High Power Factors in Full-Heuslers

Ms Saff E Awal Akhtar[1], Ms Bhawna Sahni[1], Professor Neophytos Neophytou[1]
[1]University of Warwick, United Kingdom

Electronic Transport Theory, September 16, 2026, 13:30 - 15:00

Full-Heusler (FH) Fe_2YZ compounds exhibit distinctive transport behaviour arising from their highly anisotropic, elongated (low dimensional) Γ–X conduction bands. This contrasts with the overall isotropic, bands of Half Heuslers (HHs). Such highly anisotropic bands have large transport advantages compared to isotropic bands: at the same density of states (DOS), a much larger conductivity and power factor (PF) is possible1. Here we computationally investigate the power factor of ten of Fe-based FHs materials, and two Ru-based FHs with such bands in their conduction band, and compare their power factors to representative HH compounds.

Boltzmann transport calculations are performed using the ElecTra software2, incorporating full scattering considerations (non-polar, polar phonons and ionized impurity scattering) with all relavant parameters derived ab initio. Our purpose is to explore the benefits of elongated bands, thus we ignore bipolar effects for some of the narrow bandgap materials.
We show that in these FH materials, the DOS is much larger than the DOS of typical half-Heuslers. Carrier scatterering, however, (which typically follows the DOS), does not scale proportionally, and it is actually lower than in HHs. We show that the anisotropic scattering mechanisms IIS and POP are the stronger in determining transport, for which scattering is actively strong only ‘locally’ in the Brillouin zone. This effectively allows for an increase in the apparent band degeneracy, resulting in much higher conductivities compared to typical HHs. Thus, the PF experiences a large increase, reaching values of beyond 15 (for Fe-systems) and a highest value of 24 mW/mK2 (in Ru2HfSi) due to sizeable contribution from dispersive bands as well. These values are 2- 3x compared to the PF peaks achieved in HHs (on average arounnd 8 mW/mK2).

References
1P. Graziosi, and N. Neophytou. ACS Applied Electronic Materials (2023).
2P. Graziosi, Z. Li, and N. Neophytou. Computer Physics Communications (2023).

Thermoelectric Energy Recovery in Dual-Fuel Marine Engines: Waste Heat and LNG Cold Energy Utilization

Patricia Alegría[1], Manuel Naveiro[2], Nerea Pascual[1]
[1]Public University Of Navarre, Spain, [2]Universidade da Coruña, Spain

Applications-2, September 16, 2026, 13:30 - 15:00

In the current context, where efforts are being made to reduce greenhouse gas emissions through various regulations, the maritime sector plays a key role, as it accounts for 90% of global freight transport and is responsible for approximately 3% of total greenhouse gas emissions. For this reason, the International Maritime Organization has set emission reduction targets of 50% by 2050. Achieving these goals requires the development of innovative technologies aimed at reducing CO_2 and other pollutant emissions.

One of the most effective strategies to improve ship efficiency and reduce fuel consumption, and consequently emissions, is waste heat recovery. In this context, thermoelectric generators (TEGs) emerge as a viable solution, allowing implementation without major modifications to existing ship structures and permitting to use different energy sources due to their scalability. Some studies have proposed the use of TEGs to recover waste heat from incinerators or engine exhaust gases. However, in dual-fuel ships, there is significant untapped potential not only in waste heat sources but also in the so-called cold energy, which is generated during the vaporization of liquefied natural gas (LNG) used as fuel.

Then, this work proposes and analyzes the use of thermoelectric generators to recover energy from the main residual energy sources in such engines: the waste heat of exhaust gases and engine cooling water, and the cold energy of LNG vaporization. A model has been developed for a representative vessel to evaluate the direct generation of electrical power for onboard systems. The results indicate that the potential power generation using TEGs reaches 87.54 kW, highlighting a promising research line with high development potential.

Improved thermoelectric properties in Ga-substituted p-type Fe2VAl

M.K. Moorthy[1], M. De Vos[1], C. Barreteau[1], O. Rouleau[1], **Eric Alleno**[1]
[1]Univ. Paris-Est Creteil, ICMPE-CNRS, France

Heusler-1, September 15, 2026, 13:30 - 15:00

Fe2VAl is a Heusler alloy composed of low-toxicity chemical elements. Upon n- or p-type doping, it displays maximum power factor values (PFmax = 3 – 10 mW m-1 K-2 at 300 K) equal or even larger than those of Bi2Te3. Nonetheless, the thermal conductivity is as high as 29 W m-1 K-1 in pristine Fe2VAl, an order of magnitude larger than that of Bi2Te3. Reducing thermal conductivity is thus required to reach a high ZT. Phonon point defects scattering through substitutions at V or Fe sites, by heavy chemical elements such as Ta, W, or Re has been the main pursued strategy to achieve this goal. In the present work, as a first step towards ZT > 0.2 at 300 K, we explore the effect on the thermoelectric properties of substituting Al by heavier Ga in p-type Fe2VAl.

As expected from the phonon point defects scattering in Fe2.04V0.91(Al1-xGax)1.05 (0.0 < x < 1.0), the lattice thermal conductivity lambda_L(x) at 300 K decreases with x. It forms an L-shape curve that differs from that of Si1-xGex, forming a U-shape curve. From calculations, we relate this effect to changes in the phonon spectrum. Unfortunately, in these p-type degenerate semiconductors, the power factor slightly and monotonously decreases with x. We show that this arises from the decrease in the (small) band-gap amplitude from 0.07 eV (x = 0.0) to 0.03 eV (x = 1.0). Nonetheless, the x = 0.35 concentration displays a decreased lambda_L = 8.4 W m-1 K-1 while maintaining PF = 2.6 mW m-1 K-2. This leads to improved ZT = 0.07 at 300 K.

Evolution of a Thermoelectric IIoT Platform for Continuous Furnace Monitoring

Dr. Raúl Aragonés Ortiz, Mr. Roger Malet, Mr. Andres Ibañez, Mr. Alex Prim, Dr. Mounir Amourak
[1]Alternative Energy Innovations - AEInnova, Spain, [2]UAB, , Spain, [3]ArcelorMittal Maizières Research, France

Applications-1, September 15, 2026, 11:00 - 12:15

Continuous reheating furnaces are critical assets in steel production, directly impacting energy efficiency, product quality, and operational stability.However, their harsh operating conditions—characterized by high temperatures, strong thermal gradients, and limited accessibility—make real-time monitoring challenging. Conventional instrumentation is often constrained by wiring complexity, maintenance requirements,and limited spatial resolution, leading to suboptimal process control and undetected inefficiencies [1].

This work presents an Industrial Internet of Things (IIoT) solution for high-frequency temperature monitoring in continuous furnaces, validated in a real-world deployment at an ArcelorMittal steel plant in Nador.The system enables autonomous acquisition of temperature data from eight thermocouples per furnace, with a temporal resolution of one measurement per minute,significantly enhancing process visibility compared to traditional approaches.
The proposed architecture leverages thermoelectric energy harvesting to power distributed sensing nodes, eliminating batteries and reducing maintenance in extreme environments. Data is transmitted wirelessly using low-power communication protocols and processed through edge computing, enabling real-time diagnostics and anomaly detection,including early identification of thermal deviations,refractory degradation, and combustion inefficiencies[2].
In addition,this work presents an evolution of the thermoelectric generator module incorporating a high-temperature energy storage system based on oxygen battery technology (OxyBatt). This redesign enables operation at temperatures up 400°C by overcoming the limitations of conventional energy storage systems and extending the operational range of autonomous IIoT devices in high-temperature industrial environments.The integration of energy harvesting with high-temperature storage enhances system robustness and enables more stable operation under fluctuating thermal conditions.

The results demonstrate that autonomous,high-frequency thermal monitoring is feasible in harsh steelmaking environments.Furthermore,the proposed system evolution opens new opportunities for integrating sensing and energy storage, contributing to improved energy efficiency and supporting industrial decarbonization strategies.

Bibliography
[1]E.Worrell,“Energy Efficiency Improvement and Cost Saving Opportunities for the U.S. Iron and Steel Industry,” Lawrence Berkeley National Laboratory,2008.
[2]R.Aragonés,J.Oliver,R.Malet,M Oliver-Parera,and C.Ferrer, “Model and Implementation of a Novel Heat-Powered Battery-Less IIoT”Information,vol.15, no.6,2024.

Autonomous Power Supply for Coastal Volcanic Monitoring through Geothermal Thermoelectric Generators in Intertidal Settings

Miguel Araiz[1], Leyre Catalán[1], Patricia Alegría[1], Nerea Pascual[1], Irantzu Erro[1], Laura Carlosena[1], Iñaki Górriz[1], David Astrain[1]
[1]Public University Of Navarra - Arrosadia Campus, Spain

Applications-1, September 15, 2026, 11:00 - 12:15

Continuous monitoring of active volcanoes often requires instrumentation to operate in isolated environments where conventional electrical infrastructure is unavailable. Ensuring a stable and long-term energy supply therefore represents a major challenge for remote sensing systems. Geothermal heat naturally present in volcanically active regions offers a persistent energy resource that can potentially sustain autonomous monitoring platforms.

This study presents the design and field deployment of a thermoelectric energy harvesting system that converts geothermal heat into electrical power in coastal volcanic environments affected by tidal dynamics. The proposed generator has been specifically developed to operate under the demanding conditions of intertidal zones, where equipment must tolerate repeated transitions between exposure to the atmosphere and immersion in seawater.

A prototype device has been installed in the intertidal area of Deception Island, Antarctica, to evaluate its real-world performance. Initial observations indicate that the system can sustain power generation while maintaining structural integrity under prolonged exposure to the harsh coastal volcanic environment. These results highlight the feasibility of using geothermal thermoelectric conversion as a practical energy solution for autonomous volcanic monitoring stations and other remote sensing applications located in challenging coastal settings.

Field Demonstration of Passive Geothermal Thermoelectric Generators: Long-Term Field Operation and Opportunities for Performance Improvement

Prof. David Astrain Ulibarrena[1], Dr. Miguel Araiz[1], Dra. Nerea Pascual[1], Dra. Leyre Catalán[1], Dra. Patricia Alegría[1], Dra. Irantzu Erro[1], Dra. Laura Carlosena[1]
[1]Universidad Pública de Navarra, Spain

Applications-1, September 15, 2026, 11:00 - 12:15

One of the main challenges in thermoelectric research is identifying applications with strong potential for real-world deployment, given the low conversion efficiency of thermoelectric generators. However, in environments where reliability, autonomy are critical, thermoelectric systems can become an attractive technological solution.

This work presents the field demonstration and long-term performance of two passive geothermal thermoelectric generator (GPTEG) installations designed to convert geothermal heat into electricity using thermoelectric modules combined with passive phase-change heat exchangers. These systems operate without moving components, ensuring high reliability and minimal maintenance.

The first system was installed on an active volcano on Antarctica, where geothermal heat from fumaroles is converted into electricity to power volcanic monitoring instrumentation. Continuous power supplied by the GPTEG enables geological and geothermal data to be transmitted remotely via satellite throughout the entire year, including the Antarctic winter. This is the first time that real-time remote monitoring has been achieved year-round on this volcano, representing a major advance for geological studies in Antarctica. The system produces a maximum net electrical power of 12 W and an average power of 5 W.

The second installation has been operating for more than three years in Timanfaya National Park (Canary Islands), where geothermal anomalies associated with shallow hot dry rocks are exploited. The system generates an average net electrical power of 400 W, producing 3.42 MWh per year supplied to park facilities. This generation avoids approximately 2.3 tons of CO_2 emissions per year and results in a Levelized Cost of Energy (LCOE) of 0.22 €/kWh.
The long-term operation of both systems under real environmental conditions has provided valuable data on reliability, performance stability, and operational limitations. These results are analysed to identify opportunities for improving system efficiency and design, while demonstrating the potential of passive GTEG technology for scalable deployment in geothermal environments worldwide.

Defect-Mediated Thermoelectric Properties in A14AlBi11 (A = Ca, Sr, Yb) Zintl Phases

Asooc. Prof. Umut Aydemir[1], Prof. Jeffrey Snyder[2], Mrs. Saba Sepahban Shahgoli[3]
[1]Koç University Boron and Advanced Materials Application and Research Center, Turkey,
[2]Department of Materials Science and Engineering, Northwestern University, United States,
[3]Graduate School of Sciences and Engineering, Koç University, Turkey

Zintl-2, September 16, 2026, 11:00 - 12:15

Zintl compounds adopting the Ca14AlSb11 structure type have emerged as promising high-temperature thermoelectric materials, including Yb14MSb11 (M2+= Mg, Mn, Zn), owing to their intrinsically low lattice thermal conductivity and complex electronic structures.1,2 In contrast, valence-balanced 14-1-11 Zintl phases containing trivalent cations (M3+) remain largely unexplored, as they are generally expected to exhibit intrinsic semiconducting behavior with low carrier concentrations and, consequently, limited thermoelectric performance.3,4 However, our experimental observations in some of these systems suggest unexpectedly high p-type carrier concentrations, challenging the conventional view of Zintl phases as strictly valence-precise semiconductors.

Herein, we investigate A14AlBi11 (A = Ca, Sr, Yb), a series of valence-balanced aluminobismuthide Zintl phases, to elucidate the origin of this anomalous transport behavior. Despite their nominal valence balance, electrical transport measurements reveal relatively high electrical conductivity together with moderate to high Seebeck coefficients, consistent with heavily doped, degenerate p-type behavior. Our results indicate that the unexpectedly high hole concentrations most plausibly originate from intrinsic acceptor-type point defects, particularly A-site vacancies. This defect-mediated carrier generation mechanism is fundamentally distinct from that in most other 14-1-11 compounds, where electronic transport is primarily governed by intrinsic electron imbalance rather than native defect formation. Similar behavior has been reported in other valence-balanced Zintl systems, such as AZn2Sb2,5 where stable cation vacancies were shown to control hole concentration, underscoring the broader importance of native defects in tuning transport properties. Among the investigated compositions, we introduce Sr14AlBi11 and Yb14AlBi11 as new members of this family. Particularly, Sr14AlBi11 exhibits promising thermoelectric performance, reaching a zT of approximately 0.85 at 973 K without intentional optimization. These findings highlight the untapped potential of bismuth-based 14-1-11 Zintl phases and establish defect engineering as a viable strategy for developing efficient high-temperature thermoelectric materials.

References

(1) https://doi.org/10.1021/cm060261t.
(2) https://doi.org/10.1126/sciadv.abq3780.
(3) https://doi.org/10.1039/D5TA09465H.
(4) https://doi.org/https://doi.org/10.1002/adfm.200800298.
(5) https://doi.org/10.1002/anie.201311125.

Sustainable Hybrid Thermoelectrics: Comparative Performance Analysis of Synthetic Material Integrated with Mined Waste Material and Purely Synthetic Material

Aravind Babu[1]
[1]Thermagy B.V, Netherlands

Current Modules and Beyond, September 16, 2026, 11:00 - 12:15

The commercialization of thermoelectric (TE) technology is often hindered due to the cost, scarcity and environmental impact of purely synthetic materials. This study adopts a "circular materials" approach to investigate the integration of mineral waste from mining into synthetic TE material. Rather than utilizing pure mineral phases, we use a hybrid P-Type material where specific weight percentages of mined waste are incorporated into a synthetic Tetrahedrite ($Cu_{12}Sb_4S_{13}$) material to optimize the trade-off between cost, sustainability, and conversion efficiency.

The methodology involved the synthesis of purely synthetic and hybrid powders via planetary ball milling, followed by densification with Spark plasma synthesis into discs. Thermoelectric properties like Seebeck coefficient (S), electrical conductivity (σ), and thermal conductivity (κ) were characterized across a temperature range of 25-350 °C. Material characterization of either material indicated similar ZT, pointing towards integration of mineral waste without compromising TE performance. The measured TE material properties were used in simulations to predict device-level performance. To validate these findings experimentally, the sintered discs were coated with a sputtered diffusion barrier, diced into pellets, and integrated into module assemblies. The module assembly was bonded together through a controlled thermal cycle. To evaluate experimental performance, TE modules fabricated from both pure synthetic and hybrid materials were subjected to an identical thermal gradient (ΔT), and performance curves were extracted for comparison.

This study aims to demonstrate that the strategic use of mined waste as a functional additive in P-type Tetrahedrite, paired with a suitable N-Type material, offers a viable, eco-friendly pathway for industrial waste-heat recovery. The results prove that high-efficiency energy harvesting is achievable using earth-abundant, low-toxicity materials sourced from existing industrial waste streams.

Mechanochemical Synthesis In Pb-X-S (X=Bi,Sb) Systems And Their Thermoelectric Performance

Peter Baláž[1], Dr. Nina Daneu[2], Dr. Karel Knížek[3], Dr. Emmanuel Guilmeau[4], Mia-Eussa Gauthier[4], Dr. Erika Dutková[1], Dáša Drenčaková[1]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Slovakia, [2]Jozef Stefan Institute, Slovenia, [3]Institute of Physics of Czech Academy of Sciences, Czechia, [4]CRISMAT, CNRS, Normandie University, France

Materials, September 18, 2026, 10:30 - 11:30

Development of sustainable, low-cost and clean energy sources represents one of the most important challenges for materials science. Thermoelectric materials offer the viable way to generate electricity from a temperature gradient without hazardous side products. However, their application remains limited because the best-known materials are based on toxic, scarce, and costly compounds with low chemical stability at operating conditions. To overcome these obstacles several new compounds recently emerged. Among them, metal chalcogenides1 have attracted considerable attention as potential tellurium-free alternatives.

In this work, we describe the properties and thermoelectric performance of several ternary sulphides Pb-X-S (X=Bi, Sb) synthesised via mechanochemistry. In the (Pb-Bi-S) system, aschamalmite Pb5.95Bi2.02S9.03 was documented as a product after short high-energy milling of (PbS+Bi+S) mixture2. Its low thermal conductivity values (0.38-0.5) Wm-1K-1 over the temperature range of 300 K to 525 K are lower than the values reported for similar species PbBi2S43 and Pb3Bi2S64. In (Pb-Sb-S) system several variations of composition were tested by high-energy milling for 60 min. The applied precursors (PbS+Sb+S) simulate natural minerals of plagionite group5. The ultralow thermal conductivity (0.14-0.32) Wm-1K-1 over the temperature range of 300 K to 575 K was obtained for four minerals in (Pb-Sb-S) system under study. The ultralow glass-like thermal conductivity in crystalline materials is crucial for enhancing their thermoelectric performance. Further research into optimising electrical conductivity is in progress.

This study is supported by the Slovak Research and Development Agency under Contract No. APVV-24-0353 and project SUSTENET (COST CA 24120).

1 Baláž, P.; et al.; J. Mat. Sci. 2017, 52, 11851-11890
2 Baláž, P.; et al. RSC Mechanochemistry 2025, 2, 91-99
3 Maji, K.; et al. Chem. Mater. 2024, 36, 4631-4646
4 Ohta, M.; et al. J. Mater. Chem. A 2014, 2, 20048-20058
5 Kohatsu, J.J.; Wuensch, B.J. Amer. Mineralogist 1974, 59, 1127

Fabrication of thermoelectric cementitious composites using continuous functionalized CNT-coated polymer fibers

Mr. Ali Bashiri Rezaie[1,2], George Karalis[3], Viktor Mechtcherine[1,2], Marco Liebscher[1,2]
[1]Institute of Construction Materials, Faculty of Civil Engineering, Dresden University of Technology, Germany, [2]Cluster of Excellence CARE, TU Dresden and RWTH Aachen, Germany, [3]Physics Department, School of Sciences, University of Ioannina, Greece

Emerging, September 15, 2026, 15:30 - 17:00

The transformation of concrete structures from passive energy consumers into active energy providers is a key step toward sustainable infrastructure, as their large volume enables significant cumulative energy harvesting. Thermoelectric energy harvesting in construction exploits temperature gradients arising from solar radiation and thermal flows, converting otherwise wasted heat into electricity via the Seebeck effect. Cementitious materials are promising candidates due to their relatively low thermal conductivity, ability to sustain temperature gradients, and dual functionality stemming from both electronic and ionic thermoelectric effects. Importantly, they can simultaneously serve as load-bearing elements and energy-harvesting systems, enabling seamless structural integration. Their thermoelectric performance depends on optimizing the Seebeck coefficient, electrical conductivity, and thermal conductivity. Conventional fabrication strategies rely on incorporating conductive fillers such as carbon nanomaterials or modifying the cement matrix with functional additives; however, these approaches face challenges including poor dispersion, difficulty in achieving a stable percolation threshold, and potential degradation of mechanical properties.

Herein, thermoelectric cementitious composites were fabricated using an alternative approach based on the incorporation of only two individual continuous conductive fibers twisted together, thereby eliminating the need for filler dispersion, high filler dosages, and percolation threshold optimization. The conductive fibers consist of polyethylene (PE) fibers coated with carbon nanotubes modified by tannic acid, rendering the initially insulating polymer fibers electrically conductive. The electrical conductivity of single CNT-coated fibers reaches $(1.81 \pm 0.06) \times 10^6$ S/m, while the corresponding cementitious composites exhibit a conductivity of $(3.79 \pm 1.01) \times 10^5$ S/m. Seebeck coefficients of +22.4 μV/K and +17.2 μV/K were achieved for single fibers and composite specimens, respectively, corresponding to power factors of 908.2 $\mu W/m.K^2$ and 112.1 $\mu W/m.K^2$. Despite the relatively low Seebeck coefficients, this innovative and facile approach demonstrates strong potential for developing multifunctional thermoelectric cementitious composites, representing a significant step toward sustainable and energy-efficient construction.

Low Energy Shear Vibrations of Sb2 Bilayer Driving Ultralow Lattice Thermal Conductivity in Homologous (Sb2)m(Sb2Te3)n

Shuva Biswas[1]
[1]New Chemistry Unit, Jawaharlal Nehru Centre For Advanced Scientific Research (JNCASR), India

Exotic Effects, September 16, 2026, 11:00 - 12:15

Achieving ultralow lattice thermal conductivity (κL) in topological quantum materials with fundamental understanding of its origin poses a formidable challenge in material design. Members of the (Sb2)m(Sb2Te3)n (m, n: integers) homologous series, Sb2Te3, SbTe, Sb2Te, and Sb4Te3, exhibit fascinating natural van der Waals-like heterostructure and maintain topologically protected surface states. This offers a unique platform for systematically probing the modulation of κL in conjunction with their unique local structure and lattice dynamics. Our investigation focuses on three distinct members, SbTe, Sb2Te, and Sb4Te3, of the (Sb2)m(Sb2Te3)n series, distinguished by their different stacking sequences of Sb2 bilayers (BLs) and Sb2Te3 quintuple layers (QLs). Synchrotron X-ray pair distribution function analysis reveals notable local structural signatures, distinguishing each of the compounds. Thermal conductivity measurements demonstrate a systematic reduction of κL across the series, specifically along the layered stacking direction, with Sb4Te3 exhibiting the lowest κL (~ 0.29 Wm-1K-1 at 300 K) due to enhanced phonon scattering resulting from superlattice-like heterostructure induced by the BLs, while Sb2Te3 having no BL retains the highest κL (~ 0.87 Wm-1K-1 at 300 K). Phonon modes dominated by low energy shearing vibrations of Sb2 BLs couple with acoustic phonons, reducing the phonon group velocity and thereby suppressing heat transport. This study underscores the interplay of structural modularity and low-energy selective lattice vibrations in achieving ultralow κL in topological quantum materials.

Sustainable Interfacial Engineering in Low-Cost Cu6.2Te2.3S1.7 Thermoelectrics: A Practical Step Beyond Bi2Te3

Dr Anilkumar Bohra[1], Dr Oleksandr Cherniushok[1], Dr Mykola Maksymuk[1], Dr Krzysztof T. Wojciechowski[1]
[1]Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Poland

Interfaces and Stability, September 17, 2026, 15:30 - 17:00

In large-scale energy conversion processes, about 60–70% of primary energy is typically lost, mostly as waste heat. Thermoelectric systems convert waste heat into electricity simply and efficiently, with no noise, pollution, or moving parts. Most waste heat lies below 573 K, where Bi2Te3 based material remains the leading thermoelectric material. However, its toxicity, high cost, and limited availability restrict widespread use. As a result, copper-based sulfides and selenides are receiving growing research attention as low-cost, eco-friendly alternatives. Recently the new Cu-based Cu6Te3-xS1+x material emerged as a promising eco-friendly, low-cost alternative to Bi2Te3 for low-temperature waste heat recovery. Despite its potential, issues such as interface instability, Cu migration, electrode reactions and sulfur induced degradation must be addressed to ensure practical reliability. Hence, an effective diffusion barrier for low-temperature, sulfur-containing materials is essential to prevent interfacial reactions, suppress elemental diffusion, and ensure long-term bonding.

This study systematically evaluates effective barrier materials for the Cu-based sulfide Cu6.2Te2.3S1.7 for low-temperature waste heat recovery. To achieve this, four candidate barrier materials such as Cu, Ni, Co, and Al were systematically investigated for their effectiveness. Thermoelectric material with different barrier layers were fabricated using a simple, versatile one-step sintering process. The cross-sectional interfaces of each barrier layer were analysed for compatibility, diffusion, and stability using SEM, Seebeck mapping, and contact resistance measurements. Among all the candidates, Aluminium proved the most effective diffusion barrier, enabling low-temperature bonding, suppressing interfacial reactions, and maintaining mechanical integrity in sulfur environments, while offering a low-cost, non-toxic, and scalable alternative for sustainable thermoelectric applications.

Impact of chemical heterogeneity at grain boundaries on the local thermal conductivity of Sn1-xMnxTe thermoelectrics

Florian A. Busch[1], Kyuseon Jang[1], Siyuan Zhang[1], Oluwaseyi Balogun[2], Jochen M. Schneider[3], G. Jeffrey Snyder[2], Christina Scheu[1], Eleonora Isotta[1]
[1]Max Planck Institute for Sustainable Materials, Germany, [2]Northwestern University, USA, [3]RWTH Aachen University, Germany

Chalcogenides-2, September 16, 2026, 13:30 - 15:00

Thermoelectrics are promising candidates for sustainable power generation by converting waste heat into emission-free electricity. Amongst the multiple strategies that have been applied to improve their performance, grain boundary engineering approaches have proven particularly useful to decrease the thermal conductivity and thus enhance the figure of merit. Thermal conductivity imaging has shown a local thermal conductivity suppression around grain boundaries. However, how the local chemistry and atomic arrangements at grain boundaries influence this suppression remains to be unraveled.

Electron- and laser-based analytical imaging techniques are performed on Sn1-xMnxTe materials. Electron backscatter diffraction and frequency domain thermoreflectance images of multiple grain boundaries are recorded to determine their local structural and thermal properties. High precision wavelength dispersive X-ray spectroscopy measurements are performed to determine the local chemistry. Severe chemical fluctuations are found across individual grain boundaries. A kinetic solidification model is proposed to explain the observed chemical inhomogeneity.

The excess thermal resistance of the grain boundary regions is found to positively correlate with Mn-deficient micro-segregations at the grain boundaries in Sn1-xMnxTe. A quantitative comparison of the observed segregation's magnitude indicates the local Mn deficiency to be overcompensated by Sn. This implies complex changes to the local defect structure. Our findings suggest the influence of grain boundaries on the transport properties to be composed of an interfacial and a volumetric effect. The combined effects of the atomic structure of the interface as well as the surrounding metastable micro-segregations open new opportunities to tailor transport properties in thermoelectric materials.

Electrochemically Deposited Nanostructured Bi_2Te_3 for Flexible Thermoelectric Energy Harvesting

Dr. Olga Caballero-calero[1], Mr. Joan Carrion-Ramos[1], Mr. David Lopez-Diego[1], Mr. Pablo Cerviño-Solana[1], Dr. Cristina V. Manzano[1], Prof. Marisol Martin-Gonzalez[1]
[1]Imn-cnm, Csic, Spain

Microharvesting, September 15, 2026, 13:30 - 15:00

Electrochemical deposition provides a cost effective and scalable route for synthesizing nanostructured bismuth telluride (Bi_2Te_3) suitable for low power thermoelectric energy harvesting. In this work, we demonstrate the fabrication of high quality Bi_2Te_3 films grown on rigid conductive substrates through a fully electrochemical process that enables precise control over stoichiometry, crystallographic orientation, and nanoscale morphology. By adjusting parameters such as potential, temperature, and electrolyte composition, we obtain nanostructured Bi_2Te_3 layers aiming to enhance phonon scattering while maintaining favorable electrical transport properties.

Comprehensive characterization using scanning electron microscopy, X ray diffraction, and Raman spectroscopy confirms the formation of near stoichiometric Bi_2Te_3 with well defined nanoscale features and preferred orientations. Once the material is synthesized and optimized, the films are released from their initial growth substrates and transferred onto flexible polymeric supports. This transfer process preserves structural integrity and allows the resulting thermoelectric layers to retain mechanical flexibility compatible with wearable or conformal device architectures.

Transport measurements—including Seebeck coefficient and electrical conductivity—were performed after transfer to ensure that the nanostructured films maintain their thermoelectric performance under bending and low temperature gradient conditions. The resulting flexible Bi_2Te_3 layers exhibit promising behavior for powering autonomous nodes in Internet of Things (IoT) systems and wearable electronics, where compactness, low cost, and compatibility with curved or skin mounted surfaces are essential. This approach opens new opportunities for integrating high performance Bi_2Te_3 materials into lightweight, bendable energy harvesters capable of operating under realistic ambient or body heat gradients.

Improved thermoelectric thin-film device performance via integrating optical thin films

Prof. Feng Cao[1]
[1]Harbin Institute of Technology, China

Harvesting and Sensing, September 15, 2026, 15:30 - 17:00

Thermoelectric (TE) thin-film devices have garnered considerable interest in the field of biosensing and microelectronic self-powering. However, their practical deployment is limited by intrinsically inferior electrical transport compared to their bulk counterparts, as well as by the small temperature difference typically available from low-grade and diffuse energy sources such as ambient and body heat. Here we report growth-restricted GeTe thin films with improved electrical transport performance, and further integrate optical thin films, serving as spectrally selective absorbers and radiative cooling coatings, to enlarge the temperature difference across the thermoelectric legs. The resulting increase in carrier mobility raises the room-temperature power factor of the GeTe film to 26.1 μW cm−1 K−2. Incorporated with the W-SiO2-based spectrally selective absorber and PDMS/Ag radiative coating, a circular thin-film thermoelectric device assembled by the optimized GeTe and Ag2Se thin films demonstrates a substantial temperature gradient of 22 K and an output power of 0.57 μW under AM1.5 solar illumination. We further develop a highly integrated vertical TE thin-film device comprising p-type Ge0.98Bi0.02Te and n-type Ag2Se films. When coupled with a self-cleaning solar absorber, the device efficiently captures solar energy, establishing a pronounced temperature difference of 32 K across the thermoelectric legs under outdoor conditions. This configuration delivers a high open-circuit voltage density of ~25.7 mV cm−2 and a power density of ~2.5 mW cm−2 in Shenzhen China (114.31°E, 22.59°N), due to superior room-temperature TE performance of both Ge0.98Bi0.02Te and Ag2Se films, as well as the high device integration density of ~4.4 pair cm−2. Moreover, the self-cleaning solar absorber enhances environmental resilience, enabling consistent performance even under harsh desert conditions. These findings underscore the potential of GeTe-based thermoelectric thin films for sustainable energy harvesting and power generation, particularly in extreme climates.

Data-driven design principles of tetrahedrites: Statistical analysis and experimental validation

Catarina Quiterio[1], Kalpna Rajput[1], Konstantina Iordanidou[1], Vetle Øversjøen[1], Salah Amedi[1], Daniel Marchand[1], Ana Sa[2], Paulo Luz[2], Filipe Neves[2], **Patricia Carvalho**[1]
[1]SINTEF Industry, Norway, [2]LNEG, Portugal

Measurement and Characterisation, September 17, 2026, 15:30 - 17:00

Data-driven review of design principles for thermoelectric tetrahedritesTetrahedrites are promising thermoelectric materials owing to their intrinsically low lattice thermal conductivity and earth-abundant composition. However, reported performance varies widely across the literature, and the origins of this dispersion remain unclear, hindering the development of a quantitative optimisation framework. The present work shows that this variability is largely governed by processing-related factors rather than dopant chemistry. A comprehensive meta-analysis of tetrahedrite transport properties is carried out by aggregating a literature-scale dataset of more than 8,000 datapoints from 58 independent studies on tetrahedrites synthesised by mechanochemical processing and plasma-assisted sintering. The data-driven approach is integrated with targeted experimental synthesis of samples and density functional theory calculations. Statistical analysis, after normalising for the intrinsic temperature dependence of the thermoelectric figure of merit zT, reveals that dopant identity has only a limited effect on performance. Instead, thermoelectric performance is largely affected by processing-related factors, particularly consolidation quality and microstructural porosity associated with gas evolution during sintering, which mask intrinsic transport behaviour and dopant-specific effects. The findings reconcile the broad discrepancies in reported performance and indicate that improved processing control, rather than further compositional tuning, is currently the dominant lever for enhancing zT. This shifts the optimisation paradigm for tetrahedrites and highlights the importance of stricter fabrication and reporting standards to enable rigorous benchmarking and accelerate the development of high-performance thermoelectric materials.

Near-Equilibrium Interfacial Engineering for Robust and High-Performance Bi2Te3-based Thermoelectric Generators

Mr Shanghao Chen[1], Professor Qian Zhang[1]
[1]Harbin Institute of Technology, China

Harvesting and Sensing, September 15, 2026, 15:30 - 17:00

Efficient recovery of low-grade waste heat using Bi_2Te_3-based thermoelectric materials is severely hindered by interfacial instability of n-type contacts, primarily driven by uncontrolled Se migration. Here, we utilize the interfacial reaction between metallic species and n-type $Bi_2(Te, Se)_3$ to form a thermodynamically stable binary selenide, which is employed as the contact layer. As this phase represents the equilibrium endpoint of interfacial evolution, further interdiffusion is suppressed, enabling a self-limiting reaction with strong atomic bonding and chemical stability. The resulting interface exhibits an ultralow contact resistivity below 1 μΩ cm^2 and a shear strength of 12.1 MPa. A 7-pair module fabricated with commercial Bi_2Te_3 achieves a conversion efficiency of 6.9% and a power density of 0.41 W/cm^2 at a temperature difference of 200 K. Negligible performance degradation after 500 h of aging at 500 K and 50 thermal cycles between hot-side temperatures of 393 and 493 K confirms the excellent durability of the device.

BaCuP: A Promising Layered Phosphide Thermoelectric from First-Principles and Machine-Learning Simulations

Romain Claes[1], Peter P. Russell[1], Alexander G. Squires[1], Prof. David O. Scanlon[1]
[1]University Of Birmingham, United Kingdom

Materials Theory, September 17, 2026, 13:30 - 15:00

Thermoelectric materials enable direct conversion of waste heat into electricity, yet identifying efficient, sustainable, and non-toxic compounds remains a key challenge [1,2]. Here, we investigate the thermoelectric potential of the layered 1-1-1 phosphide BaCuP using first-principles calculations and machine-learning interatomic potentials.

The electronic structure of BaCuP features a small indirect band gap of 0.19 eV and strongly anisotropic valence-band dispersion arising from Cu–P derived states, which favours in-plane hole transport. Defect calculations reveal that BaCuP is intrinsically p-type, dominated by copper vacancies under Cu-poor conditions, yielding hole concentrations slightly above the thermoelectric optimum. Among several doping strategies explored, La substitution on the Ba site emerges as the most effective route to tune carrier concentration toward the optimal range while preserving the favourable Cu–P electronic structure.

On the thermal side, BaCuP exhibits a comparatively low lattice thermal conductivity within the 1-1-1 phosphide family [3], driven by strong anharmonic phonon scattering enhanced by the heavy Ba cation. Notably, higher-order anharmonic effects play a significant role in this material and should be considered when assessing thermal transport in related compounds. Combining electronic and thermal transport, La-doped BaCuP is predicted to reach a peak averaged figure-of-merit $zT \approx 0.65$ at 700–800 K, with in-plane values approaching unity. Transport anisotropy remains one of the primary limitation, with excellent in-plane performance offset by poor out-of-plane response. Further reductions in lattice thermal conductivity through nanostructuring could push the average zT beyond 0.8, establishing BaCuP as one of the most promising phosphide thermoelectrics reported to date.

[1] A. Firth, B. Zhang, and A. Yang, Applied Energy 235, 1314–1334 (2019).
[2] G. J. Snyder and E. S. Toberer, Nature Materials 7, 105–114 (2008).
[3] R. J. Quinn and J.-W. G. Bos, Journal of Materials Chemistry A 11, 8453–8469 (2023).

Maximizing thermoelectric performance in Fe2VAlM_x (M=W, Ti) thin films by synergistic combination of chemical ordering and controlled doping

Dr. Andres Conca[1], J.M. Domínguez-Vázquez[1], Olga Caballero-Calero[1], Ketan Lohani[1], Miguel A. Tenaguillo[1], Cristina V. Manzano[1], Alfonso Cebollada[1], Marisol Martín-González[1], Antonio M. Márquez[2], Jose J. Plata[2], Ernst Bauer[3]
[1]Instituto de Micro y Nanotecnología, IMN-CNM, CSIC (CEI UAM+CSIC), Spain, [2]Dpto. de Química Física, Facultad de Química, Universidad de Sevilla, Spain, [3]Institute of Solid State Physics, TU Wien, Austria

Zintl/Heusler-3, September 17, 2026, 15:30 - 17:00

The Fe_2VAl family of Heusler alloys shows a large potential with tunable properties via doping with additional elements such as Ti, Ta, Si or W [1-3]. The doping allows the fabrication of p- and n-type alloys, which simplifies thermoelectric device fabrication.

We experimental and theoretically investigate the combined effects of chemical ordering and finely tuned doping on optimizing the thermoelectric properties of sputter-deposited Fe_2VAl thin films. We synergistically combine long-range chemical order control with doping engineering, we reproducibly enhance both the average power factor (PF) and the dimensionless figure of merit (zT) of Fe_2VAl-based thin films.

We first demonstrate that $L2_1$ chemical ordering stabilizes a narrow-gap electronic structure on Fe_2VAl, leading to a four-fold increase in zT compared to chemically disordered films [4]. Subsequent tungsten doping in $L2_1$ $Fe_2V_{0.8}W_{0.2}Al$ n-type films yields a twofold rise in PF and tenfold improvement in zT compared to undoped Fe_2VAl, driven by electronic structure modulation and enhanced phonon scattering [5]. Finally, co-deposition of Fe_2VAl and W or Ti at 900ºC produces off-stoichiometric, chemically ordered, n- and p-type films, respectively, achieving maximum PF and zT values of 2200±300μW/m·K² and 0.3±0.05 on W-doped co-deposited films and 1250±190μW/m·K² and 0.12±0.05 on Ti-doped co-deposited films respectively.

Acknowledgements
Financial support by MICIU (ThermHeus TED2021-131746B-I00) and ERC Advanced Grant POWERbyU (ERC-2021-ADG-101052603), Spanish MICIU/AEI/10.13039/501100011033 and “European Union Next Generation EU/PRTR” (grants PID2022-1380630B-I00, and TED2021-130874B-I00) is acknowledged.

References

[1] Nishino, Y. IOP Conference Series: Materials Science and Engineering, IOP Publishing, 142001 (2011).
[2] [2] K. Renard, et al., Journal of Applied Physics, 115 (3), 033707 (2014).
[3] [3] B. Hinterleitner, et al., Nature, 576 (7785), 85-90 (2019).
[4] J. M. Domínguez-Vázquez, et al. , J. Mater. Chem. A Mater., 2025, 13, 24716–24726.
[5] J. M. Domínguez-Vázquez, et al. , J. Mater. Chem. A, 2026, Advance Article https://doi.org/10.1039/D5TA09938B

High-Performance Fully Flexible Self-Supported Thermoelectric Generator from Bi2Se3 and Cu3BiS3 Based Composites

Mr. Surajit Das[1], Dr. Anuja Datta[1]
[1]Indian Association For The Cultivation Of Science, India

Organics and Hybrids, September 15, 2026, 11:00 - 12:15

Owing to the rapid development of multifunctional and small-scale portable electronic systems, the development of efficient self-powered devices is highly essential. Flexible thermoelectric (TE) materials and devices have attracted increasing attention because of their ability to convert thermal energy directly into electrical power and are regarded as promising power sources for the rapidly growing field of wearable microelectronic devices. Inorganic-organic composites are promising for micro devices owing to their robustness, cost-effective fabrication and flexibility. In this work, we synthesized rhombohedral (space group $R\bar{3}m$) Bi2Se3 (BS) nanocrystals by a simple reflux-method and fabricated free-standing n-type films using BS nanocrystals/polyvinylidene fluoride (PVDF) composites. Subsequently, we investigated temperature dependent TE properties of optimized BS/PVDF composites exhibiting a Seebeck coefficient (S) of -232 μV/K and an electrical conductivity (σ) of 0.210 S/cm at 373 K. In conjunction, we fabricated p-type TE composite film using Cu3BiS3 nanocrystals/PVDF following the similar method that exhibited a S and σ ~37 μV/K and ~0.298 S/cm, respectively. Multi-pair self-supported n-p device were fabricated using PI as substrates for the free-standing TE films. A 15- pair device generated a maximum Voc of 320 mV with a 17.7 μA Isc that corresponds to 1.4 μW output power for ΔT = 80 K. Bending test demonstrates the excellent mechanical flexibility of both the individual TE legs and the TEG, with the small variation in internal resistance even after 2000 bending cycles. The experimental result was further verified using theoretical simulation and finally for proof-of-concept demonstration for waste-heat energy harvesting, the 15-pair device was used across various ambient heat sources resulting in measurable voltage and current generation.

[1] S. Das et al. APL Electronic Devices 2025, 1, 026113.
[2] C. Dun et al. ACS Appl. Mater. Interfaces 2015, 7, 7054

Grain boundary engineering for high temperature stable Mg2Si-based thermoelectric materials

Johannes de Boor[1,2], Amandine Duparchy[1], Saya Guadarama[1], Kyuseon Jang[3], Eleonora Isotta[3], Siyuan Zhang[3], Christina Scheu[3], Eckhard Müller[1,4]
[1]German Aerospace Center, Germany, [2]University of Duisburg-Essen, Institute of Technology for Nanostructures and CENIDE, Germany, [3]Max Planck Institute for Sustainable Materials, Germany, [4]Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry and ZfM/LaMa, Germany

Zintl-1, September 15, 2026, 15:30 - 17:00

Alternatives to state-of-the-art bismuth telluride are required to unlock further applications of thermoelectric devices in thermal management and power generation. Magnesium-based TE materials like MgAgSb, Mg3(Sb,Bi)2 and Mg2(Si,Sn) are some of the most promising candidates due to excellent performance, low cost, and environmental compatibility. However, n-type Mg2(Si,Sn) and Mg3(Sb,Bi)2 suffer from an instability of the functional properties due to the loss of loosely bound Mg, which causes a change in the previously optimized carrier concentration due to the formation of intrinsic point defects. This limits the maximum application temperatures for TE modules from these materials and even questions long term stability at room temperature.

We have previously shown that the degradation mechanism for these materials comprises the diffusion of Mg along grain boundaries and its sublimation off or consumption in chemical reactions at the surface, depending on the surrounding atmosphere. Based on this we have evaluated several organic and inorganic additives for their inhibition effect on Mg diffusion and can show that usage of the right additive can decelerate the degradation of high-performance n-type Mg2(Si,Sn) by three orders of magnitude at 500 °C; preliminary experiments even indicate chemical material stability at 600 °C. We have employed transport data analysis of differential experiments (variation of additive amount and processing parameters) in combination with advanced microstructural characterization by TEM to disclose the inhibition mechanism, providing guidelines to transfer this to further material systems. We also show that the stabilizing effect of the additives does not require the often-employed ball milling route for synthesis but is also compatible with an upscalable melting route.

With this we overcome a major challenge which has to this day prevented industrial scale fabrication of high performance, high temperature stable Mg-based thermoelectric materials.

Nanostructural Modifications in Ti-doped NbxTa1-xFeSb Half-Heusler Thermoelectrics

Dr. Andreas Delimitis[1], Dr. Panagiotis Mangelis[2], Prof. Theodora Kyratsi[2]
[1]Aristotle University Of Thessaloniki, Greece, [2]University of Cyprus, Cyprus
Zintl/Heusler-3, September 17, 2026, 15:30 - 17:00

Half-Heuslers (HHs) are among the most promising thermoelectrics for medium- to high-temperature applications, combining favourable electronic transport, thermal stability and good mechanical robustness. Among p-type HHs, NbFeSb-TaFeSb alloys have predominantly shown strong potential and compositional tuning of the transition metal sublattice has emerged as an effective route for improving thermoelectric performance. Partial substitution of Nb by Ta can alter microstructure and transport behaviour, while Ti doping can optimize electronic performance and influence phonon scattering-related mechanisms.

In this context, nanoscale characterization is essential for understanding how alloying modifies local structure. The present study focuses on the impact of dopant and host ions on morphology, defect configuration, strain state and chemical homogeneity of mechanical alloying prepared Ti-doped NbxTa1-xFeSb, by advanced electron microscopy (STEM HAADF, Geometric Phase Analysis -GPA).

Combined Nb-Ta alloying and Ti doping brings upon a ~15% particle size reduction, down to 172 nm, on average, for Nb0.5Ti0.1Ta0.4FeSb. HRTEM and GPA confirmed the absence of pronounced lattice distortions, even in the regions of extended structural defects, such as {111} stacking faults. This suggests that any local chemical variations are rather small and do not significantly affect the average strain state. HAADF-STEM images confirmed, in general, the expected HH structure; however, confined regions with partially occupied vacancy sites also detected locally. HAADF image simulations proved that this is a priori initiated by Nb/Ta intermixing in undoped NbxTa1-xFeSb and maintained after Ti incorporation. These observations suggest that Ti affects the nanostructure through particle size reduction, defect formation and lattice site intermixing, while preserving the overall HH crystal matrix. Since defect engineering and nanoscale structural modifications are known to widely influence phonon transport in HHs, these features are highly relevant for interpreting performance enhancement in such materials.

European Union’s Horizon Marie Skłodowska-Curie Actions program HIPERT under grant agreement No 101150392 is acknowledged.

Stabilizing Mg2(Si,Sn) Thermoelectric Materials by Suppressing Mg Sublimation Using Aerogels and Atomic Layer Deposition

Miss Radhika Ravindra Deshpande[1,2], Amin Bahrami[1], Marina Schwan[2], Fabian Henn[2], Pascal Vöpel[2], Kornelius Nielsch[1,4,5], Johannes de Boor[2,3]
[1]Leibniz Institute of Solid State and Materials Science (IFW), Germany, [2]Institute for Frontier Materials on Earth and in Space, German Aerospace Centre (DLR), Germany, [3]Institute of Technology for Nanostructures (NST) and CENIDE, Faculty of Engineering, University of Duisburg-Essen, Germany, [4]Institute of Materials Science, Technische Universität Dresden, Germany, [5]Institute of Applied Physics, Technische Universität Dresden, Germany
Zintl-2, September 16, 2026, 11:00 - 12:15

Mg_2X (X =Si, Sn)- based solid solutions are attractive materials for mid- to high-temperature waste heat recovery, but long-term stable thermoelectric generators (TEG) remain challenging to realize. Despite their excellent thermoelectric (TE) performance, Mg_2X materials suffer from Mg loss, which alters the carrier concentration via intrinsic point defects and reduces the figure of merit by >50% within hours to days at the target operating temperature of 450 °C.
To address this, aerogels were explored as mass-transport barriers. Both the aerogel composition (SiO_2 vs. carbon) and pore-size distribution were varied to understand their influence on the local Mg chemical potential and the driving force for sublimation. Stability was assessed via electrical transport measurements after annealing for one week at ~450 °C. SiO_2 aerogels proved unsuitable due to reactivity with Mg, while carbon-based aerogels showed potential in reducing Mg loss. Samples encapsulated in mesoporous carbon aerogels (2-50 nm) retained near-pristine transport properties, consistent with limited vapor diffusion once pore sizes fall below the Mg mean free path. The stabilization remains limited, however, pointing toward the need for further optimization of the encapsulation design. As an alternative, atomic layer deposition (ALD) was explored. After annealing at ~450 °C, coated samples show improved stability with <2% change in both Seebeck coefficient and electrical conductivity at room temperature, compared to significant degradation in unprotected samples (~97% and ~91%, respectively). This demonstrates that Mg sublimation can be effectively suppressed at the material surface. Both approaches aim to decouple the TE material from its environment by maintaining a high Mg chemical potential. While ALD provides a direct surface barrier, aerogels also offer the potential benefit of reducing radiative heat losses. Overall, the results indicate that Mg loss is governed by coupled transport and reaction processes, suggesting that addressing both will be key to achieving long-term stability in Mg_2X -based TEG.

Additive Manufacturing of Ni-Based Thermoelectric Materials for Waste Heat Recovery

Aayush Dobhal[1], Karolin Amstein[1], Heiko Reith[1], Ran He[1], Julia Kristin Hufenbach[1], Kornelius Nielsch[1], Pingjun Ying[1]
[1]Leibniz Institute for Solid State and Materials Research (IFW Dresden), Germany
Additive Manufacturing, September 18, 2026, 10:30 - 11:30

Thermoelectric generators convert waste heat into electricity but are limited by conventional manufacturing methods that restrict design flexibility and scalability. Additive manufacturing, particularly laser powder bed fusion (LPBF), offers a solution by enabling the direct fabrication of complex customised geometries. In this study, we successfully fabricated cuboid thermoelectric legs from n-type $Cu_{60}Ni_{40}$ and p-type $Ni_{90}Cr_{10}$ (at.%) using LPBF. We systematically investigated the effects of laser scan speed and power on density, as well as the impact of laser scan speed on microstructure and thermoelectric performance. Higher scan speeds increased porosity, reduced grain size, and significantly lowered thermal conductivity. By modifying process parameters, $Cu_{60}Ni_{40}$ achieved a 62% reduction in thermal conductivity, with a peak zT of 0.21 at 673 K. Additionally, a module assembled using the LPBF-fabricated legs achieved a maximum conversion efficiency of 0.8% at a temperature difference of 419 K. These results demonstrate the potential of LPBF to not only fabricate components with complex geometries, but also to tailor their thermoelectric properties, opening new opportunities for thermoelectric leg design and module fabrication.

Toward Efficient and Earth-Abundant Thermoelectrics: Anion-Tuned Cu2FeSnS4-xSex

Ms Hanna Donyk[1], Oleksandr Cherniushok[1], Dariusz Wieczorek[2], Bartlomiej Wiendlocha[2], Krzysztof Wojciechowski[1], Taras Parashchuk[1]
[1]Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Poland, [2]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland

Chalcogenides-1, September 15, 2026, 11:00 - 12:15

Many high-performance thermoelectric (TE) materials rely on toxic or critical elements, motivating the development of materials based on earth-abundant elements. Diamond-like chalcogenides, such as Cu2FeSnS4-xSex, are promising candidates for TE applications due to their chemical flexibility and intrinsically low lattice thermal conductivity. Here, we systematically investigate the Cu2FeSnS4-xSex (x = 0-4) solid-solution series to elucidate the role of anion substitution in coupling crystal structure, lattice dynamics, and transport properties. This system is a suitable model for studying anion substitution effects in diamond-like chalcogenides owing to its stannite-derived structure and composition-dependent transport properties. Sulfur/Selenium substitution strongly modifies the crystal symmetry and lattice parameters, driving a structural evolution toward a pseudocubic state at elevated temperatures ($c/2a \rightarrow 1$ near 773 K). This evolution enhances band degeneracy near the band edges and significantly influences the electronic structure.

First-principles calculations confirm semiconducting behavior and reveal large density-of-states effective masses ($m^* \approx 3.7\text{-}4.6$ me for S-rich and mixed compositions), consistent with the experimentally observed high Seebeck coefficient (220-300 μV K-1) and carrier concentration (~10^{20} cm-3). In parallel, the lattice thermal conductivity is intrinsically low and decreases from 1.5-1.8 W·m-1·K-1 at room temperature to ~0.7 W·m-1·K-1 at 773 K. Debye–Callaway analysis shows that point-defect scattering induced by S/Se substitution is the dominant mechanism for reducing phonon transport in intermediate compositions. Despite structural instability in Se-rich samples, the thermoelectric transport properties remain stable over the investigated temperature range.

By combining structural characterization, transport measurements, phonon-transport modeling, and first-principles calculations, we establish clear structure-phonon-transport relationships in diamond-like quaternary chalcogenides. These results demonstrate that anion substitution is an effective strategy for simultaneously tuning crystal structure, electronic structure, and thermal transport, providing a rational framework for designing efficient and earth-abundant thermoelectric materials.

This work was funded by the National Science Center (Poland) under the research project “OPUS-26” UMO 2023/51/B/ST11/00329.

Diffusion-Controlled Interfacial Evolution in Ti Contacts to n-type Half-Heusler

Mr Anjan Karmakar[1], Mr Philippe Masschelein[1], Dr Ioannis Petsagkourakis[2], Dr Gwladys Steciuk[1], Ms Sylvie Migot[1], Dr Ilayda Terzi[1], Mr Arthur Wieder[1], Dr Christophe Candolfi[1], Pr Bertrand Lenoir[1], Soufiane Eloualid[1]
[1]Institut Jean Lamour, Université De Lorraine, France, [2]Research Institutes of Sweden, Sweden
Heusler Modules, September 17, 2026, 13:30 - 15:00

Although n-type half-Heusler compounds such as $Zr_{0.4}Hf_{0.6}NiSn_{0.98}Sb_{0.02}$ are highly promising for thermoelectric applications, the interfacial structure between metal electrodes and these materials remains poorly understood. This work investigates the Ti/$Zr_{0.4}Hf_{0.6}NiSn_{0.98}Sb_{0.02}$ junction and its evolution under thermal treatment.

The interface is characterized by the formation of a complex multi-layered reaction zone, including an ultra-thin $SnTi_3$-rich interlayer acting as the effective diffusion barrier. In contrast, thicker Ti–Sn–(Hf,Zr) reaction layers develop but do not prevent further Ti-driven interfacial growth. Detailed TEM and STEM-EDS analyses reveal that the interfacial evolution is mainly governed by Ti diffusion, which becomes progressively limited by the formation of $SnTi_3$-type phases.

After annealing at 600 °C, the interfacial structure remains relatively stable, with limited compositional evolution. However, the growth of the reaction layers follows diffusion-controlled kinetics, which may impact the long-term electrical performance of the contact.

These results demonstrate that $SnTi_3$ plays a key role in controlling interfacial diffusion, providing important insights for designing stable and low-resistance Ti-based contacts for half-Heusler thermoelectric devices.

Wearable Thermal Management System Based on Thermoelectric Device and Textile Heat Exchanger

Carlo Fanciulli[1], Giovanna Latronico[1], Fabio Lazzari[1], Gennaro Rollo[2], Ilaria Improta[2], Marco Fiume[2], Marino Lavorgna[2], Simona Del Ferraro[3], Vincenzo Molinaro[3]
[1]CNR - ICMATE, Italy, [2]CNR - IPCB, Italy, [3]INAIL - DiMEILA, Italy

Harvesting and Sensing, September 15, 2026, 15:30 - 17:00

Rising energy and climate challenges have spurred interest in energy-efficient personal thermoregulation. As thermal comfort varies, research targets personalized solutions to improve comfort and cut energy use. Personal cooling systems can lower air conditioning demand saving individual comfort and provide portable relief for outdoor workers.

This work presents a system developed for SMART-SHIRT project (SMART materials and technologies for thermal-stress & physio-monitoring SHIRT), aimed at improving thermal regulation for workers in thermal-stressful environments. The system integrates sensors within a t-shirt to capture biometric data in real time, activating a thermoelectric cooling unit to prevent critical thermal stress.

The design employs an innovative 3D textile heat exchanger while maintaining comfort and mobility. Current efforts focus on lightweight, unobtrusive integration, and a benchmark setup is being developed to evaluate thermal management performance.

Optimizing textured structure of polycrystalline SnSe thermoelectric material by solvent-regulated cold sintering

Xin Feng[1], Václav Ocelík[1], Horatio Cox[1,2], Jacob Bass[1], Graeme R Blake[1]
[1]Zernike Institute for Advanced Materials, University Of Groningen, Netherlands, [2]Groningen Cognitive Systems and Materials Center (CogniGron), University of Groningen, Netherlands

Emerging, September 15, 2026, 15:30 - 17:00

SnSe has emerged as a highly promising thermoelectric material due to its layered crystal structure, highly anharmonic bonding, ultralow phonon group velocity, and favorable electronic band structure, which together yield exceptional electrical transport performance and extremely low thermal conductivity.

However, the record high thermoelectric performance is typically realized in single crystals, whose fabrication complexity and limited long-term reliability hinder large-scale deployment compared with polycrystalline counterparts. Moreover, spark plasma sintering (SPS), one of the most widely used consolidation techniques for polycrystalline samples, requires bulky equipment, high temperatures and significant energy input, constraining its scalability for practical manufacturing.

This talk will introduce our strategy to enhance the anisotropic alignment of polycrystalline SnSe grains using the solvent-regulated cold sintering process (CSP) in order to obtain ceramic samples that are single-crystal-like in terms of anisotropy. In this approach, nano-scale features are well-preserved, while the interfacial friction between SnSe nanosheets is markedly reduced by introducing a mixed solvent with low polarization and surface tension during CSP treatment. This reduction in friction promotes particle rearrangement and facilitates the formation of a highly oriented structure. Furthermore, this process effectively transforms inter-particle grain boundaries into predominantly low-angle grain boundaries that act like dislocation walls, facilitating charge transport while scattering phonons. The resulting bulk materials exhibit comparable, or even superior, in-plane electrical performance to those processed by SPS, highlighting CSP as a promising, energy-efficient and scalable alternative for fabricating high-performance SnSe-based thermoelectric materials.

Unraveling Complex Crystal Structures and Cation Ordering in Cu-Sn-Se Thermoelectric Compounds

Mia-eussa Gautier[1], Minati Tiadi[1], Animesh Bhui[1], Carmelo Prestipino[1], Bin Zhang[2], Xioayuan Zhou[2], Julien Varignon[1], Philippe Boullay[1], Emmanuel Guilmeau[1]
[1]Laboratoire de cristallographie et Sciences des Matériaux, Université de Caen Normandie, ENSICAEN, CNRS, Normandie Univ, France, [2]College of Physics and Institute of Advanced Interdisciplinary Studies, Chongqing University, China

Materials, September 18, 2026, 10:30 - 11:30

In recent years, copper-rich sulfides have attracted increased interest as thermoelectric materials due to their low-cost and environmentally benign nature, as compared to state of art selenides and tellurides. Within the Cu-Sn-S phase diagram, several compounds have been reported, including Cu2SnS3, Cu22Sn10S32, Cu5Sn2S7, exhibiting promising thermoelectric properties. [1] Variations in the Cu/Sn ratio give rise to different cationic ordering and crystal structures, often derived from the sphalerite-type structure, and lead to diverse electrical and thermal transport behaviors.

In parallel, compounds in the Cu-Sn-Se system such as Cu2SnSe3, or Cu5Sn2Se7, also display interesting thermoelectric properties. However, their crystal structures remains poorly investigated and understood; they are also highly sensitive to non-stoichiometry effect and synthesis conditions. [2]

To gain deeper insight into the crystal chemistry and transport properties in the Cu-Sn-Se system, we have investigated a series of compounds by varying the S/Se and Cu/Sn ratio. Our study also aims to elucidate the impact of the synthesis conditions on the cationic ordering. By using advanced structural characterization techniques, such as 3D electron diffraction (3D ED) and HAADF-STEM analyses, we have elucidated the complex crystal structure of a new compound in the Cu-Sn-Se system. Combining structural and transport properties characterizations, in relation with first principles calculations, we clarify the relationships between crystal structures and thermoelectric properties in the Cu-Sn-Se system.

[1] L. Le Gars et al, Chem. Mater. (2025), 37, 5271−5285 and references therein.
[2] Y. Zhou et al, Materials Today Physics, (2018), 7, 77-88, and references therein.

Highly stabilized thermoelectric performance in natural mixed minerals

Zhenhua Ge[1]
[1]Kunming University Of Science And Technology, China

Emerging, September 15, 2026, 15:30 - 17:00

Excellent thermoelectric materials can be obtained by various synthesis procedures and optimization strategies, and the elaborately designed composition and microstructure benefit thermoelectric parameter decoupling. Herein, a high-performance mixed natural mineral (CQB), composed by chalcocite, quartz, and bismuthinite, enables direct thermoelectric energy conversion. The network of quartz layers is embedded into the matrix and blocks Cu ion long-range migration by producing the natural rheostat and voltage division circuit. The thermoelectric performance, mechanical strength, and electrical stability of natural minerals are found to be highly superior to the artificially synthesized Cu2S material. Learning from nature, a strategy for blocking mobile Cu+ ions in Cu-based superionic conductors is proposed. Various Cu-based superionic conductors, composited with insulating macroscale glass sheets, have been designed and fabricated, showing highly enhanced electrical stability while maintaining good thermoelectric properties. These findings provide a deep understanding of the role of macroscopic insulating materials in improving the electrical stability of superionic conductors.

Electrical Characterization of Encapsulated Vertically Aligned Silicon Nanopillars Obtained via Metal-Assisted Chemical Etching

Dr. Federico Giulio[1], Professor Dario Narducci[1]
[1]University Of Milano-Bicocca, Dept. of Materials Science, Italy

Organics and Hybrids, September 15, 2026, 11:00 - 12:15

Nanostructuration significantly reduces the thermal conductivity of crystalline silicon, increasing the thermoelectric figure of merit to 0.8 at room temperature in silicon nanopillars (SiNPs). Metal-assisted chemical etching (MACE), an electroless metal catalyzed and localized process, enables the production of dense, vertically aligned, and cost-effective SiNPs. Furthermore, MACE may be extended to remove the residual bulk Si membrane, leading to the formation of self-standing SiNP aggregates, we named Si nanofelts (SiNFs). These unique structures allow the fabrication of macroscopic thermoelectric legs, transferring nanoscale advantages to the macroscale. However, SiNPs remain quite fragile when subjected to shear stress. In addition, for their utilization in thermoelectric devices, it is mandatory to fabricate low-resistance metal contacts on the SiNP tips.

To these aims, both supported SiNPs and SiNFs (with a doping level of 10^{15} and 10^{18} cm-3) were embedded in a polymer matrix through spin-coating. We used poly-hydroxypropyl methacrylate (poly-HPMA) which is thermally and mechanically stable and fills completely the space between the pillars without modifying their orientation. Following thermal polymerization, reactive sputter etching, in oxygen and argon atmosphere, was employed to remove excess polymer and expose the pillar tips for metallization. Subsequently, a 4 nm chromium adhesion layer and 500 nm of copper were deposited using e-beam evaporation. The current-voltage curves of supported SiNPs and SiNFs display a linear behavior across all silicon doping levels and types, due to the high density of surface defects injected during prolonged etching exposure. Furthermore, the electrical fill factor was measured to exceed 20%, fully comparable with the visual fill factor estimated via SEM. Our results confirm the potential use of SiNFs for the fabrication of silicon-based thermoelectric devices with output power densities and cooling performances comparable to those of telluride-based devices.

Design and Scaling of Additively Manufactured Thermoelectric Heat Exchangers Using Lattice Structures

Sumner Gubisch[1], Dr. Saniya LeBlanc[1]
[1]The George Washington University, United States

Additive Manufacturing, September 18, 2026, 10:30 - 11:30

Heat exchangers are essential across a vast array of applications, ranging from automotive cooling to building climate control. As their global presence multiplies, the energy required to operate these systems continues to rise, necessitating more efficient and multifunctional designs. Thermoelectrics present a promising avenue for direct integration with heat exchangers, enabling simultaneous energy harvesting from the pre-existing thermal gradients within the device. Traditional manufacturing techniques, however, are ill-suited for this integration, as they typically yield flat thermoelectric modules that conflict with complex heat exchanger geometries. Additive manufacturing overcomes this limitation by enabling the creation of custom, conformal thermoelectric structures that build directly into the device. To physically realize this concept, this study details the fabrication of a novel heat exchanger prototype using fused filament fabrication (FFF). By using a custom PLA-based filament with 5% silver selenide powder by weight, Protopasta conductive filament, and standard Bambu Lab PLA, thermoelectric, conductive, and insulating materials are all combined into one manufacturing process to produce a complete device. Thus, this work represents the first additively manufactured thermoelectric heat exchanger printed entirely in one continuous operation. Building upon this initial prototype, this study also explores device scalability by presenting a next-generation heat exchanger design that incorporates both n-type and p-type thermoelectric materials. Computational simulations evaluate the effects of volumetric scaling on power output across the single-material baseline and the new n/p-type configurations. Scaling analyses show that doubling the device volume lowers the power density from 1.67 kW/m^3 to 1.32 kW/m^3. However, combining alternating n-type and p-type lattices increases the overall power output by almost eight times. This strategic integration effectively counters volume-scaling losses, unlocking the traditional benefits of thermoelectrics for advanced, three-dimensional heat exchangers.

Composite thermoelectric samples made via cold-press sintering based on PEDOT:PSS aerogels

Dr. Savvas Hadjipanteli[1], Dr. Panagiotis Mangelis[1], Dr. Ujwala Ail[2], Dr. Zia Ullah Khan[2], Prof. Reverant Crispin[2], Prof. Theodora Krasia-Christoforou[1], Prof. Theodora Kyratsi[1]
[1]University of Cyprus, Department of Mechanical and Manufacturing Engineering, Cyprus,
[2]Linköpings Universitet, Department of Science and Technology, Sweden

Composites, September 17, 2026, 11:00 - 12:15

Organic thermoelectric (TE) materials have been gaining attention as a new alternative for low-temperature TE systems. Conducting polymers in particular show various inherent advantages such as low thermal conductivity, abundance, ease of synthesis and processing, cost-effectiveness and suitability for more sustainable device fabrication. In addition to their easily tuneable electrical properties, via various doping methods and additives, their intrinsic mechanical flexibility is also a significant advantage, since it enables the development of increasingly complex device architectures. Among these polymers, PEDOT:PSS (poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate)) is an excellent candidate for TE applications. It has a relatively high electrical conductivity that is easily enhanced via secondary doping with organic solvents, since they cause morphological changes. Therefore, increasing carrier mobility with better π-π stacking. This polymer, in the form of aerogel microparticles, can exhibit more robust design choices and diversify from the usual thin films. More importantly, this may enable the cold sintering of inorganic particles via the polymer matrix and make for a more cost-effective approach.

In this study, thermoelectric composite pellet samples from PEDOT:PSS aerogels and inorganic additives were made via cold press. The PEDOT:PSS aerogels were obtained via a freeze-drying method from solutions of PEDOT:PSS, mixed with various NFC (nanofibrillated cellulose) concentrations for mechanical stability. The effect of various additives on the TE performance was systematically investigated, including organic solvent dimethyl sulfoxide (DMSO), inorganic classic TE material (Bi,Sb)2Te3, half-Heuslers (Nb,Ta,Ti)FeSb and Ti(Fe,Co,Ni)Sb to increase the Seebeck coefficient. While keeping in mind the sign of the Seebeck coefficient for TE compatibility. The samples were studied in terms of Seebeck coefficient, electrical and thermal conductivity measurements.

Conduction Band Convergence and Modular Nanostructures: Driving High Thermoelectric Performance in n-Type PbSe

Mr. Indrajit Haldar[1], Ms. Vaishali Taneja[1], Mr. Naveen Goyal[2], Dr. Mohammad Ubaid[3], Dr. Debattam Sarkar[1], Mr. Dinesh Kumar Kedia[4], Dr. Kumar Saurabh[1], Prof. Surjeet Singh[4], Dr. Koushik Pal[3], Prof. N. Ravishankar[2], Prof. Kanishka Biswas[1]
[1]New Chemistry Unit, International Centre for Materials Science and School of Advanced Materials, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), India, [2]Materials Research Centre, Indian Institute of Science, India, [3]Department of Physics, Indian Institute of Technology Kanpur, India, [4]Department of Physics, Indian Institute of Science Education and Research, Pune, India

Chalcogenides-1, September 15, 2026, 11:00 - 12:15

n-type lead chalcogenides showing high thermoelectric performance are rare due to the larger energy offset between the two lowest energy conduction bands minima, leaving ample opportunity to modulate electronic structure for improving their thermoelectric performance. Here, we present a remarkable thermoelectric figure of merit (zT) of ~1.8 at 873 K in n-type PbSe doped with MoCl5 by modulation of the conduction bands, while simultaneously suppressing the phonon transport. Doping MoCl5 in PbSe induces notable convergence of conduction bands and an increased density of states near the Fermi level, mainly due to the contribution of Mo 4d orbital hybridized with the Se 4p-Pb 6p. This results in an improved Seebeck coefficient, despite maintaining a high n-type charge carrier concentration resulting in an excellent power factor (σS2) of ~21 μW cm−1 K−2 at 873 K for PbSe + 1 mol% MoCl5. When the solid solution limit of the doping exceeds, it forms unique modular nano-heterostructures (5-30 nm) of PbSe-MoSe2 misfit layered compounds embedded in PbSe matrix. These nano-heterostructures significantly intensify phonon scattering, leading to an ultralow lattice thermal conductivity (κ_{lat}) of 0.20 W m-1 K-1 at ~725 K in PbSe + 1 mol% MoCl5 sample.

Point-Defect Modulation as a Design Strategy for Optimizing Thermoelectric Transport in Half-Heusler Compounds

Dr. Ran He[1]
[1]IFW-Dresden, Germany

Heusler-1, September 15, 2026, 13:30 - 15:00

Half-Heusler compounds are leading thermoelectric materials for medium- to high-temperature applications, yet their performance is fundamentally limited by the strong coupling between electronic transport and lattice thermal conductivity. Recent advances demonstrate that deliberate modulation of point defects, such as vacancies, antisites, interstitials, and aliovalent substitutions, offers an effective pathway to decouple these transport channels. In this presentation, I discuss how controlled defect chemistry, combined with tailored synthesis and processing routes, enables simultaneous tuning of carrier concentration, scattering mechanisms, and phonon transport in half-Heusler systems. Beyond isolated defects, the interaction between point defects and hierarchical microstructures introduces multiscale phonon scattering while preserving favorable electronic characteristics. Structural characterization and theoretical insights reveal that managing intrinsic defect populations can mitigate carrier compensation, stabilize desirable electronic states, and enhance phonon suppression without severely compromising carrier mobility. These results establish point-defect modulation as a general design principle for half-Heusler thermoelectrics, providing a coherent framework for rational materials optimization and guiding the development of next-generation thermoelectric materials.

Power factor optimization and thermal conductivity reduction in selected sulfides

Sylvie Hebert[1], Laura Agnarelli[1], Serge El Haber, Ramzy Daou[1], Denis Pelloquin[1], Antoine Maignan[1], Anustup Mukherjee[2], Alaska Subedi[2]
[1]Laboratoire Crismat, CNRS, Ensicaen and Unicaen, France, [2]Laboratoire CPHT, Ecole Polytechnique, France

Materials, September 18, 2026, 10:30 - 11:30

Sulfides constitute a rich playground to investigate transport properties and study the parameters that can tune thermoelectric properties. Large ZT values have already been observed in sulfides with different crystallographic structures [1]. Also large power factors can be obtained, as for example in the CoS2 pyrite [2], this power factor being moreover strongly enhanced at low temperatures in the ferromagnetic state. More recently, the shandite with kagome layers which exhibit magnetic frustration has also emerged as a promising candidate for thermoelectric applications, both for longitudinal and transverse effects [3]. These examples show that a subtle interplay between the electronic and magnetic properties can be beneficial for thermoelectric properties.

In the case of pyrites, the thermal conductivity is too large and the possibility to reduce it will be discussed [4]. Also, in thiospinels and related structures, the different ways to optimize the power factor by modifying the doping or the magnetic ground state will be presented.

[1] : A. Powell, J. Appl. Phys. 126, 100901 (2019); Fu-Hua Sun et al., Journal of Materiomics 10 (2024) 218e233.
[2] : Ulises Acevedo Salas et al., Phil. Trans. R. Soc. A 377, 20180337 (2018).
[3] : Chenguang Fu et al., Adv. Mater. 31, 1806622 (2019) ; Panagiotis Mangelis et al., ACS Appl. Energy Mater. 3 (2020) 2168–2174 ; R. Daou et al., Solid State Sciences 149, 107454 (2024).
[4] : L. Agnarelli et al., J. Phys. Condens. Matter 37, 415701 (2025).

From material to device: impact of microstructure on oxidation and stability of skutterudites

Arige Hodroj[1], Mathieu Pasturel[2], Valerie Bouquet[2], Carmelo Prestipino[3], Ruchi Bhardwaj[4], Eric Alleno[4], Philippe Masschelein[1], Soufiane El Oualid[1], Bertrand Lenoir[1], Christophe Candolfi[1]
[1]Université de Lorraine, CNRS, Institut Jean Lamour, France, [2]Univ Rennes, CNRS, France, [3]Univ Normandie Caen, CNRS, France, [4]Univ Paris Créteil, CNRS, ICMPE, France
Interfaces and Stability, September 17, 2026, 15:30 - 17:00

Skutterudites based on $CoSb_3$ have demonstrated promising performance in thermoelectric modules in the mid-temperature range (600–800 K). Nevertheless, their long-term stability remains limited by oxidation in air at operating temperatures, which impacts their reliability. Oxidation is influenced by multiple factors, including chemical composition and microstructure, the latter being governed by the synthesis route. In this work, n-type $In_xCo_4Sb_{12}$ skutterudites synthesized via melting/annealing [1] and magnesioreduction [2] are compared.

While exhibiting similar thermoelectric performance ($ZT \approx 1.1$), these materials display markedly different thermal stabilities and oxidation behaviors. In this presentation, we show that these differences are directly related to microstructural features controlling diffusion processes, oxide formation, and degradation mechanisms. Aging experiments performed at 650 K in air further highlight these effects.

To further assess their impact at the device level, n-type legs obtained from both synthesis routes are integrated into thermoelectric modules. The resulting devices are evaluated under operating conditions, enabling a direct comparison before and after aging. In parallel, protective coatings deposited by dip-coating are applied at both material and module levels, and their effectiveness in limiting oxidation-induced degradation is assessed.

[1] Benyahia M. et al., J. Alloys Compd., 735 (2018) 1096-1104
[2] Le Tonquesse S. et al., J. Alloys Compd., 796 (2019) 176-184

Machine Learning Interatomic Potentials for Microstructural Defects in SnSe and SnTe

Guojing Huang[1], Prof. Dr. rer. nat. Gerhard Dehm[1], Dr.-Ing. Tobias Brink[1]
[1]Max Planck Institute for Sustainable Materials, Germany

Machine Learning, September 15, 2026, 13:30 - 15:00

Understanding thermal transport in materials with complex microstructures is essential for improving thermoelectric performance. Efficient thermoelectrics require high electrical conductivity and low thermal conductivity to maximize the figure of merit zT. Achieving this decoupling is challenging. One promising strategy is to reduce lattice thermal conductivity through microstructural engineering. Grain boundaries (GBs) can scatter phonons and reduce thermal conductivity, while the impact on electrical conductivity can be tuned [1]. The atomic structure, chemistry, and transport impact of different GBs remain incompletely understood and controversial. Systematic investigations using density functional theory (DFT) are difficult due to the large length and time scales required to describe a realistic microstructure.

To overcome those computational limitations, we developed machine learning interatomic potentials (MLIPs) for the thermoelectric materials SnSe and SnTe. Training datasets were generated using the ASSYST approach [2], which systematically samples crystal structures to provide diverse and unbiased coverage of the configurational space including defects and metastable phases. A range of MLIPs were constructed using the Atomic Cluster Expansion (ACE) and Graph ACE (GRACE) frameworks [3], enabling different tradeoffs between accuracy and computational efficiency. We extensively validated the models against DFT for a range of physical properties, including elastic constants, point defect energetics, grain boundary energies, and lattice thermal conductivity.

The resulting MLIPs enable large-scale simulations of grain boundaries and defects beyond the reach of DFT, allowing investigation of lattice heat transport and defect structures/phases relevant to thermoelectric materials. In this presentation, we will present the development and validation of the MLIPs and discuss their first applications to defects and grain boundaries in SnSe and SnTe, highlighting their influence on lattice thermal transport.

[1] Bueno Villoro et al., Adv. Energy Mater. 13 (2023): 2204321
[2] Poul et al., npj Comput. Mater. 11 (2025): 174
[3] Bochkarev et al., Phys. Rev. X 14 (2024): 021036

Metallization routes for low resistance contacts in p-type (Nb,Ta)FeSb half-Heuslers: experimental characterization and thermoelectric modeling

Dr. Panagiotis S. Ioannou[1], Dr. Panagiotis Mangelis[1], Dr. Oleksandr Horniichuk[2], Dr. Radoslaw Chmielowski[2], Dr. Seyedmohammad Mortazavinatanzi[3], Dr. Savvas Hadjipanteli[1], Dr. Theodora Kyratsi[1]
[1]Department of Mechanical Engineering, University of Cyprus, Cyprus, [2]IMRA Europe SAS, France, [3]ParsNord Thermoelectric Filial, Denmark

Heusler Modules, September 17, 2026, 13:30 - 15:00

Half-Heusler (HH) compounds have attracted considerable attention as thermoelectric materials due to their favorable transport properties and high-temperature stability. Selected members with promising room temperature properties are increasingly considered as sustainable alternatives to Bi_2Te_3-based systems, owing to their abundance, low toxicity, reduced reliance on critical raw materials as well as thermal and mechanical stability. However, their implementation in efficient modules requires stable, low-resistance electrical contacts. Metallization is a multi-step process involving surface pre-treatment of thermoelectric legs (e.g., polishing, planarization, cleaning), where processing parameters critically affect interface quality and contact resistance.

In this work, sputtering and sintering metallization routes for p-type (Nb,Ta)FeSb-based HH materials are investigated through interface characterization, contact resistance, and bonding strength measurements, and their impact on device performance is evaluated via thermoelectric modeling. Specifically, (Nb,Ta)FeSb HH compounds are synthesized by mechanical alloying, followed by Ni/Cu metallization using physical vapor deposition and two-step sintering approaches. Interfacial characteristics are examined using high-resolution cross-sectional scanning electron microscopy, combined with elemental and grain mapping via energy-dispersive X-ray spectroscopy (EDX) and electron backscatter diffraction (EBSD). Interdiffusion phenomena and microstructural modifications induced by thermal processing are also analyzed. Electrical contact resistance is experimentally assessed using the scanning probe method (SPM), demonstrating the potential for low-resistance contacts. In addition, the bonding strength of metallized HH legs is evaluated as a function of surface preparation and metallization conditions. The influence of contact resistance on device-level performance is further assessed through thermoelectric power generation simulations using COMSOL Multiphysics®.

Discovery of Resonant-Like Doping in Mg3Sb2 for High-Efficiency Thermoelectrics

Navita Jakhar[1], Sharona Horta[1], Ke Xiao[1], Ankit Kumar[2], Maria Ibanez[1]
[1]Institute of Science and Technology Austria, Austria, [2]University of Warwick, United Kingdom
Zintl-1, September 15, 2026, 15:30 - 17:00

The development of sustainable, high-performance thermoelectric (TE) materials is critical for efficient green energy harvesting. Among emerging candidates, Mg3Sb2-based compounds offer significant promise due to their earth-abundant constituents, low-cost synthesis, and high thermoelectric performance. In this work, we present a band-engineered n-type Mg3Sb2 system via dilute doping incorporation, achieving simultaneous enhancement in the figure of merit (zT), device efficiency, and material stability. We identify a resonant-like dopant in n-type Mg3Sb2, which suppresses Mg vacancy defects, leading to increased carrier concentration, preserving the higher electrical conductivity. Additionally, it introduces electronic states near the Fermi level, enhancing the density of states and improving the Seebeck coefficient with minimal detriment to the electrical conductivity. This results in an enhanced power factor across the entire temperature range. Further reduction in lattice thermal conductivity is achieved by introducing excess Mg, which promotes nanoprecipitate formation and enhances phonon scattering. Owing to these synergistic effects, a peak zT of 1.94 is obtained at 720 K. A single-leg device fabricated from the optimized material demonstrates a maximum conversion efficiency above 12% and an output power of 170 mW under a 439 K temperature gradient. This study provides a scalable strategy combining resonant-like band engineering and defect control for advancing high-performance, stable thermoelectric materials.

Probing Local Electrical Properties at Thermoelectric–Electrode Interfaces via Correlative KPFM and Seebeck Microprobe Techniques

Dr. Subhra Sourav Jana[1], Ms. Sarah E. Beck[2], Mr. H Myja[3], Prof. Gerd Bacher[4], Prof. Eckhard Müller[5], Prof. Wolfgang Mertin[6], Prof. Johannes de Boor[7]
[1]Institute for Frontier Materials on Earth and in Space,German Aerospace Center (DLR), Köln, Germany, [2]Institute of Electronic Materials and Nanostructures (WET) & CENIDE, Universität Duisburg-Essen, Germany, [3]Institute of Electronic Materials and Nanostructures (WET) & CENIDE, Universität Duisburg-Essen, Germany, [4]Institute of Electronic Materials and Nanostructures (WET) & CENIDE, Universität Duisburg-Essen, Germany, [5]Institute for Frontier Materials on Earth and in Space,German Aerospace Center (DLR), Germany, [6]Institute of Electronic Materials and Nanostructures (WET) & CENIDE, Universität Duisburg-Essen, Germany, [7]Institute for Frontier Materials on Earth and in Space, German Aerospace Center (DLR), Germany

Measurement and Characterisation, September 17, 2026, 15:30 - 17:00

High interfacial resistance at metal–thermoelectric (TE) contacts leads to significant efficiency losses in thermoelectric devices, yet its microscopic origin remains poorly understood. This enhanced resistance has been attributed to several factors, including Schottky barrier formation, interfacial phase formation, and metal diffusion into the thermoelectric material. Understanding the relative contributions of these effects requires direct insight into the local electronic structure at the interface, which governs charge transport. To address this, we employ a correlative approach combining Kelvin Probe Force Microscopy (KPFM) and Transient Potential Seebeck Microprobe (TPSM), supported by microstructural analysis using SEM/EDX. Using the Ag/n-Mg_2Si system as a model interface, we show that Ag diffusion leads to the formation of an interfacial Ag–Mg–Si composite layer, strongly modifying the local electronic structure. KPFM measurements reveal a potential barrier of ~0.6 eV at the interface and a continuous Fermi level shift of ~0.23 eV within Mg_2Si towards the contact, consistent with the Ag diffusion profile. We have found an excellent agreement between the change in Fermi level measured by KPFM and the calculated variation of the Fermi level with respect to the conduction band edge derived from Seebeck coefficients measured by TPSM. To establish this relation, both single parabolic band (SPB) and two-parabolic-band (2PB) models are employed to determine the position of the Fermi level relative to the band edge. These results establish a direct link between interfacial chemistry, local band structure, and transport properties, and demonstrate a correlative approach towards resolving the origin of contact resistance in thermoelectric materials.

Quantifying the Effect of Lateral Heat Flux Heterogeneity on the Output of Anisotropic Thermoelectric Heat Flux Sensors

Dr Filip Janasz[1], Dr. Iurii Dolganov[2], Prof. Stephan Leyer[2]
[1]Meerstetter Engineering GmbH, Switzerland, [2]University of Luxembourg, Luxembourg
Applications-3, September 17, 2026, 11:00 - 12:15

Anisotropic thermoelectric heat flux sensors, including transverse and tilted-layer architectures, are calibrated under one-dimensional thermal boundary conditions that assume spatially uniform heat flux normal to the sensing surface. In practice, thermal fields are often multidimensional and may contain lateral heat flux components. Although these sensors have been extensively studied for materials, fabrication, and dynamic performance, the effect of lateral heat flux heterogeneity on the measured output has not been systematically quantified. Here, this effect is investigated using coupled heat transfer and thermoelectric finite element simulations. A representative sensor cross-section embedded in a surrounding medium is analysed under steady-state conditions. The normal heat flux through the sensing surface is held constant, while controlled heterogeneity is introduced by applying lateral heat flux at one side of the surrounding domain. A dimensionless heterogeneity parameter, $H=q\parallel/q\perp$, is introduced, where $q\parallel$ is the imposed lateral heat flux and $q\perp$ is the normal heat flux.
The simulations show that lateral heat flux heterogeneity produces a systematic bias in the output voltage. Owing to the inclined sensing layers, the sensor geometry generates an in-plane thermoelectric response component even under normal loading. The imposed lateral heat flux perturbs this generated response and may therefore either enhance or reduce the measured signal. Depending on the orientation of the sensing layers relative to the imposed lateral flux, the bias is additive or subtractive. When expressed as a normalized signal ratio, the response follows a single functional relationship with H, indicating that, within the linear material regime, the relative bias is governed primarily by the heterogeneity ratio rather than the absolute heat flux magnitude.

These results provide a quantitative basis for assessing measurement errors when sensors calibrated under one-dimensional conditions are deployed in multidimensional thermal fields, and they guide calibration and design strategies for reducing sensitivity to lateral heat flux disturbances.

Retarding moisture-induced chemical degradation of Yttrium Tellurides by tailoring grain boundary chemistry

Kyuseon Jang[1], Dr. Jamil Ur Rahman[2], Dr. Su-Hyun Yoo[3], Prof. Chanwon Jung[4], Dr. Eric Woods[1], Dr. Ruben Bueno Villoro[1], Prof. Kornelius Nielsch[2], Prof. Yonghyuk Lee[5], Prof. Pyuck-Pa Choi[6], Dr. Ran He[2], Dr. Siyuan Zhang[1], Prof. Christina Scheu[1]
[1]Max Planck Institute for Sustainable Materials, Germany, [2]IFW Dresden, Germany, [3]Korea Research Institute of Chemical Technology, Republic of Korea, [4]Pukyong National University, Republic of Korea, [5]Dongguk University, Republic of Korea, [6]KAIST, Republic of Korea

Interfaces and Stability, September 17, 2026, 15:30 - 17:00

Grain boundary engineering has been widely applied to enhance thermoelectric performance, as it critically governs both charge and phonon transport. However, its potential to improve chemical stability remains far less explored. Y2Te3 is an emerging n-type thermoelectric material, first identified via machine learning-guided material screening in 2021. Despite the promising thermoelectric performance of Y2Te3 owing to its intrinsically low thermal conductivity, the instability upon air exposure remains a key challenge. Here, through a detailed mechanistic study, we show that the chemical degradation of Y2Te3 is driven by H2O, rather than O2, and that tailoring grain boundary chemistry via minor Bi addition effectively suppresses this chemical degradation under ambient conditions. Scanning transmission electron microscopy and atom probe tomography reveal that H2O preferentially infiltrates along grain boundaries, triggering oxidation into Y–O–H phases and causing chemo-mechanical breakdown of the matrix. Remarkably, incorporating only ~1 at.% of Bi retards this process by its segregation to the grain boundary and impedes long-range H2O diffusion, and simultaneously yields a two-fold increase in thermoelectric performance. These findings establish multifunctional grain boundary engineering as a potential strategy to achieve sustainability in thermoelectrics.

Mechanistic insight into phase formation and fast processing of Cu doped thermoelectric half-Heusler TiNiSn

Dr Blair Kennedy[1], Dr Aaron Naden[1], Dr Clemens Ritter[2], Dr Jan-Willem Bos[1]
[1]EaStCHEM School of Chemistry, University of St Andrews, United Kingdom, [2]Institut Laue-Langevin, France

Zintl/Heusler-3, September 17, 2026, 15:30 - 17:00

Half-Heusler's (HH's) are leading contenders for thermoelectric power generation and cooling. Traditional XYZ HH materials are characterised by large electronic power factors, $S^2\sigma$, but limited by high lattice thermal conductivity which compromises the materials figure of merit zT. The best performing n-type composition for HH's is XNiSn (X = Ti, Zr, Hf), with zT values exceeding unity. From this family the most suitable alloy for widespread application is TiNiSn, due to both its precursors availability and cost. Furthermore, doping with abundant Cu can both optimise electronic performance and lower lattice thermal conductivity.

In this contributed talk, we highlight our recent investigations into the scalable solid-state synthesis of TiNiCuySn and its thermoelectric properties. In-situ Neutron powder diffraction reveals that the formation of TiNiSn relies on the melting of Sn at ~231 °C and Ni-Sn binaries at ~745 °C. Importantly, we identify that the reaction is complete after ~14 hours, not requiring week(s) long processes. These results allowed oxidation to be minimised, facilitating a 50 % increase in material PF and zT, achieving zT = 0.9 at 773 K.

Strategies reducing thermal conductivity in ZnO films

Misha Khalid[1], Boguslaw Nozdryn[1], Hadiqa Naaz[1], Carlos J. Tavares[2], Michał Pawlak[1]
[1]Institute of Physics, Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University, Poland, [2]Centre of Physics of Minho and Porto Universities (CF-UM-UP), University of Minho, Portugal

Phonons, Fundamental Aspects, September 18, 2026, 10:30 - 11:30

Transparent oxide thermoelectric thin films are promising for energy-harvesting applications requiring both optical transparency and thermal-to-electical conversion, including smart windows, displays, and optoelectronic devices [1,2]. This work presents a comparative study of magnetron-sputtered and ion-implanted ZnO:Sb thin films together with plasma-assisted molecular beam epitaxy-grown ZnO:Cd,Eu epitaxial films. The aim is to clarify how fabrication route influences crystallinity, defect structure, dopant distribution, and thermal transport [3,4]. In ZnO:Sb films, the Sb concentration range of 0.1-0.5 modified the Seebeck coefficient, crystallite grain size, diffraction peak broadening, lattice parameters, resistivity, carrier concentration, electron mobility, and the thermoelectric figure of merit, ZT. Thermal conductivity measurements yielded cross-plane values of 4.14-6.92 W□m-1□K-1 by FDTR and in-plane values ranged from 7.88 to 12.46 W□m-1□K-1 by PTR, confirming anisotropic heat transport. In ZnO:Cd,Eu films, with dopant concentrations of 1.3/0.3 and 1.5/0.5, XRD confirmed a-oriented ZnO, SEM showed continuous interfaces, SIMS verified dopant incorporation, and cross-plane thermal conductivity spanned about 3.7-6.3 W□m-1□K-1. These results clearly demonstrate that dopant incorporation and growth method strongly govern phonon scattering, structural quality, and heat transport in transparent ZnO-based thin films.

References

[1] H. F. Faria, J. M. Ribeiro, T. Boll, and C. J. Tavares, “Thermoelectric and Structural Properties of Transparent Sb-Doped ZnO Thin Films,” Coatings 13(4), 735 (2023).
[2] H. F. Faria, J. M. Ribeiro, F. V. N. B. de Carvalho, I. M. M. da Silva, L. P. Cardoso, and C. J. Tavares, “Enhancing transparent thermoelectric properties of Sb-doped ZnO thin films,” Journal of Physics and Chemistry of Solids 170, 110890 (2022).
[3] H. F. Faria et al., “The influence of Sb doping on the local structure and disorder in thermoelectric transparent ZnO:Sb thin films,” Journal of Alloys and Compounds (2023).
[4] M. Suchea et al., “Sb-implanted ZnO ultra-thin films,” Materials Science in Semiconductor Processing 69, 32-35 (2017).

Au-Ni thin film thermoelectrics

Jan Koenig[1], Mike Benkendorf[1], Uwe Vetter[1], Olivia Hermes[1], Andreas Mahlke[1], Markus Bartel[1]
[1]Fraunhofer IPM, Germany

Novel Material Directions, September 17, 2026, 11:00 - 12:15

Au-Ni alloys were investigated as bulk materials by Garmroudi et al., Sci. Adv. 9, eadj1611 in 2023 and showed high power factors. As early as 1967, William T. Hicks filed a patent for a "thermoelectric alloy of gold and nickel" for use in thermocouples and thermoelectric devices. Nowadays, high costs for gold make the employment of bulk materials made from Au-Ni alloys less attractive. This is not the case for thin-film components, as the process costs dominate the material costs. Therefore, we investigated the formation of co-sputtered Au-Ni films as well as Au-Ni-multistacks. The thermoelectric properties of these films were investigated regarding the Au-Ni composition and the temperature dependency. Depending on the deposition high power factors are obtained for certain compositions. The results will be presented and discussed regarding future applications.

SPIRIT - Sustainable Power Integration and Recovery of Industrial Thermal Waste

Ms. Jovana Kovacevic[1], Dr. Illia Serhiienko[1], Prof. Andrej Pustogow[1]
[1]TU Wien, Institute of Solid State Physics, Austria

Applications-1, September 15, 2026, 11:00 - 12:15

The SPIRIT project (Sustainable Power Integration and Recovery of Industrial Thermal Waste) aims to improve industrial energy efficiency by converting low-temperature waste heat (<200 °C) into electricity using thermoelectric generators (TEGs). Its core is to use the innovative Flex-TEG (TEGnology), which is a flexible, modular and lightweight TEG that can be easily installed on existing equipment such as pipes, boilers and exhausts, adapting to curved and irregular surfaces. As a solid-state technology, Flex-TEG operates without moving parts, with no direct emissions and minimal maintenance. Its performance and scalability are enabled by newly developed tellurium-free, cost-effective thermoelectric materials, supporting economically viable deployment in industrial environments. SPIRIT follows a stepwise development path, starting with laboratory testing and optimisation of TEG components and system design. Laboratory work at TU Wien focuses on performance and stability testing to refine the technology before field validation under real operating conditions in an industrial biomass plant (Acciona). This approach targets up to 3% additional energy recovery and prepares the modular concept for transfer to other industrial waste-heat sources, including waste-to-energy, chemicals, steel and district heating.

Melt-mixed thermoplastic polymer/CNT composites for energy generation through the thermoelectric effect

Beate Krause[1]
[1]Leibniz-institut Für Polymerforschung Dresden Ev: Leibniz-institut Fur Polymerforschung Dresden Ev, Germany

Composites, September 17, 2026, 11:00 - 12:15

In the context of the current urgent energy problems, one approach to improve the energy efficiency of equipment or systems is waste heat recovery. Waste heat is a by-product of many production processes and, if not reused, is released into the atmosphere or water. By using the Seebeck or thermoelectric (TE) effect, a net zero emission of energy transfer from heat to electrical energy can be achieved if suitable electrically conductive materials are used.
This paper presents results on the development of novel, energy-efficient and environmentally friendly thermoelectric materials based on electrically conductive polymer/carbon nanotube (CNT) composites that can be used as TE generators to directly convert waste heat into thermoelectric power. The factors influencing the thermoelectric properties of melt-mixed thermoplastic composites with multi- and single-walled CNTs were investigated. The influences of carbon nanotube types and grades, polymer matrix materials, filler content and processing conditions on electrical conductivity, the Seebeck coefficient, the power factor and the thermoelectric figure of merit of the nanocomposites are investigated. In order to produce composites with n-type transport behavior, we show ways to obtain materials with negative Seebeck coefficients, especially by adding suitable additives during the melt mixing process. Finally, thermoelectric demonstrators were built consisting of p- and n-type polymer composite strips and their performance was evaluated. Even though the TE values achieved are still significantly below those of conventional materials, the results show that such conductive polymer composites are promising and can in principle be used for TE applications.

Thanks for the financial support of the EU Commission project GlaS-A-Fuels (Grant Agreement No. 101130717, HORIZON-EIC-2023-PATHFINDEROPEN-01)

Dopant-induced bandstructure and power factor modifications in NbFeSb and NbCoSn

Dr Sumit Kukreti[1], Dr Rajeev Dutt[1], Prof. Neophytos Neophytou[1]
[1]School of Engineering, University of Warwick, United Kingdom

Electronic Transport Theory, September 16, 2026, 13:30 - 15:00

Alloying is used to optimize carrier concentration and tailor electronic bandstructure in thermoelectrics. We investigate computationally multiple dopants (Ti, Zr, Hf, Ta, and Sn) in two prominent half-Heusler (HH) materials, n-/p-type NbFeSb and NbCoSn, and quantify how alloying translates into bandstructure and power factor (PF) changes.
We compute alloyed supercells and unfold their energy surfaces. We then analyse the conduction/valence-band splittings near the band edges, and extract density-of-states (mDOS) and conductivity effective masses (mcond) using the EMAF code1. The PF is calculated using ElecTra2,3.

We show that alloying results in: a) band splittings of degenerate bands, and b) 'fragmented' bands and energy surfaces. A larger change in lattice parameter typically results in larger splittings, larger changes in mDOS and mcond, and larger PF changes. For example, for p-type NbFeSb, the initial degenerate L-valley valence bands split by up to ~ 0.1 eV with Hf and Zr dopants, while Ta splits them only by 0.01 eV. This reduces mDOS from 4.25 m0 for pristine NbFeSb, to 2.8 m0 for Hf and 2.6 m0 for Zr, compared to 3.86 m0 for Ta doping. Similarly, for NbCoSn, a splitting of ~ 0.04 eV for Hf and Zr is observed, whereas for Ta it is 0.01 eV. The computed PF at 300 K decreases much more for Hf- and Zr-doped systems compared to their Ta-doped counterparts. For instance, the PF in Hf-doped NbFeSb reduces by > 30%, whereas for Ta-doping only by 5%.

These results show that alloying-caused band splitting can reduce the PF and provide understanding for dopant selection and band-engineering strategies in HH thermoelectrics.

1. P. Graziosi et al, ACS Applied Energy Materials 3, 5913–5926 (2020).
2. P. Graziosi et al, 'ElecTra code' Computer Physics Communications 287, 108670 (2023).
3. R. Dutt et al. J. Mater. Chem. A 14, 10332- (2026).

Ab initio thermoelectric transport calculations of high entropy materials

Dr. Ankit Kumar[1], Dr. Bhawna Sahni[1], Prof. Neophytos Neophytou[1]
[1]University Of Warwick, United Kingdom

Materials Theory, September 17, 2026, 13:30 - 15:00

This work presents an efficient ab initio framework to evaluate transport properties across a progression of material complexity, from the half-Heusler (HH) TiCoSb to the double HH $Ti_2FeNiSb_2$, and further to the high-entropy $Ti_4Hf_4Fe_3Co_2Ni_3Sb_8$. We use Boltzmann transport through the ElecTra code [1], considering the full energy/ momentum dependence of the bands and the scattering rates using first-principles extracted parameters –no such method exists for alloys on ab initio basis.

Our results show that the electronic structure and transport properties are strongly influenced by atomic disorder, which increases significantly with configurational entropy, particularly in high-entropy alloys (HEA) where disorder is inherently present. For example, we quantitatively assess the influence of atomic disorder on $Ti_2FeNiSb_2$ and $Ti_4Hf_4Fe_3Co_2Ni_3Sb_8$ transport and show that the PF fluctuates by 50% just by changing the arrangement of Fe/Ni.

Using the example of the HEA $Ti_4Hf_4Fe_3Co_2Ni_3Sb_8$, we quantitatively show that although it exhibits ultra-low lattice thermal conductivity (κl), compared to the conventional HH, its power factor suffers even more. This negative trade-off makes zT improvements hard to reach in high-entropy materials. However, the extent of this effect depends sensitively on the choice of alloying elements as well as their lattice sites. Alloying elements which do not alter the electronic structure near the band edge of the host compound, such as XNiZ (X= Ti, Zr,Hf; Z = Si, Ge, Sn) will not degrade the PF significantly, but reduce κl to lead to higher zT (in general alloying at 4a site for p-type and 4c cite for both n- and p- in the HH).

Overall, these findings contribute to a deeper understanding of how atomic disorder affects the electronic states in high-entropy alloys and offer design guidance for these materials for possible zT performance advancement over the HH compound.

References

[1] ElecTra code, Computer Physics Communications, 287, 2023, 108670.

Sustainable Solution Processing of High-Performance PbTe

Abayomi Lawal[1], Dr. Sharona Horta[1], Dr. Krishnendu Maji[1], Francesco Milillo[1], Dr. Christine Fiedler[1], Dr. Tobias Kleinhanns[1], Dr. Navita Jakhar[1], Aiswarya Rayaroth[1], Prof. Shengduo Xu[2], Prof. Maria Ibáñez[1]
[1]Institute of Science and Technology Austria, Austria, [2]Hong Kong Polytechnic University, People's Republic of China

Nanomaterials, September 17, 2026, 13:30 - 15:00

Waste heat represents a vast, underutilized energy resource, and thermoelectricity offers a direct pathway for converting this waste heat into useful electricity. Despite this promise, widespread thermoelectric implementation has been hindered by production costs stemming from energy-intensive manufacturing processes and high-purity material requirements. PbTe, despite its high thermoelectric performance, remains confined to niche applications such as space exploration due to conventional "top-down" synthesis methods involving high-temperature melting, grinding, and re-densification.

We address this sustainability challenge through a room-temperature, solution-based "bottom-up" synthesis utilizing thiol-amine chemistry, drastically reducing energy consumption without sacrificing performance. Our approach incorporates a facile post-synthetic Na doping strategy that leverages the porous microstructure of the synthesized PbTe particles, which provides extensive surface area for Na^+ adsorption followed by a short sintering step. This method effectively tunes the charge transport to p-type, overcoming the bipolar nature of pristine PbTe while creating a multi-scale phonon scattering network that significantly suppresses lattice thermal conductivity. The optimized Na-doped PbTe achieves a peak figure of merit zT of 2.48 at 823K, a performance comparable to conventional solid-state techniques but with substantially reduced production costs.

To further enhance the sustainability and cost-effectiveness of our method, we developed a strategy to reuse waste solvents from the initial reaction over twelve consecutive synthesis cycles, maintaining high synthesis yields and reproducible zT values throughout. Our overall synthetic approach demonstrates the potential to reduce solvent waste in solution-processed thermoelectric materials, while maintaining high synthesis yield and final material performance.

Dual High Performance ZrCoBi-based Half-Heusler Module for Thermoelectric Generation

Assoc. Prof. Xiaofang Li[1], Dr. Xin Bao[1], Dr. Sichen Duan[1], Prof. Li Yin[1], Prof. Qian Zhang[1]
[1]Harbin Institute of Technology (Shenzhen), China

Heusler Modules, September 17, 2026, 13:30 - 15:00

Half-Heusler (HH) alloys, renowned for their excellent mechanical properties and good thermal stability, have garnered extensive attention as high-temperature TE materials in recent years. ZrCoBi stands as a half-Heusler alloy with high zT in both polarities. But due to its complex and difficult preparation process, subsequent investigations have been limited, and dedicated efforts are required to further enhance its TE properties and obtain dual high modules. Beyond the intrinsic TE performance of the material, high-performance TE modules also require well-matched contact layer materials and appropriate bonding techniques to minimize parasitic losses arising from electrical and thermal resistances, while ensuring robust operational stability. Therefore, the identification of suitable contact layers and the development of reliable joining technologies for ZrCoBi-based modules are crucial for advancing their TE performance.

Here we examine ZrCoBi half-Heusler materials as a case study and find Hf-dual-partitioning in (Zr, Hf)Co(Bi, Sn): lattice substitution coupled with elemental nanophase precipitation, which could make a partial decoupling of electron and phonon transport, thereby synergistically optimizing the zT. As a result, we achieve a high peak zT ~1.3 at 973 K and an average zT ~0.88 across a temperature range of 300-973 K in Zr0.85Hf0.15CoBi0.87Sn0.13. To circumvent the thermal damage to TE materials caused by high-temperature brazing, we developed a reliable TLPB (Transient Liquid Phase Bonding) encapsulation method based on the Cu–Sn phase diagram for half-Heusler materials, enabling low-temperature bonding and high-temperature service. Using optimized ZrCoBi as the p-type leg and (Ti, Zr, Hf)Ni(Sn, Sb) as the n-type leg, the fabricated module achieved a simultaneous high η of 14% and ω of 3.1 W cm-2 under a temperature difference of 673 K. Our work underscores the significant potential of ZrCoBi-based TE materials for hig-temperature TEG applications.

Atomic Layer Deposited Cu Incorporation Enables Enhanced Thermoelectric Performance in n-Type Mg3(Sb, Bi)2

Jun Li[1]
[1]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Zintl-1, September 15, 2026, 15:30 - 17:00

Thermoelectric (TE) materials with high efficiency near room temperature are crucial for low-temperature waste-heat recovery and solid-state cooling applications. Among them, Mg3(Sb, Bi)2-based Zintl compounds have emerged as leading n-type materials due to their intrinsically low lattice thermal conductivity and favorable electronic structure. However, their performance is still constrained by the relatively low carrier mobility in the low-temperature regime because of the dominated grain-boundary charge scattering, which limits the achievable power factor and thus the overall figure of merit (zT). Hereby, we proposed an interface modification strategy based on powder atomic layer deposition (pALD) of metallic Cu to enhance the carrier mobility of n-type Mg3(Sb, Bi)2. The ALD-Cu addition is found to be beneficial for improving carrier mobility by promoting grain growth, compensating Mg deficiencies at some of the grain boundaries (particle boundaries), and thereby mitigating the interfacial transport barriers. Metallic Cu was precisely deposited on TE powders without introducing oxygen-or water-based precursors, thereby avoiding surface oxidation and degradation of the powders. Simultaneously, despite the more than twofold increase in grain size, the formation of Cu-rich domains near particle boundaries acts as effective phonon-scattering centers, leading to a lower lattice thermal conductivity. Benefiting from this synergistic modification of electrical and thermal transport, both peak and average zT over 303–573 K were enhanced by 14% and 13.3%, respectively. This work demonstrates a feasible metallic pALD approach for interface modification and establishes a new strategy to decouple transport parameters in n-type Mg3(Sb, Bi)2-based alloys for near room temperature applications.

Geometry-Driven Design of Thermoelectric Coolers via Topology Optimization

Mr Haiyang Li[1], Prof. Jae Sung Son[1]
[1]POSTECH, South Korea

Applications-3, September 17, 2026, 11:00 - 12:15

Topology optimization (TO) has emerged as a powerful design methodology for enhancing thermoelectric device performance beyond the limitations of conventional geometries. In this work, we present a geometry-driven optimization framework for Peltier coolers, focusing on improving key cooling metrics including the coefficient of performance (COP), cooling capacity (Qc), and maximum temperature difference (ΔT).

A coupled electro-thermal finite element model of a thermoelectric unicouple was developed, and density-based TO with SIMP interpolation was employed to systematically redistribute material within a fixed design domain. Three independent objective functions—maximizing COP, Qc, and ΔT—were investigated under realistic thermal and electrical boundary conditions. The results reveal that the optimal geometry strongly depends on the selected objective, leading to distinct structural features. In particular, COP- and ΔT-optimized designs exhibit pronounced necked or hourglass-like geometries that enhance thermal resistance and suppress parasitic heat leakage, whereas Qc optimization favors bulkier structures to accommodate higher current flow.

Performance evaluation demonstrates that topology-optimized geometries significantly outperform conventional cuboid designs, achieving substantial improvements in COP and ΔT across a wide operating range, while improvements in Qc remain limited due to inherent trade-offs between electrical and thermal transport. Furthermore, by incorporating geometry optimization and advanced fabrication strategies such as 3D printing, the proposed approach enables practical realization of complex architectures with simultaneous gains in performance and cost efficiency, with COP improvements approaching ~20%.

These findings highlight that there is no universal optimal geometry for thermoelectric cooling; instead, objective-specific design strategies are essential. The present study provides fundamental insights into the interplay between geometry, heat transfer, and electrical transport, offering a scalable pathway for designing high-performance Peltier cooling systems.

P-type to n-type transition in excitonic insulator Ta2NiSe5 and its thermoelectric transport

Prof. Huili Liu[1], Mr. Qiang Feng[1], Ms. Jiayi He[1], Mr. Zhefeng Wang[1]
[1]ShanghaiTech University, China

Zintl/Heusler-3, September 17, 2026, 15:30 - 17:00

Excitonic insulator, as an emerging correlated electron system in solid state physics, is narrow-gap semiconductor or semimetal with electron-hole interaction. Ta2NiSe5 is semiconducting material with a small bandgap, and has excitonic insulator transition around ~326 K with optical excitation gap of ~0.16 eV. Whereas, few of literatures reported thermoelectric properties of the excitonic insulator compounds. In this work, we synthesized single crystalline excitonic insulator of Ta2NiSe5 with variable tantalum contents, via chemical vapor transport technique, and carried out the measurements of their thermoelectric properties at low temperature. It is found that a transition of p-type to n-type occurs by varying the tantalum contents, where the Seebeck coefficients change from positive to negative ~450 uV/K at temperature range of 100-150 K, respectively. In those crystals, thermal conductivities are changing at the range of 1.5 - 11.5 W/m-K at room temperature, due to the defects from sample to sample. The carrier mobility can reach to ~27.6 cm^2/V-s, with carrier concentrations at the range of ~10^14 - 10^21 /cm^3. Those findings provide a platform to understand fundamental physics of thermoelectric transport in the excitonic insulator compounds, and shed light on potential applications in next generation electronics.

Thermoelectric Figure-of-Merit: from Electrons to Ions

Prof. Weishu Liu[1]
[1]Southern University Of Science And Technology, China

Exotic Effects, September 16, 2026, 11:00 - 12:15

Thermoelectrics directly converts thermal energy into electricity using electrons or ions as carriers. Seeking a high ZT within the space of temperature and dopants becomes a major task for the electronic thermoelectrics. Here, we show the theoretical connection between the ZTmax and materials parameter B*, and discuss the critical factors. Next, we present the thermoelectric figure of merit ZQ for constant heat-flux boundary, explaining that the thermoelectric boundary can redefine the figure of merit. Finally, we willdiscuss the ionic thermoelectrics, and present that the electrical working mode is another importance factor to define the figure of merit. Ions could not pass through the electrode, resulting in a completely different electrical operating mode compared with the e-TE counterpart. Consequently, a new i-TE figure-of-merit is proposed, i.e., ZTΔ, in which a general conductivity ε/τ is defined. An optimized efficiency equation as a function of ZTΔ and working condition function is outlined. The newly ZTΔ, composed of thermopower S, general conductivity ε/τ, thermal conductivity κ, and working temperature range TΔ, showing a good linearconnection with experimentally measured efficiency. Generally, we show that the thermoelectric performance is strongly influenced by the thermal boundary condition and the electrical working mode, and impact the materials chosen.

Competing effects of electron scattering in materials with low-dimensional band structures

Øven A. Grimenes[1], Kristian Berland[1], Ole Martin Løvvik[2,3]
[1]Norwegian University of Life Sciences, Norway, [2]SINTEF, Norway, [3]University of Oslo, Norway
Electronic Transport Theory, September 16, 2026, 13:30 - 15:00

Predicting thermoelectric properties of materials using density functional theory and Boltzmann's transport equations has been the topic of many studies. The vast majority of these were based on the constant relaxation time approximation (CRTA), in which the electrons are assumed to scatter at a fixed rate. This approximation has proven useful for rationalizing experimental results on specific materials, and screening studies have identified several new materials with beneficial transport parameters. However, it is well known that CRTA is a coarse approximation, not reflecting materials' response properties nor the role of scattering space. This is particularly important for complex band structures.

We have investigated the thermoelectric properties of CsK2Sb and Na2TlSb by including electron-phonon and impurity scattering mechanisms as implemented in the AMSET code, benchmarked with ab initio electron-phonon scattering calculated in VASP. The two materials feature electronic band structures akin to those of low-dimensional materials. The energy isosurfaces ("Fermi surfaces") of CsK2Sb are tubular, resembling those of 2D systems. Na2TlSb exhibits a hollow box-like isosurface, similar to 1D systems. CRTA-based studies have established that such band structures give rise to promising transport parameters due to a rapid increase of the electronic density of states in the relevant energy window, as well as high Fermi velocities. However, this could be reversed by the large available space for electron scattering, potentially leading to high scattering rates and degraded transport parameters. A detailed analysis of the electron scattering revealed that this did not happen. Most of the scattering space required large momentum transfers, depicted by the elongated isosurfaces in reciprocal space. This led to small scattering matrix elements and thus high electron relaxation times. Combined with very low lattice thermal conductivity, this resulted in a maximal figure of merit of $zT = 2.8$ for CsK2Sb and $zT = 4.4$ for Na2TlSb.

Chalcogenide-based Flexible Thermoelectric Films and Devices for Multifunctional Applications

Yao Lu[1]
[1]Southern University of Science and Technology, China

Microharvesting, September 15, 2026, 13:30 - 15:00

Thin-film thermoelectric (TE) generators and coolers present promising solutions for self-powering of wearable electronics and thermal dissipation of chips, respectively. In recent years, chalcogenide-based TE materials, have garnered ever-increasing attention due to their exceptional TE performance near room temperature. However, their brittleness and rigidity are far-flung and agelong challenges for flexible applications. To address this issue, we developed bottom-up and top-down approaches to prepare Ag2Se and Bi2Te3-based films.

The “bottom-up” approach was employed to prepare inorganic TE films, utilizing atoms, ions, or molecules as the “building blocks”. Through this method, a range of Ag2Se-based films were fabricated via a process involving chemically template-assisted synthesis, vacuum filtration, and subsequent hot-pressing. Notably, the Ag2Se/MXene composite film exhibited a high power factor of 2100 μW m-1 K-2 at 300 K. A Bending test demonstrated the exceptional flexibility of this hybrid film. The as-assembled flexible TE device generated a maximum power density of 24.2 W m-2 at a temperature difference of 30 K. Additionally, multifunctional TE devices with rapid responsiveness hold great potential as wearable/portable energy supply, cooler and sensor applications.

The “top-down” method involves the fabrication of bulks by traditional melting and annealing processes, followed by slicing or exfoliating into thin sheets or nanosheets. Employing this technique, we demonstrated the good pliability of 1000 bending cycles and high power factors of 4200 (p-type) and 4600 (n-type) μW m-1 K-2 in Bi2Te3-based films that were exfoliated from corresponding single crystals. This unprecedented bendability in single crystal films was ascribed to the in-situ observed staggered-layer structure that was spontaneously formed during the fabrication to promote stress propagation whilst maintaining good electrical conductivity. Our flexible generator showed a high normalized power density of 321 W m-2 with a temperature difference of 60 K, surpassing other reported film-based TE devices by an order of magnitude.

Optimizing performance of printed flexible origami thermoelectric generator via non-stoichiometry and sulfur inclusion

Nan Luo[1]
[1]Karlsruher Institut für Technologie, Germany

Microharvesting, September 15, 2026, 13:30 - 15:00

Thermoelectric generators (TEGs) for energy harvesting are increasingly appealing when it comes to battery-free Internat of Things devices, where battery lifetime is inherently limited. However, achieving high performance, good mechanical stability, and scalable manufacturing simultaneously remains challengeing. Here, we report a high performance flexible fully printed origami TEG through non-stoichiometry and sulfur substitution. With 2at.% sulfur substitution, the Ag2(Se1-xSx)1.05-based n-type film reaches a power factor of 16 μWcm−1 K−2 at 360 K. The origami TEG delivers a maximum power output of 907 μW at a temperature difference of 80 K, correaponding to a power density pd of 21 W m−2 (corresponding to 800 μW g−1), which is twice that of our previously reported origami-TEGs. Based on this device, we futher fabricate a TEG module that consists of 10 origami devices. Without a heat sink, the module generates a voltage of 2V on a 460K hotplate, sufficient to directly power an LED. With body temperature, it could power a Bosch sensor when integrated with a power controller. These results demontrate high potential of printed origami TEGs for practical low-grade heat harvesting applications.

Nonlinear transverse transport in Weyl-Kondo semimetals

Monika Lužnik[1], Mathieu Taupin[1], Xinlin Yan[1], Andrey Prokofiev[1], Léo Mangeolle[2,3], Gwenvredig Le Roy[1], Silke Paschen[1]
[1]Institute of Solid State Physics, TU Wien, Austria, [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, Germany, [3]Munich Center for Quantum Science and Technology, Germany

Novel Material Directions, September 17, 2026, 11:00 - 12:15

Transverse thermoelectrics exploiting the Nernst effect are attracting growing interest because they enable a simplified module design based on a single material [1]. Large Nernst responses can result from the Berry curvature in materials with nontrivial electronic band topology such as topological semimetals, which have thus emerged as promising candidates [2]. Unfortunately, the practical application of transverse thermoelectric devices is limited by the high magnetic fields typically needed to induce sizable Nernst effects [1]. An alternative approach could utilize the nonlinear Nernst effect in the absence of external fields [3], as recently realized in a 2D system [4]. Here, we investigate this approach in a 3D material, a Weyl-Kondo semimetal [5]. In such systems, strong electronic correlations lead to the formation of Weyl nodes near the Fermi level, thereby significantly enhancing Berry curvature effects [6–10].

The work was supported by the European Research Council (ERC Advanced Grant 101055088 “CorMeTop”), the Austrian Science Fund (FWF grants SFB F86 “Q-M&S”, I5868-N/FOR5249 “QUAST”, 10.55776/COE1 “quantA”), and the Air Force Office of Scientific Research (AFOSR project No. FA8655-24-1-7018).

[1] T. Feng et al., Next Energy 3, 100105 (2024).
[2] Y. Pan et al., Next Energy 2, 100103 (2024).
[3] C. Zeng et al, Phys. Rev. B 100, 245102 (2019).
[4] H. Liu et al., Nat. Nanotechnol. 20, 1221–1227 (2025).
[5] M. Lužnik et al., submitted.
[6] S. Dzsaber et al., Phys. Rev. Lett. 118, 246601 (2017) .
[7] H.-H. Lai et al., Proc. Natl Acad. Sci. USA 115, 93-97 (2018).
[8] S. E. Grefe et al., Phys. Rev. B 101, 075138 (2020).
[9] S. Dzsaber et al., Proc. Natl Acad. Sci. USA 118, e2013386118 (2021).
[10] D. M. Kirschbaum*, M. Lužnik* et al., J. Phys. Mater. 7, 012003 (2024): * joint first author.

Design and Integration Framework for Thermoelectric Technologies in Buildings

Dr Reshma krishnan Madathil[1], Ms Amaya Acarregui Padilla[1], Prof Cesar Martin Gomez[1]
[1]Universidad de Navarra, Spain

Applications-3, September 17, 2026, 11:00 - 12:15

Buildings account for nearly 40% of global energy consumption and carbon emissions, making them a central focus of sustainable energy policies. Thermoelectric (TE) technology is a solid-state, refrigerant-free solution capable of heating, cooling, power generation, and waste heat recovery; however, it is still not widely used in mainstream building practice. A key reason for this is not materials performance alone, but the absence of a clear, shared workflow that enables architects, mechanical engineers, electrical engineers, TE specialists, and facility managers to collaborate effectively using this technology.

This work introduces a six-phase Design and Integration Framework for Building-Integrated Thermoelectric Systems (BITES), grounded in materials science, building engineering, and architectural integration research. The framework covers the complete system lifecycle: (1) building characterization and energy assessment, (2) multi- stakeholder integration strategy and technology selection, covering TE cooling, hybrid PV-TE systems, and waste heat recovery, (3) regulatory compliance pathways addressing fire safety, electrical standards, and energy codes, (4) construction and installation, (5) operation, performance monitoring, and maintenance, and (6) end-of-
life management, including material recovery and waste reduction.

Each phase includes discipline-specific decision tools such as technology selection matrices, regulatory compliance checklists, and troubleshooting guides. The framework draws on experimental data from our group´s building-integrated TE prototype development activities (1-4), ensuring that decisions are grounded in validated performance benchmarks.

The framework addresses a critical translational gap: while laboratory-scale TE research continues to advance, no standardized protocol currently exists to guide multi- disciplinary teams from early planning through to installation and end of use. By establishing a common working methodology for different specialists, the proposed framework makes thermoelectric integration more accessible at a larger scale and supports zero-carbon building goals.

Investigating microstructural effects in the lattice thermal conductivity and thermoelectric properties of Cu2+yZn1-ySnSxSe4-x alloys

Marcelo Augusto Malagutti[1,2], Prof. Eleonora Isotta[2], Prof. Himanshu Nautiyal[3], Prof. Umberto Anselmi-Tamburini[4], Dr. Andrea Chiappini[5], Dr. Sebastian Bette[1], Prof. Robert Dinnebier[1], Prof. Narges Ataollahi[2], Prof. Paolo Scardi[2]
[1]Max Planck Institute, Germany, [2]University of Trento, Italy, [3]Manipal University Jaipur, India, [4]University of Pavia, Italy, [5]Laboratory and Fondazione Bruno Kessler, Italy
Phonons, Fundamental Aspects, September 18, 2026, 10:30 - 11:30

Kesterite compounds of the form Cu_2+yZn_{1-}ySnS_xSe_{4-x} (CZTSSe) have attracted considerable interest as sustainable thermoelectric materials due to their earth-abundant composition and intrinsically low lattice thermal conductivity. However, several studies on polycrystals report an unexpected trend in which the selenide exhibits higher lattice thermal conductivity than the sulphide, contrary to expectations based on atomic mass and lattice stiffness. In this work, we investigate the origin of this behaviour and shed light on how microstructural, chemical, and structural features affect the thermoelectric performance across the CZTSSe compositional series. First-principles calculations indicate that the intrinsic lattice dynamics favour lower lattice thermal conductivity in Se-rich compositions. In contrast, experimental results show that microstructural effects dominate phonon transport in polycrystalline samples. In particular, larger porosity, smaller grain size, and reduced grain connectivity strongly suppress the lattice thermal conductivity in sulphide-rich compounds, leading to an apparent inversion of the expected CZTS–CZTSe thermal conductivity trend. Electronic transport analysis reveals an increase in weighted mobility above the order-disorder phase transition temperature, observed across all compositions and resulting in improved performance. This effect is attributed to the band convergence effect related to the increased structural symmetry promoted by Cu-Zn disorder, approaching a where the kesterite assumes a pseudo-cubic structure. Despite the lower intrinsic carrier mobility in sulphide-rich compositions, their suppressed lattice thermal conductivity results in comparable thermoelectric performance across the series, with zT values up to ~0.5 at 723 K. These results demonstrate that microstructural effects can outweigh intrinsic chemical trends and play a critical role in determining thermal transport and thermoelectric performance in kesterite materials.

The important role of Ti doping in the thermoelectric efficiency improvement of p-type (Nb,Ta)FeSb-based half-Heusler phases.

Dr Panagiotis Mangelis[1], Michal Rybski[2], Panagiotis S. Ioannou[1], Andreas Delimitis[3], Janusz Tobola[2], Theodora Kyratsi[1]
[1]Department of Mechanical and Manufacturing Engineering, University of Cyprus, Cyprus, [2]Faculty of Physics and Applied Computer Science, AGH University, Poland, [3]Department of Physics, Aristotle University of Thessaloniki, Greece

Zintl/Heusler-3, September 17, 2026, 15:30 - 17:00

The group of half-Heusler (HH) has attracted considerable research interest, since these materials exhibit promising electrical transport properties but also exceptional mechanical properties and thermal stability at high temperatures.

HH materials of general formula Nb0.6-xTixTa0.4FeSb were synthesized by mechanical alloying. The role of Ti doping is investigated by both experimental and theoretical approaches. Powder X-ray diffraction Rietveld refinements and Transmission Electron Microscopy analyses confirm the HH phases and the incorporation of Ti atoms in the crystal structure. Electrical transport properties measurements indicate that Ti substitution induces an effective hole doping, increasing significantly the electrical conductivity. However, the increase in hole concentration is accompanied by a moderate decrease in Seebeck coefficient, keeping the values of heavily doped phases at relatively high levels.

Interestingly, DFT calculations using the KKR-CPA method to account for such a complex chemical disorder, reveal new aspects related with the role and contribution of Ti in the formation of electronic structure of (Nb,Ta)FeSb system in the vicinity of the Fermi level (EF). Ti substitution seems to contribute to the sharpness enhancement of total electronic Density of States (DOS) close to EF, since Ti presents a higher and sharper DOS than those of Nb and Ta. According to Mott relation, this probably affects positively the thermopower of heavily doped phases. Theoretical estimations of Seebeck coefficient based on the electronic DOS support this evidence.

Moreover, Ti substitution in combination with the Nb/Ta alloying and nano-structuring effect induces an effective phonon scattering, strongly reducing the lattice thermal conductivity. As a result, a powerful enhancement of ZT is achieved for the Ti-rich phases, highlighting the multiple role of Ti in the improvement of thermoelectric performance of MVFeSb-based HH phases.

This work is part of European Union’s Horizon Marie Skłodowska-Curie Actions Postdoctoral Fellowship program HIPERT with grant award No 101150392.

Understanding the mechanisms behind Zn-diffusion in Zn4Sb3 thermoelectric materials for long term material stability

Dominique Mattlat[1], Dr. Siyuan Zhang[1], Prof. Christina Scheu[1], Jun Li[2], Dr. Amin Bahrami[2]
[1]Max Planck Institute for Sustainable Materials, Germany, [2]Leibniz Institute for Solid State and Materials Research Dresden (IFW), Germany

Measurement and Characterisation, September 17, 2026, 15:30 - 17:00

Thermoelectric (TE) devices can either generate clean energy by converting thermal energy into electrical power by using a temperature differential or use electrical power to create a temperature differential. The microstructure of thermoelectric materials is crucial for their conversion efficiency, as it determines their thermoelectrical properties. Zn4Sb3 is a promising thermoelectric material for mid temperature (150 - 400 °C) energy recovery applications, but is prone to Zn-whisker growth by Zn ion diffusion due to phase transitions at elevated temperatures.

These modifications may cause degradation and instabilities in thermoelectric materials over time which in turn lead to changes in thermoelectric properties. To characterize such changes in situ using(scanning) transmission electron microscopy ((S)TEM), electrical biasing at elevated temperatures was performed on the sample using a MEMS chip. Operando measurements are made during the trigger of phase decomposition and Zn ion diffusion. The observations are utilized to relate the mechanisms of Zn diffusion in the material.

In situ (S)TEM observation showed the combination of biasing and elevated temperatures (200 - 250 °C) leads to Zn diffusion and the formation of Zn voids. During electrical biasing, the Zn voids shrink or grow depending on the direction of the applied potential. The observation of Zn diffusion is further related to the local microstructures of Zn4Sb3. Furthermore, Zn precipitation is observed which results in the degradation of properties.

Fermi-level Engineering and Band gap Renormalization for High Performance Bi-doped Mg2Si0.6Sn0.4 Solid Solution for Thermoelectric Application

Mr. SARAN Mayilsamy[1,2], V Vijay[3], C. Kanagaraj[3], M Navaneethan[3], P. Justin Jesuraj[1,2], J. Archana[1]
[1]Center of Excellence in Materials for Advanced Technologies, SRM Institute of Science and Technology, India, [2]Department of Physics and Nanotechnology, SRM Institute of Science and Technology, India, [3]Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, India

Zintl-1, September 15, 2026, 15:30 - 17:00

Thermoelectric technology is revolutionizing energy conversion applications in power generation and active thermal management. Lead-free magnesium tin silicide-based system is emerging as a promising alternative due to its eco-friendly thermoelectric properties and tunable electronic structure. Here, we report the Bi doping in Mg2Si0.6Sn0.4 solid solutions effectively modulates the band structure by Burstein-Moss effect shift (ΔE_"BM") to the Fermi energy and introduces rigid-band carrier tunning (Band filling effect). Supported by DFT findings, the incorporation of heavy element Bi activates a lattice-dynamical pathway for synergistic carrier-phonon manipulation, dominated by the alloy-induced point defects. As a result, a record high TE figure of merit (zTMax) of 1.6 @753 K is achieved, driven by a superior power factor of (PFMax) of 3 mW. m-1 K-2 via carrier band engineering, and suppressed lattice thermal conductivity of (κ_Ph) of 1.02 W. m-1 K-1 arising from multiscale phonon distortion defects. Furthermore, a higher zTAvg=0.95 enables a theoretical conversion efficiency of 11.3% under a ΔT=400 K, highlighting a new paradigm toward high-performance energy conversion materials.

Keywords: Fermi-level engineering, carrier-phonon decoupling, alloy induced point defect, figure of merit.

Nanocrystalline Si Thin Films Grown by Low-Temperature E-Beam Evaporation for Thermoelectric Applications

Mr. Antonio Mazzacua[1], Claude Alfonso[2], Chaymaa Boujrouf[2], Stefano Frabboni[3], Gian Carlo Gazzadi[3], Dario Narducci[1]
[1]University of Milano Bicocca, Dept. of Materials Science, Italy, [2]Aix Marseille University, CNRS, IM2NP, France, [3]University of Modena and Reggio Emilia, Department of Physics, Informatics and Mathematics, Italy

Nanomaterials, September 17, 2026, 13:30 - 15:00

It is known that single-crystalline silicon is a poor thermoelectric material due to its high thermal conductivity κ. Much effort has been spent to decrease its κ while keeping its electrical conductivity unchanged. The other way around, Si figure of merit can be increased by enhancing the power factor in nanocrystalline Si (κ ≈ 10 W/mK) by energy filtering (EF), namely enabling hot carrier transport only by engineering potential barriers. We reported how this can be achieved in CVD-grown heavily boron-doped nanocrystalline Si thin films, where the precipitation of SiBx at grain boundaries (GBs) sets the charge-carrier filter. An unprecedented power factor of ≈ 30 mW/mK^2 was observed. However, it was observed how the presence of H dissolved into Si (as a by-product of silane degradation) complexes boron, decreasing the amount of dopant available to precipitate at GBs.

In this presentation we will discuss how low-temperature electron beam (e-beam) evaporation technique may be used to prepare hydrogen-free nanocrystalline Si thin films.
Doping was attempted via co-deposition at room temperature with a Silicon-Boron (SiB) alloy on oxidized Si substrates followed by high-temperature annealing, mimicking the process implemented in CVD-grown thin films. TEM analyses and Atomic Probe Tomography (APT) confirmed boron incorporation and diffusion in the film but reported a low crystallization degree. To solve this problem, the effect of post-deposition annealing on different substrates (oxidized Si and sapphire) was investigated with XRD, Raman spectroscopy and TEM analysis. Full crystallization was obtained on oxidized Si after annealing for 8 hours at 475°C followed by a high-temperature thermal treatment of one hour at 900°C. The same process led to 85% of crystalline fraction on sapphire.

Thermoelectric properties of co-deposited and ion implanted thin films will be compared, in view of the activation of the EF effect to enhance material's figure of merit.

Enhanced thermoelectric power factor by transition metal substitution in the Kagome metal Ni3Sn

Kim-Isabelle Mehnert-Birk[1], Saff E. Awal Akhtar[2], Dr Blair F. Kennedy[1], Dr Ankit Kumar[2], Prof Neophytos Neophytou[2], Dr Jan-Willem G. Bos[1]
[1]University Of St Andrews, United Kingdom, [2]University of Warwick, United Kingdom
Novel Material Directions, September 17, 2026, 11:00 - 12:15

Metallic thermoelectric materials offer promise in terms of elemental abundance and avoiding rare or toxic elements. Recent studies have shown possibilities to design metallic alloys like Ni-Au with ultra-high power factor PF = 34mWm-1K-2.[1] The Kagome metal Ni_3Sn is of particular interest, showing a strong asymmetry in electronic density of states g(E) and thereby a high Seebeck coefficient S.[2]

In our work, we replace Ni by Co (hole doping) and Cu (electron doping), which changes the position of the Fermi level EF.[3] Co substitution leads to a doubled S = -55µVK-1 and a high PF = 5mWm-1K-2 at 800K, while Cu substitution lowers S. We present a theoretical framework using overlapping electron-like dispersive and hole-like heavy bands to capture the experimental trend and reproduce S(T) in near-quantitative manner. Inclusion of inter- and intra-band scattering allows the electrical conductivity to be captured as well. Finally, a large sample of $Ni_{2.9}Co_{0.1}Sn$ was synthesised to examine the impact of ingot texturing. This enabled reliable electronic and lattice thermal conductivities to be calculated. The lattice contribution is in good agreement with estimates from velocity of sound measurements. A highest zT = 0.12 at 800K was found for the $Ni_{2.9}Co_{0.1}Sn$ sample.

In this oral contribution, the results from our experimental and modelling study into the tuneability of the thermoelectric properties of the Kagome metal Ni_3Sn will be presented.

1 F. Garmroudi et.al. Science Advances, 2023, 9, eadj1611.
2 F. Garmroudi et.al. Physical Review X, 2025, 15, 15.021054.
3 submitted K.-I. Mehnert-Birk et.al. Journal of Materials Chemistry A, 2026.

Accessible thermoelectrics characterization at room temperature and observed anisotropy in polycrystalline SnSe materials

František Mihok[1], Viktor Puchý[2], Karel Saksl[1]
[1]Technical University In Košice, Slovakia, [2]Institute of Materials Research, SAS, Slovakia
Measurement and Characterisation, September 17, 2026, 15:30 - 17:00

Thermoelectric generators (TEGs) offer reliable solid-state power for applications ranging from space missions to autonomous terrestrial systems, yet their long-term stability often suffers from mechanical stress in conventional heterojunctions. Tin selenide (SnSe) stands out as a promising homojunction thermoelectric material combining high efficiency with reduced interfacial stress. In our work, we present low-cost, modular instruments for accessible room-temperature thermoelectric characterization and demonstrate their capabilities to study anisotropic behavior in polycrystalline SnSe doped with Bi, Ag, and In.

One of the instruments can simultaneously measures the Seebeck coefficient and electrical conductivity using a four point geometry, while the second employs the Van der Pauw configuration for precise characterization of electrical conductivity in regular bulk 3D samples. The device is also equipped to perform measurements under magnetic field allowing for determination of Hall coefficient, charge carrier concentration and mobility. Both devices are built from readily available components and 3D printed parts, supported by fully documented open-source control and acquisition software. Validation against established systems confirmed accurate and reproducible measurements, demonstrating that reliable thermoelectric assessment can be achieved without specialized instrumentation, allowing more research groups to pursue thermoelectrics.

Polycrystalline SnSe samples were synthesized via powder metallurgy and mechanochemistry. Powders were consolidated by spark plasma sintering (SPS), producing a layered microstructure with pronounced crystallographic orientation. Such texture induces measurable anisotropy, particularly along and perpendicular to the sintering axis. Doping with Bi revealed polarity switching from p-type to n-type conduction above 0.5 at.% while maintaining comparable electrical and Seebeck coefficients. Ag and In doping further highlighted complex charge-carrier compensation effects and emphasized the strong influence of dopant type and concentration on anisotropic conduction pathways. Through anisotropic engineering and careful dopant selection we found homojunction pair capable of reaching up to 1.6 V/K.

Design of PN-junctions for energy converters.

Dr. Joaquin Gabriel Miranda[1], Dr. Sara Ghomi[1], Dr. Nallagatla Venkata Raveendra[1], Dr. Gerhard Span[2]
[1]Silicon Austria Labs, Villach, Austria, [2]Silicon Austria Labs, Austria, [3]Silicon Austria Labs, Austria, [4]LAMBDA Wärmepumpen GmbH, Austria

Current Modules and Beyond, September 16, 2026, 11:00 - 12:15

Many industrial processes dissipate significant amounts of energy as heat, which can be recovered and converted into electricity using a PN-junction-based thermoelectric device. In this work, we compute and measure the electrical current and output voltage associated with the dynamics of electron-hole pairs due to the response to temperature gradients in devices using large-area PN-junctions. This thermally generated charge mechanism has been previously proposed [1] and is similar to the one developed for hot-carrier photovoltaic energy converters [2]. Our multiphysics modeling considers explicitly the interplay between heat transfer and electron-hole recombination in graded designed carrier concentration materials which create a built-in potential gradient that assists the separation of electrons and holes. Since these hot-carriers should be transported to metal contacts before they dissipate their energy back into the materials, besides the traditional metal contacts, we include carrier-selective contacts to their respective PN materials that allow the optimal flow of one type of carrier. We discuss, together with the experimental validation, the complex interrelationships of this multilayer system, the optimized geometry and operational regimes as well as potential commercialization prospects.

[1] Ruben Chavez, Gerhard Span, et al, J. Phys. D: Appl. Phys. 51 014005 (2017).
[2] Robert T. Ross; Arthur J. Nozik, J. Appl. Phys. 53, 3813 (1982).

Thermoelectric Transport in Monolayer and Bilayer MoS2

Yunhao Mo[1]
[1]King's College London, United Kingdom

Exotic Effects, September 16, 2026, 11:00 - 12:15

Two-dimensional materials are promising thermoelectric materials due to quantum confinement effects that can enhance the power factor [1,2]. In this work, the phonon-limited thermoelectric transport properties of monolayer and bilayer MoS_2 are investigated using a combination of first-principles calculations and analytical modelling. Electronic band structures, phonon dispersions and electron–phonon coupling matrix elements on a coarse grid in the reciprocal space are obtained using density functional theory and density functional perturbation theory implemented in the QUANTUM ESPRESSO and EPW codes [3,4]. To perform calculations of electron-phonon matrix elements on dense reciprocal space grids, an analytical framework based on the deformation potential approximation is developed. Using parameters extracted from first-principles calculations, and by solving the Boltzmann transport equation in the relaxation time approximation, the electrical conductivity, Seebeck coefficient, and power factor are evaluated. The results show that bilayer MoS_2 exhibits an enhanced power factor compared with monolayer MoS_2 due to the presence of an additional conduction-band valley at the Λ point.

[1] L. D. Hicks and M. S. Dresselhaus, Physical Review B 47, 12727 (1993)
[2] K. Hippalgaonkar et al., Physical Review B 95, 115407 (2017)
[3] I. Carnimeo et al., Journal of Chemical Theory and Computation 19, 6992 (2023)
[4] H. Lee et al., npj Computational Materials 9, 156 (2023)

Thermoelectric properties of Nb/W doped ScN multilayer structures

Dr. Joris More-chevalier[1], Dr. U. D. Wdowik[2], Dr. J. Martan[3], Pr. X. Portier[4], Dr. S. Cichoň[1], Dr. P. Levinský[1], Pr. D. Legut[2], Dr. E. de Prado[1], Dr. J. Pokorný[1], Dr. M. Novotný[1], MSc D. Prokop[1], Dr. L. Fekete[1], Dr. J. Lančok[1]
[1]Fzu - Institute Of Physics Of The Czech Academy Of Sciences, Czech Republic, [2]bIT4Innovations, VSB - Technical University of Ostrava, Czech Republic, [3]New Technologies Research Centre (NTC), University of West Bohemia, Univerzitni 8, Czech Republic, [4]Centre de Recherche sur les Ions, les matériaux et la photonique, France

Materials, September 18, 2026, 10:30 - 11:30

Scandium nitride (ScN) shows promising thermoelectric properties that can overcome certain limitations of group III(A) nitride semiconductors for various applications. In this study, ScN/Sc1-xNbxN and ScN/Sc1-xWxN multilayers were deposited on MgO (001) substrates using DC magnetron sputtering in an ultra- high vacuum (UHV) system. The Nb dopant concentration ranged from x = 0. 004 to 0. 05, while the W dopant varied from x = 0. 005 to 0. 12. Quantum-mechanical calculations using density functional theory simulated the effects of replacing Sc with Nb or W on thermoelectric properties, showing good agreement with experimental results. Material characterization, including X-ray diffraction and transmission electron microscopy, was performed to elucidate doping-induced changes in the multilayers. A clear improvement in the Seebeck coefficient (S) was observed with Nb and W doping across this temperature range. The ScN layer exhibited an S value of- 60 μV/K at 800K, which is increased to -110/-115 μV/K at 800K for Sc1-xNbxN layers with x varying from 0. 004 to 0. 02, and to -100/-106 μV/K at 800K for Sc1-xWxN layers with x from 0. 005 to 0. 013. However, the higher electrical resistivity with both dopants indicates a slight decrease in conductivity. Resistivity displayed semimetal behavior with temperature for all layers. Specifically, the resistivity increases from 0. 4 mΩ·cm at 800K for pure ScN to between 2.2 mΩ·cm and 0. 6 mΩ·cm at 800K, depending on Nb concentration, and between 2.5 and 1. 2 mΩ·cm at 800K, depending on W concentration. This decrease in conductivity is counterbalanced by a reduction in thermal conductivity from approximately 10 W·m-1·K-1 to about 4 W·m-1·K-1 and 2 W·m-1·K-1 at room temperature with Nb and W doping, respectively. Nevertheless, these reductions lead to an enhancement of the thermoelectric properties when compared to ScN and its multilayers.

Flexible Cellulose-Based Insulated Metal Substrates for Thermoelectric Modules

Seyedmohammad Mortazavinatanzi[1,2], Puria Puria Mahmoudi Nezhad[1], Zia Ullah Khan[2], Reverant Crispin[2]
[1]ParsNord Thermoelectric Filial, Sweden, [2]Laboratory of Organic Electronics, Department of Science and Technology, Linköping Universit, Sweden

Organics and Hybrids, September 15, 2026, 11:00 - 12:15

Flexible electronic substrates are widely used in modern electronics; however, applications such as flexible thermoelectric generator (TEG) modules place particularly stringent demands on thermal stability, dielectric performance, and reliable operation under high-temperature processing conditions. Conventional materials, including polyimide- and paper-based substrates, often fall short in meeting these requirements. In this work, we present the development of a flexible insulated metal substrate (IMS) based on a cellulose-derived microfibrillated nanocomposite matrix, designed to address these limitations. The substrate incorporates a coated dielectric layer based on hexagonal boron nitride (h-BN), enabling enhanced electrical insulation and thermal robustness while retaining the inherent advantages of cellulose-based materials. The developed IMS withstands reflow soldering temperatures up to 300 °C without degradation in performance, overcoming a key barrier for paper-based electronics. The dielectric layer thickness can be tailored between 10 µm and 100 µm depending on the required breakdown voltage, allowing optimization of insulation properties for different device requirements. This tunability supports integration into applications where both electrical reliability and mechanical flexibility are essential. To demonstrate its practical relevance, the substrates were evaluated in flexible thermoelectric generator (TEG) configurations, showing stable electrical insulation and reliable operation under relevant conditions. These results highlight the potential of the developed IMS as a cellulose-based, sustainable alternative for flexible thermoelectric modules.

Multichannel Power Conditioning System for TEG Arrays Under Non-Uniform Temperature Distribution Using a Modified Sine-Cosine MPPT Algorithm

Mr Mirosław Mrozek[1,2], Prof. Mariusz Malinowski[2], Dr. Wojciech Mizak[1]
[1]Łukasiewicz Research Network – Institute For Sustainable Technologies, Poland, [2]Warsaw University of Technology, Poland

Applications-2, September 16, 2026, 13:30 - 15:00

Thermoelectric generators (TEGs) are a promising solution for waste-heat recovery from continuous industrial processes. However, in real-world installations, non-uniform temperature distribution across the TEG array surface causes variations in the electrical characteristics of individual modules, reducing energy harvesting efficiency in conventional single-channel power conditioning systems.

This work presents a multichannel DC–DC boost converter system with independent maximum power point tracking (MPPT) for individual TEG channels, designed for operation under non-uniform temperature conditions. The MPPT is based on a modified sine-cosine algorithm (SCA), a population-based metaheuristic capable of determining the global maximum power point under multi-peak P(V) characteristics. Such characteristics may arise in TEG arrays equipped with bypass diodes, used to limit energy losses in the event of failure or degradation of individual modules. Under these conditions, conventional MPPT methods such as P&O may become trapped in a local maximum. Unlike typical metaheuristic applications reported in the literature, the algorithm has been adapted for online operation, i.e. continuous real-time monitoring and tracking of the maximum power point with a reduced number of agents and iterations.

The proposed modification of the SCA has been tailored for microcontroller implementation and addresses the definition of the agent search space, the exploration–exploitation balancing mechanism, and the estimation of TEG source parameters. The adopted solutions enable continuous energy harvesting without interrupting system operation.

The algorithm was verified experimentally on a hardware prototype with a DC–DC boost converter fed by a source replicating the electrical characteristics of a TEG array. The results confirm fast convergence to the global maximum power point and high tracking effectiveness. The hardware implementation also reveals practical design considerations that are typically not apparent in purely simulation-based studies.

Keywords: thermoelectric generator, waste heat recovery, MPPT, sine-cosine algorithm, DC–DC boost converter, non-uniform temperature, bypass diodes, metaheuristic optimisation.

Defect Complexity-Induced Local Bonding Reconstruction Enables Synchronized Thermoelectric Performance in V0.9Fe0.5Co0.5Sb-based Half-Heusler Thermoelectrics

XUE NAN[1], Kei Hayashi[1], Chen Chen[2], Md All Amin Newton[2], Hezhang Li[2], Jing-Feng Li[2], Yuzuru Miyazaki[1]
[1]Tohoku University, Japan, [2]Tsinghua University, China

Heusler-1, September 15, 2026, 13:30 - 15:00

Decoupling weighted mobility (μw) and lattice thermal conductivity (κlat) remains a central challenge in thermoelectric materials, as structural disorder that suppresses phonon transport typically degrades carrier transport. Half-Heusler compounds (HHs), characterized by a XYZ cubic structure and a tunable 18-electron configuration, provide an ideal platform for investigating the interplay between lattice dynamics and electronic structure. A non-stoichiometric 18-electron system, V0.9Fe0.5Co0.5Sb, is designed to host Vanadium vacancies (Vv), interstitials (Fei and Coi), and compositional fluctuations, giving rise to strain fields and dislocation networks.

Multiscale microstructural observations reveal that various defects, including Vv, Fei and Coi, introduce pronounced lattice distortions, strain fields, and dislocation networks, which give rise to multiscale phonon scattering. These defects are further analyzed using representative defect models by first-principles calculations, with bonding characteristics resolved through electron localization function, deformation charge density, and crystal orbital Hamilton population analyses [1]. The Vv –Sb interaction exhibits largely delocalized electronic states, providing effective pathways for carrier transport. In contrast, V–Fei and V–Coi interactions induce local lattice distortions and bonding anharmonicity, further enhancing phonon scattering.

Further tuning of the Fe/Co ratio on V0.9Fe0.5+xCo0.5-xSb HHs leads to an unusual transport response in Fe-rich compositions, where κlat is suppressed alongside an enhancement in μw. This unexceptional behavior is attributed to a refined grain size with high density of large angle grain boundary, together with promoted carrier delocalization in V-Fe electronic framework for ever-increasing electrical conductivity. The maximum zT of 0.72 at 973 K, is obtained in V0.9Fe0.6Co0.4Sb samples, with a simulated maximum efficiency of 6.03 % on its single-leg module.

These results show that phonon and carrier transport can be regulated through distinct aspects of disorder, providing a route to decouple μw and κlat and achieving balanced thermoelectric performance.

References
[1] X. Nan et al., Sci. Adv. 11, 2375-2548 (2025).

Transitioning Thermoelectricity from Static to Dynamic

Prof. Dario Narducci[1]
[1]Univ. of Milano Bicocca, Dept. Materials Science, Italy

Current Modules and Beyond, September 16, 2026, 11:00 - 12:15

The efficiency and output power density of thermoelectric generators (TEGs) are fundamentally linked to material properties through the figure of merit (ZT) via Domenicali's equation. While materials research has pursued notable efficiency gains over the last twenty years, the fundamental physics governing dynamic TEG operation has remained largely elusive. This is primarily due to the mathematical complexity of Domenicali's time-dependent nonlinear differential equation. Recently, we derived an exact analytical solution to this equation, revealing that time-modulated operation can tremendously boost TEG efficiency, effectively doubling a material's inherent figure of merit. This discovery opens new opportunities for thermoelectricity, unlocking a realm of dynamic energy conversion and providing a theoretical rationale for controversial computational and experimental results reported over the last decade. After outlining the analytical approach used to solve the time-dependent Domenicali's equation, this presentation focuses on how enhanced dynamic efficiency impacts practical applications. We first demonstrate how a strategic choice of time modulation can lead to dynamic enhancements that more than double the effective ZT. Furthermore, we show that dynamic operation causes an even larger enhancement of power output when accounting for the temperature dependence of all transport coefficients, specifically highlighting the critical role of the Thomson coefficient. We also showcase how dynamic operation may be implemented even when harvesting from sources natively releasing heat at a constant rate. This suggests that dynamic harvesting is a general, innovative paradigm for thermoelectricity and a vital guide for the search for new thermoelectric materials. Finally, we elaborate on the prospects of dynamic thermoelectric generation and its impact on heat harvesting at both the macro and microscale.

Recycling of Bi2Te3 based thermoelectric modules: progress for the recovery of bismuth and tellurium

Vicente Pacheco[1], Benjamin Balke-Grünewald[2], Roland Binninger[3], Sabrina Unmüßig[3]
[1]Fraunhofer Institute For Manufacturing Technology And Advanced Materials IFAM, Germany, [2]Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS, Germany, [3]Fraunhofer Institute for Physical Measurement Techniques IPM, Germany

Emerging, September 15, 2026, 15:30 - 17:00

Commercial thermoelectric modules (TE-modules) are based on n-Bi2(Te0.97Se0.03) and p-(Bi0.2Sb0.8)2Te3 alloys. The scarcity of the elements forming these alloys and the toxicity of tellurium demand the development of a recycling technology. However, in Europe special regulations for the recycling of TE-modules do not exist, and they are included in the rules for recycling e-waste. This could change soon due to the current geopolitical situation. The world's largest producer of Bismuth and Tellurium is China. On February 4, 2025, China announced export controls on certain items, including Bismuth and Tellurium, and some of their compounds, classifying them as "dual-use" items (meaning they have both military and civilian applications). In this contribution, we will present part of the progress made in the RecycleTEAM project. From the perspective of module recycling, degradation effects under long-term operation are of great importance. To assess such effects under application-relevant conditions, a customized measuring station for Peltier modules was developed. The station combines full characterization with thermal cycling capability within a single setup, eliminating remounting errors. Two commercial modules were characterized and cycled to validate the station; further investigations at higher cycle numbers are ongoing to quantify module aging. The mechanical separation of the TE-module components was done by electro-hydraulic fragmentation or thermal disassembly flowed by certain sieving processes and eddy current separation technology. The separation of the n- and p-type TE-legs was done by a half-automated XRF-sorting process. The separation of tellurium from a piece made of melted n- and p-alloys (1:1 mass) was successfully done by using selective evaporation. For this purpose, it was constructed a distillation apparatus equipped with three sliding cold fingers. The EDX analysis shows an enrichment of tellurium (95 at %) in the condensed phase. The sample remaining in the crucible is enriched in Bismuth (up to 69 at %).

Topological thermoelectrics for solid state cooling

Professor Yu Pan[1]
[1]Chongqing University, China

Novel Material Directions, September 17, 2026, 11:00 - 12:15

Thermoelectric effects enable the direct conversion between thermal energy and electrical energy, and has broad application potential in areas such as thermoelectric power generation, solid-state cooling, and precise temperature control. Classic thermoelectric materials mainly focus on heavily doped narrow bandgap semiconductor materials, whose thermoelectric performance is limited above room temperature (> 300 K). So far, further enhancement of thermoelectric performance at low temperatures (<300 K) faces signiffcant challenges, severely re-stricting the application of thermoelectric materials in low-temperature solid-state cooling. In recent years, the surge of topological quantum materials has triggered many novel thermoelectric transport behaviors, especially the signiffcantly enhanced low-temperature thermoelectric performance under magnetic ffelds, providing new opportunities to greatly improve low-temperature thermoelectric performance. This talk will introduce how linear band dispersion and the resulted ultrahigh mobility, as well as Berry curvature could enhance the magneto-Seebeck and (anomalous) Nernst effects.

References

[1] Y. Pan*, B. He, X. Feng, F. Li, D. Chen, U. Burkhardt, C. Felser*, Magneto-thermoelectrics toward high figure of merit in Bi88Sb12 topological insulator, Nat. Mater. 2025.
[2] Y. Pan*, B. He, T. Helm, D. Chen, W. Schnelle, C. Felser*, Ultrahigh transverse thermoelectric power factor in flexible Weyl semimetal WTe2, Nat. Commun. 2022.
[3] S. Wu, Y. Pan*, X. Wang, T. Xie, S. Zheng, Y. Liu, W. Li, Z. Zhou, B. Ruan, X. Lu, G. Wang*, X. Zhou*, Dirac Fermion and Phonon Coupling Toward Giant Nernst Thermoelectric Performance in Topological Semimetal TaSb2. Adv. Mater. 2025.
[4] H. Hu, X. Feng, Y. Pan*, V. Hasse, H. Wang, B. He*, C. Felser*, Multipocket synergy towards high thermoelectric performance in topological semimetal TaAs2, Nat. Commun. 2025.
[5] Y. Pan*, C. Le, B. He, S. J. Watzman, M. Yao, J. Gooth, J. P. Heremans, C. Felser*, Giant anomalous Nernst signal in the antiferromagnet YbMnBi2, Nat. Mater. 2022.

Cu-based chalcogenides for reliable near-room-temperature thermoelectric cooling

Dr. Hab. Taras Parashchuk[1], Dr. Oleksandr Cherniushok[1], Dr. Adrianna Lis[1], Dr. Mykola Maksymuk[1], Prof. G. Jeffrey Snyder[2], Prof. Krzysztof T. Wojciechowski[1]
[1]Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Poland, [2]Department of Materials Science and Engineering, Northwestern University, USA

Chalcogenides-2, September 16, 2026, 13:30 - 15:00

Thermoelectric (TE) cooling technologies are attracting increasing attention for solid-state thermal management; however, their broader deployment remains constrained by the limited availability of efficient, stable, and scalable materials operating near room temperature. State-of-the-art solutions are still dominated by Bi2Te3-based alloys, which suffer from toxicity concerns and rely on high tellurium content, limiting their sustainability and large-scale applicability. In this context, the development of alternative TE materials with comparable performance and improved environmental compatibility represents a critical challenge. Copper-based chalcogenides are promising candidates due to their cost-effectiveness, environmental friendliness, and intrinsically low lattice thermal conductivity. However, conventional binary Cu2X systems undergo superionic phase transitions near or above room temperature, leading to microstructural evolution and unstable transport properties, which limits their applicability in cooling devices.

Here, we report a new family of Cu-based materials with a Cr3Si-type structure (space group I-43d), developed as a platform for thermoelectric cooling. The materials exhibit high thermal and structural stability without phase transitions, along with reproducible transport properties. Through compositional tuning of the Te/S ratio in Cu6Te3-xS1+x ($0 \leq x \leq 1$), the electronic structure is optimized, leading to a strong increase in the Seebeck coefficient from 9 to 200 μV K-1, associated with an enhanced DOS effective mass (from ≈0.2me to >1.0me). Combined with ultralow lattice thermal conductivity (≈0.24-0.26 W m-1 K-1 at 300 K), this results in significantly improved power factors and a high thermoelectric performance with $zT \approx 1.1$ at ≈500 K. These results highlight Cu6Te3-xS1+x as a promising, stable, and cost-effective candidate for near-room-temperature thermoelectric cooling.

Acknowledgments
The research was funded by the Foundation for Polish Science (FNP) under the First-Team programme, project no. FENG.02.02-IP.05-0012/25, co-financed by the European Union under the European Funds for a Modern Economy Programme (FENG 2021-2027).

[1] O. Cherniushok, T. Parashchuk, G. J. Snyder, K. T. Wojciechowski, Adv. Mater. 2025, 2420556.

Nanowire-Bundled Grain Boundaries in Thermoelectric Materials

GwangMin Park[1], Dr. Seunghyeok Lee[2], Jinseok Hong[4], Seokho Nahm[4], Dr. Seung-Hyub Baek[2], Dr. Jin-Sang Kim[2], Prof. Seung-Yong Lee[4], Prof. Seong Keun Kim[1]
[1]KU-KIST Graduate School of Converging Science and Technology, South Korea, [2]Electronic and Hybrid Materials Research Center, Korea Institute of Science and Technology, South Korea, [3]Department of Materials Science and Chemical Engineering, Hanyang University, , South Korea, [4]Division of Materials Science and Engineering, Hanyang University, South Korea
Nanomaterials, September 17, 2026, 13:30 - 15:00

Improving thermoelectric material performance is essential for energy harvesting and solid-state cooling applications. This study demonstrated a novel structure of Bi_2Te_3-based thermoelectric materials with ZnO nanowire-bundled grain boundaries, realized via atomic layer deposition (ALD) and subsequent spark plasma sintering (SPS). The ZnO nanowires formed at the interfaces due to the rearrangement of the ALD-grown ZnO ultrathin layer over Bi0.4Sb1.6Te3 powder, driven by localized heating during the SPS process and the anisotropic nature of ZnO. The nanowire-bundled interfaces enhanced phonon scattering, thereby reducing lattice thermal conductivity while maintaining excellent electronic transport. This structural innovation achieved a high figure-of-merit, zTmax = 1.69 ± 0.09 at 373 K and an average zT of 1.55 over the range of 300–473 K. A thermoelectric module fabricated with 127 p–n pairs achieved a record-high conversion efficiency of 6.57% at a temperature difference of 163 K. These findings highlight the potential of nanowire-bundled interfaces to enhance the thermoelectric material performance and pave the way for scalable next-generation energy conversion technologies.

What Makes a Diffusion Barrier Effective for Colusite?

Swagata Patra[1], Soufiane El Oualid[1], Bertrand Lenoir[1], Christophe Candolfi[1], Philippe Masschelein[1], Emmanuel Guilmeau[2], Gaëlle Riou[2]
[1]Institut Jean Lamour, University Of Lorraine, France, [2]CRISMAT, CNRS, Normandie Univ, ENSICAEN, UNICAEN, France

Interfaces and Stability, September 17, 2026, 15:30 - 17:00

The integration of sulfur-containing thermoelectric materials into functional devices remains limited by interfacial instability during thermal processing. In particular, elemental diffusion and chemical interactions at metal–thermoelectric interfaces can significantly alter local composition, leading to degradation of electrical contact and device performance. The selection of suitable diffusion barrier materials is therefore critical to ensuring interfacial stability under operating conditions.

In this work, we will discuss the choice of diffusion barrier for colusite ($Cu_{26}V_2Sn_6S_{32}$)[1] based on the properties such as the coefficient of linear thermal expansion (CLTE). The microstructure and phase composition of the joint area as well as the electrical contact resistance, were investigated in the as-fabricated state and after prolonged annealing. The results indicate that significant metal–sulfur interactions can occur during thermal processing, potentially leading to the formation of metal sulfides and modification of the local composition of colusite. These reactions influence both the mechanical stability and electrical contact properties of thermoelectric modules. These findings highlight the complex interplay between diffusion kinetics, interfacial phase formation, and transport properties.

[1] K. Suekuni et al. Interaction between Cu–S-Based Sphalerite-like Frameworks and Interstitial Cations in Colusite-Based Thermoelectric Materials, ACS Applied Energy Materials, 2025, 8 (6), 3563.

Gamma-Irradiation-Induced γ⟶α MgAgSb solid-state phase transformation: Mechanisms and Implications

António Pereira Gonçalves[1], Beatriz A. Santos[1], Leonor Gonçalves[1], Pedro de Almeida Silva[1], Pedro Santos[2]
[1]CeFEMA, DECN, Instituto Superior Técnico, Univ. Lisboa, Portugal, [2]C2TN, DECN Instituto Superior Técnico, Univ. Lisboa, Portugal

Zintl-1, September 15, 2026, 15:30 - 17:00

Gamma irradiation can significantly induce materials structural modifications by interacting high-energy photons with the atomic lattice, which create defects such as vacancies, interstitials, and defect clusters. Energy is transferred to the lattice via ionization and subsequent atomic displacements, with the accumulation of defects enhancing the atomic mobility by lowering activation barriers for diffusion. Therefore, when a metastable phase is exposed to sufficient irradiation, the equilibrium phase can nucleate at defect sites and grow through defect migration and recombination. The transformation kinetics depends on the irradiation dose, dose rate, temperature, and intrinsic material properties, such as crystal structure and bonding characteristics.

MgAgSb is a promising p-type thermoelectric material due to its low toxicity (compared to Bi2Te3) and intrinsic low thermal conductivity, which leads to high performance near room temperature. Its efficiency is governed by a favorable combination of moderate Seebeck coefficient, high electrical conductivity, and low lattice thermal conductivity that yield figures of merit, zT, >1 at ~300–525 K. However, MgAgSb exhibits three solid-state phases: α, β, and γ. The low-temperature α-phase possesses a complex tetragonal structure, which is responsible for the best thermoelectric performance due to its strong phonon scattering and optimized carrier transport. While the α to β-phase is easily reversible, the α to γ-phase transformation is not, requiring very long annealing times at 573 K.

In this work, we present preliminary results in the effect of gamma irradiation on the γ⟶α-phase transformation of MgAgSb materials prepared by induction melting. High irradiation levels lead to a significant reduction of the γ metastable phase, promoting its transformation to the α-phase. A discussion of the fundamental mechanisms underlying the gamma-induced γ⟶α phase transformation will be presented.

This work was partially supported by Horizon Europe Marie Skłodowska-Curie Actions programme “MaGnesium Alloys for effICient solId stAte cooliNg”, grant agreement ID 101227508.

Structural order and thermoelectric transport in the substitution topological insulators Sb2SeyTe3-y (y = 0.3–2)

Shailja Sharma[1], Vicente Pacheco[2], Raul Cardoso-Gil[3], Golam Haider[1], Markus König[3], Oleg Janson[1], Kornelius Nielsch[1], Nicolas Perez[1]
[1]Leibniz Institute for Solid State and Materials Research Dresden, Germany, [2]Fraunhofer Institute for Manufacturing Technology and Advanced Materials, Germany, [3]Max Planck Institute for Chemical Physics of Solids, Germany

Phonons, Fundamental Aspects, September 18, 2026, 10:30 - 11:30

The thermoelectric transport properties of Sb2SeyTe3-y (y = 0.3,..., 2) single crystals were determined in the temperature range of 2 - 380 K. The distribution of the substituent Se atoms between lattice sites was investigated using single crystal X-ray diffraction, indicating that Sb2SeTe2 is an ordered phase and determines a turning point in all electric and thermoelectric properties of the series. The observed selective occupation of lattice sites may explain the phase separation limit for the ternary compositions with Se contents above about y = 2. High crystalline order was further evidenced in thermal conductivity and Raman spectroscopy measurements across the sample series. All the prepared materials showed p-type character at room temperature. However, the addition of Se until y =1 increases the contribution of electrons to transport, as evidenced by the Seebeck coefficient, indicating n-type character for Sb2SeTe2 below about 143 K. The electronic structure, calculated using observed lattice parameters and site occupancies, resulted in (1;000) $\mathbb{Z}2$ index for all compositions indicative of a strong topological insulator. Sb2SeTe2 has the largest band-gap of the series, 0.31 eV. As for thermoelectric performance, the n-type Sb2SeTe2 and p-type Sb2Se0.3Te2.7 have comparable power factor at temperatures around 50 K.

Record Thermoelectric Performance at Room Temperature Via Electrodeposited Films of Silver Selenide (Ag2Se) and Copper Selenide (Cu2Se)

Elena Pérez-Picazo[1], Miguel Ángel Tenaguillo[1], Ketan Lohani[1], Marisol Martín-González[1], Cristina V. Manzano[1]
[1]Instituto de Micro y Nanotecnología, IMN-CNM, CSIC (CEI UAM+CSIC) Isaac Newton, Spain
Nanomaterials, September 17, 2026, 13:30 - 15:00

Thermoelectric materials based on chalcogenides have attracted growing interest for the efficient conversion of waste heat into electricity, especially near room temperature (RT)[1-3]. In this work, we report record thermoelectric performance at RT in electrodeposited Ag2Se and Cu2Se films achieved through controlled microstructural engineering. By tuning the electrodeposition potential, we modulate composition, morphology, and crystal structure, allowing us to directly correlate microstructure with thermoelectric response. For Ag2Se, the optimized films reach an exceptionally high room-temperature (RT) power factor (PF) of 7655 ± 1578 μW·m-1·K-2, exceeding all previously reported n-type semiconductors at RT. Combined with a low out-of-plane thermal conductivity (k) of 0.79 ± 0.16 W·m-1·K-1, this leads to an apparent figure of merit zT = 2.89 ± 0.83, assuming isotropic transport. This outstanding performance originates from a dense granular Ag1.92Se microstructure with strong orthorhombic (200) texture and minimal secondary phases. Cu2Se films also show a substantial enhancement, achieving a record PF of 1130 ± 233 μW·m-1·K-2 and a k of 0.89 ± 0.18 W·m-1·K-1, resulting in apparent zT = 0.38 ± 0.10 at RT. This corresponds to a fivefold improvement over previous electrodeposited Cu2Se films and is comparable to state-of-the-art values obtained using more complex vacuum-based techniques. The optimized Cu1.88Se films show compact elongated grains and a predominantly cubic structure with preferred (111) orientation. Thus, this work reveals how specific microstructures influence and optimize the thermoelectric performance of these materials.

REFERENCES
[1] H. Liu, et al., Materials Letters 2013, 93, 121-124. https://doi.org/10.1016/j.matlet.2012.11.058.
[2] J. A. Perez-Taborda et al., Advanced Energy Materials 2018, 8, 1702024. https://doi.org/10.1002/aenm.201702024.
[3] C. V. Manzano et al., Sustainable Energy & Fuels 2021, 5, 4597-4605. https://doi.org/10.1039/D1SE01061A.

Laser Powder Bed Fusion of $Bi_{0.5}Sb_{1.5}Te_3$ Thermoelectric Legs: Processing, Interfaces, and Performance

Mr. Mateusz Pindel[1], Dr. Taras Parashchuk[1], Dr. Piotr Ledwig[1], Dr. Hubert Pasiowiec[1], Dr. Mykola Maksymuk[1], Dr. Grzegorz Cios[2], Prof. Beata Dubiel[1], Prof. Krzysztof Wojciechowski[1]
[1]AGH University of Kraków, Poland, [2]AGH University of Kraków, Academic Centre for Materials and Nanotechnology, Poland

Additive Manufacturing, September 18, 2026, 10:30 - 11:30

Laser powder bed fusion (LPBF) offers a promising route toward simplified fabrication of thermoelectric elements, but its application to Bi_2Te_3-based materials remains challenging because of narrow processing windows, defect formation, and limited understanding of metal–thermoelectric interfaces. Here, we investigate LPBF processing of $Bi_{0.5}Sb_{1.5}Te_3$ and relate volumetric energy density (VED), microstructure, texture, and transport properties to the performance of thermoelectric legs.

A first LPBF screening over VED = 4.8–9.5 J mm^{-3} showed that low energy input leads to lack-of-fusion porosity and vertical pore channels, whereas higher VED suppresses large pores but promotes cracking, delamination, and keyhole-type defects. Based on this analysis, two parameter sets with VED values of 5.6 and 6.0 J mm^{-3} were selected for detailed characterization. XRD, Lotgering factor, SEM, and EBSD show that LPBF samples remain single-phase and weakly textured in contrast to strongly textured PECS reference material.
The LPBF samples exhibit Seebeck coefficients comparable to PECS, but lower electrical conductivity (720–1120 S cm^{-1} versus 1400–2200 S cm^{-1} for PECS) and higher thermal conductivity (1.12–1.29 W m^{-1} K^{-1} versus 0.9 W m^{-1} K^{-1} in the best PECS orientation), resulting in ZT values of 0.41–0.52 compared with 1.1 for the textured PECS benchmark. At the same time, preliminary SEM observations for the LPBF sample processed at 6 J mm^{-3} reveal very good cohesion at the Ni/Bi_2Te_3 interface due to local remelting and interpenetrating, hook-like Bi_2Te_3 features anchored in the Ni substrate. This distinctive interfacial microstructure is promising for improving contact integrity relative to conventionally joined PECS elements.

For reference, the best PECS leg reached a device-level conversion efficiency of 7.2%. Overall, the present results establish LPBF as a viable emerging route for fabrication of $Bi_{0.5}Sb_{1.5}Te_3$ thermoelectric legs.

Accelerating the Discovery of Thermoelectric Skutterudites through Efficient Chemical Space Exploration

Jose J. Plata[1], Victor Posligua[1,2], Elena R. Remesal[1], Antonio M. Marquez[1]
[1]Universidad de Sevilla, Spain, [2]I-FIM, National University of Singapore, Singapore

Machine Learning, September 15, 2026, 13:30 - 15:00

One of the primary challenges in discovering novel thermoelectric materials lies in the exploration of large chemical spaces. Traditional trial-and-error experimental methods are often slow and cost-prohibitive for navigating these spaces. Consequently, computational approaches—such as high-throughput density functional theory calculations and machine learning methods—have emerged as indispensable tools for accelerating the screening and identification of promising candidates by predicting desired properties within vast compositional landscapes. Here, we present two approaches for exploring new thermoelectric materials using the skutterudite prototype. By creating an experimental database and developing a machine learning model, we have been able to predict the thermoelectric figure of merit, zT, for skutterudites, thereby enabling the rapid screening of thousands of potential candidates [1]. Alternatively, we used two high-throughput DFT-based approaches to explore the synthesizability of high-entropy skutterudites [2].

[1] Posligua, Victor, et al. "Deep Learning Framework for Accurate Prediction and High-Throughput Search of the Thermoelectric Figure of Merit in Skutterudites." J. Mater Chem A (2026)

[2] Plata, Jose J., et al. "High-Entropy Skutterudites as Thermoelectrics: Potential Synthesizability, Enhanced Stability, and Band Convergence via the Cocktail Effect." PRX Energy 5.1 (2026): 013008.

Zn-induced topological phase transition and thermoelectric enhancement in SnTe

Kacper Pryga[1], Bartlomiej Wiendlocha[1]
[1]AGH University of Krakow, Faculty of Physics and Applied Computer Science, Poland
Exotic Effects, September 16, 2026, 11:00 - 12:15

SnTe has been recently revisited from the thermoelectric perspective as a lead-free analogue of PbTe, while simultaneously possessing a range of other unique properties, such as being the first reported example of a topological crystalline insulator [1]. Unfortunately, despite the same crystal structure and similar band structure as in PbTe, large energy offset between valence band maxima and high carrier concentration in the pristine SnTe severely limits its thermoelectric performance. Consequently, multiple band engineering strategies often need to be utilized to improve the ZT and among various impurities, Zn doping has been experimentally reported to enhance the performance of p-type samples i.a. through introduction of a resonant state [2].

In this work, we show how Zn-induced band modifications allow for a controllable topological phase transition and simultaneously enhance the thermoelectric performance. Those findings are supported by calculations obtained using two complementary methods based on DFT: KKR-CPA and the supercell approach while the study of the transport properties was performed within the Kubo-Greenwood formalism. We show that doping with Zn introduces a resonant-like state in the conduction band of the system, enhancing n-type thermopower. At the same time, valence band is also extensively modified, as doping-induced band convergence and flattening increases p-type Seebeck coefficient in a wide carrier concentration range and delays the onset of bipolar effect. Evolution of the band structure under zinc's influence heavily depends on the impurity concentration and at sufficient level, a trivial band ordering is restored from a topological crystalline insulating state. This makes Zn a universal dopant capable of tuning the topological and thermoelectric properties.

[1] T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nature Communications 3, 982 (2012).
[2] D. Bhat and U. Shenoy, Materials Today Physics 11, 100158 (2019).

Thermoelectric Composites Based on Chalcogenide Particles and Organic Charge-Transport Molecules

Dr Kaspars Pudzs[1], Mrs Adriana Maurucaite[1], Dr Bejan Hamawandi[1], Mr Oskars Bitmets[1], Ms Renate Celmodejeva[1], Dr Muhammet S. Toprak[2]
[1]Institute of Solid State Physics, University of Latvia, Latvia, [2]Department of Applied Physics, KTH Royal Institute of Technology, Sweden

Composites, September 17, 2026, 11:00 - 12:15

Growing interest in sustainable energy technologies has intensified research into hybrid thermoelectric (TE) materials that combine inorganic TE compounds with carbon-based nanostructures and conducting organic species. In such systems, the organic phase serves not only as a structural binder for inorganic nanoparticles but also as a medium enabling efficient charge-carrier transport between discrete particles.

Achieving high TE performance in hybrid systems requires careful alignment of energy levels—specifically, the electron affinities and ionisation potentials of the organic molecules and the work functions of the inorganic nanoparticles—to minimise interfacial contact barriers and facilitate charge transport.

This study explores glass-forming, low-molecular-weight organic compounds as functional components for next-generation sustainable hybrid TE materials. Well-defined p-type Sb_2Te_3 and n-type Ag_2Se nanoparticles were synthesised via energy-efficient microwave-assisted routes to ensure controlled morphology and narrow size distribution. These were combined with commercially available, solution-processable small molecules commonly used as charge-transport layers in OLED and OPV technologies.

The electronic structure of the TE nanoparticles and organic compounds was characterised via photoelectron yield spectroscopy. Hybrid film morphology was examined using scanning electron microscopy. Charge-transport behaviour was further evaluated using Hall effect measurements, which provided insight into carrier concentration and mobility. Thermoelectric performance was assessed by measuring the Seebeck coefficient and electrical conductivity, enabling calculation of the TE power factor.

Anomalous Nernst Effect and Transverse Thermoelectric Conversion in Co2MnAl-Based Heusler Magnets

Sheng Qian[1], Dr. Mengzhao Chen[1], Prof. Tiejun Zhu[1], Prof. Chenguang Fu[1]
[1]State Key Laboratory of Silicon and Advanced Semiconductor Materials School of Materials Science and Engineering, Zhejiang University, China

Novel Material Directions, September 17, 2026, 11:00 - 12:15

Topological magnets, in which electronic band topology is intertwined with spin configurations, have demonstrated extraordinary transport phenomena that are highly promising for transverse thermoelectric applications. This work reports a significantly enhanced ANE in polycrystalline bulk Co2MnAl1-xSix, enabled by synergistic tuning of atomic ordering and Fermi level via Si substitution. A large anomalous Nernst thermopower of 4.9 μV K−1 and an anomalous Nernst conductivity of 1.46 A m−1 K−1 at 300 K are obtained in Co2MnAl0.69Si0.31. Furthermore, A centimeter-sized bulk Nernst thermoelectric generator has been developed using Co2MnAl0.69Si0.31 as the legs, which delivers an output voltage of 2.2 mV and a maximum power of 7.7 μW under a temperature difference of 15 K. These results highlight the potential of scalable, high-performance polycrystalline topological magnets for transverse thermoelectric applications and pave the way for practical integration of ANE-based devices.

Enhanced Lattice Symmetry via Mn Doping Boosts Electrical Transport Performance in Rhombohedral GeSe Thermoelectric Materials

Yuting Qiu[1]
[1]Beihang University, China

Chalcogenides-1, September 15, 2026, 11:00 - 12:15

Low-symmetry thermoelectric material GeSe exhibits inherently low thermal conductivity but suppressed electrical transport properties. Here, we demonstrate that Mn doping in AgBiTe2-alloyed rhombohedral GeSe introduced band engineering and further significantly enhanced lattice symmetry. Mn-induced resonant energy levels enhanced the density of states effective mass and significantly optimized the Seebeck coefficient. Crucially, elevated lattice symmetry reduced deformation potential and weakened phonon-electron coupling, triggering a 185% surge in carrier mobility despite a ~1.2-fold increase in the effective mass. The synergistically optimized Seebeck coefficient and electrical conductivity enabled the high-symmetry (GeMn0.005Se)0.9(AgBiTe2)0.1 sample to achieve a record average power factor of ~17 μW cm-1K-2 over 300–673 K while retaining low lattice thermal conductivity. Consequently, A maximum ZT of ~1.50 at 673 K and an average ZT of ~0.94 (300–673 K) were achieved, yielding a single-leg thermoelectric conversion efficiency of ~6.1% under a temperature difference of 325 K. This lattice symmetry manipulation through rational doping provided a universal pathway to promote phonon-electron decoupling and enhanced thermoelectric performance in low-symmetry thermoelectric materials.

Simple physics-based correction of CRTA predictions towards ab-initio accuracy thermoelectric transport

Mr Nirmal Kumar Ramalingam[1]
[1]University Of Warwick, United Kingdom

Machine Learning, September 15, 2026, 13:30 - 15:00

Accurate prediction of thermoelectric transport properties is fundamentally limited by the complex interplay of energy-dependent scattering mechanisms, which are not captured within the widely used constant relaxation time approximation (CRTA). While CRTA enables efficient high-throughput screening, it introduces arbitrary errors in electrical conductivity and power factor (PF) predictions, whereas fully ab-initio approaches are computationally demanding and not scalable.

In this work, we develop a physics-informed framework to systematically correct CRTA predictions towards ab-initio transport accuracy. Using Half-Heusler (HH) materials and transport calculations from the ElecTra Boltzmann transport code [1] with detailed scattering included, we first show that polar optical phonon (POP) and ionized impurity scattering (IIS) largely determine their conductivity and PF trends by over 70% [2, 3]. We compute the electronic conductivity and PF for 80 materials using CRTA, for 40 materials including POP+IIS scattering, and for 12 materials using fully ab-initio scattering including acoustic and optical phonons, which is computationally extremely expensive.

Using these data sets and statistical correlations involving simple physics-based quantities, such as valley/band degeneracies, effective masses, dielectric constants, and phonon energies, we identify as a first step a simple correction, ε_0/mDOS to the CRTA that can provide the results for the conductivity and PF of the POP+IIS limited transport with 60-70% accuracy. As a second step, we identify a further correction from the POP+IIS results to the full ab initio calculation that includes ADP+ODP+POP+IIS, as (mDOS·ε_0)/(mcond·ω) Combining these two steps together, we show that an overall correction of (ε_0^2/mcond · ω) , applied to the CRTA conductivity and PF can provide results close to the full an initio calculation with less than 16% error.

References

[1] Graziosi et al., Comput. Phys. Commun. (2023)

[2] Dutt et al., J. Mater. Chem. A (2026)

[3] Sahni et al., Mater. Horizons (2025)

Toward High-Efficiency Micro-Thermoelectric Cooling: The Role of Leg Height Optimization

Heiko Reith[1], Nithin B. Pulumati[1,2], Adhiraj Sundar[1,2], Kornelius Nielsch[1,2]
[1]Leibniz-institute For Solid State And Materials Research (IFW Dresden), Germany, [2]TU Dresden, Faculty of Mechanical Engineering, Germany

Microharvesting, September 15, 2026, 13:30 - 15:00

Micro-thermoelectric coolers (µTECs) are emerging as effective solutions for localized hotspot management in miniaturized electronic systems, enabling high cooling performance with seamless on-chip integration. In this work, we present a fabrication and design strategy based on electrochemical deposition (ECD) that enables scalable, cost-effective fabrication of µTECs with precise control over geometry and material composition.

A height-optimization approach is introduced to enhance device performance by increasing packing density and cooling power while significantly reducing the consumption of toxic and expensive thermoelectric materials. µTECs were fabricated using photolithography combined with ECD of $Bi_2(Te_xSe_{1-x})_3$ (n-type) and Te (p-type). Nitrogen injection into the electrolyte minimizes oxygen incorporation, resulting in reduced contact resistance and improved thermoelectric performance. The optimized devices achieve a maximum temperature difference of 10.8 K for area-optimized and 10.5 K for height-optimized µTECs at room temperature, increasing to 21 K at 343 K for height-optimized devices. Notably, material usage is reduced by up to 75% without compromising performance. Finite element simulations further predict cooling power densities in the order of several hundred W cm^{-2}, highlighting the strong potential of the proposed design.

These results demonstrate that height-optimized µTECs represent a compact, efficient, and scalable solution for high-density integration, offering significant advantages for advanced thermal management in next-generation electronic and microsystem applications.

Increasing the thermoelectric performance of MgAgSb by fine-tuning the MgAg synthesis

Mr Theo Renard[1], Amandine Duparchy[1], Thibault Carabeuf[1,2], Eckhard Müller[1,3], Johannes de Boor[1,4]

[1]German Aerospace Center (DLR), Germany, [2]European Space Agency (ESA), European Astronaut Centre (EAC), Germany, [3]Justus Liebig University Giessen, Germany, [4]University of Duisburg-Essen, Germany

Zintl-2, September 16, 2026, 11:00 - 12:15

Predictable transport properties and a reproducible performance of thermoelectric (TE) materials are essential for scaling-up TE device fabrication for large scale applications . Mg-based TE materials represent a good alternative for low temperature thermoelectrics due to their performance and as they are environmentally friendly compared to the commercial BiTe. In the case of MgAgSb, excellent material and device properties have been reported, but the consistent fabrication of high-performance material remains a challenge as even small amounts of secondary phases can drastically decrease the TE performances. To reduce the formation of secondary phases a two-step synthesis is commonly employed with MgAg synthesized first, then MgAgSb synthesized from precursors MgAg and Sb. While it is clear that the purity and spatial homogeneity of the intermediate MgAg has an influence on the phase constitution of MgAgSb, this is usually not studied.

In this study, the synthesis of MgAg has been improved by increasing the sintering time and reducing the Ag powder size. This ensures that the latter is single phase and homogeneous. We show that increasing the phase purity with the correct Mg to Ag ratio impacts the phase constitution of MgAgSb. From this, improvements of our synthesis route allowed an improvement of MgAgSb phase purity and an increase of the figure of merit by 20%, directly linking MgAg synthesis and MgAgSb performances.

Furthermore, as MgAg is not a line compound but has an extended phase width, knowing the exact Mg to Ag ratio is necessary to tune the final MgAgSb composition precisely. For that, a new characterization method has been developed, combining chemical analysis as a calibration tool and X-ray diffraction combined with Rietveld refinement to directly link the lattice parameters to the Mg to Ag ratio. This allows us to fine-tune the TE performances by minimizing the secondary phases formation.

Evaluation of TE-Catalyst Driven CO_2 Hydrogenation under Non-Pressurized Reaction Conditions

Ali Mohammad Nia[1], Aliasghar Enkeshafi[1], Kjeld Peterson[2], Peter Kjær Kristensen[2], Alireza Rezaniakolaei[1]
[1]AAU Energy, Aalborg University, Denmark, [2]Department of Materials and Production, Aalborg University, Denmark

Emerging, September 15, 2026, 15:30 - 17:00

Climate change and green fuel production are among the most significant challenges over the last few decades, and many researchers have conducted trials to address these challenges. CO_2 hydrogenation is one solution that may affect both areas simultaneously. However, there are some challenges to reducing the cost of products like green fuel. One of the challenges is the high energy required to activate CO_2 due to a lack of efficient catalyst materials. Therefore, developing catalyst materials with enhanced performance is crucial for hydrogenating CO_2 under mild conditions, particularly at lower pressures.

Thermoelectric materials are capable of converting temperature gradients into electrical potential. This process can elevate the Fermi level at the catalyst surface, thereby facilitating electron transfer and enhancing reaction rates. In the proposed system, the requisite temperature gradient could be generated by the hybridization of the reactor with water electrolysis. This configuration facilitates in situ production of hydrogen, sustains the necessary thermal gradient for thermoelectric operation, and efficiently dissipates the excess heat produced by the exothermic hydrogenation reaction.

An experimental setup has been established at Aalborg University to evaluate this concept. This setup incorporates a TE-assisted catalyst that has been specifically developed for the hydrogenation of CO_2. The primary objectives are to enhance reaction rates and reduce operating pressure, thereby enabling the development of more compact and energy-efficient reactor designs for the conversion of CO_2.

The results demonstrated that the TE-catalyst material is able to increase the reaction rate of the CO_2 hydrogenation process by approximately 50%. Trials also confirmed that P-type and N-type thermoelectric materials have different effects on CO_2 hydrogenation, based on changes in electron transfer and variations in the reaction surface Fermi level.

The findings of this study highlight the potential of thermoelectric-assisted catalysis in fostering sustainable fuel production and in mitigating industrial emissions.

Energy storage system integrated with low temperature gradient thermoelectric generator for self-powering industrial sensor platforms

Alireza Rezaniakolaei[1], Ali Mohammadnia[1], Ali Enkeshafi[1]
[1]Aalborg University, Denmark

Applications-1, September 15, 2026, 11:00 - 12:15

Sensor platforms need electrical power to operate, while providing perpetual energy source for such devices in a great challenge. In this work a conceptual energy storage system has been developed to harness thermal energy to power sensor platforms at low temperature difference between the heat source and environmental ambient. The multidisciplinary design of the thermoelectric energy storage system, consisting of a high-power density thermoelectric module, a power converter with low startup voltage, a natural convection cooled based heatsink, a charging circuit, and an electric storage unit, is built, and tested under steady state and unsteady thermal conditions to investigate potential of energy storage for supplying sensor platforms. Results of this study show that the energy storage system proposed in this work successfully provide required electrical power for the sensor platform device at temperature difference of 10.6 °C between the heat source and ambient and with, only, 5.98 °C temperature difference across the thermoelectric module. At higher wall temperatures, 98 °C, the thermoelectric energy storage system provides up to 30 times more than power required by the sensor platform considered in this study. Investigation of the developed system under the cold-start and thermal relaxation conditions show that this system has high potential to charge the energy storage unit, used for supplying sensor platform devices, within short time during the cold-start stages and a long time in thermal relaxation stages.

Improved performances of Fe2VAl-based thermoelectric modules

Geoffrey Roy[1,2], Michael Parzer[3], Fabian Garmroudi[4], Pawel Ziolkowski[5], Thomas Konegger[6], Pascal J. Jacques[1], Ernst Bauer[3]
[1]Institute of Mechanics, Materials, and Civil Engineering, IMAP, Belgium, [2]Thermo Power SRL, Belgium, [3]Institute of Solid State Physics, Austria, [4]Materials Physics Applications – Quantum, Los Alamos National Laboratory, USA, [5]German Aerospace Center (DLR) – Institute of Materials Research, Germany, [6]Institute of Chemical Technologies and Analytics, Austria

Heusler Modules, September 17, 2026, 13:30 - 15:00

Thermoelectric (TE) materials enable direct heat to electricity conversion and are promising candidates for sustainable energy harvesting. For practical implementation, they must combine high efficiency with low cost, non toxicity, and scalable fabrication. In this work, we enhance the TE performance of low cost Fe_2VAl based full Heusler compounds through a synergistic strategy combining heavy element doping and controlled off stoichiometry. The optimized materials achieve an average figure of merit of $zT \approx 0.3$ over 300–500 K.
To demonstrate reproducibility and technological relevance, we fabricate and characterize a complete thermoelectric module (TEM) based on the optimized compounds. Scaled up batches produced by hot pressing show TE properties consistent with laboratory scale samples, with only a slight increase in electrical resistivity due to the absence of post annealing. The excellent mechanical workability of Fe_2VAl based materials enables direct brazing of the TEM legs onto copper electrodes, yielding robust modules with ultra low contact resistances ($< 6\ \mu\Omega\cdot cm^2$).
A 36 leg TEM was assembled and tested in two independent laboratories under both vacuum and ambient conditions. The device delivers output power exceeding 3 W and achieves conversion efficiencies above 1.2% across 300–673 K, representing among the highest reported performance values for Fe_2VAl based generators. These results highlight the strong potential of this material system for scalable thermoelectric energy harvesting applications.
Finally, a modelling approach based on intrinsic material properties was used to analyse module performance, revealing significant opportunities for further improvement through optimized thermal contacts.

Processing and Doping Effects in P3HT for High-Performance Organic Thermoelectric Modules

Mina Saeidnia[1], Sajid Muhammad[1], Marcello Franzini[2], Luca Cavinato[2], Simone Galliano[2], Claudia Barolo[2], Andrea Reale[1]
[1]Department of Electronic Engineering, CHOSE—Centre for Hybrid and Organic Solar Energy, University of Rome Tor Vergata, Italy, [2]Department of Chemistry, University of Turin, Italy
Organics and Hybrids, September 15, 2026, 11:00 - 12:15

Organic thermoelectric (TE) materials based on conjugated polymers have attracted increasing attention as candidates for flexible, lightweight, and low-cost energy harvesting. However, their performance remains limited by the difficulty of simultaneously optimizing charge carrier concentration, molecular ordering, and long-term stability. Because thermoelectric efficiency depends on the interdependent relationship between electrical conductivity and Seebeck coefficient, precise control over doping and microstructure is essential [1].

In this work, we systematically investigate the combined influence of dopant chemistry and solution-processing methods on poly(3-hexylthiophene) (P3HT). A variety of dopants, including LiTFSI, F4TCNQ, and Lewis acids, is explored to tailor charge transport and electronic structure. LiTFSI is found to promote enhanced molecular ordering and induce polaron formation, facilitating improved charge transport within the polymer matrix [2]. Molecular doping with F4TCNQ further increases charge carrier concentration, while Lewis-acid-based systems provide additional pathways toward improved doping efficiency and enhanced thermal and operational stability, in line with recent developments in dopant design [3].
To enable scalable fabrication, solution-based deposition techniques such as blade coating and drop casting are employed, allowing systematic control over film thickness, uniformity, and dopant distribution. The results demonstrate that both doping strategy and processing conditions play a critical role in defining film morphology and, consequently, thermoelectric properties, emphasizing the importance of structure–property relationships in organic TE systems .

Finally, optimized materials are implemented in prototype thermoelectric modules. Device design considerations include control of film uniformity, leg geometry, and interfacial electrical connections, enabling efficient charge transport across the module. This integrated approach bridges materials development and device engineering, providing a viable pathway toward scalable and stable organic thermoelectric technologies for practical energy harvesting applications.

References:
1. DOI: 10.1016/j.ccr.2026.217639
2. DOI: 10.1002/adfm.202106991
3. DOI: 10.1021/acsenergylett.4c01278

Unveiling low temperature thermal transport in AgGaTe2-AgInTe2 chalcopy-rite solid solutions

Dr. Aryan Sankhla[1], Dr. Peter Thorup[1], Mr. Jacob Kammer Nielsen[1], Prof. Bo Brummerstedt Iversen[1]
[1]Department Of Chemistry, Aarhus University, Denmark

Phonons, Fundamental Aspects, September 18, 2026, 10:30 - 11:30

Recent studies on silver-based tetrahedrally bonded chalcogenides, AgGa1-xInxTe2, have demonstrated promising thermoelectric performance (zT = 1.6-1.8) at elevated temperatures (T = 750 - 850 K), driven by an ultralow thermal conductivity (κ=0.1-1 W/m-K between 300 - 850 K). This behavior is attributed to weak Ag–Te bonding, which promotes strong coupling between acoustic-to-low lying optical phonons, resulting in reduced sound velocity and Debye temperature (and frequencies) compared to state-of-the-art thermoelectrics. While κ(T) measured at high temperatures highlight phonon-phonon scattering due to weak bonding interactions, the role of distinct phonon scattering mechanisms remain unelucidated. To address this, we synthesized AgGa1-xInxTe2 solid solutions (x = 0-1), performed high-resolution synchrotron X-ray diffraction (SR-XRD) at room temperature, and measured thermal conductivity and heat capacity from 2 K to 300 K. An analysis of SR-XRD revealed nearly pure composition but with asymmetric peaks, that originates from compositional phase width associated particularly with AgInTe2, that favours formation of multiple solid solution phase compounded by preferential Ga/In occupation to neutralize charge imbalance. Multiphase Le Bail fitting enables good agreement with SR-XRD data and a quantification of subtle variations in unit cell volume across multiple disordered phases. Thermal transport measurements show a systematic effect of alloying, with AgGa0.5In0.5Te2 exhibiting more than two-fold reduction in κ(T) compared to the end members. A further analysis of C_P/T^3 (T) showed the expected extremum for all compositions around T≈10 K (the Boson peak) but with an increase in its height and a decrease of full-width of half maximum with increasing x (In-content) that cannot be solely attributed to the Einstein-like independent oscillations of weakly bonded Ag and Te atoms. Therefore, with this study, we unravel an unequivocal description of thermal transport in AgXTe2 (X: Ga/In) materials that adds new knowledge for advancing the optimization of these materials.

Optimisation of Silicon Germanium alloys performances developed by Laser Powder Bed Fusion

Dr Guillaume Savelli[1], Dr Alizée Thomas[1], Bastien Marchais[1], Tanguy Obringer[1]
[1]CEA-Liten, France

Additive Manufacturing, September 18, 2026, 10:30 - 11:30

If the use of additive manufacturing (AM) processes is mainly focused on metals and polymers materials, it has been applied to thermoelectric (TE) materials for few years. These processes can offer some advantages compared to standard sintering methods (such as SPS, HIP, etc.): complex shapes at both materials and devices level, new possible materials microstructures, simplified manufacturing processes for TE devices, etc. Among the various AM methods, Laser Powder Bed Fusion (LPBF) stands out as a promising approach for printing complex metal parts and can be used for TE materials, as it has already been the case for bismuth telluride [1], Half-Heusler [2] or SiGe [3].

Our work presents the optimization of silicon germanium alloys TE material developed by LPBF. As most of TE materials manufactured by this technique, SiGe alloys present structural defaults due to hot craking, limiting their TE properties. We developed a specific process, based on the combination of the use of an heating plate and annealing steps to improve their TE performances. Thanks to this optimization, ZT similar to the state-of-the-art has been achieved, but using less germanium content (Si85Ge15 for our work compared to Si80Ge20 for the SoA). We will present here how the combination of these thermal optimizations increase their TE properties.

References
[1] R. Zhan, J. Lyu, D. Yang et al., Mater. Today Phys., 24, 100670 (2022).
[2] Y. Yan, W. Genga, J. Qiu et al., RSC Adv., 8, 15796-15803 (2018).
[3] M. Baudry, G. Savelli, G. Roux, Mater. Sci. Eng. B, 298, 116897 (2023).

Acknowledgments
This work was supported by the French National Research Agency within the project FASTE (Grant Agreement n° ANR-22-CE50-0021) and by the European Union under @HorizonEU research and innovation program within the project STARTREC (Grant Agreement n° 101160663).

Powder Aerosol Deposition of Bi_2Te_3: Thermoelectric Properties from Thick Films to Bulk Like Samples

Dr. Daniela Schönauer-Kamin[1], Daniel Paulus[1], Jaroslaw Kita[1], Ralf Moos[1]
[1]University of Bayreuth, Department of Functional Materials, Germany

Composites, September 17, 2026, 11:00 - 12:15

Bismuth telluride (Bi_2Te_3) is one of the most relevant thermoelectric materials for room temperature applications, making scalable, flexible, and cost efficient fabrication routes highly attractive. Powder aerosol deposition (PAD) is a room temperature fabrication method that enables the rapid processing of thermoelectric materials such as Bi_2Te_3 and calcium cobaltite directly from the starting powder. The technique offers exceptionally high deposition rates while avoiding high-temperature processes during film formation.

Using PAD, dense Bi_2Te_3 films with controlled composition (undoped, n-type, and p-type) can be fabricated ranging from conventional µm-thick coatings to bulk-like PAD samples with thicknesses in the mm-range. This technology enables the production of thick-film and bulk thermocouples in a single manufacturing process, which allows for a high flexibility in film thickness.

The focus of this work is on the systematic investigation of the morphological, structural, and thermoelectric properties of both µm-thick and bulk-like Bi_2Te_3 films processed by PAD. The influence of the PAD-induced microstructure is studied, as well as the effect of post deposition annealing, which is characteristic for PAD-processed materials. This annealing step is typically used to reduce microstrain in the PAD-films and to improve carrier transport properties while maintaining the dense film morphology and the microstructure.

The thermoelectric performance is characterized as a function of temperature over the relevant operating range. Seebeck coefficient, electrical conductivity, thermal conductivity, and Hall measurements are used to determine the charge carrier concentration and mobility of charge carriers, with a particular emphasis on anisotropic transport properties. Structure-property relationships are investigated by comparing µm-thick and bulk PAD Bi_2Te_3 samples before and after thermal annealing and in dependence on temperature. This provides insights into the potential of PAD as a versatile fabrication process for thermoelectric materials across different thickness scales.

Energy-selective transport as a strategy to minimize the Lorenz number in metallic thermoelectrics

Dr. Illia Serhiienko[1], Dr. Fabian Garmroudi[2], Prof. Dr. Andrej Pustogow[1]
[1]TU Wien, Vienna, Austria, [2]Los Alamos National Laboratory, United States
Electronic Transport Theory, September 16, 2026, 13:30 - 15:00

In metallic thermoelectrics, the figure of merit reduces to zT≈S^2/L in the electron-dominated regime. While thermoelectric optimization still relies primarily on enhancing the Seebeck coefficient S, the Lorenz number L becomes the second key parameter controlling performance. Yet, comparatively little attention has been paid to strategies for suppressing L below its Sommerfeld value. Within the Boltzmann transport, L can be expressed in terms of the variance of carrier energies relative to the chemical potential, L ~ Var(E - μ), implying that narrowing the energy distribution of conducting carriers provides a direct route to lowering L.

Here, we develop a general framework for energy-selective transport in metals and show how strongly energy-dependent scattering can be used to control the Lorenz number. Building on recent observations of enhanced thermopower in Ni3Ge [1] and Ni3In [2], we identify a common principle: interband scattering with strong energy dependence creates an effective transport window, leading to enhanced carrier asymmetry and an increased Seebeck coefficient. This behavior is promoted by flat-band features in the electronic structure, which strongly modify the scattering phase space near the Fermi level. We further extend this concept to systems hosting two flat bands separated by an energy scale W. We show that such a configuration can generate a boxcar-like transport distribution function, selectively suppressing carrier contributions outside a narrow energy window. This reduces Var(E - μ) and thus suppresses the Lorenz number significantly below its Sommerfeld value without strongly compromising the electrical conductivity. These results establish energy-selective transport engineering as a general strategy for approaching the ideal transport distribution in metallic thermoelectrics.

References
[1] F. Garmroudi et al., Energy filtering–induced ultrahigh thermoelectric power factors in Ni3Ge. Sci. Adv. 11, eadv7113 (2025).
[2] F. Garmroudi et al., Topological Flat-Band-Driven Metallic Thermoelectricity. Phys. Rev. X 15, 021054 (2025).

Hybrid Thermoelectrics as a Platform for Printable Wearable Energy Harvesting Systems

José F. Serrano-Claumarchirant[1], Bejan Hamawadi[2], Oliver Fenwick[3], Muhammet Toprak[1]
[1]Royal Institute of Technology, KTH, Sweden, [2]Institute of Solid State Physics, ISSP, Latvia, [3]School of Engineering and Materials Science, SEMS-QMUL, United Kingdom

Applications-3, September 17, 2026, 11:00 - 12:15

The demand for portable electronic devices has increased enormously in recent years due to their integration into flexible substrates, which are easy to incorporate into clothing. Therefore, the development of wearable thermoelectric generators (wTEGs) requires materials that simultaneously exhibit high thermoelectric performance, mechanical flexibility, and compatibility with scalable fabrication techniques. Hybrid thermoelectrics, combining organic and inorganic components, have emerged as a promising strategy to meet these demands by leveraging the intrinsic advantages of each material class.

In this work, we present a unified approach to the design and fabrication of printable hybrid thermoelectric systems that integrates advances in organic conductive polymers and inorganic nanostructured materials. On the organic side, the thermoelectric properties of polymer-based systems are tailored through sequential post-processing strategies that optimize electrical conductivity, carrier concentration, and charge transport by controlling composition and morphology. These developments enable the fabrication of flexible and solution-processable thermoelectric elements compatible with inkjet printing.

Building on this foundation, hybrid thermoelectric inks are formulated by incorporating inorganic thermoelectric nanoparticles into polymer matrices engineered to provide suitable rheological properties for additive manufacturing. This approach allows the fabrication of thermoelectric architectures via printing techniques, while maintaining mechanical compliance and enhancing thermoelectric performance through synergistic effects between phases. Across both material systems, device geometries are optimized using finite element modeling to maximize thermal gradients and electrical output under wearable operating conditions. The resulting strategy establishes a general framework for developing hybrid, printable thermoelectric generators that bridge the gap between high-performance inorganic materials and flexible organic systems.

High-Performance 14-1-11 Thermoelectrics via Sb-Induced Carrier Tuning in Ca14AlBi11-xSbx

Saba Shahgoli[1], Jeffrey Snyder[2], Umut Aydemir[3]
[1]Graduate School of Sciences and Engineering, Koç University, Türkiye, [2]Department of Materials Science and Engineering, Northwestern University, USA, [3]Department of Chemistry, Koç University, Türkiye

Zintl/Heusler-3, September 17, 2026, 15:30 - 17:00

Zintl phases in the 14-1-11 family are promising high-temperature thermoelectric materials because of their intrinsically low lattice thermal conductivity and chemically tunable electronic structure.1 However, precise control of carrier concentration in Bi-based 14-1-11 compounds remain a critical challenge for optimizing their thermoelectric performance.2,3 Here, Ca14AlBi11-xSbx (x = 0, 1, 3, 5) compounds were synthesized to investigate the effect of isovalent Sb-for-Bi substitution on charge and thermal transport. Structural characterization confirms retention of the tetragonal 14-1-11 framework upon Sb incorporation. Transport measurements show that Sb substitution reduces the hole concentration and significantly enhances the Seebeck coefficient while preserving relatively high weighted mobility, suggesting that Sb-for-Bi substitution primarily tunes the intrinsic defect chemistry rather than degrading carrier transport, thereby highlighting defect-mediated carrier tuning as a promising strategy for controlling electronic properties in 14-1-11 compounds.4 The accompanying suppression of thermal transport leads to a marked improvement in TE performance. Among the investigated compositions, Ca14AlBi8Sb3 exhibits the best performance, reaching a peak TE figure of merit, zT, of ~1.35 at 973 K and maintaining a high average zT across the measured temperature range, placing it among the best-performing high-temperature p-type TE materials reported to date. Device-level analysis further predicts a device ZT of ~0.6 and a maximum conversion efficiency approaching 10% at 973 K, highlighting the strong potential of this system for mid-to-high-temperature waste heat harvesting module applications.

References

(1) https://doi.org/10.1021/cm060261t.
(2) https://doi.org/10.1021/acs.inorgchem.7b01548.
(3)https://doi.org/https://doi.org/10.1016/j.mtadv.2020.100094.
(4) https://doi.org/10.1002/anie.201311125.

Electron and Phonon Transport Properties of The Single-crystalline TiCoSb - based Half-Heuslers

Ye Sheng[1], Professor Fu Yuhao[2], Professor Zhang Qian[1], Professor Mao Jun[1]
[1]Harbin Institute of Technology (Shenzhen), China, [2]Jilin University, China

Heusler-1, September 15, 2026, 13:30 - 15:00

Half-Heuslers are promising for medium- to high-temperature thermoelectric power generation, but their polycrystalline forms typically suffer from defect-dominated electron scattering, limiting performance. Here, we report the successful growth of high-quality TiCoSb-based single crystals exceeding 1 cm in size. Leveraging enhanced electron mobility, n-type Ti1−xNbxCoSb single crystals achieve an average power factor of ~37 μW cm-1 K-2 between 307 and 973 K. Additionally, Hf alloying expands the weighted scattering phase space and intensifies anharmonic scattering, significantly reducing lattice thermal conductivity. Through Nb/Ta co-doping and Hf alloying, a peak zT above 1.0 is attained, surpassing polycrystalline (Ti, Zr, Hf)CoSb- and ZrCoBi-based materials. A single-leg device fabricated from these crystals demonstrates a heat-to-electricity conversion efficiency of ~10.2% at a temperature difference of 700 K.

Furthermore, we synthesized two TiCoSb single-crystal variants with identical stoichiometry but distinct atomic occupancies: pristine TiCoSb with an ideal MgAgAs-type structure, and a defective variant containing ~4% Co interstitials at the 4d site and ~4% vacancies at the 4c site. Remarkably, the defective crystal exhibits a dramatic reduction in thermal conductivity (~3.9-6.5 W m-1 K-1) compared to the pristine one (~118-188 W m-1 K-1). Co-site disorder does not introduce localized states or avoid-crossing behavior in the phonon dispersion. Instead, it increases the scattering phase space, enhancing anharmonic scattering and drastically reducing phonon lifetimes. These findings elucidate the microscopic mechanism of defect-dominated phonon scattering in half-Heuslers.

Toward flexible and conformable thermoelectric energy harvesting based on poly(vinylidene fluoride) with Bi2S3 and Bi2Te3

Diana Sotelo[1,2], Nikola Peřinka[1], Alberto Oleaga[3], Arantza Mendioroz[3], Agustín Salazar[3], Davide Spirito[1], Senentxu Lanceros-Méndez[1,4,5]
[1]BCMaterials - Basque Center for Materials, Applications and Nanostructures, Spain, [2]Departamento de Electricidad y Electrónica, Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU., Spain, [3]Departamento de Física Aplicada, Escuela de Ingeniería de Bilbao, Universidad del País Vasco UPV/EHU, Spain, [4]IKERBASQUE, Basque Foundation for Science, Portugal, [5]Physics Centre of Minho and Porto Universities (CF-UM-UP), and Laboratory of Physics for Materials and Emergent Technologies, LapMET University of Minho, Portugal
Composites, September 17, 2026, 11:00 - 12:15

Flexible and conformable thermoelectric polymer composites are gaining significant interest for energy harvesting applications, particularly in low-power and autonomous systems. However, achieving efficient charge transport while maintaining processability remains a major challenge.

In this work, polyvinylidene fluoride (PVDF) composites with chalcogenides, bismuth sulfide (Bi_2S_3) and bismuth telluride (Bi_2Te_3), were developed using a processing route based on 1,3-Dimethyl-3,4,5,6-Tetrahydro-2(1H)- Pyrimidinone (DMPU) solvent, enabling the fabrication of flexible thin films with reduced environmental impact. Their thermal and electrical properties were tailored for thermoelectric device applications.

The influence of filler type, concentration (up to 90 wt% nominal), and processing conditions (curing temperature and substrate) on the electrical, dielectric, thermo-mechanical and thermoelectric properties was systematically investigated. The results reveal a strong dependence of charge transport on filler chemistry and microstructure. The Seebeck coefficient increases with filler content in semicrystalline PVDF composites. PVDF/Bi_2Te_3 composites exhibit significantly higher electrical conductivity (up to ~10 S/m) and stable positive Seebeck coefficients (~20–160 μV/K), indicating efficient thermoelectric performance. In contrast, PVDF/Bi_2S_3 composites show lower conductivity and a negative Seebeck coefficient, enabling for p-n type devices.

Dielectric analysis highlights interfacial polarization and concentration-dependent behavior consistent with percolation phenomena at high concentrations (≥75 wt%). Morphological characterization confirms the role of particle dispersion, agglomeration, and anisotropic transport pathways. Furthermore, differences between in-plane and cross-plane measurements demonstrate the directional dependence of electrical transport. Further, the thermo-mechanical characteristics of the materials demonstrate their compatibility with flexible and conformable electronic applications.

This work indicates that alternatively processed PVDF/chalcogenide composites are promising candidates for flexible and conformable thermoelectric applications and provides insight into structure–property relationships in polymer-based thermoelectric systems and highlight their potential for self-powered devices in environmental monitoring and low-power electronics.

Multiphysics simulation of germanium-tin thermophotovoltaics

Ignatii Zaitsev[2], Costanza L. Manganelli[2], Christian Wenger[2], Davide Spirito[1]
[1]Bcmaterials - Basque Center For Materials, Applications And Nanostructures, Spain, [2]IHP - Leibniz Institute For High Performance Microelectronics, Germany

Emerging, September 15, 2026, 15:30 - 17:00

Thermophotovoltaic energy conversion uses narrow-gap semiconductors to convert radiation from hot bodies into electrical power. This mode of energy harvesting from heat may be advantageous with respect to thermoelectrics especially in case when heat transfer by conduction can be difficult or mechanically unstable, and found application with concentrated sunlight or power plants. Narrow gaps semiconductors are needed to absorb efficiently long wavelength radiation, yet they present challenges in terms of availability and degradation of performance with temperature. Germanium-tin alloys (GeSn) have recently been developed into a high-quality materials suitable for photonics and compatible with CMOS processing.
In this work, we address its application to thermophotovoltaics. We present a comprehensive simulation based on finite element modelling (FEM) that includes thermal, optical and electrical properties of GeSn as a function of its Sn content, temperature dependence of the various parameters and the 3D geometry of the heater/photovoltaic cell system. Our model includes indirect recombination processes, multilayer generation dynamics and thermal equilibrium between the emitter and cell. In a cylindrical geometry, the simulated efficiency is predicted up to 6.5% power conversion efficiency with 0.11 W/cm² power generated, at an optimal heater temperature of around 1100 K. We discuss strategies for improving device efficiency, such as the use of selective emitters. This modelling framework enables in-depth theoretical exploration of Ge-based materials under varying strain, composition and temperature.

Finally, a comparison of thermophotovoltaic with thermoelectric and combined energy harvesting is presented.

Development of Thermoelectric Generators with a Manufacturing-Friendly Design for Stationary and Mobile Applications

Arne Stumpf[1], Julian Schwab, Christopher Fritscher, Timo Knobelspies, Matthias Helmich, Marc Rosenbeck, Martin Kober, Frank Rinderknecht, Tjark Siefkes
[1]German Arospace Center, Germany

Applications-2, September 16, 2026, 13:30 - 15:00

Thermoelectric generators (TEG) have so far mainly been used in space travel as a reliable source of power generation - however, a broad terrestrial application has not become established until now. With rising energy prices and growing pressure for energy efficiency, the utilisation of waste heat is becoming increasingly important. This opens up new prospects for TEGs, which can now develop new fields of application beyond the boundaries of space travel. A key factor for the practical implementation of the technology is the cost-benefit factor: it evaluates the technical advantages of a measure in economic terms and often forms the decisive basis for the decision on its technical feasibility. Both in thermal industrial processes and in some mobile applications, TEGs offer great potential for increasing overall efficiency, provided they achieve a good cost-benefit ratio. In this presentation, the development of cost-efficient mobile and stationary TEGs for a wide range of applications will be presented using concrete examples: pellet stoves, melting furnaces and trucks. The TEGs are based on a generic, production-friendly design that has already been tested in mobile applications and has now been transferred to stationary systems and further optimised. The presentation provides an overview of diverse and new applications with successful integration of TEGs in a wide range of power from W to kW. The presentation thus emphasises the high technical and economic potential of thermoelectric generators in various areas of power generation.

From Height-Optimized to Upscaled Micro-Thermoelectric Generators for Autonomous IoT Applications

Adhiraj Sundar[1,2], Dr Heiko Reith[1], Professor Kornelius Nielsch[1,2]
[1]Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Germany,
[2]Institute of Materials Science, Technische Universität Dresden, Germany

Harvesting and Sensing, September 15, 2026, 15:30 - 17:00

Micro-thermoelectric generators (µTEGs) are promising energy harvesters for autonomous low-power Internet of Things (IoT) systems, where compact device footprint and sufficient electrical output under small temperature gradients remain key challenges. Our MEMS-based fabrication approach combines lithographic patterning with electrochemical deposition (ECD) of thermoelectric materials, enabling precise control of device geometry and dense thermocouple integration.

Building on our previously reported ECD-based µTEG platform, numerical modelling and experimental optimization of the relative thermoelectric leg heights were used to improve device performance and material utilization. The resulting height-optimized µTEG achieved a normalized power density of 25.1 µW cm^{-2} K^{-2}, demonstrating the potential of geometry optimization for compact thermoelectric energy harvesting and its applicability toward powering low-power autonomous sensor systems.

The present work extends this approach toward device-level scaling, investigating strategies to increase thermocouple integration and improve utilization of the available active area while maintaining compatibility with the established fabrication route. Upscaled µTEG structures are fabricated and electrically characterized to evaluate the scalability of the approach. These developments provide a pathway toward higher-output µTEGs for autonomous IoT applications.

High-performance Mg2SiSn-based thermoelectrics with superior compression strength and elastic resilience

Jing Tang[1,2], Ran He[2], Kornelius Nielsch[2], Yue Chen[1]
[1]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China, [2]Leibniz Institute for Solid State and Materials Research, Germany

Zintl-1, September 15, 2026, 15:30 - 17:00

The growing demand for sustainable energy solutions has intensified interest in thermoelectric materials capable of efficiently converting heat into electricity while maintaining robust mechanical performance. Here, we investigate Mg2Si1-xSnx-based thermoelectrics, which combine superior compressive strength, high elastic limits, and cost-effectiveness compared with conventional Mg-based systems. These materials retain structural integrity under high compressive loads, ensuring stable operation in device applications. Additionally, the high elastic limits enable Mg2Si1-xSnx to recover the original dimension within the elastic region. To enhance performance, indium and antimony co-doping was employed to suppress lattice thermal conductivity and optimize carrier concentration simultaneously. As a result, this work achieves a peak zT of ~1.7 at 700 K, and a two-pair module with p-type MgAg0.97Sb0.99 delivered a thermoelectric efficiency of ~7.3% at temperature difference of 300 K. The demonstrated balance of mechanical robustness, high conversion efficiency, and sustainability positions Mg2Si1-xSnx as a promising n-type candidate for near-room to mid-temperature energy conversion applications, particularly in scenarios requiring durable and mechanically resilient thermoelectric devices.

Synergistic Enhancement of Bi2Te3/Sb2Te3–PMMA Thermoelectric Generators via

Dithiol-Assisted Conductivity and FEM-Based Geometry Optimization

Prof. Muhammet Toprak[1], Dr. José Francisco Serrano-Claumarchirant[1], Dr. Bejan Hamawandi[1,2], Dr. Adem Björn Ergül[1]
[1]KTH Royal Institute of Technology, Department of Applied Physics, Sweden, [2]Institute of Solid State Physics, University of Latvia, Latvia

Organics and Hybrids, September 15, 2026, 11:00 - 12:15

There is increasing interest in thermoelectric (TE) films based on pre-synthesized nanoparticles, enabling conformal coatings for harvesting waste heat from complex and curved surfaces. A key challenge remains the development of scalable and reproducible routes for high-quality n- and p-type materials, together with controlled integration into functional devices. In this work, we report the synthesis of n- and p-type bismuth–antimony telluride (Bi_2Te_3–Sb_2Te_3) nanostructures using a scalable microwave-assisted bottom-up approach, enabling precise control over composition, morphology, and surface chemistry. Dithiol-assisted surface modification is employed to enhance interparticle transport and improve electrical connectivity within the nanoparticle network. The influence of synthesis conditions on microstructure and transport-relevant properties is systematically investigated, highlighting the role of nanoscale design in governing thermoelectric performance.

Hybrid inks are formulated by integrating the synthesized nanoparticles with a PMMA matrix, enabling robust and processable systems for thick-film fabrication via doctor blading. The resulting hybrid films exhibit tunable electrical transport under applied temperature gradients, with performance strongly influenced by nanoparticle dispersion and interfacial interactions within the polymer matrix.

Based on the optimized material systems, thermoelectric generators (TEGs) are fabricated using printed n- and p-type legs. Finite element method (FEM) simulations, incorporating experimentally obtained material parameters, are employed to guide device design. This approach enables geometry optimization beyond conventional symmetric architectures, resulting in enhanced power output.

The combined strategy of scalable nanoparticle synthesis, hybrid material design, and FEM-guided device optimization demonstrates a viable pathway toward high-performance, conformal thermoelectric generators.

Beyond Flexible Devices: the System Challenge

Dr Richard Tuley[1], Dr Cevriye Koz[1], Mr Richard Lydiard[1], Dr Rajeshkumar Mohanraman[1], Mr Yeremi Perez-Ramirez[1], Dr Eleni-Chrysanthi Stefanaki[1]
[1]European Thermodynamics Ltd, United Kingdom

Harvesting and Sensing, September 15, 2026, 15:30 - 17:00

The largest commercial success of thermoelectric devices is in bulk Peltier devices rather than generation systems. Yet their design has not substantially changed in decades. We report flexible and stretchable Peltier devices which have the opportunity to open up new applications, enabling easier installation onto irregular or changing surfaces, such as the potential for better integration and proximity with people, e.g. in wearable devices. A flexible device allows the use of a curved surface, while a significantly stretchable device additionally allows conforming with more complex surfaces and movement.

We report a 27 K cooling effect between a solid surface and air, using a flexible, stretchable device and a rigid forced convection heat sink. The device demonstrated good flexibility, with resistance change <5% after bending to a 9mm radius, and average failure under tension at 31% strain. Repeated, cyclic tensile stress at lower strains showed no loss in performance, with resistance change <5% after 1000 cycles of 4mm tensile and compressive lateral displacement. However, to take advantage of this flexible module in a real application, a flexible heat sink coupled to the module is required to form a true flexible system. We discuss the challenges and initial approaches to create a flexible heat sink using an egg-box flexible geometry, demonstrating a cooling effect of 8 K.

Structure-Property Relationships in Thermoelectric Copper-Iron Sulfides

Dr Paz Vaqueiro[1], Dr Shriparna Mukherjee[1], Dr Sebastian Long[1], Shoeb Athar[1], Prof Anthony Powell[1], Dr Krishnendu Maji[2], Prof Emmanuel Guilmeay[2]
[1]Department of Chemistry, University of Reading, United Kingdom, [2]Laboratoire de Cristallographie et Sciences des Matériaux, Université de Caen, France

Chalcogenides-1, September 15, 2026, 11:00 - 12:15

Metal sulfides are attractive candidates for thermoelectric applications because sulfur is abundant and widely available. While p-type sulfides containing Earth-abundant elements with figures of merit that approach or surpass unity, are known (e.g. Cu_2S, tetrahedrites), the thermoelectric performance of n-type sulfides generally lags behind. In addition, many of the best performing n-type sulfides, such as PbS and $AgBi_3S_5$, contain toxic or scarce elements. In this context, tetragonal chalcopyrite, $CuFeS_2$, has attracted significant interest as a potential n-type thermoelectric material composed of Earth-abundant elements. However, its relatively high thermal conductivity ($\kappa \approx 8$ W m^{-1} K^{-1} at 300 K) results in a low thermoelectric figure of merit ($ZT \leq 0.4$).

A small number of studies have reported chalcopyrite with significantly reduced thermal conductivity ($\kappa \approx 1.5$ W m^{-1} K^{-1} at 300 K), through sulfur deficiency or via substitution with In or Al. This marked decrease in thermal conductivity has been attributed to cation disorder and the formation of a “cubic chalcopyrite” phase. Here, we present our results on two closely related metal-rich sulfides, cubic talnakhite ($Cu_{17.6}Cu_{17.6}S_{32}$ = $Cu_{1.1}Fe_{1.1}S_2$) and tetragonal mooihoekite ($Cu_9Fe_9S_{16}$ = $Cu_{1.125}Fe_{1.125}S_2$). Neutron diffraction and synchrotron X-ray diffraction data, combined with DSC, reveals the coexistence of multiple phases. Thermoelectric measurements are consistent with n-type semiconducting behaviour with low thermal conductivity, comparable to that of “cubic chalcopyrite”. Diffraction data collected as a function of temperature, shows that talnakhite coexists with chalcopyrite from room temperature up to ~500 K, with the chalcopyrite fraction increasing rapidly with temperature. These results suggest that the low thermal conductivity for “cubic chalcopyrite”, talnakhite and mooihoekite may be related to the coexistence of closely-related phases, with numerous grain boundaries.

3D elastic inorganic thermoelectric network for body heat energy harvesting

Dr. Xiaodong Wang[1,2], Professor Jun Mao[1], Professor Feng Cao[1], Professor Qian Zhang[1]
[1]School of Materials Science and Engineering, Harbin Institute of Technology (Shenzhen), China, [2]Institute of Special Environments Physical Sciences, Harbin Institute of Technology (Shenzhen), China

Harvesting and Sensing, September 15, 2026, 15:30 - 17:00

The rigid and brittle nature of inorganic thermoelectric materials poses a fundamental challenge for their application in flexible wearable devices. Here, we address this issue by constructing three-dimensional (3D) elastic inorganic networks that efficiently harvest body heat. Using a facile and scalable two-step dip-coating method, we first fabricated an ultra-lightweight Ag_2Se thermoelectric sponge with a density of 0.28 g cm^{-3}. This 3D network exhibits an extremely low thermal conductivity of 0.04 W m^{-1} K^{-1}, a high tensile elongation (>100%), and a room-temperature figure of merit zT of 0.1. A thermoelectric jacket prototype assembled from this material demonstrates an output power of 4 μW cm^{-2}, rivaling advanced bulk-based flexible generators. To further enhance performance, we developed a pure inorganic Ag_2Se nanowire aerogel via a polymer-crosslinker-free synthesis, achieving a record zT of 0.17 for inorganic thermoelectric aerogels with tunable porosity (95–99%). Subsequently, a biomimetic hierarchical organic/inorganic composite aerogel was constructed, enhancing the compressive strength by nearly an order of magnitude while maintaining excellent thermoelectric properties. A vertical prototype device based on this composite delivers a high specific power output of 76 μW g^{-1} at a temperature difference of ~60 K. Our work provides a design strategy for next-generation flexible thermoelectrics by decoupling electrical, thermal, and mechanical transport in all-inorganic 3D networks.

Plastic deformation and metalworking for inorganic thermoelectric materials

Professor Tianran Wei[1]
[1]Shanghai Jiao Tong University, China

Interfaces and Stability, September 17, 2026, 15:30 - 17:00

Brittleness poses a critical bottleneck that limits the low-cost manufacturing and diversified application of inorganic thermoelectric materials. In this talk, I report our progress on this issue in three aspects. (i) We discovered or created a series of room-temperature ductile thermoelectric materials, such as Ag2(S, Se, Te), enabling efficient processing at ambient temperature. (ii) For room-temperature brittle materials, we established a temperature-dependent plasticity model based on the physical picture of “easy to slip, difficult to cleave”. This model identified a range of thermoelectric semiconductor materials with excellent plasticity below ~200 °C. We thereby enabled warm metalworking techniques for these materials, which yielded high-quality, free-standing foils and high-performance thermoelectric film devices. (iii) Focusing on classic thermoelectric materials like PbTe, we systematically investigated the dependence of mechanical properties on temperature and loading rate, preliminarily established the mechanical constitutive relationship for compressive behavior, and constructed a mechanical processing diagram.

Theoretical study of the electronic structure, thermoelectric properties and electronic correlations in pristine and doped GeMnTe2

Dariusz Wieczorek[1], Bartlomiej Wiendlocha[1]
[1]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland
Materials Theory, September 17, 2026, 13:30 - 15:00

In this work we analyze the electronic structure, electronic correlations, and transport properties of disordered GeMnTe2, which has been experimentally shown to be a good thermoelectric material with a large effective mass of carriers. We focus on the interplay of atomic disorder, possible electronic correlations on the Mn d-shell and magnetism on its transport properties.

This material crystallizes in a cubic NaCl-type structure with Ge and Mn atoms randomly occupying the Na site [1,2] and should be rather denoted as Ge0.5Mn0.5Te. Because of the lower amount of Ge, it is cheaper and easier to obtain than GeTe [4]. Due to disorder and the formation of Ge vacancies, it has low lattice thermal conductivity and high carrier concentration which can be additionally controlled via doping [1,3,5].

Our theoretical calculations of the Bloch spectral functions allow us to quantify the strong effect of intrinsic disorder on the electronic structure. Transport calculations within the Kubo-Greenwood approach allow us to take the disorder-induced scattering into account in the analysis of the transport properties. Doping effects are further analyzed for the dopants already reported in the literature as well as new ones to search for new possibilities to improve thermoelectric properties of this material.

Due to the presence of Mn d-shells, the ferromagnetic character will also be taken into account [2]. Because of these orbitals and the high reported density of states effective mass (~9 me) [5], the electronic correlations in this material will also be studied to check if they have influence on thermopower in GeMnTe2.

[1] Zhou, B. et al., Sci. China Mater. (2019), 62
[2]Sichen Duan et al., Research. (2021),2021
[3] Jinfeng Dong et al., J. Mater. Chem. A, (2019), 7
[4] Lei Gao et al., Materials Today Communications, (2023), 37
[5] Jinfeng Dong et al., J. Am. Chem. Soc. 2023, 145

Enhancing the Thermoelectric Performance of Cu_2SnSe_3 through Structural Ordering Control

Arthur Wieder[1], Petr Levinský[2], Pierric Lemoine[1], Erik Elkaim[3], Jaafar Ghanbaja[1], Gwladys Steciuk[1], Sylvie Migot[1], Christine Clément[1], Ghouti Medjahdi[1], Lionel Aranda[1], Bernard Malaman[1], Ilayda Terzi[1], Bertrand Lenoir[1], Soufiane El Oualid[1], Christophe Candolfi[1]
[1]Université de Lorraine, CNRS, Institut Jean Lamour, France, [2]FZU – Institute of Physics of the Czech Academy of Sciences, Czech Republic, [3]Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin BP 48, 91192, France

Chalcogenides-1, September 15, 2026, 11:00 - 12:15

Cu_2SnSe_3 has recently emerged as a promising candidate for high-temperature thermoelectric applications due to the combination of its tuneable electronic properties and low lattice thermal conductivity. Its structure consists of corner-sharing tetrahedral networks, in which cationic disorder and the spatial arrangement of tetrahedral motifs can give rise to various lattice symmetries, ranging from an ordered, low-symmetry monoclinic phase to a disordered, high-symmetry cubic phase. As the coexistence of these polymorphs may strongly influence the charge carrier transport, controlling this aspect by tuning the synthesis conditions is essential. In this study, we demonstrate the detrimental influence of structural disorder at the sub-µm length scale on charge carrier transport. Precession-assisted electron diffraction tomography and synchrotron X-ray diffraction reveal that annealing below 673 K triggers phase coexistence, and the resulting structural disorder promotes charge carrier trapping in the induced impurity band, resulting in hopping conduction at low temperatures. In contrast, annealing above 873 K restores a single structural motif and conventional valence-band-like transport. Consequently, enhanced hole mobilities are achieved, yielding optimum ZT values of about 0.55 at 673 K, representing the highest value reported so far for undoped Cu_2SnSe_3.

Electronic structure, transport and lattice dynamics of a novel Cu-based thermoelectric chalcogenide Cu6+yTe3-xS1+x: theoretical study.

Andrzej P. Kądzielawa[1], **Bartlomiej Wiendlocha**[1]
[1]AGH University of Krakow, Faculty of Physics and Applied Computer Science, Poland
Materials Theory, September 17, 2026, 13:30 - 15:00

A recently discovered novel phase of γ-$Cu_6Te_{2.3}S_{1.7}$ [1] belonging to a family of copper chalcogenides, $Cu_{6+\gamma}Te_{3-x}S_{1+x}$, has emerged as a promising alternative to Bi_2Te_3-based compounds, exhibiting excellent performance near room temperature. Experiments report a large thermopower of 200 μV/K at room temperature and an ultralow lattice thermal conductivity of 0.2-0.25 $W{\cdot}m^{-1}{\cdot}K^{-1}$, resulting in a thermoelectric figure of merit zT approaching 1.1 at 500 K.

In this work, we present a comprehensive theoretical study of the electronic structure and transport properties of this family of materials using density functional theory combined with Boltzmann transport calculations. A particular challenge of this system is its complex crystal structure, which contains not only Te/S disorder but also partially occupied overlapping Cu sublattices, which exclude the application of coherent potential approximation. Accurately capturing this disorder requires the construction of large supercell models with up to ~160 atoms, making the calculations computationally demanding.

In a series of structures we analyze the effects of Te - S substitution and Cu disorder on the electronic band structure, density of states, carrier effective masses and thermopower. The results reveal significant band-structure modifications, including features favorable for enhanced thermopower. Calculated transport properties indicate that the interplay between band complexity and disorder is key to achieving high performance.
While the main focus is on electronic transport, we also initiated lattice dynamics studies to understand the origin of ultralow thermal conductivity.

These findings provide insight into the mechanisms governing thermoelectric behavior in $Cu_{6+\gamma}Te_{3-x}S_{1+x}$ and offer guidance for further optimization through compositional tuning and doping.

Acknowledgements:
We acknowledge Polish high-performance computing infrastructure PLGrid for awarding this project access to the LUMI supercomputer, owned by the EuroHPC Joint Undertaking, hosted by CSC (Finland) and the LUMI consortium through PLL/2025/09/018916.

References:
[1] O.Cherniushok et al., Adv. Mater. 37, 2420556 (2025).

From Incommensurate Structure to Transport Functionality in Fe–Ge Nowotny Chimney–Ladder Phases

Prof. Dr. Krzysztof Wojciechowski[1], Oleksandr Cherniushok[1], Kcper Pryga[1], Raisa Tahiyah[2], Taras Parashchuk[1], Yaroslav Tokaychuk[3], Lev Akselrud[3], Bartlomiej Wiendlocha[1], Roman Gladyshevskii[3], Alexandra Zevalkink[2], Yuri Grin[4]
[1]AGH University of Krakow, Poland, [2]Michigan State University, USA, [3]Ivan Franko National University of Lviv, Ukraine, [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Germany
Exotic Effects, September 16, 2026, 11:00 - 12:15

Nowotny Chimney–Ladder (NCL) phases in the Fe–Ge system exhibit the unusual coexistence of degenerate electronic transport and phonon-glass-like lattice thermal conductivity, yet the structural origin of this transport functionality remains unresolved. In particular, the relation between the incommensurate crystal framework, local bonding, and thermoelectric transport has not been established within a single physically consistent picture.

Here, we combine synchrotron diffraction, transport and Hall measurements, elastic characterization, chemical-bonding analysis, and first-principles calculations to identify the structure–property relations of the Fe–Ge NCL phase near the nominal Fe_2Ge_3 composition. We show that samples prepared as Fe_2Ge_3 crystallize as an incommensurately modulated phase close to $FeGe_{1.52}$. To connect this structural complexity with transport behavior, a three-dimensional commensurate approximant, $Fe_{27}Ge_{41}$, was derived and used as an interpretive model for electronic-structure calculations.

The results reveal that the slight Ge excess accommodated by the incommensurate framework shifts the Fermi level into the conduction band and produces a carrier concentration on the order of 10^{21} cm^{-3}, consistent with Hall measurements and explaining the degenerate n-type behavior without invoking extrinsic donor defects. At the same time, real-space bonding analysis shows that the structure is governed by a three-dimensional network of heteroatomic Fe–Ge interactions, without homoatomic Fe–Fe or Ge–Ge bonds, and with pronounced bonding inhomogeneity. Despite high elastic moduli and only moderate anharmonicity, the lattice thermal conductivity remains low, about 1.8 W m^{-1} K^{-1} at 300 K, indicating ultrashort phonon mean free paths imposed by the structurally inhomogeneous incommensurate framework.

These findings show how transport functionality in Fe–Ge NCL phases emerges directly from incommensurate structure: slight stoichiometric imbalance governs the electronic ground state, while bonding inhomogeneity suppresses lattice heat transport. More broadly, the work establishes a structure-to-functionality perspective for understanding and designing complex thermoelectric materials.

Improved Thermoelectric Properties of p-Type Mg3Sb2 via Cation Site Confinement for all-Mg3Sb2-Based Module Application

Dr. Xiao Xu[1], Dr. Ran He[1], Prof. Kornelius Nielsch[1]
[1]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Zintl-2, September 16, 2026, 11:00 - 12:15

Mg3Sb2-based materials have recently increased the likelihood of challenging the dominance of Bi2Te3-based modules in the commercial market, owing to the reported high-performance Mg3Sb2 n-type compounds, their high elemental abundance, and nontoxic nature. However, the inferior thermoelectric performance of p-type Mg3Sb2 hinders the development of a robust all-Mg3Sb2-based module. Here, we developed a strategy to ensure that sufficient dopants occupy the Mg site, thereby refining the optimized carrier concentration. The confined migration of Mg atoms was directly studied using a transmission electron microscope with atomic-resolved spherical aberration correction, and the corresponding effects on transport properties were verified by the temperature dependent characterizations, especially beneficial in high temperature area, eventually, the significant improvement of peak ZT at 723 K and average ZT from 323 to 723 K can be achieved in our p-type Mg3Sb2 specimens. Based on the optimization of p-type materials, a single-stage, all-Mg3Sb2-based module with 2 pairs of the same-parent legs was constructed, and a high efficiency of ~ 7% at a temperature gradient of 380 K was demonstrated. The competitive energy conversion performance promotes the practical application of all-Mg3Sb2-based generators.

Acknowledgments
This work was financially supported by the HORIZON EUROPE Climate, Energy and Mobility (INFERNO 101160642).

Machine learning-enabled design and optimisation of thermoelectric devices: from generators to coolers

Dr Ruomeng Huang[1], **Haoji Yang**[1]
[1]University Of Southampton, United Kingdom

Machine Learning, September 15, 2026, 13:30 - 15:00

Thermoelectric (TE) technologies, including generators (TEGs) and coolers (TECs), offer compelling solutions for energy harvesting and thermal management. However, device performance is governed by complex, strongly coupled interactions between material properties, geometry, contact effects, and operating conditions, making design and optimisation computationally demanding when relying on conventional modelling approaches. Here, we present an overview of our work on machine learning (ML)-enabled modelling and optimisation of thermoelectric devices, spanning bulk and segmented TEGs, hybrid PV–TEG systems, and TECs. In these studies, artificial neural networks (ANNs) are trained on high-fidelity datasets generated from three-dimensional multiphysics simulations, achieving prediction accuracies exceeding 99% while delivering orders-of-magnitude speed-up (up to 10^5×) compared to finite element methods (FEM).

For TEGs, ANN-based models capture the effects of geometrical design, contact resistance, and operating conditions, enabling rapid prediction of power density and efficiency. Coupling with genetic algorithms (GAs) allows efficient optimisation of device architecture under varying thermal conditions [1]. This approach is further extended to segmented TEGs using iterative training, improving prediction fidelity for high-performance configurations without increasing dataset size [2]. At the system level, ML models of hybrid PV–TEG systems demonstrate the capability to handle coupled multi-physics interactions and environmental variability for enhanced energy conversion [3]. For TECs, ANN–GA frameworks enable fast prediction and optimisation of cooling performance under dynamic boundary conditions, including varying heat flux and ambient environment, supporting adaptive thermal management [4].

Overall, this work establishes ML as a powerful surrogate modelling tool for thermoelectric device design, enabling rapid optimisation, multi-objective analysis, and scalable deployment across energy and electronics applications.

Reference

1. Appl. Energy, 305 (2022) 117800.
2. Energy AI, 12 (2023) 100225.
3. Case Stud. Therm. Eng., 61 (2024) 105053.
4. Appl. Therm. Eng., 285 (2026) 129224.

Combining CALPHAD with low-temperature sintered nano-silver forms a powerful technology chain for design and fabrication of high-performance thermoelectric generators

Li Yin[1], Feng Cao[1], Jun Mao[1], Qian Zhang[1]
[1]Harbin Institute of Technology, China

Interfaces and Stability, September 17, 2026, 15:30 - 17:00

The design of thermoelectric contact layers and the limitations of connection technology restrict the development of high-performance thermoelectric materials to high-efficiency thermoelectric generators. A wide variety of thermoelectric materials have very different physical and chemical properties and require different welding temperatures. Therefore, a general thermoelectric module interface design and preparation technology, which can improve the efficiency of device development, is highly anticipated. Silver nanoparticles have a low melting point and exhibit high stability in their sintered bulk form, so we have adopted them for the interface connection design in fabricating low-, medium-, and high-temperature thermoelectric modules. A record-high conversion efficiency of ~11% at the temperature difference of 550 K was achieved for the PbTe-based module. Additionally, we proposed an efficient contact materials screening strategy based on thermodynamically CALPHAD (CALculation of PHAse Diagram) method. A record high efficiency of ~11% at the temperature difference of 430 K has been first achieved for full Zintl-based thermoelectric module. The thermal aging and thermal cycle experiments proved the long-term reliability of the Mg2Ni/Mg3Sb2-xBix interface and the nano-silver low-temperature sintering joints. Our work greatly accelerates the development of advanced modules for thermoelectric power generation.

Fabrication of robust hBN-Encapsulated Graphene Sensors: A Path to Practical Johnson Noise Thermometry

Mrs Mahjabeen Fatima Yousafzai[1], Amir Mehrnejat[1], Daniel Burrow[1], Paul Bramley[3], Declan Tucker[2], Robert Crabtree[3], Jonathan Pearce[2], Ivan J. Vera Marun[1]
[1]Department of Physics and Astronomy, University of Manchester, United Kingdom, [2]National Physics Laboratory, United Kingdom, [3]Plum Park Estate, United Kingdom
Measurement and Characterisation, September 17, 2026, 15:30 - 17:00

Accuracy and precision are crucial in thermal measurements across many research disciplines, both academic and industrial. Considering this, robust temperature sensors that do not suffer from a calibration drift, particularly in harsh environments, are essential. This is the main advantage of a Johnson noise thermometry (JNT), which exploits the thermal electronic noise produced by electrical resistors to determine true thermodynamic temperature directly [1,2]. Herein, we discuss the potential of hexagonal boron nitride (hBN) encapsulated graphene as the temperature sensing element for practical JNT operation. By leveraging robustness, exceptionally high electron mobility, and thermally sensitive conductivity of hBN encapsulated graphene [3,4], we intend to develop a sensor that is accurate over broad range of temperatures (up to 1200 °C) and under ionizing radiation. This exploratory research is part of a collaboration between NPL, Metrosol and UoM. A key barrier to industrial implementation is the probe and sensor element, which needs to operate at temperatures up to 1200 °C or higher [5], while maintaining specific properties such as mechanical robustness and minimal electrical leakage.

Herein, we demonstrate the fabrication and comprehensive electrical characterization of an hBN-encapsulated graphene-based sensor with 1D edge (Pt) contacts, which endured annealing in an O_2 environment up to 700 °C. Through systematic Raman spectroscopy, AFM, SEM, and transport measurements before and after high-temperature annealing (up to 700 °C in oxidizing atmosphere), we establish that Pt contacts significantly outperform other metals such as Au, Pd, Cr, Ti in thermal stability [6]. We present Dirac curves, carrier mobility, and four-probe transport measurements under varying magnetic fields, demonstrating that hBN encapsulation combined with Pt edge contacts and protective capping layer effectively prevents oxidative degradation while preserving graphene transport properties. These results unlock new measurement windows for extreme-environment sensing and transforms practical JNT from a Physics concept to a real-world application.

Further evidence on practicality of utilising hBN encapsulation in thermoelectric devices is provided by characterising an air-sensitive 2D magnet [7] even after weeks of exposure to ambient condition with negligible (if any) degradation. As figures of merit, we report on Seebeck and thermomagnetic Nernst coefficients measured below and above room-temperature. The stability of the thermoelectric signals directly reflect device coupling to thermal gradients and serves as a validation that employing these device architectures can also be promising in increasing the efficiency of sensors and in waste-heat management.

References
[1] Nyquist, H. (1928). Physical review, 32(1), p.110.
[2] Bramley, P., et al. (2020). Measurement Science and Technology, 31(5), p.054003.
[3] Kretinin, A.V., et al. (2014). Nano letters, 14(6), pp.3270-3276.
[4] Wang, L., et al. (2013). Science, 342(6158), pp.614-617.
[5] Pearce, J.V., et al. (2020). In EPJ Web of Conferences, 225, p. 03001.
[6] Wang, Jingjing, et al, (2025) Nanoscale 17.2, 16848-16858.
[7] Zhang G. et al, Nat Commun 13, 5067 (2022).

Giant ZT enhancement in rhombohedral GeTe-based thermoelectric materials

Dr. Jincheng Yu[1], Dr. Xiaodong Liu[2], Dr. Yilin Jiang[3], Prof. Yu Pan[1], Prof. Xiaoyuan Zhou[1], Prof. Jing-Feng Li[3]
[1]Chongqing University, China, [2]University of Liverpool, UK, [3]Tsinghua University, China
Chalcogenides-2, September 16, 2026, 13:30 - 15:00

GeTe is a highly attractive p-type thermoelectric (TE) material, however, its peak figure of merit (ZT) is typically attained in the high-temperature cubic phase, where the inevitable phase transition raises concerns over interfacial instability during operation. Therefore, developing high-performance rhombohedral GeTe below the phase transition temperature represents a more viable path toward practical applications. Herein, we propose a facile nanocomposite strategy to enhance the TE performance of rhombohedral GeTe by incorporating high-modulus TiB_2 nanoparticles into $Ge_{0.94}Bi_{0.05}Te$ matrix. We demonstrate that the nanoparticle-induced interfacial constraint effect contributes to increasing longitudinal elastic modulus and decreasing equivalent deformation potential. These merits cancel the negative effects of increased interfacial potential barrier caused by grain refinement and unfavorable band bending, accounting for improved carrier mobility. In addition to introducing nanoparticle scattering, these TiB_2 inclusions form heterogeneous interfaces that promote charge depletion and generate substantial thermal resistance, concurrently suppressing the heat transfer by carriers and phonons. Consequently, an extraordinary ZT of 2.66 at 613 K and a superior average ZT of 1.29 (300~613 K) are obtained in the rhombohedral GeTe-based composite. This work shows a paradigm for synergistically optimizing the electrical and thermal transports of emerging TE systems with nanoinclusions.

Three-dimensional flexible thermoelectric network for energy harvesting and sensing

Prof. Qian Zhang[1]
[1]Harbin Institute of Technology, China

Applications-3, September 17, 2026, 11:00 - 12:15

We develop a three-dimensional flexible thermoelectric (TE) network for energy harvesting and sensing. Organic and carbon-based aerogels have traditionally dominated thermoelectric (TE) research, yet their performance remains limited ($zT < 0.1$ at 300 K). In this work, we present a stepwise synthesis strategy for the first high-performance n-type inorganic aerogel. The optimized aerogel, with 95% porosity, achieves a power factor of 34.8 μW m^{-1} K^{-2} and an ultralow thermal conductivity of 0.061 W m^{-1} K^{-1}, resulting in zT values of 0.17 at 300 K and 0.24 at 383 K. A vertical TE generator prototype incorporating six aerogel legs delivers a gravimetric power output of 76 μW g^{-1} under a temperature difference of ~60 K. To overcome mechanical brittleness, a bioinspired polyimide-encapsulated aerogel was developed, achieving a compressive strength of 1.4 kPa while maintaining excellent TE performance. This work provides a generalizable design strategy for flexible, high-performance inorganic aerogels, enabling new opportunities for lightweight and wearable energy harvesting applications. We also report a monolithic bimodal sensor based on a three-dimensional Ag2Se thermoelectric network that enables simultaneous and decoupled detection of temperature and pressure within a single device. The sensor demonstrates a high temperature sensitivity of −122.7 μV K−1 with a fast response time of ~0.14 s, and a high pressure sensitivity of −2.94% kPa−1 with a fast response time of about 0.08 s, indicating excellent signal isolation between the two sensing channels. When combined with deep learning, the sensor enables a real-time intelligent sorting system that achieves 96% recognition accuracy across nine materials, outperforming single-mode sensing approaches. This work provides an integrated multimodal sensing solution that advances the deployment of embodied AI in complex environments.

Atomic to Nanoscale Chemical Fluctuations: The Catalyst for Enhanced Thermoelectric Performance in High-Entropy Materials

Kunpeng Zhao[1], Xun Shi[2]
[1]Shanghai Jiao Tong University, China, [2]Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Zintl-2, September 16, 2026, 11:00 - 12:15

High-entropy materials have expanded the frontier for discovering uncharted physicochemical properties. The phenomenon of chemical fluctuation is ubiquitous in high-entropy materials, yet its role in the thermoelectric field is often overlooked. Herein, we designed and synthesized a series of (Mg0.94-nYb0.26Sr0.26Znm)(MgnCd0.69Zn0.69-mNax)(Sb1.74Ca0.26) samples characterized by ultrahigh configurational entropy. These samples exhibit a homogeneous single-phase structure at macroscopic and microscopic scales, yet display notable chemical fluctuations at the atomic to nanoscale. These fluctuations, along with the unusual atomic occupations, lead to an exceptionally low lattice thermal conductivity akin to that of amorphous materials. Combining the optimized carrier concentration and well-maintained carrier mobility, we ultimately achieved a high zT value of 1.2 at 750 K, outperforming most previously reported AB2Sb2-type Zintls. This study underscores that the atomic to nanoscale chemical fluctuations are the crucial catalyst for the enhanced thermoelectric performance in high-entropy materials.

Poster Presentations

Enhancing Thermoelectric Figure of Merit (zT) in β-Ag2Se via Aliovalent Doping

Ms Aradhana Acharya[1]
[1]PhD Student, India

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

High-performance thermoelectric materials are essential for efficient low-temperature (300–400 K) heat energy harvesting, with n-type Ag_2Se being a promising candidate. To further enhance the thermoelectric figure of merit (zT) of Ag_2Se, aliovalent doping has emerged as a key strategy.[1,2] For instances, β-Ag_2Se doped with Zn resulted in zTmax to be 1.3 at 393 K.[3] However, achieving wet-chemical aliovalent doping of Ag_2Se at ambient temperatures has proven challenging. In this work, we report a record-high zTmax of 1.57 at 398 K for an optimally Cd(II)-doped Ag_2Se sample, specifically in the structurally phase-pure $Ag_{1.98}Cd_{0.02}Se$, which was successfully synthesized via an aqueous-based method at room-temperature (300 K). The $Ag_{1.98}Cd_{0.02}Se$ sample also exhibited an impressive average zTavg of 1.12 over the temperature range of 315–400 K.[4] Density functional theory (DFT) calculations for both the pristine and doped samples revealed significant changes in the electronic band structures, including notable modulations in the density of states near the Fermi energy, particularly for the Ag-3d states. The remarkable thermoelectric performance of $Ag_{1.98}Cd_{0.02}Se$ is attributed to an optimization of charge carrier induced by the Cd(II)-doping.

Reference
1. D. Li, J. H. Zhang, J. M. Li, J. Zhang, X. Y. Qin, Mater. Chem. Front. 2020, 4, 875.
2. S. Ahmad, P. Sarkar, P. Bhatt, S. Bhattacharya, M. Navaneethan, R. Basu, R. Bhatt, A. Bohra, A. K. Debnath, K. P. Muthe, S. Vitta, A. Singh, Appl. Phys. Lett. 2022, 121, 173905.
3. Y. Abusa, P. Yox, G. Viswanathan, J. Opare-Addo, A. Sarkar, V. Kyveryga, E. Smith, O. I. Lebedev, K. Kovnir, J. Am. Chem. Soc. 2024, 146, 11382.
4. A. Acharya, S. Nagaraja, N. Hassan, K. Tarafder, N. Ballav, Small 2025, 21, 2411498.

Thermoelectric properties of mechanochemically doped Cu0.6Ag1.4Se sample series

Mgr. Dáša Drenčaková[1], Dr. Marcela Achimovičová[1], Dr. Emmanuel Guilmeau[2], Prof. Jaroslav Briančin[1], Dr. Viktor Puchý[3]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Slovakia, [2]CRISMAT, CNRS, Normandie University , France, [3]Institute of Materials Research, Slovak Academy of Sciences, Slovakia
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Eucairite (CuAgSe), a ternary copper(I)–silver selenide, belongs to a class of metal chalcogenides with highly attractive functional properties. A distinctive feature of CuAgSe is its switch between n type and p type conductivity associated with a phase transition1. This, combined with its extremely low thermal conductivity and high carrier mobility, makes CuAgSe a very promising thermoelectric material, particularly in the low to mid-temperature range. Environmentally friendly synthesis routes are becoming increasingly important in thermoelectric materials research. Ball milling represents a simple, solvent-free, one-pot method that operates at room temperature and ambient pressure, significantly reducing processing time. The present study investigates how doping with various amounts of zinc or iron affects the thermoelectric properties of non stoichiometric $Cu_{0.6}Ag_{1.4}Se$. Previous publications differ in the stoichiometry, dopants, and synthesis methods used, yet consistently report substantial changes in the thermoelectric behaviour of doped CuAgSe2,3. Mechanochemical syntheses of $Cu_{0.6}Ag_{1.4}Se$ doped with 3, 6, and 10 % Zn or Fe at the Cu site were performed using a planetary ball mill starting from elemental powders. XRD analysis confirmed that the reactions were completed after only 7 minutes of milling. The resulting powders were consolidated into pellets using spark plasma sintering (SPS). Phase composition, morphology, specific surface area, mean particle size, and thermoelectric properties of the samples were subsequently examined.

Acknowledgement
This work was supported by the Slovak Grant Agency VEGA (02/0036/23) and the Slovak Research and Development Agency (APVV-24-0353).

1 Han, C. et al. J. Am. Chem. Soc. 2014, 136, 17626–17633.
2 Nguyen, T. H. et al. J. Alloys Compd. 2021, 852, 157094.
3 Qiu, P. F. et al. J. Mater. Chem. A 2015, 3 (44), 22454–22461.

Synthesis, Characterization, and Thermoelectric Properties of Copper Bismuth Sulphides.

Nasir Alzzahrani[1]
[1]University Of Reading, United Kingdom

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

In recent years, significant attention has been directed toward metal Sulphides as promising thermoelectric materials. Their low cost, environmental friendliness, and high natural abundance make them highly attractive candidates for future commercial thermoelectric applications. Our recent investigations have focused on materials in the Cu-Bi-S family, which includes Cu3BiS3. Initial synthesis of the stoichiometric phase by high-temperature methods, revealed the presence of approximately 3 wt.% elemental bismuth impurity. Refinement of the reactant composition by introducing bismuth deficiency, resulted in the successful formation of phase-pure $Cu_3Bi0.94S_3$. This material exhibits an exceptionally low thermal conductivity of k = 0.38 W m^{-1} K^{-1} at 298 K. Furthermore, on increasing the temperature, the thermal conductivity decreases to a minimum of k = 0.29 W m^{-1} K^{-1} at 423 K, before rising again at higher temperatures. Substitution of copper by silver, leads to a further reduction of up to 26 % in the thermal conductivity.

DSC data indicate that the minimum in thermal conductivity is associated with a phase transition. This is supported by variable-temperature powder neutron diffraction which reveal an orthorhombic-to-orthorhombic transition, involving a change from full occupancy of 4-fold sites by copper/silver to partial occupancy of 8-fold sites. This, together with the increasing atomic displacement parameters, appears to indicate the onset of appreciable ionic mobility. This is further evidenced by ionic conductivity data. Seebeck coefficient data suggest a p–n crossover in charge carriers occurs on heating. The impact on the electrical transport properties of hole doping induced by copper deficiency in Cu3-xBi0.94S3, and substitution with Ni and Se has also been investigated.

A Battery-Free, Waste-Heat-Powered IIoT Architecture for Real-Time Steam Trap Diagnostics

Dr. Raúl Aragonés Ortiz[1,2], Roger Malet[1,2], Andres Ibañez[1], Alex Prim[1], Joan Mulet[1], Kaku Saito[3], Leonardo de Freitas Leucas[3], Paulo Henrique Ferreira[4]
[1]Alternative Energy Innovations - AEInnova, Spain, [2]UAB, Spain, [3]Petrobras, Brazil, [4]Petrobras, Brazil

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The large-scale deployment of Industrial Internet of Things (IIoT) systems is constrained by a fundamental bottleneck: reliable and sustainable power supply for distributed sensing in harsh industrial environments. Battery-dependent solutions introduce maintenance costs, safety risks, and environmental impact, limiting scalability—particularly in energy-intensive sectors [1]. This work presents a novel, fully autonomous IIoT architecture for real-time steam trap monitoring, powered exclusively by waste heat recovery. The proposed system builds upon recent advances in battery-less, heat-powered IIoT systems for industrial applications, demonstrating their feasibility in demanding environments [2].

The system exploits thermoelectric generators (TEGs) to convert residual thermal energy from steam infrastructure into electrical power, enabling continuous, battery-less operation of sensing, edge processing, and wireless communication. The device integrates multi-modal sensing—combining temperature differential (ΔT) analysis and ultrasonic detection—with embedded edge intelligence to enable robust, in-situ classification of steam trap conditions. Unlike conventional solutions, which rely on low-frequency data transmission due to energy constraints, the proposed system supports high-resolution monitoring without compromising energy autonomy. Data is transmitted via LoRaWAN, ensuring long-range, low-power connectivity suitable for large-scale industrial deployment.

The architecture was validated in a real-world pilot at a Petrobras thermoelectric facility of Cubatao (Brazil). Experimental results demonstrate accurate detection of steam leakages and abnormal operating regimes under varying conditions.

By eliminating batteries and minimizing infrastructure requirements, the solution reduces operational costs and enhances safety in hazardous environments. This work establishes a new paradigm for scalable, energy-autonomous IIoT systems in industrial applications.

Bibliography

[1]T. Pirson and D. Bol, “Assessing the embodied carbon footprint of IoT edge devices with a bottom-up life-cycle approach,” Sustainable Computing: Informatics and Systems, Elsevier, 2021.
[2] R. Aragonés, R. N. Alegret, J. Oliver, and C. Ferrer, “Autonomous Battery-Less Vibration IIoT Powered by Waste Heat for Chemical Plants Using NB-IoT,” IEEE Sensors Journal, vol. 22, no. 15, pp. 15448–15456, Aug. 2022.

Correlation between Seebeck Coefficient and Chemical Species in PEDOT:PTSA supported on PET fibers.

Dr. Hideki Arimatsu[1], Mr. Ryo Takagi[2], Mr. Yuki Osada[3], Prof. Takuya Fujima[4]
[1]Tokyo City University, Japan, [2]Tokyo City University, Japan, [3]Tokyo City University, Japan, [4]Tokyo City University, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric materials based on poly(3,4-ethylenedioxythiophene) (PEDOT) are promising for flexible thermoelectric applications, although their performance is insufficient for practical use. In our previous work, we demonstrated that PEDOT-based thermoelectric materials, when fabricated on polyethylene terephthalate (PET) fibers with p-toluenesulfonic acid (PTSA), achieved both positive and negative Seebeck coefficients with magnitudes reaching several mV/K while maintaining high electrical conductivity [1]. This distinctive thermoelectric property strongly correlated with the distortion of PEDOT molecular chains. Furthermore, it has been proposed that residual additives, such as PTSA and sodium persulfate (SPS), within the PEDOT network contribute to its thermoelectric properties [2], [3]. This study investigated the impact of residual additives within the material on the thermoelectric properties of felt-supported PEDOT:PTSA.

The samples were prepared by polymerizing PEDOT and loading it with PTSA onto felt fabrics (100% PET) in a reaction solution containing EDOT, SPS, and PTSA, which were dispersed in purified water. The resulting materials were analyzed using Raman spectroscopy and X-ray photoelectron spectroscopy (XPS), and their thermoelectric properties were assessed by measuring their Seebeck coefficient and sheet resistivity.

The XPS S2p spectra indicated that the proportions of sulfonate and sulfate species in the samples varied depending on the composition of the reaction solution. When the relative amount of sulfate species derived from SPS increased with respect to PEDOT, the Seebeck coefficient shifted from positive to negative. On the other hand, the sheet resistance tended to increase with increasing sulfonate content derived from PTSA.

References

[1] H. Arimatsu, Y. Osada, R. Takagi, T. Fujima, Materials 18 (2025) 838.
[2] H. Arimatsu, Y. Osada, R. Takagi, T. Fujima, Polymers 13 (2021) 3518.
[3] H. Arimatsu, Y. Osada, R. Takagi, Y. Ohira, T. Hijikata, T. Fujima, Materials 18 (2025) 619.

Mechanochemical synthesis as a unique tool to tackle some challenges in thermoelectrics: A case study of copper sulfide

Matej Baláž[1], Saba Sepahban Shahgoli[2], prof. Dr. Umut Aydemir[2]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Slovakia, , Slovakia, [2]Koç University Boron and Advanced Materials Application and Research Center (KUBAM), Türkiye
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

High-energy ball milling is very often used among the thermoelectrics community. However, not all researchers really acknowledge and grasp the great potential that the mechanochemical process offers1. Being much more than just a mere homogenization technique, it enables the synthesis of desired products in a solvent-free manner and introduces the effect of nanostructuring, which is so important for TE performance later on. The present contribution will briefly showcase the current state-of-the-art of mechanochemistry and illustrate a few examples of successful synthesis of TE-suitable sulfides formed mostly from Earth-abundant elements in our laboratory2. In the end, the possibility to prepare copper sulfides (well-known TE materials) via a mixing-induced self-propagating reaction will be demonstrated3. The combustive way for preparing TE materials is known, however, the process is ignited by a high temperature4. In our case, only high-speed mixing of the elements is required. The contribution will conclude with the open question why the successfully synthesized material exhibits zT value of 0.05 at 625 K, which is about half of that reported in 5. Much better performance of copper sulfides can be achieved via doping6. This study is supported by the Slovak Research and Development Agency under Contract No. APVV-24-0353.

References

1. Stolar, T., et al., Chem 2026, 12.
2. Baláž, P., et al., ACS Sust. Chem. Eng. 2021, 9, 2003-2016.
3. Baláž, M., et al., ChemRxiv, 2026, https://chemrxiv.org/doi/full/10.26434/chemrxiv-2025-l4n3s-v2.
4. Su, X., et al., Nat. Comm. 2014, 5, 4908.
5. Ge, Z.-H., et al., Adv. Energ. Mater. 2016, 6, 1600607.
6. Yan, X., et al., Journal Adv. Ceram. 2024, 13, 641-651.

Passive control of heat flux using a thermoelectric module

Mr Rachid BELRHITI NEJJAR[1], Mr Fabien Giovannelli[1], Mr Etienne Lemaire[1], Mr Guillaume Nataf[1], Mr Lionel Haumesser[1]
[1]University Of Tours, BLOIS, France

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Modulating heat flux is a crucial step toward developing a new computing paradigm based on thermal currents, capable of overcoming the main limitations of conventional electronics such as excessive energy consumption and overheating [1]. A promising approach involves the use of thermal diodes. In this context, thermoelectric modules provide an effective solution, theoretically allowing the passive modulation of heat flux by a factor of (1+ZT), without additional electrical energy input and using a simple load resistor [2].

Two main boundary conditions are reported in the literature. The first assumes a constant temperature difference (ΔT) while varying the thermal conductivity using a load resistance [3]. However, this approach still lacks experimental validation. The second assumes a constant input heat flux with fixed output temperature, leading to a variation of ΔT depending on the load resistance [2]. In this work, we investigate both cases. With constant ΔT, our homemade device yields a heat flux variation reaching 48% of the theoretical value. Under constant heat flux conditions, experimental results demonstrate variations in the distribution of Peltier and Fourier heat fluxes, while Joule losses are neglected .

Modulating the total heat flux paves the way for the development of thermal diodes, whilst variations in heat flux distribution offer new possibilities for adaptive cooling applications.

References

[1] G.F.Nataf et al., Nat Rev Mater 9, 530–531, (2024).
[2] G.Min, Energy Environ. Sci., 15, 356, (2022).
[3] A. Massaguer Colomer et al., Applied Energy 154 ,709–717, (2015).

Modified PEDOT:PSS composite polymer for fabrication of Sb2Te3 nanoparticle based thermoelectric hybrid materials

Oskars Bitmets[1], Kaspars Pudzs[1], Bejan Hamawandi[1]
[1]Institute Of Solid State Physics, University Of Latvia, Latvia

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Hybrid thermoelectric materials can be made from nanoparticles and polymers. However, most polymers have insulating properties and high electrical resistance. The presence of the insulating material may cause an additional barrier between thermoelectric nanoparticles, affecting the charge carrier transport and creating nonconducting regions in the hybrid material. PEDOT:PSS is one of the most popular and widely studied polymers with a high electrical conductivity. Unfortunately, PEDOT:PSS tends to form a crystalline structure, resulting in a fragile hybrid material with a high chance of crack and defect formation. Additionally, PEDOT:PSS tends to dominate the Seebeck coefficient, which affects the thermoelectric power factor.

In this work, we have created a hybrid thermoelectric material from Sb2Te3 nanoparticles and a modified composite polymer consisting of PEDOT:PSS and PEO. The composite polymer's properties were tuned further with NaBH4. The hybrid materials Seebeck coefficient, specific electrical conductivity and power factor has been determined. Structure of the material was studied with scanning electron microscopy. Ionization energies were determined with electron emission spectroscopy, to characterize the compatibility of Sb2Te3 nanoparticles and PEDOT:PSS composite polymer.

Results show that adding PEO to PEDOT:PSS improves the quality of the hybrid films and prevents crack formation. Seebeck coefficient of PEDOT:PSS was successfully tuned by dedoping. Modified PEDOT:PSS leaves a lesser impact on Seebeck coefficient and can be used in preparation of hybrid materials, resulting in improved power factor values. The formation of Sb2Te3 percolation network was observed.

Acknowledgment
This work was supported by the Latvian Council of Science project No. lzp-2023/1-0456.

A methodology to correlate local chemistry with electronic and phononic transport in thermoelectrics

Florian A. Busch[1], Eleonora Isotta[1], Kyuseon Jang[1], Siyuan Zhang[1], Oluwaseyi Balogun[2], Jochen M. Schneider[3], G. Jeffrey Snyder[2], Christina Scheu[1]
[1]Max Planck Institute for Sustainable Materials, Germany, [2]Northwestern University, USA, [3]RWTH Aachen University, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric generators bear the prospect to enhance the production of emission free electricity by converting heat to electricity. Especially grain boundary engineering approaches have yielded good results in enhancing the figure of merit by lowering the thermal conductivity in multiple cases. Our previous investigations indicate synthesis-induced chemical inhomogeneities in the grain boundary region to largely influence the transport properties. A holistic framework of local chemical influences on the transport properties in thermoelectrics remains to be fully developed.

Electron- and laser-based analytical imaging techniques are performed on Sn1-xMnxTe and Mg3Sb2-yBiy materials to explore the effect of chemistry on the thermal (κ) and electrical conductivity (σ) of individual grain boundaries, respectively. Frequency domain thermoreflectance experiments and micro-scale four-point probe measurements are performed to determine the local κ and σ. The results are discussed as a function of composition, based on high precision wavelength dispersive X-ray spectroscopy mappings.

Chemical inhomogeneities, such as micro-segregations, are found to largely influence the local transport properties. Our findings expand the preexisting knowledge of κ suppression at grain boundaries by consideration of the distribution of dopants within the material. Our pathway and findings outline the importance of high-precision chemical analyses for accurately discussing thermal and electrical transport in thermoelectrics.

THERMOELECTRIC PROPERTIES AND BONDING ANALYSIS ON NATURALLY OCCURRING TENNANTITE FROM COPIAPO, CHILE

Dr. Raúl Cardoso-Gil[1], Dr. Patricio Vargas[2], Mrs. Nubia Caroca-Canales[1], Dr. Danny Guzman[3], Dr. Igor Veremchuk[1,4], Prof. Yuri Grin[1]
[1]Max-Planck-Insitut CPfS, Desden, Germany, [2]Universidad Técnica Federico Sta. María, Chile, [3]Universidad de Copiapó, Copiapó, Chile, [4]Helmholz-Zentrum Dresden-Rossendorf, Germany
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The mineral tennantite with chemical composition Cu10(Fe, Zn)2As4S13 is a member of the tetrahedrite-group. It crystalizes cubic in the space group I-43m, with lattice parameters a = 10.190 Å and two formula units per unit cell. Natural intergrowths of well-formed crystals show grey-black colour and metallic lustre[1,2].

Tetrahedrite self is an Antimony-based mineral and, due to its natural abundance, attracted special attention for thermoelectric application[3]. As observed in the calculated electronic density of states of tetrahedrite and tennantite, these show similar and appropriate electronic conditions for a potential thermoelectric material. In this context, mineral samples of tetrahedrite-tennantite, e.g. minerals containing different Sb/As ratios, and from different mineral deposits, have been also studied concerning their thermoelectric properties[4].

The atomic arrangement in tennantite provides an interesting framework for controlling thermoelectric properties. The presence of different elements leads to bonding inhomogeneity. At the same time, the presence of arsenic with an electron lone pair may influence defects in the crystal lattice, thereby directly affecting the heat transport properties.

With the aim to gain further insights into the relationship between crystal-chemistry and thermoelectric properties, our investigation is focussed in a naturally occurring tennantite from Copiapó - Chile, with the chemical composition Cu9.9(1)Fe0.46(2)Zn1.65(1)As3.69(3)Sb0.25(1)S13.1(1). We studied its crystal structure, performed chemical bonding analysis, and characterized its thermoelectric properties – Seebeck coefficient, electrical resistivity and thermal conductivity– topics addressed in this work.

Literaure
[1] www.mindat.org
[2] Pauling, L.; Neuman, E.W. The Crystal Structure of Binnite, (Cu,Fe)12As4S13, and the Chemical Composition and Structure of Minerals of the Tetrahedrite Group. Z.Kritallgr. 1934, 54.
[3] Chetty, R.; Bali, A.; Mallik, R.C. Tetrahedrites as thermoelectric materials: an overview. J.Mater.Chem. C3, 2015, 12364.
[4] Levinsky, P., Vaney, J.-B.; Candolfi, C., Dauscher, A.; Lenoir, B.; and Hejtmánek, J. Electrical, Thermal, and Magnetic Characterization of Natural Tetrahedrites-Tennantites of Diferent Origen. J.Elec.Mat.45, 2016, 1351.

Processing of thermoelectric intermetallic compounds for a waste heat harvesting module

Xinxi Huang[1], Alessandro Difalco[1], Edoardo Berardino, Marcello Baricco[1], Carlo Fanciulli[2], Alberto Ferrario[3], Stefano Boldrini[3], **Alberto Castellero**[1,3]
[1]University of Turin, Italy, [2]CNR-ICMATE, Italy, [3]CNR-ICMATE, Italy
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Large-scale production of thermoelectric (TE) generators requires the use of materials affordable in terms of supplying and cost, with reproducible as well as reliable thermoelectric and thermophysical properties.

In this work, we selected two categories of materials for the assembling of TE modules to be used in different temperature ranges:
- Half Heusler alloys for medium/high temperature (400-600 °C);
- ZnSb and Zn4Sb3 intermetallic compounds for medium/low temperature (RT-400°C).

Half Heusler alloys were selected in order to guarantee thermomechanical and thermoelectric compatibility between the n and p legs of the module. Therefore, various processing routes (e.g. arc-melting of elemental metals, rapid solidification by melt-spinning, ball milling, sintering, isothermal annealing) were employed in order to optimize thermoelectric and mechanical properties by the refinement of the microstructure of the synthesized alloys.
In the case of ZnSb and Zn4Sb3 intermetallic compounds, the effect of extrinsic doping and self doping on the thermoelectric properties of has been investigated by using raw materials with different purity and by changing the ratio between the constituent elements. The final target is to reach a conversion efficiency comparable to that of commercial systems, currently based on toxic and critical raw materials, such as Te.

Samples produced by the different processing routes were characterized in terms of structural, microstructural, thermal, mechanical and thermoelectric properties. The effect of the process on the microstructure (e.g., grain boundaries densities), transport and mechanical properties is studied. Materials with optimized properties were selected for assembling lab-scale thermoelectric generator prototypes.

A. Castellero, S. Boldrini, A. Ferrario and C. Fanciulli acknowledge financial support from Ricerca di Sistema Elettrico Nazionale PROGETTO PTR_25_27_CNR_1_4 – “Materiali e dispositivi di frontiera per applicazioni energetiche" (CUP: D13C25002440001).
Authors from Università di Torino acknowledge support from the Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023-2027" (CUP: D13C22003520001).

Thermoelectric and electric properties of CuI:Ag and PEDOT composites

Renāte Čelmodejeva[1], Bejan Hamawandi, Oskars Bitmets, Kaspars Pudzs
[1]Institute of Solid State Physics, University of Latvia, Latvia

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Hybrid organic-inorganic composites based on conductive polymers are promising materials for thermoelectric energy conversion near room temperature due to their low thermal conductivity and tuneable electrical transport properties. In this work, composites based on silver-doped Copper Iodide (CuI:Ag) particles and conductive polymer PEDOT were investigated using both water-based and anisole-based systems.

Composites with varying CuI:Ag content were prepared in the form of films and pellets, allowing evaluation of the influence of composition, processing route, and morphology on thermoelectric performance. Electrical conductivity, Seebeck coefficient and Power Factor were determined for all samples.

The anisole-based films showed a pronounced increase in Seebeck coefficient with increasing particle content, for 80% CuI:Ag content Seebeck is the highest. Electrical conductivity remained low, resulting in low Power Factor. In contrast, anisole-based pellet samples exhibited significantly higher Seebeck coefficients at value 2019 $uV \cdot K^{-1}$, which improved thermoelectric response even though the conductivity is pretty low.

For water-based PEDOT film composites, electrical conductivity increased from 512 $S \cdot m^{-1}$ for pure polymer to a maximum of 670 $S \cdot m^{-1}$ at 40% CuI:Ag content, followed by a gradual decrease at higher particle loading. The Seebeck coefficient increased continuously with CuI:Ag concentration. The highest power factor for thin films was observed at 60% CuI:Ag .
Water-based pellet samples demonstrated a different behaviour. Pure CuI:Ag pellets showed a Seebeck coefficient of 1326 $uV \cdot K^{-1}$ with low conductivity of 4 $S \cdot m^{-1}$, which also gave the highest Power Factor of 7 $W \cdot m^{-1} \cdot K^{-1}$.

The results demonstrate that thermoelectric properties strongly depend on composite composition, polymer matrix, and sample morphology. Water-based PEDOT composites provide higher electrical conductivity in films, whereas pellet processing significantly enhances Seebeck response and Power Factor.

Acknowledgement: The Latvian Council of Science funded this research, grant number lzp-2023/1-0456 "Advancing Sustainable Thermoelectric Hybrid Systems Utilizing Glass-Forming Low Molecular Weight Compounds".

Self-nanostructuring advances thermoelectric copper selenide

Dr. Chen Chen[1]
[1]Tsinghua University, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Copper selenide (Cu2Se), as a superionic conductor, exhibits extraordinary research value by virtue of the “liquid like” migration behavior of Cu ions. However, its inherent Cu vacancies and mobile Cu ions strongly scatter charge carriers, thereby limiting carrier mobility. Under the action of temperature and electric fields, directional long range migration of Cu ions leads to metal deposition and structural degradation, and these factors collectively hinder the device fabrication process based on Cu2Se. Here we show a construction strategy of self-nanostructures (pore-precipitate pairs), by building coherent interfaces with high lattice matching degree in the Cu2Se system and inducing the generation of a two dimensional hole gas (2DHG), thereby achieving coordinated optimization of thermoelectric performance and service stability. In studies based on density functional theory (DFT), it has been confirmed that the formation of 2DHG effectively enhances carrier mobility and electrical conductivity. Meanwhile, the self-nanostructures induced by in situ reactions can significantly enhance phonon scattering and effectively restrict the long range migration of copper ions. Ultimately, this material achieves a peak ZT value of 3.34 at 973 K, attains a high average ZT of 1.66 over the wide temperature range of 432 - 973 K, and obtains a highly stable thermoelectric conversion efficiency of approximately 12 % at ΔT = 530 K, setting a new record for the comprehensive thermoelectric performance of this system. This strategy provides a new paradigm for the scientific construction of high performance thermoelectric materials.

A universal approach to high-performance thermoelectric module design for power generation

Jinxuan Cheng[1]
[1]Harbin Institute of Technology (shenzhen), China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Because most thermoelectric modules are fabricated using traditional welding processes, optimal efficiency is difficult to achieve. Although the nano-silver sintering process can provide an efficient approach to connect the electrodes and thermoelectric legs, its applicability is restricted to the metallization layer based on Ag, Pt, and Au. As a promising solution, transient liquid phase bonding (TLPB) enables the realization of full-compound joints with high melting points, even at low bonding temperatures. Given that this method can be guided by phase diagrams, it has great potential to facilitate the realization of high conversion efficiency in various mid- and high-thermoelectric modules. In this work, a highperformance, single-stage, seven-couple germanium telluride (GeTe)/Mg3Sb2 module is fabricated at 533 K via TLPB, and the module realizes an hmax of 15.1% and a power density of 0.73 W cm−2 at a DT of 473 K. Additionally, the module's performance remained nearly unchanged throughout 150 h of service, with a hot-side temperature of 773 K and a cold-side temperature of 300 K. Guided by phase diagrams, the assembly of the low- (Bi2Te3-based) and high-temperature (half-Heusler-based) modules has also been realized. We provide a promising and general route in the assembly of full-temperature-range (300–1,073 K) thermoelectric devices.

Evaluation of Contact Engineering Strategies for Achieving Low Electrical Resistance in n-Type Mg_3Sb_2-Based Thermoelectrics

Oleksandr Horniichuk[1], Panagiotis Ioannou[2], Seyedmohammad Mortazavinatanzi[3], Theodora Kyratsi[2], Radoslaw Chmielowski[1]
[1]Imra Europe SAS, , France, [2]Department of Mechanical and Manufacturing Engineering, School of Engineering, University of Cyprus, Cyprus, [3]ParsNord, Sweden

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

n-Type Mg3Sb2-based Zintl compounds are promising mid-temperature thermoelectrics due to their high power factor, low lattice thermal conductivity, and earth-abundant chemistry. However, device integration is hindered by the difficulty of forming mechanically stable, low-resistance contacts, a challenge amplified by Mg volatility and strong interfacial reactivity that can increase contact resistance.

In this context, several approaches – including electrochemical deposition and one- and two-step SPS processes employing different diffusion barriers – were explored to achieve high-quality electrical contacts on Mg3Sb2-based materials.

The contact interfaces were examined by SEM/EDX, including elemental mapping to assess interdiffusion and reaction layers. Electrical contact resistivity was determined using a scanning probe method, and mechanical robustness was evaluated through mechanical bonding strength measurements. This workflow enabled the identification of the most suitable contact configuration for device integration.

Correlation of Electronic Structure and Thermoelectric properties of Cr(Mo, V)Nx Thin Films Studied by Synchrotron and Lab-based X-ray Spectroscopy

Susmita Chowdhury[1,2], Victor Hjort[2], Dr. Rui Shu[2], Dr. Grzegorz Greczynski[2], Dr. Arnaud le Febvrier[1,2], Dr. Per Eklund[1,2], Dr. Martin Magnuson[1,2]
[1]Inorganic Chemistry, Department of Chemistry-Ångström Laboratory, Uppsala University, Sweden, [2]Thin Film Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Chromium-based nitrides are used in hard, resilient coatings and show promise for thermoelectric applications due to their combination of structural, thermal, and electronic properties. Here, we investigate the electronic structures and chemical bonding correlated to the thermoelectric properties of epitaxially grown chromium-based multicomponent nitride Cr(Mo, V)Nx thin films. The small amount of N vacancies causes Cr 3d and N 2p states to appear at the Fermi level and reduces the band gap in Cr0.51N0.49. Incorporating holes by alloying of V in N-deficient CrN results in an enhanced thermoelectric power factor with marginal change in the charge transfer of Cr to N compared with Cr0.51N0.49. Further alloying of Mo, isoelectronic to Cr, increases the density of states at the Fermi level due to hybridization of the (Cr, V) 3d and Mo 4d-N 2p states in Cr(Mo, V)Nx. This hybridization and N off-stoichiometry result in more metal-like electrical resistivity and reduction in Seebeck coefficient. The N deficiency in Cr(Mo, V)Nx also depicts a critical role in reduction of the charge transfer from metal to N site compared with Cr0.51N0.49 and Cr0.50V0.03N0.47. In this study, we envisage ways for enhancing thermoelectric properties through electronic band engineering by alloying and competing effects of N vacancies.

Thermoelectric properties of defective scandium nitride nanostructures from first principles

Luigi Cigarini[1], Urszula Danuta Wdowik[1], Dominik Legut[2,1]
[1]It4innovations, Všb – Technical University Of Ostrava, Czech Republic, [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The thermoelectric properties of scandium nitride (ScN) thin films vary significantly with the experimental conditions [1,2]. In this context, it is well established that structural defects and chemical impurities play a crucial role, affecting the thermoelectric performance of ScN nanostructures [3,4]. Nevertheless, the underlying transport mechanisms and how they are affected remain unclear. Reported measurements show large variability, but strategies to enhance efficiency often yield conflicting results [4,5]. Recent progress has demonstrated the possibility of significantly reducing thermal transport in ScN thin films [6,7]; however, achieving an effective improvement in thermoelectric efficiency requires that this reduction is not neutralized by a decrease in the power factor.

In this presentation, using the Landauer approach, we analyze how different types of imperfections alter electronic and thermal transport in the ScN lattice. We analyze two types of defects: those that are commonly present and those that can be intentionally introduced to tailor transport properties. Among the latter, we examine the effects of the intentional substitution of scandium atoms with other transition metals, such as niobium, tungsten, and magnesium [8]. Among the former, we identify two dominant classes with opposing effects: (i) contiguous nitrogen vacancies, which enhance electrical conductivity but reduce the magnitude of the Seebeck coefficient (S), and (ii) oxygen substitutions coupled with nearby stacking faults, which increase the magnitude of S while hindering electrical conductivity [9].

References:

[1]. Phys. Rev. Mater. 3, 020301 (2019).
[2]. J. Mater. Chem. C 4, 3905 (2016).
[3]. Phys. Rev. B 86, 195140 (2012).
[4]. Phys. Rev. B 97, 085301 (2018).
[5]. J. Appl. Phys. 115, 153508 (2014).
[6]. Appl. Surf. Sci. Adv. 25, 100674 (2025).
[7]. ACS Appl. Energy Mater., 5 (9), 11025 (2022).
[8]. L. Cigarini et al., in preparation.
[9]. Appl. Surf. Sci. Adv. 31, 100923 (2026).

Thermoelectric performance of Ag2Se films grown by Pulsed Hybrid Reactive Magnetron Sputtering (PHRMS) on glass and flexible substrates

Andres Conca[1], Jose Maria Domínguez-Vázquez[1], Ketan Lohani[1], Alfonso Cebollada[1], Marisol Martín-González[1]
[1]Instituto de Micro y Nanotecnología, IMN-CNM, CSIC (CEI UAM+CSIC), Spain
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Ag_2Se is one of the best-performing thermoelectric materials, particularly near the RT range, however most of the works are on bulk form while studies on thin films remain scarce. Here we present a study on Ag_2Se thin films, deposited by our own developed technique of Pulsed Hybrid Reactive Magnetron Sputtering (PHRMS)1. In this technique, Ag continuous deposition by sputtering methods is combined with pulsed Se deposition, for which an electrically actuated pulsed effusion cell is used.

In this work we have grown, on solid and flexible substrates, Ag_2Se thin films by PHRMS methods with a wide range of compositions, from Ag-rich to Se-rich, optimising the stoichiometry to maximise the thermoelectric performance. We present comprehensive structural and thermoelectric results of Ag_2Se thin films, correlating single β-phase crystallization to thermoelectric performance maximisation. Here we obtain highest PF values of 4000 $\mu W/(m \cdot K^2)$ surpassing actual values from the literature [1,2], that could yield world record values of zT at RT of any previous thermoelectric material.

Acknowledgements: Financial support of ERC Advanced Grant POWERbyU (ERC-2021-ADG-101052603) is gratefully acknowledged.

References
1 J. A. Perez-Taborda, et al. , Adv. Energy Mater., 2018, 8, 8.
2 D. Yang, et al. , Nat. Commun., 2024, 15, 923.

Influence of low-, mid- and high-temperature thermoelectric materials on Radioisotope Thermoelectric Generators (RTGs) design and performance

Stylianos Kyrimis[1], Pawel Ziolkowski[1], Christian Stiewe[1], Eckhard Müller[1,3], Johannes de Boor[1,2]
[1]German Aerospace Center, Germany, [2]3Institute of Technology for Nanostructures (NST) and CENIDE, University of Duisburg-Essen, Germany, [3]Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry and ZfM/LaMa, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Lunar exploration requires a reliable supply of electrical power, independent of solar irradiation availability, which can be provided by Radioisotope Thermoelectric Generators (RTGs). RTGs contain a radioisotope heating unit coupled with thermoelectric modules (TEMs). Thermal insulation covering all free surfaces causes most of the source heat to flow through the TEMs which convert part of the transmitted heat into electricity through the Seebeck effect. The RTG's performance is driven by the temperature difference between the TEM's hot side and its cold side, connected to radiator fins attached to the outer RTG surface. Because of the complex interdependencies of the design parameters, optimizing the RTG design necessitates multi-parametric computational tools which can holistically model the system behaviour. We developed a thermoelectric network model which represents the RTG as a circuit of thermal resistors and thermoelectric elements. By solving the heat transfer equation, the temperature difference across all components can be calculated while evaluating the thermoelectric heat balance equation provides an estimate of the RTG's performance. The network model is coupled with a Finite Element Analysis (FEA) model for in-depth analysis and validation. Employing thermal boundary conditions typical for the lunar surface, we optimized the RTG design to maximise its gravimetric power density while respecting the deployed TEM's hot-side temperature limit. Three optimized RTG designs are compared, produced using literature data for low- (Bi2Te3 or Mg-based, <600 K), mid- (Half-Heusler (HH) or Skutterudites (SKD), <900 K), and high-temperature (SiGe, >900 K) TEMs. Mid-temperature TEMs lead to increased power densities and smaller RTGs, while for high-temperature TEMs care must be taken to avoid overheating the RHU. Understanding the TEM's influence can guide engineering decisions towards next-generation, high-performance RTG designs.

Impact of side chain substituents on the thermal conductivity of hydrocarbonated polymers assessed by molecular dynamics simulations.

Sir Louis Duhayon[1], Professor Claudio Melis[2], Professor Jérôme Cornil[1]
[1]University of Mons, Laboratory for chemistry of novel materials (CMN), Belgium, [2]Departement of physics, University of Cagliari, Cittadella Universitaria, Italy

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Understanding heat propagation is a key parameter for improving the performance of thermoelectric devices. While most studies focus on inorganic materials, organic materials—particularly polymers—have received far less attention. Different parameters such as crystallinity [2] and chain length [3] are known to strongly affect the thermal conductivity, however the influence of polymer side-chain substituents remains poorly explored. In this work, we use the Approach-to-Equilibrium Molecular Dynamics (AEMD) method to investigate how the chemical nature of substituents modulates the thermal conductivity. The AEMD method consists in applying hot and cold thermostats to two halves of a supercell (Fig.1 a)) and monitoring the exponential decay of the temperature difference during relaxation [1]. By applying Fourier's law and a appropriate fitting procedure, the thermal conductivity $\kappa(L)$ (L, the supercell length) of the supercell is obtained. After the extrapolation of $\kappa(L)$ to different lengths using the linear relationship, $1/(\kappa(L))=1/(\kappa(\infty))(1+ \Lambda/L)$ (with Λ, a typical length of the heat transport in the material) [1], we determine the bulk thermal conductivity and estimate the phonon mean free path [4]. Thanks to this approach we have highlighted significant differences in the thermal behavior of crystalline polyethylene (PE), polypropylene (PP) and polystyrene (PS) chains. The method is currently being extended to other polymeric structures (as amorphous PE, PP and PS systems).

[1] C. Melis, R. Dettori, S. Vandermeulen, and L. Colombo, Eur. Phys. J. B, Vol. 87 (2014). Art. no. 119.
[2] H. Chen, J. Mater. Process. Des., Vol. 7, No. 3 (2023), pp. 43–51.
[3] X. Wei and T. Luo, Phys. Chem. Chem. Phys., Vol. 21, (2019), pp. 15523–15530.
[4] D. P. Sellan, E. S. Landry, J. E. Turney, A. J. H. McGaughey, and C. H. Amon, Phys. Rev. B, Vol. 81 (2010), Art. no. 214305.

An ab initio method for extracting mode-specific deformation potentials in thermoelectric materials

Dr. Rajeev Dutt[1], Dr. Bhawna Sahni[1], Dr. Yao Zhao[1], Dr. Ankit Kumar[1], Dr Sumit Kukreti[1], Ms Saff-E-Awal Akhtar[1], Mr. Yuji Go[1], Prof. Zhen Li[2], Dr. Patrizio Graziosi[3], Prof Neophytou Neophytos[1]
[1]School of Engineering, University of Warwick, United Kingdom, [2]Beihang University, China, [3]School of Materials Science and Engineering, Institute of Nanostructured Material, CNR, Italy
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Accurate prediction of electronic transport is central to the discovery of high-performance thermoelectrics. For this, solutions of Boltzmann Transport Equation (BTE) are needed. These involve scattering rates, which typically need deformation potentials (DP). Traditionally, DP theory is applied using several methods: volume-strain, which relies on band edge shifts under uniform dilation, and the rigid-ion approximation, which assumes a static shift during atomic displacement. While these methods offer simplicity, they often inaccurate and overlook the phonon mode specifics complexity. Modern workflows that utilize exhaustive ab initio matrix element sampling provide high accuracy, but encounter significant computational bottlenecks.

In this work, we bridge this gap by utilizing density functional perturbation theory to extract deformation potentials with high efficiency and physical precision. By selectively sampling the momentum-space regions and phonon branches most relevant to electronic scattering, we reduce the required matrix element evaluations by several orders compared to fully ab initio scattering rate calculations. This targeted approach allows for a precise decomposition of scattering mechanisms, successfully distinguishing between acoustic and optical contributions as well as intra-valley and inter-valley transitions.

To demonstrate the scalability and accuracy of the method, we apply this method to a set of 13 half-Heusler compounds, elaborate on the effect of individual phonon modes and discuss how these affect factors such as intra- versus inter-band/valley scattering and the relative strength of acoustic/optical/polar modes. The extracted deformation potentials are subsequently integrated into BTE using ElecTra for accurate evaluation of the mobility, and thermoelectric properties [1]. Such calculations provide a detailed understanding of the internal scattering and transport in materials, essential for optimization directions. They can form the basis of test sets upon which accurate machine learning predictions can be make upon scaling to larger material sets.

References :
[1] P. Graziosi, Z. Li, N. Neophytou, Comput. Phys. Commun., 287, 108670 (2023).

Harnessing Chemical Short-Range Ordering in a Cation-Disordered, Mechanically Resilient AgMnSnBiTe4 Multi-Component Thermoelectric Alloy

Mr Sri Sai Samhitha Gadhavajhala[1], Dr Veera Prabu Kannan[1], Mr Jorlit John[1], Dr. Slyvain Le Tonquesse[2], Prof. Bhuvanesh Srinivasan[1]
[1]Thermal Energy Materials Group, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, India, [2]Laboratorie CRISMAT, France

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The performance of thermoelectric materials can be strategically tuned by balancing atomic order and disorder. In this study, a multi-component quaternary telluride, AgMnSnBiTe4, is developed by alloying AgBiTe2, MnTe, and SnTe, wherein substantial configurational cationic disorder is intrinsic, alongside the emergence of chemical short-range ordering, deviating from a fully random solid solution. The presence of chemical short-range ordering sustains coherent charge transport by preserving locally correlated electronic pathways, yielding a nearly temperature-independent power factor over 300–523 K. Concurrently, the random occupation of Ag, Mn, Sn, and Bi at equivalent lattice sites induces local lattice distortions and structural anharmonicity, which enhance phonon scattering and suppress lattice thermal conductivity. AgMnSnBiTe4 further exhibits notable mechanical resilience, combining high hardness with fracture toughness comparable to benchmark tellurides. These attributes highlight a rare convergence of mechanical robustness with decoupled electronic and thermal transport. The results demonstrate how the interplay between configurational cationic disorder and chemical short-range ordering can be leveraged to optimize coupled physical properties, establishing a framework for designing high-entropy/multi-component thermoelectric materials beyond the paradigm of complete chemical randomness.

The presentation is based on our published paper in Acta Materialia:
S. S. S. Gadhavajhala, V. P. Kannan, J. John, S. Le Tonquesse, B. Srinivasan, Harnessing chemical short-range ordering in a cation-disordered, mechanically resilient $AgMnSnBiTe_4$ multi-component thermoelectric alloy, Acta Mater. (2026) 122222.
https://doi.org/10.1016/j.actamat.2026.122222

Multiphysics Modeling of Trap-Assisted Thermoelectric Generation in Reverse-Biased PN-Junctions

Dr. Sara Ghomi[1], Dr. Venkata Raveendra Nallagatla[1], Dr. Gerhard Span[2], Dr. Joaquín Miranda[1]
[1]Thin Film Technologies, Silicon Austria Labs GmbH. High Tech Campus Villach, Austria,
[2]LAMBDA Wärmepumpen GmbH. Perlmooserstraße 2, Austria

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Industrial systems dissipate large amounts of energy as low-grade heat, motivating the development of thermoelectric devices capable of harvesting thermal energy at moderate temperatures [1]. Unlike conventional Seebeck thermoelectric generators, which rely on a temperature gradient, the proposed concept converts thermal lattice energy into electrical power through thermally activated carrier generation and separation in the depletion region of a reverse-biased PN junction [2].

In this work, we present a comprehensive multiphysics modelling framework for trap-assisted carrier generation cooling in reverse-biased PN-junction devices. The simulation platform is implemented in COMSOL Multiphysics and couples semiconductor drift–diffusion transport with heat transfer physics. The model explicitly incorporates relevant microscopic generation and recombination mechanisms under reverse-bias conditions, accounting for device-level effects such as contact properties and device geometry. When generation dominates recombination, the junction operates as a thermally driven carrier generator, locally absorbing heat from the lattice. Systematic parametric studies evaluate the influence of material properties, and device design on thermoelectric performance. The simulations reveal key design trade-offs between carrier generation, recombination losses, and carrier extraction efficiency, identifying optimal device parameters that enhance thermally generated carrier transport.

This work establishes a computational design framework for reverse-biased thermoelectric devices and provides quantitative guidelines for device optimization targeting industrial waste heat harvesting and thermal management applications.

References
[1] Ruben Chavez, Gerhard Span, et al, J. Phys. D: Appl. Phys. 51 014005 (2017).
[2] Robert T. Ross; Arthur J. Nozik, J. Appl. Phys. 53, 3813 (1982).

On the validity of temperature dependent exponents for complex electronic structure materials

Yuji Go[1], Rajeev Dutt[1], Bhawna Sahni[1], Neophytos Neophytou[1]
[1]University Of Warwick, United Kingdom

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The scattering exponent approximation is a common method employed to identify the dominant internal material electronic scattering processes which limit transport and conductivity in experimental measurements. For this, the mobility versus temperature data are fit to an exponent function of temperature as μ∝T^s. Literature values of s = -1.5 indicate acoustic/optical (ADP/ODP) phonon scattering, s = -0.5 indicates polar optical phonon (POP) scattering, and s = 1.5 indicates ionized impurity scattering (IIS). These values are defined using various assumptions, most importantly using a single, parabolic band for its electronic structure. However, typical thermoelectric materials often involve complex electronic structures.

Here we examine the validity of the scattering exponent approximation for thermoelectric materials. We take 13 half-Heusler materials (n-type and p-type, thus 26 different electronic structures), for which transport is calculated fully ab initio using ElecTra [1]. We extract the temperature dependent mobility exponents in the range of 300 K – 900 K for various densities, including all ADP, ODP, POP and IIS. We show that the electronic structure complexities make the exponents deviate substantially from nominal values, at a degree where we cannot infer the underlying scattering process. At low densities, the exponents vary from s = −2.5 to −1 between materials, indicating ADP/ODP, although POP is the strongest (nominal s = −0.5). At higher densities, they tend to increase slightly towards s = −0.5, despite transport becoming IIS-dominated (nominal s = 1.5). We show that the reduction is caused mainly by the ODP/POP emission onsets, while the variation due to variations in their electronic structures and their phonon energies; in fact we find a linearly negative dependence of s to the phonon energy [2].

References

[1]Patrizio Graziosi et al, 'ElecTra code'. Computer Physics Communications, 287, 2023, 108670.
[2]Yuji Go et al, Physical Review B, under review.

Strategies for incorporating alloy scattering in the calculation of the thermal conductivity of solid solutions

Mr Tom Ord[1], Dr Antonio Marquez[2], Dr Jose Plata[2], **Dr Ricardo Grau-Crespo**[1]
[1]Queen Mary University of London, United Kingdom, [2]University of Seville, Spain

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Solid solutions often exhibit significantly reduced lattice thermal conductivity due to alloy disorder, but incorporating alloy scattering into predictive calculations remains a practical bottleneck, particularly when one seeks a balance between accuracy and computational cost. In this work, we outline and compare several complementary strategies to include alloy scattering within Boltzmann transport calculations for phonons, using PbTe–PbSe as a representative case study. The approaches combine a virtual-crystal-like host description, built from composition-dependent force constants and volumes, with additional disorder-induced scattering terms, and special quasi-random structures. The emphasis is on workflow design, validation checks, and identifying the minimum level of disorder information required to obtain useful trends across compositions.

Evaluating Reproducibility of Density and Thermoelectric Properties in Additively Manufactured Silver Selenide

Sumner Gubisch[1], Dr. Saniya LeBlanc[1]
[1]The George Washington University, United States

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The energy sector has long viewed thermoelectric materials as promising due to their ability to generate electricity from heat. Traditional manufacturing, however, has limited their adoption to niche applications due to their low efficiency and non-conformal geometries. Additive manufacturing techniques, particularly Laser Powder Bed Fusion (LPBF), offer dynamic new approaches for fabricating bulk thermoelectric devices. LPBF's layer-by-layer process enables the ability to construct thermoelectrics into complex geometries. The process of repeated melting and solidification of the material could enable control over the micro- and nanostructure, allowing for the fabrication of preferential structures that can increase thermoelectric efficacy. This study investigates the LPBF production of silver selenide, a highly promising thermoelectric candidate chosen for the congruent melting behavior of its constituent elements. The primary objective is to evaluate the impact of this manufacturing process on the material's resulting structural and functional properties. Fifteen rectangular specimens were fabricated using identical LPBF process parameters. Density, Seebeck coefficient, and electrical conductivity were measured to evaluate the repeatability of the manufacturing process. This study works to help establish a statistical baseline for these functional properties, which is a critical milestone in validating LPBF as a reliable manufacturing route for thermoelectric materials. This process consistency paves the way for tuning thermoelectric microstructures and overcoming the geometric limitations of traditional manufacturing.

A validated segregated finite-element solution strategy for thermoelectric module simulation in Elmer FEM

Lukas Gupfinger[1], Christoph Beisteiner[2], Maximilian Fruhmann[1], Nadine Kleinbruckner[1], Oliver Maier[1], Vinzenz Ober[1], Peter Zellinger[1]
[1]K1-MET GmbH, Austria, [2]Beisteiner Printronics e.U., Austria

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Accurate numerical simulation of thermoelectric (TE) modules requires the robust solution of strongly coupled thermal and electrical transport equations with temperature-dependent material properties. Monolithic solution approaches may suffer from convergence issues and high computational cost, particularly for large temperature gradients and nonlinear material behaviour. In this work, a segregated finite-element solution strategy for coupled TE problems is implemented in the open-source software Elmer FEM and validated experimentally at module level.

The transport equations for heat and electrical current, including the Seebeck and Peltier effects, govern the TE characteristics between temperature and electric potential in any material. They are solved sequentially within an iterative coupling framework. Temperature-dependent material parameters, depicting the Thomson effect, are taken from literature for commercially available Bi2Te3-based materials. The proposed approach is assessed with respect to numerical stability, convergence behaviour, and computational efficiency.

Experimental validation is performed using a dedicated test rig for a complete TE module, allowing controlled hot- and cold-side boundary conditions and clamping forces. Measured voltage-current characteristics, output power, and temperature distributions are compared with simulation results over a range of operating conditions.

The numerical model reproduces the experimentally observed trends and absolute values with good agreement. Remaining deviations are discussed in terms of interface resistances and heat losses. The presented segregated solution strategy demonstrates improved robustness for nonlinear TE simulations while maintaining physical accuracy at the module scale. Owing to its implementation in Elmer FEM, the approach is fully transparent and reproducible, providing a practical and extensible framework for the simulation and design of TE devices.

Effect of Amino Acid Doping on the Thermoelectric Properties of PEDOT:PSS : A Numerical Study

Dr. Barış Oğuz Gürses[1], Şeyma Özkan[1,3], Dr. Bekir Özkan[1], Dr. Mert Şener[2], Dr. Gökhan Gürlek[1]
[1]Ege Universitesi, Turkey, [2]Balıkesir Universitesi, Turkey, [3]Dokuz Eylül Universitesi, Turkey
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

PEDOT:PSS is a promising thermoelectric material due to its high conductivity, solution processability, and stability[1]. Its biocompatibility with dopants like amino acids suits biointegrated and wearable applications[3]. However, performance is a concern. This study used symmetry-adapted perturbation theory (SAPT) at the SAPT0/def2-SVP level with Psi4 to find amino acid dopants for PEDOT:PSS. All 20 standard amino acids were assessed in zwitterionic forms for binding affinity with poly(styrenesulfonate) (PSS^-). Structures were generated using RDKit and optimized with MMFF94. For each amino acid–PSS pair, multiple geometries were tested, and the best configuration was chosen. SAPT energy decomposition divided interactions into electrostatic, exchange-repulsion, induction, and dispersion. A scoring system emphasized binding mechanisms: 0.7|E_elst| + 0.3|E_ind| for charged amino acids, 0.6|E_ind| + 0.4|E_disp| for neutral ones. Positively charged amino acids showed the strongest binding. Lysine (−61.67 kcal/mol, score = 45.70) and arginine (−51.08 kcal/mol, score = 39.01) were top candidates, with >80% of binding energy from electrostatic attraction. Neutral amino acids showed 3–8 times weaker binding, while negatively charged ones showed strong repulsion (Asp: +46.38 kcal/mol; Glu: +40.70 kcal/mol) due to charge–charge repulsion with PSS^-. These results identified lysine and arginine for experimental validation.1-Luo, P., Dong, S., Liang, L., Kuang, F., Du, C., Ye, Z., & Chen, G. (2026). Highly Sensitive Thermoelectric Fabric of PEDOT: PSS/SWCNT@ PU Composite Fibers for Body-Temperature Monitoring and Fever Alarming. Advanced Materials, 38(9), e18506.2-Alam, J., Xu, X., Adu, P. C. O., Meng, Q., Zuber, K., Afshar, S., ... & Ma, J. (2024). Enhancing thermoelectric performance of PEDOT: PSS: A review of treatment and nanocomposite strategies. Advanced Nanocomposites, 1(1), 16-38.3- Chamria, D., Alpha, C., & Adhikari, R. Y. (2023). Phenylalanine-assisted conductivity enhancement in PEDOT: PSS films. ACS omega, 8(8), 7791-7799.

Sustainable Hydrothermal Synthesis of Copper Iodide featuring Near Room Temperature Thermoelectric Properties

Bejan Hamawandi[1,2], Adrianna Lis[3], Kaspars Pudzs[1], Inga Pudza[1], Alexei Kuzmin[1], José F Serrano-Claumarchirant[2], Oskars Bitmets[1], Sedat Ballikaya[4], Muhammet S. Toprak[2]
[1]Institute of Solid State Physics, University of Latvia, Latvia, [2]Department of Applied Physics, KTH Royal Institute of Technology, Sweden, [3]Faculty of Materials Science and Ceramics, AGH University of Science and Technology, Poland, [4]Department of Engineering Science, Istanbul University-Cerrahpasa, Turkey

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Copper iodide (CuI) is regarded as a promising p-type thermoelectric (TE) material because of its high carrier mobility, non-toxicity, and the abundance of earth elements. In this study, we introduce an eco-friendly, cost-effective hydrothermal synthesis process for CuI performed at room temperature. This approach eliminates the need for hazardous solvents and high-temperature steps, supporting the sustainability of large-scale production of TE materials. Phase-pure γ-CuI was synthesized and then doped with elements such as silver, thereby tailoring its charge-transport properties. Structural and morphological characteristics were investigated using X-ray diffraction (XRD), Synchrotron radiation X-ray absorption spectroscopy (XAS), and scanning electron microscopy (SEM), confirming high crystallinity and a uniform grain distribution. Compositional analysis confirmed successful dopant incorporation without secondary-phase formation.

The thermoelectric transport properties were examined for different cold-pressed and sintered pellets of synthesized CuI. Modulating the carrier concentration via doping led to a notable increase in the Seebeck coefficient. Consequently, the power factor and overall thermoelectric efficiency were evaluated close to room temperature. These findings indicate that hydrothermally synthesized, doped CuI is a promising, eco-friendly material for low-temperature energy-harvesting applications.

Role of Electrodes in Liquid and Gelified Thermoelectrochemical Redox Systems for Waste-Heat Recovery Applications

Momna Haq[1], Andrea Reale[1], Edoardo Marchini[2], Rita Boaretto[2], Stefano Caramori[2], Stefano Carli[3], Claudia Barolo[4]
[1]Department of Electronic Engineering, CHOSE - Centre for Hybrid and Organic Solar Energy, University of Rome Tor Vergata, Italy, [2]Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara, Italy, [3]Department of Environmental and Prevention Sciences — DEPS, University of Ferrara, Italy, [4]Department of Chemistry and NIS Interdepartmental Centre, University of Turin, Italy

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermogalvanic cells (TGCs) have emerged as a promising technology for converting low-grade thermal energy into electricity. Liquid electrolytes are no doubt effective in terms of better ionic conductivity, but they often face leakage and rigidity issues, which restrict their use in wearable applications. However, gel electrolytes have emerged as an ideal solution, especially when ionic liquids are incorporated into the gel matrix. Cobalt-based electrolytes are known for high entropy, stability, and tunable redox properties, which promise to enhance thermogalvanic cells performance. But they are limited by the use of suitable solvents and specific electrode materials. Recent research in TGCs has focused on optimizing electrode materials, electrolyte composition, and device engineering [1].

We present a liquid and gel electrolyte-based TGC device using Platinum (Pt) and PEDOT-based electrodes on both Glass-FTO and PET-ITO. Our reference devices based on 100 mM Co(II)/Co(III) liquid and Gel electrolytes based on PVDF formulation have shown a Seebeck coefficient ranging from 400 µV/K to 1000 µV/K across different electrode materials. We verified that the activation time of PEDOT is dependent on the type of catalyst being used. PEDOT-based electrodes were fabricated using both spray-coating and electrodeposition techniques, and Pt electrodes were fabricated through the spin coating technique. We also investigate other types of polymeric matrix for gel formulation, other electrode materials, targeting the upscaling of the device from single TGC cells to a full TGC module in a unipolar, mono-leg design, both on rigid and flexible substrates. Further, we present preliminary results to explore other redox couples like I^{-3}/I^{-} or Fe(II)/(III) to have both p-type and n-type systems, which will make it easier to assemble a module in the near future.

Grain boundary engineering enables stable and efficient Mg3(Sb,Bi)2 thermoelectric materials

Dr. Zizhuang He[1], Dr. Hezhang Li[2], Dr. Chen Chen[1], Prof. Jing-Feng Li[1]
[1]State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering, Tsinghua University, China, [2]Department of Precision Instrument, Tsinghua University, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

$Mg_3(Sb,Bi)_2$ has attracted considerable interest as an emerging thermoelectric material for both power generation and electronic cooling. Despite substantial gains in its thermoelectric figure of merit (zT) in recent years, critical challenges persist-, including secondary-phase refinement, elemental precipitation, and interfacial mismatch. In this work, we incorporated copper selenide into the $Mg_3(Sb,Bi)_2$ matrix to engineer grain-boundary phases in situ, yielding a zT above 2 at 798 K. Moreover, the as-prepared sample exhibits orders-of-magnitude improvement in resistance to moisture and oxygen degradation relative to the pristine matrix. This enhancement arises primarily from Mg-Cu and Mg-Se enrichment formed at grain boundaries, which modulates both carrier concentration and mobility. Benefiting from the simultaneous enhancement of the power factor, suppression of lattice thermal conductivity, and improved environmental stability, the zT increases across the entire measured temperature range. Consequently, a single-leg device attains a conversion efficiency of 14% with robust cycling stability.

From self-modulation to modulation doping in Bi2O2Se

Jiří Hejtmánek[1], Antonín Sojka[2], Karel Knížek[1], Petr Levinský[1], Jiři Navrátil[1,2], Jan Zich[2], Pavlína Ruleová[2], Tomáš Plecháček[2], Čestmír Drašar[2]
[1]FzU - Institute Of Physics Of The Czech Academy Of Sciences, Prague 6, Czech Republic,
[2]University of Pardubice, Faculty of Chemical Technology, Czech Republic

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Keywords:
Bi_2O_2Se, Charge carrier mobility, Modulation doping, Composite material

Abstract:
The Bi_2O_2Se phase can be considered to have separate "doping " (Se layer) and "electrically conducting" (Bi_2O_2 double layer) parts represents a “natural” electronic composite (1). This material exhibits high carrier mobility through a process referred to as self-modulation doping, which is an internal analogue of the conventional modulation doping induced by an extraneous phase. Unlike conventional doping, both of these processes do not compromise the carrier mobility. The high potential of modulation doping in Bi_2O_2Se is fostered by its huge permittivity, which strongly suppresses ionized impurity scattering resulting in the low-temperature electron mobility as large as 10^4 to 10^6 cm^2/Vs for samples self-doped by Se vacancies (1,2). This motivates the exploration of creating artificial electronic composites - heterogeneous materials, in which the doping is realized due to the presence of an extraneous phase. We presume that such a heterostructure of “dopant” and “recipient” would benefit both simultaneously: (i) strongly suppressed carrier scattering compared to classical doping, and (ii) increased stability of Bi_2O_2Se grain boundaries (3). In this respect we will attempt to provide guidance on selecting the appropriate “dopant” phases to form chemically stable “pairs” with Bi_2O_2Se.

Acknowledgments:
Authors acknowledge for financial support of Czech Science Foundation (Project No. 22-05919S), project TERAFIT (CZ.02.01.01/00/22_008/0004594) and Ministry of Education, Youth and Sports of the Czech Republic (grant LM2023037).

References:
(1) H. Fu, J. Wu, H. Peng, B. Yan, Phys. Rev. B, 97, 241203(R) (2018), doi.org/10.1103/PhysRevB.97.241203.
(2) A. Sojka et al., Computational Materials Science, 243, 113138 (2024), doi.org/10.1016/j.commatsci.2024.113138.
(3) S. Xu et al., Angew. Chem. Int. Ed., 59, 17938 (2020), doi.org/10.1002/ange.202006745.

High Power Density up to 2.2 W/cm² in Cryogenic Thermoelectrics for Commercial Vehicle Applications

Matthias Helmich[1], Timo Knobelspies[1], Christopher Frischter[1], Jonah Schnüll[1], Martin Kober[1], Christian Stiewe[2], Frank Rinderknecht[1], Tjark Siefkes[1]
[1]German Aerospace Center, Germany, [2]German Aerospace Center, Germany
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Liquid hydrogen is a promising fuel for heavy commercial vehicles that use fuel cells or hydrogen engines, for example. However, challenges persist: cryogenic hydrogen must be heated and vaporized before use, it remains more expensive than conventional fuels, and fuel cell systems face difficulties with heat dissipation due to low temperature gradients. It has been demonstrated that a cryo-thermoelectric generator (Cryo-TEG) effectively recovers waste heat from cooling water of a fuell cell, thereby reducing the thermal load on the cooling system. This heat is converted into electrical energy, which is utilized by the drivetrain, increases system efficiency, lowering hydrogen consumption and operating costs. As the heat is transfered into the liquid hydrogen, its temperature rises, ensuring that hydrogen reaches a gaseous state for safe fuel cell or engine operation.

A series of experiments were conducted on Bi_2Te_3 thermoelectric modules on a module test bench at cold-side temperatures of down to -150 °C and hot-side temperatures between 0 °C and 300 °C to evaluate their potential. The tests achieved electrical power densities of up to 2.2 W/cm², thereby demonstrating considerable potential for cost-effective enhancing efficiency in liquid hydrogen-powered commercial vehicles. The present analysis, when considered in conjunction with the findings of Helmich et al. (2025), as reported in ICT Sendai, indicates that the implementation of a Cryo TEG has the potential to result in a substantial reduction in fuel consumption, thereby leading to significant cost savings in heavy vehicles with fuel cells or hydrogen engines. Beyond power generation, the TEG ensures safe operation by heating cryogenic hydrogen to the required temperature. Taking all factors into consideration, including energy recovery, safety and cost, this technology enables the development of a cost-effective system with a amortization period of under one year. This makes it a viable solution for sustainable heavy-duty transportation.

Power Hardware-in-the-Loop (Power-HIL) System for Thermoelectric Generators (TEGs) to Optimize and Validate MPPT Algorithms with Health Monitoring

Dustin Henneberg[1], Dr. Florian Liebetrau, Christopher Fritscher, Julian Schwab, Martin Kober, Frank Rinderknecht
[1]German Aerospace Center, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

A critical component of thermoelectric generator (TEG) systems is power electronics and associated algorithms, which increasingly handle complex tasks such as health monitoring, fault detection, and strategy selection [1]. To enable early collaboration between TEG developers and power electronics or software engineers, Power Hardware-in-the-Loop (Power-HIL) systems [2] are used. These systems replicate the TEG's thermal behavior, operational dynamics, and fault scenarios via a real-time simulator and power amplifier, connecting to the device under test (DUT) through electrical terminals. This enables comprehensive validation of control algorithms and system behavior under realistic conditions before physical deployment.

The Power-HIL system supports three applications:
a) Small-Signal Behavior: Assessing MPPT algorithm reliability, accuracy, and interaction under various configurations; validating health monitoring.
b) Large-Signal Behavior: Enabling fast real-time simulation of complex operational strategies; simulating faults to evaluate robustness.
c) Model Level (Digital Twin): Enhancing digital twin fidelity for small- and large-signal behavior to improve simulation realism and prediction.

This work focuses on integrating TEG models and realizing the electrical terminal characteristics control-theoretically. The power electronics are based on [3], also used in MPPT TEG systems, enabling cost-effective, scalable, and modular development.

Acknowledgments: Funded by the Federal Ministry for Economic Affairs and Energy under SPEKTRUM (grant no. 03EN4105A).

References:
[1] Carstens, J.H.H., Gühmann, C., Reuss, H.C., Schauer, T. Control and Optimization of a DC-DC Converter for Thermoelectric Generators. Technische Universität Berlin (2016).
[2] De Carne, G., Müller, K., Schmidt, A., Fischer, T., Klein, R. "Power Hardware-in-the-Loop for Electrical Systems: From Research Experience to Guidelines for Industrial Testing," IEEE Open Journal of Power Electronics, vol. 7, pp. 822–842, 2026, doi: 10.1109/OJPEL.2026.3666762.
[3] Liebetrau, F., Schwab, J., Knobelspies, T., Kober, M., Weber, C., Rinderknecht, F. (2024), "Microinverter for thermoelectric generators for combined feed-in to AC grids and low-voltage battery storage systems," ICT/ECT 2024, p. 428. International Thermoelectric Society.

Electronic structure of $Na_xIn_\gamma Ge_{136-\gamma}$ type-II clathrate: carrier tuning via In substitution and Na filling control

Naomi Hirayama[1]
[1]The University of Osaka, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

P-type doping in type-II clathrates has remained a challenging issue, despite its importance for thermoelectric applications. Most type-II clathrates exhibit n-type behavior, and stable hole doping has not yet been well established.

In this study, we investigate the electronic structure of an In-substituted Ge-based type-II clathrate ($Na_xIn_\gamma Ge_{136-\gamma}$) using first-principles calculations. In substitution at the framework sites is expected to introduce hole carriers, while Na guest atoms, which are essential for structural stability, act as electron donors.

By systematically varying the Na content, we examine how the electronic structure evolves under carrier compensation between holes introduced by In substitution and electrons supplied by Na. This study provides insight into carrier tuning through the interplay between framework substitution and guest filling.

Effects of processing routes, multiphase system engineering and doping on the properties of ZnSb thermoelectric alloy

Xinxi Huang[1], Carlo Fanciulli[2], Stefano Boldrini[3], Alberto Ferrario[3], Alberto Castellero[1,3]
[1]University of Turin, Chemistry Department, Italy, [2]CNR – ICMATE, Lecco Unit, Italy, [3]CNR – ICMATE, Padova Unit, Italy

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

ZnSb is a promising p-type thermoelectric material below 700 K, thanks to low toxicity, abundance and affordability compared to conventional thermoelectric systems.
To improve the thermoelectric properties of the stoichiometric, pristine compound, three possible strategies can be combined:
- Microstructural refinement by non-equilibrium processing (i.e., rapid solidification, ball milling) is expected to decrease lattice thermal conductivity by increasing phonon scattering.
- Off-stoichiometry approach allows for multiphase composites (e.g., ZnSb matrix decorated with Sb-rich secondary phase), potentially having the advantage of exhibiting intermediate properties and increasing phonon scattering.
- Concerning doping, depending on the solubility limit of the dopant in the system, different scenarios will occur. On the one hand, if it dissolves in the system, it will affect Seebeck coefficient and electrical conductivity. Consequently, the power factor improves by optimizing carrier concentration. On the other hand, thermal conductivity will be affected: nanostructures scatter phonons, lowering lattice thermal conductivity. In the best-case scenario, the two effects coexist.

The effects of the different strategies have been investigated to obtain p-type legs for a thermoelectric module, having reliable transport and mechanical properties.
Master alloys were synthesized via melting and quenching. Since master alloys exhibit high porosity and low density compared to the theoretical value, two different processing routes were followed. On the one hand, master alloys were ground and the powders sintered by open die pressing (ODP). On the other hand, the starting elements were molten by induction and rapidly solidified by melt-spinning. The flakes obtained were ground to powder and sintered by ODP.

The samples obtained were characterized in terms of structural, microstructural, mechanical and thermoelectric properties and the results compared to relate the effects observed to the preparation process. This approach promotes a deeper understanding of the material, supporting the design of a production process able to take advantage of the different solutions tested.

Thermoelectric properties of NiCu fabrics covered with ZnO nanorods for wearable power generator

Hiroya Ikeda[1], Koki Kato[1], Sei Iijima[1], Palanisamy Rohini[2], Veluswamy Pandiyarasan[2], Kazushi Ikeda[3], Yasuhiro Hayakawa[1], Hiromu Hamasaki[1]
[1]Shizuoka University, Japan, [2]IIITDM, , India, [3]NAIST, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

For developing wearable power generators, we have investigated the thermoelectric properties of ZnO nanorods grown on conductive NiCu fabrics. ZnO nanostructures were formed on NiCu fabrics using two-step microwave-assisted solvothermal synthesis, where some seeds of ZnO were fixed on the fabric in the first step and ZnO nanorods grew up in the second step. In this study, we repeated the growth process (second step) for making the ZnO nanorod longer. It was observed by scanning electron microscope (SEM) and X-ray diffraction analyses that the fabric surface is fully covered with dense hexagonal-ZnO-nanorods growing vertically. We could evaluate the diameter and height of nanorods from the SEM images, which indicated that both structural parameters increase linearly by repeating the growth process. The Seebeck coefficient was evaluated by measuring the thermoelectromotive force (TEMF) under temperature gradient applied to the sample in plane. The evaluated Seebeck coefficients of the samples have negative values, indicating n-type semiconductor. In addition, the Seebeck coefficient was found to be enhanced by repeating the growth process because of an increase in the total volume of ZnO nanorods. On the other hand, the electrical conductivity was hardly influenced by the repeat count of growth process. This fact suggests that the electrical conductivity is mainly ruled by the NiCu fabric substrate. As a result, the power factor of the ZnO/NiCu-fabric was improved by repeating the growth process.

Toward Printable Thermoelectric Materials Based on AgSbTe2 Chalcogenides

Mohd Ishtiyak[1], Dr. Bastian Weinert[1], Dr. Md. Mofasser Mallick[2], Prof. Uli Lemmer[2], Prof. Stefanie Dehnen[1]
[1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany, [2]Light Technology Institute, Karlsruhe Institute of Technology, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The increasing global demand for energy and the abundance of wasted thermal energy have driven significant research efforts toward thermoelectric materials capable of converting heat gradients directly into electricity. Along with high thermoelectric performance, printing-based fabrication is now attractive because it offers a scalable route to lightweight, low-material-waste, and potentially flexible devices, unlike conventional bulk thermoelectric that are usually rigid and less suitable for large-area or shape-adaptable applications. AgSbTe2 is therefore interesting not only as a high-performance bulk thermoelectric, but also as a potential candidate for printed energy-harvesting devices. Among medium-temperature thermoelectric materials, AgSbTe2 has drawn strong attention because of its rock-salt-derived structure, cation disorder, and intrinsically low lattice thermal conductivity of about 0.5–0.7 $Wm^{-1}K^{-1}$. It is a narrow-bandgap indirect semiconductor, and its complex electronic structure is characterized by Te-5p dominated dispersive valence states together with mixed cations Ag/Sb-derived conduction states. Spin–orbit coupling and the presence of closely spaced valence bands make this system especially interesting. In AgSbTe2-based compositions, reduced energy separation between valence bands can promote band convergence, while heavier valence-band features can increase the density-of-states effective mass; both effects are beneficial for improving the Seebeck coefficient, power factor, and ultimately the thermoelectric figure of merit. We have synthesized a few reported and new dopant based AgSbTe2 that are highly promising thermoelectric materials using standard solid-state synthesis. The doped-AgSbTe2 powders are subsequently processed into printable thermoelectric inks through controlled particle size reduction and dispersion in appropriate solvent–binder systems. The resulting inks exhibit suitable rheological behavior for printing and are deposited onto flexible Kapton substrates using solution-based printing approaches. Post-printing thermal treatment is employed to promote interparticle connectivity, enabling mechanically flexible thermoelectric films while maintaining favorable transport properties. This combined materials-to-device strategy provides a practical pathway toward flexible thermoelectric generators for waste-heat recovery applications.

Constructing Magnetic Semiconductors to Enhance Thermoelectric Material Performance

Dr. Baohai Jia[1]
[1]Southern University Of Science And Technology, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric materials enable the direct conversion between thermal gradients and electric potential, exhibiting significant application potential in waste heat recovery and sustainable energy fields. Conventional strategies based on electron–phonon interactions have approached a practical bottleneck, posing severe constraints on further substantial enhancements in thermoelectric conversion efficiency. Spin-related effects offer novel pathways for boosting thermoelectric performance, encompassing mechanisms such as magnon-drag, spin entropy, etc. Nevertheless, current spin-mediated thermoelectric enhancements remain largely restricted to ferromagnetic materials or specific material systems, underscoring an urgent demand for universally applicable strategies that transcend distinct material categories. In this study, we construct a magnetic semiconductor system by incorporating magnetic elements into the tradditoional thermoelectric material through manganese substitution. Through precise manipulation of Ruderman–Kittel–Kasuya–Yosida (RKKY) exchange interactions between localized magnetic moments and itinerant charge carriers, local nanoscale ferromagnetic domains were constructeded. These localized ferromagnetic regions generate pronounced spin-fluctuation effects that contribute substantial spin entropy at elevated temperatures, consequently leading to a marked enhancement of the Seebeck coefficient. Simultaneously, the resultant magnetic nanoclusters serve as effective scattering centers for phonon transport, significantly suppressing the lattice thermal conductivity. This approach provides a novel and broadly applicable strategy, rooted in spin manipulation, for overcoming the performance bottlenecks of thermoelectric materials.

Thermoelectric properties of co-doped PbTe single crystals

Nikola Kanas[1,2], I. Longkumer[3], P. Tatarko[3], V.E. Slynko[4], E.I. Slynko[4], G.M. Stojanović[1], M. Romcevic[5], N. Romcevic[5], W.D. Dobrowolski[6]
[1]University of Novi Sad, Faculty of Technical Sciences, Serbia, [2]Tegmatica Ltd, 23300 Kikinda, Serbia, [3]Institute of Inorganic Chemistry, Slovak Academy of Sciences, Slovakia, [4]Institute of Materials Science Problems, Ukrainian Academy of Sciences, Ukraine, [5]Institute of Physics Belgrade, University of Belgrade, Serbia, [6]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Tellurides are state-of-the-art thermoelectric materials, with PbTe-based compounds standing out for their exceptional stability in ambient air and their wide operating temperature range. Enhancing the thermoelectric performance of these monocrystalline materials through solid solution formation or targeted doping has emerged as a promising strategy.

In this study, we investigate the structural evolution and thermoelectric behavior of PbTe-based crystals with systematically varied chemical compositions, such as Pb1-x-ySixGdyTe, and Pb1-xSixSezTe1-z. Crystal growth and phase stability were examined, while thermoelectric properties were assessed through measurements of the Seebeck coefficient, electrical conductivity, and thermal conductivity. Thermal stability was further evaluated using thermo-gravimetric analysis (TGA), with particular attention to the influence of dopant type and concentration. Complementary structural and microstructural characterization was performed using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy. The results reveal clear correlations among dopant chemistry, structural features, and thermoelectric performance, highlighting pathways to optimize efficiency and durability. These findings not only advance the fundamental understanding of PbTe-based thermoelectrics but also underscore their strong potential for practical applications and commercialization in energy conversion technologies.

Preparation of NbCoSn via 4-probe melting and Properties of NbCoSn

Miss SHRIKHA KARUPPIAH[1], Dr Blair Kennedy[1], Dr Jan-Willem Bos[1]
[1]EaStCHEM School of Chemistry, University of St Andrews, United Kingdom

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Half-Heusler materials are intermetallic alloys that demonstrate a good balance between thermoelectric performance and thermal stability. Their high power factor and robust mechanical properties make them suitable for thermoelectric applications - particularly at high temperatures. NbCoSn is one such composition within this family, with promising potential for both n-type and p-type doping, which makes it ideal for use in thermoelectric devices. Achieving phase-pure NbCoSn, however, remains challenging. This is mainly due to large melting point mismatch between Nb, Co, and Sn, which can lead to compositional inhomogeneity and the formation of secondary phases. As phase purity and microstructure can strongly influence transport properties, optimising the synthesis route of this composition is necessary.

In this work, 4-probe arc melting was used to synthesise NbCoSn. 4-probe melting affords better melt uniformity in comparison to conventional single-probe arc melting. Samples are largely pure after melting, with high melting point Nb-Sn binaries present. Subsequent ball milling and hot pressing improves phase purity compared to annealed ingots, indicating that annealing alone is insufficient for complete homogenisation. This poster will give an overview of the impact of varying synthesis conditions on phase purity, microstructure, and the resulting thermoelectric properties of NbCoSn and appropriately doped samples.

Advancing precision in Hall effect through localized heating with a compact design

Dinesh Kumar Kedia[1], Dr. Navita Jakhar[1], Prof. Surjeet Singh[1]
[1]Indian Institute of Science Education and Research Pune, India

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

We have developed a versatile, fully automated Hall measurement setup for operations between room temperature and 750˜K and in magnetic fields up to ±10˜kOe. Our compact sample holder design, with localized heating and minimal heat loss, delivers precise temperature stability (better than ±10˜mK at 750˜K) and low power consumption (20–25˜W). The setup is housed within a 26˜mm air gap between the pole pieces of an electromagnet. The sample holder, enclosed in a quartz tube for a controlled atmosphere, accommodates various sample shapes and sizes and can be contacted using adjustable pressure-point contacts. Despite its compact size, bulk thermoelectric samples measuring up to 10˜mm laterally can be analyzed successfully. A phase-sensitive lock-in technique and electromagnetic shielding ensure excellent sensitivity, allowing nano-volt Hall signal measurements in high-carrier-concentration samples. We have successfully applied this setup to diverse materials, including lightly doped germanium (10ˆ14˜cmˆ(−3)), degenerate semiconductors from the half-Heusler family (10ˆ21˜cmˆ(−3)), and superionic thermoelectrics (10ˆ18˜cmˆ(−3)), demonstrating its versatility and reliability. Our results align well with those from commercial systems where available.[1] We also studied the bipolarity in self-doped Ag2Te using the two-carrier model and Hall and MR data from our setup.

[1] D.K. Kedia, N. Jakhar, S. Singh, Rev. Sci. Instrum., 96, 033906 (2025).

TEG-Integrated Cookstove for Institutional Use Across Sub-Saharan Africa

Cevriye Koz[1], Tibor Toro[1], Yeremi Perez[1], Anna Bengtsson[2], Anders Vestin[2], Richard Tuley[1], Kevin Simpson[1]
[1]European Thermodynamics Ltd, United Kingdom, [2]Zemission AB, Sweden
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Access to reliable electricity remains a major challenge across Sub-Saharan Africa, with approximately 600 million people lacking access according to the IEA. In addition, charcoal burning stoves release CO and particulate-matter (linked to >4M deaths/year); the WHO has declared pollution caused by unclean cooking as “the world’s largest single environmental health risk”. This work presents the development of an institutional cookstove integrating a thermoelectric generator (TEG) with an energy harvesting system to provide simultaneous cooking, off-grid power generation and enables a fan to reduce combustion pollution. The system incorporates custom-engineered TEGs with bismuth telluride thermoelectric materials optimized for the operating conditions of biomass cookstoves.

Experimental results from a demonstration unit show that during the pyrolysis phase of cooking, the TEG modules generate up to 9.1 W of electrical power. With a power conditioning (energy harvesting) efficiency of approximately 90%, around 8.2 W is available for useful output. A portion of this energy (1.8 W) is consumed by combustion air fan to enable clean cooking and a cooling pump for TEGs, resulting in a net power output of approximately 6.4 W during peak operation. Total energy stored in the battery after the pyrolysis phase reaches up to 3.8 Wh. This net output is sufficient to support low-power applications such as LED lighting and mobile phone charging, providing added value in off-grid institutional settings such as schools or community kitchens.

The results demonstrate the feasibility of integrating thermoelectric energy harvesting into institutional cookstoves, offering a scalable solution that addresses both clean cooking needs and energy access challenges.

Acknowledgments
The authors acknowledge project partner, Emerging Cooking Solutions, and funding support from INNOVATE UK.

Thermoelectric properties of thin films of Hf-doped ScN

Petr Levinsky[1], Joris More-Chevalier[1], Urszula D Wdowik[2], Jiri Martan[3], Xavier Portier[4], Stanislav Cichon[1], Dejan Prokop[1,5], Dominik Legut[2], Esther de Prado[1], J Pokorny[1], J Bulir[1], M Novotny[1], L I Gregora[1], L Fekete[1], J Lancok[1]
[1]FZU - Institute of Physics of the Czech Academy of Sciences, Czech Republic, [2]IT4Innovations, VSB - Technical University of Ostrava, Czech Republic, [3]New Technologies Research Centre (NTC), University of West Bohemia, Czech Republic, [4]Centre de Recherche sur les Ions, les matériaux et la photonique, France, [5]Faculty of Mathematics and Physics, Charles University, Czech Republic

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Transition metal nitrides have attracted growing interest for their thermoelectric properties, among other characteristics. We examine scandium nitride in the form of thin layers doped with Hf. A series of ScN films with different level of Hf doping was prepared where Hf was either homogeneously distributed or confined to Hf-rich layers separated by Hf-free ScN, effectively forming multilayered samples. The samples were deposited on MgO(001) substrates by DC magnetron sputtering in ultra-high vacuum. Thermoelectric measurements were carried out from room temperature to 750 K and compared with theoretical calculations. These were complemented by structural and chemical characterization performed using X-ray diffraction, energy-dispersive X-ray spectroscopy, Raman spectroscopy, and atomic force microscopy. All samples display metallic behavior: the electrical resistivity ρ increases moderately with temperature, while the magnitude of the Seebeck coefficient |S| rises nearly linearly and doubles between room temperature and 750 K. Negative S values indicate electrons as the dominant carriers.

Thermoelectric properties of p-type BaSn0.5(Fe,Co,Ti)0.5O3

Damian Lewoc[1], Tadeusz Miruszewski[1], Maria Gazda[1], Sebastian Wachowski[1], Aleksandra Mielewczyk-Gryń[1]
[1]Institute of Nanotechnology and Materials Engineering, Gdańsk University of Technology, Poland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Barium stannate is an interesting member of the perovskite oxides. Undoped $BaSnO_3$ is a wide-gap semiconductor with a bandgap larger than 3.1 eV [1]. The presence of oxygen vacancies compensated by the reduction of Sn4+ into Sn2+ causes n-type conductivity. Its electrical properties can be further modified by Ba- and/or Sn- cation substitution with iso- or aliovalent elements. Dominant charge-carrier concentration in doped stannates is a complex function of dopant type, partial pressures of oxygen and water-vapour, and temperature. As a result, they may conduct electrons, holes, oxygen ions, or protons, which make these materials mixed ionic-electronic conductors (MIECs). Moreover, they can exhibit a high Seebeck coefficient, which makes them promising thermoelectric materials. In this work, we report on the thermoelectric properties of barium stannate substituted with Fe, Co and Ti.

Ceramic samples were prepared using the solid-state reaction method. The following compositions were prepared: (1) $BaSn_{0.5}Fe_{0.5-x}Co_xO_3$, where x =0.4, 0.3, 0.25, 0.2 and 0.1, and (2) $BaSn_{0.5}Fe_{0.15}Co_{0.15}Ti_{0.2}O_3$ and $BaSn_{0.5}Fe_{0.2}Co_{0.2}Ti_{0.1}O_3$. X-ray diffraction studies confirmed the cubic perovskite structure (Pm-3m) of the materials. Electrical and thermoelectric properties were measured using 4-wire DC method as a function of pO_2, pH_2O, and temperature. It was found that the total electrical conductivity in $BaSn_{0.5}Fe_{0.1}Co_{0.4}O_3$ at RT is 0.1 S/cm which is four orders of magnitude higher than that in undoped $BaSnO_3$ [2].

Bibliography

[1] B. C. Luo, J. Zhang, J. Wang, and P. X. Ran, “Structural, electrical and optical properties of lanthanum-doped barium stannate,” Ceram. Int., vol. 41, no. 2, Part B, pp. 2668–2672, Mar. 2015, doi: 10.1016/j.ceramint.2014.10.080.
[2] S. Upadhyay, O. Parkash, and D. Kumar, “Synthesis, structure and electrical behaviour of lanthanum-doped barium stannate,” J. Phys. Appl. Phys., vol. 37, no. 10, p. 1483, Apr. 2004, doi: 10.1088/0022-3727/37/10/011.

Challenges in the design and development of a customised microinverter for

thermoelectric generators for feeding into AC grids and SELV DC grids.

Florian Liebetrau[1], Dustin Henneberg[1], Julian Schwab[1], Martin Kober[1], Frank Rinderknecht[1]
[1]DLR e.V., Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Due to the relatively simple technical implementation, the use of thermoelectric generators is primarily focused on supplying DC grids and consumers in the Safety Extra Low Voltage (SELV) range, for example 12V, 24V or even 48V. [1-3] The integration of thermoelectric generators into standard AC grids has so far been the exception. The reasons for this are:

a) the incompatibility of the inputs of existing PV micro-inverters with the output characteristics of thermoelectric generators (high open-circuit voltages of the TEGs, excessively high start-up voltages of the MPPT controllers in the PV inverters)

b) the need for galvanic isolation of the thermoelectric generators from the AC grid, with the associated complexity in hardware and software and the resulting high development costs.

This publication addresses the topic using a micro-inverter for TEGs that has been developed, built and tested. The micro-inverter can be connected to and operated with both the AC mains and SELV DC systems, enabling flexible power supply with corresponding prioritisation. Key aspects of this work are:

-Design of the DC input stages for TEGs
-Control voltage supply for the micro-inverter
-Implementation of galvanic isolation using a special planar transformer design
-Challenges in the implementation of the control software

In addition to explaining how the various technical aspects are implemented, the relevant measurement results are also presented.

Se/S anion engineering of Cu6.4Te2.2Se1.8−xSx as a low-tellurium thermoelectric material for cooling applications

Adrianna Lis[1], Oleksandr Cherniushok[1], Krzysztof T. Wojciechowski[1], Taras Parashchuk[1]
[1]AGH University Of Krakow, Faculty of Materials Science and Ceramics, Poland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric materials for near-room-temperature cooling applications are predominantly based on Bi2Te3 compounds. However, their high tellurium content limits large-scale application due to cost and limited elemental availability. In this context, copper-based chalcogenides have emerged as promising low-cost alternatives with intrinsically low thermal conductivity and favorable thermoelectric transport properties. Nevertheless, their highest thermoelectric performance is typically achieved well above room temperature, which limits their use in solid-state cooling.

In this work, Se/S anion engineering was applied to the Cu6.4Te2.2Se1.8−xSx system to shift its optimal thermoelectric performance toward lower temperatures. Increasing sulfur content progressively modifies the phase balance within the system and strongly affects the electronic and thermal transport properties. Sulfur substitution increases the room-temperature Seebeck coefficient from approximately 15 to 151 μV·K−1 while reducing the thermal conductivity from about 0.9 to 0.2 W·m−1·K−1. Transport analysis indicates that this improvement is associated with a reduction in carrier concentration, an increase in the effective mass, and an enlarged estimated transport band gap, without substantial deterioration of electronic transport. As a result, the optimized Cu6.4Te2.2Se0.5S1.3 composition reaches a room-temperature zT approaching 0.5, while the highest thermoelectric performance within the Cu6.4Te2.2Se1.8−xSx series reaches $zT \approx 1.25$ at 450 - 500 K.
The enhanced low-temperature thermoelectric properties result in promising cooling performance. Numerical simulations predict ΔT_{max} values of approximately 53 K at 298 K and 78 K at 348 K, together with $COP_{max} \approx 2.6$ at $\Delta T = 10$ K. These results demonstrate that Se/S anion engineering is an effective strategy for extending low-tellurium Cu-based chalcogenides from mid-temperature energy conversion toward near-room-temperature solid-state cooling applications.

Acknowledgment
The research was funded by the Foundation for Polish Science (FNP) under the First-Team programme, project no. FENG.02.02-IP.05-0012/25, “EcoCool: Eco-Friendly Semiconductor Cooling Solution with Dual-Use Applications”, co-financed by the European Union under the European Funds for a Modern Economy Programme (FENG 2021-2027).

Numerical Modelling of Silicon Nano-grain Materials

Ms Yaqi Liu[1], Mr Keitaro Nakamura[1], Ms Moeka Sato[1], Prof Mitsuhiro Matsumoto[1], Mr Nobuhiko Kajinami[2], Ms Misaki Hanaoka[2], Mr Manabu Iwakawa[2]
[1]Kyoto University, Japan, [2]Mitsubishi Electric Corporation, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

We have developed a numerical simulation scheme for thermoelectric devices with nano-scale structures [1]. For the phonon transport, we adopted the Boltzmann transport equation (BTE) with the relaxation-time approximation; to treat the various types of nanostructures, the volume of fluid (VOF) scheme, which is conventionally used in multi-phase flows, was extended to properly trace the phonon fluxes near interfaces. The electron transport is evaluated with a simple electric network model since the spatial scale of our target systems (typically 10-1000 nm) is larger than the mean free path of electrons. We have successfully investigated the thermoelectric properties of silicon thin films with nano-scale holes of various shapes [2].
In this study we focus on grain structures of silicon nano-crystalline systems, the properties of which have been experimentally investigated [3] in some details. To investigate phonon transport of these systems, proper treatment of the phonon scatterings on the grain boundaries (GBs) are essential. We have developed a simple scheme of GB modelling, which utilizes a Voronoi diagram analysis based on various seed particle arrangements to prepare appropriate distributions of grain sizes and shapes. Partial transmissions/reflections are assumed on GBs; specular and diffusive reflections are also considered.

In this presentation, we report how GBs reduce the effective thermal conductivity and discuss its grain size dependence.

[1] Y. Takahara et al., “Phonon transport simulation with an extended VOF scheme for nano-structured thin film,” Applied Physics Letters, 124, 172204 (2024).
[2] N. Kajinami et al., “Si thin film with nanohole structures to improve thermoelectric performance Part 1: Effects of shape and arrangement in periodic holes,” J. Heat Mass Transfer, 148, 012501 (2026).
[3] E. Isotta et al., “Heat transport at silicon grain boundaries,” Advanced Functional Materials, 34, 2405413 (2024).

Heavy-element-doped Chromium Nitride Thin Films for Thermoelectric Properties

Yi-Ling Lo[1,3], Arnaud le Febvrier[1], Erik Lewin[1], Per Eklund[1,2,3]
[1]Inorganic Chemistry, Department of Chemistry — Ångström Laboratory, Uppsala University, Sweden, [2]Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden, [3]Wallenberg Initiative in Materials Science for Sustainability (WISE), Sweden

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

In contrast to its common use as a hard coating, chromium nitride (CrN) has more recently been studied as a thermoelectric material. In this context, heavy-element doping or alloying has been used to influence the electrical and thermal conductivities of CrN, motivated by the fact that the significant atomic mass contrast between heavy elements and Cr may increase phonon scattering.[1,2] Doping with tantalum (Ta) and hafnium (Hf) provides a mechanism to tune the carrier concentration while promoting phonon scattering.

Here, CrN thin films were deposited by direct-current reactive co-sputtering onto c-plane sapphire substrates at temperatures from 600 to 925 °C. Three Cr targets were used, one pure and two alloyed with 7 at.% Ta and 7 at.% Hf, at magnetron powers of 80–115 W in an Ar/N_2 atmosphere of 30–60% N_2 flow. The synthesis of CrN thin films focused on maintaining the single-phase rock-salt (NaCl-type) cubic structure while incorporating 0 to 7 at.% of the heavy-element dopants.

Structural analysis by XRD revealed that all films retained the NaCl-type cubic structure and that a secondary phase, Cr_2N, emerged at low Ta-doping (1.5 at.%). Conversely, 1.5 at.% Hf-doping was observed to refine the surface morphology and slightly increase the Seebeck coefficient. Higher doping concentrations (7 at.%) induced significant lattice expansion and led to a decrease of the Seebeck value. Overall, the Seebeck coefficient exhibited a range from +80.4 to -103.3 μV/K, showing a transition of CrN from n-type to p-type semiconductor. These results highlight the importance of heavy-element doping for influencing the thermoelectric properties in CrN thin films.

References:
[1] G. J. Snyder and E.S. Toberer Nature Materials, 7(2), 105-114 (2008)
[2] M. Mukherjee et al. Journal of Materials Chemistry. C, 1(35), 12524-12555 (2022)

Glass-Like Thermal Conductivity in n-type Pb-Sb-Sn-based Sulfide Mineral: Interstitial Rattling and Soft Phonon Modes

Krishnendu Maji[1], Naruse Takuya[2], Susumu Fuji[2], Maria Ibáñez[1]
[1]Institute of Science and Technology Austria, Austria, [2]Kyushu University, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Crystalline compounds with intrinsically low thermal conductivity play a pivotal role in the advancement of thermoelectrics and thermal barrier coatings. Investigating the fundamental origins of such low thermal conductivity and its correlation with chemical bonding and crystal structure is essential for developing highly efficient thermoelectric materials.

In this study, we synthesized an earth-abundant n-type Pb-Sb-Sn-based ternary sulfide mineral, achieving an exceptionally low κ_{lat} of ~0.41–0.48 W m^{-1} K^{-1} across a temperature range of 300–663 K. The low temperature (2 K) study indicates that this compound shows glass-like thermal conductivity. Atomic refinement and structural investigation indicated significant atomic displacement parameters (ADPs) associated with lead and atimony, implying inherent rattling-like behavior. The electron localization function (ELF) shows that these atoms are weakly bounded, forming low-energy Einstein-like vibrational modes. Additionally, low-temperature heat capacity (Cp) measurements and temperature-dependent Raman spectroscopy supported the presence of these soft optical modes. Density functional theory (DFT) calculations of phonon dispersion reveal that bonding hierarchy and collective rattling of weakly bound atoms generate these low-energy optical phonons. These optical modes interact with heat-carrying acoustic phonons, lowering their lifetimes and suppressing lattice thermal conductivity.

Dimensional Evolution of Phonon Scattering Mechanism in Bi2Se3 Thin films near room temperatue

Mr. Saptak Majumder[1], Mr. Gireesh Kandappanthodi[2], Mr. Hemanth Singh[3], Dr. Dinesh Kumar Shukla[3], Dr. Vinayak B. Kamble[1]
[1]School of Physics, IISER Thiruvananthapuram, India, [2]Zernike Institute for Advanced Materials, University of Groningen, Netherlands, [3] UGC-DAE Consortium for Scientific Research, University Campus, India

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Phonons, the quanta of lattice vibrations, play a central role in governing thermal transport in crystalline solids. Their scattering, arising from intrinsic lattice anharmonicity as well as extrinsic sources such as point and extended defects, leads to a reduction in lattice thermal conductivity. Temperature-dependent Raman spectroscopy on single crystals of Bi2Se3 up to 333 K reveals dominant three-phonon scattering across all Raman-active modes, with a finite contribution from four-phonon processes for the out-of-plane mode. To disentangle intrinsic and extrinsic scattering contributions, thin films were grown on polycrystalline SiO2 and crystalline GaAs (00l) substrates. A systematic evolution of phonon scattering is observed with decreasing thickness (~20–180 nm), with thinner films on GaAs exhibiting a pronounced enhancement of higher-order (quartic) anharmonic interactions. These results demonstrate that dimensional confinement provides an effective route to tune intrinsic lattice anharmonicity, particularly for out-of-plane vibrational modes in layered materials for systematic electron-phonon decoupling in thermoelectric materials

Thermoelectric Properties of Ag_2Se-Based Composites Incorporating Organic Small Molecules

Ms Adriana Maurucaite[1], Dr. Bejan Hamawandi[1], Dr. Raitis Grzibovskis[1], Dr. Kaspars Pudzs[1]
[1]Institute Of Solid State Physics, University Of Latvia, Latvia

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The move towards more sustainable energy practices in today's world has fueled the search for alternative and renewable energy sources, one of which is the use of thermoelectric generators (TEG). There are many strategies to improving TEGs, such as nano structuring and doping. This work focuses on improving thermoelectric performance and applications of inorganic and organic materials, by creating composite films, made from silver selenide nanoparticles, dispersed in an organic matrix. Inorganic part is responsible for high electrical conductivity and Seebeck coefficient, while the organic component offers advantages such as elasticity and lower thermal conductivity.

Silver selenide is n-type thermoelectric material and is well suited for use in room temperature. For the organic component, organic small molecules, that are typically used in organic light emitting diodes as charge transport and host materials, are used. This work utilizes electron transporting materials OXD-7 (1,3-bis[2-(4-tert-butylphenyl)-1,3,4-oxadiazo-5-yl]benzene), TAZ (3-(4-Biphenyl)-4-phenyl-5-tert -butylphenyl-124-triazole) and PBD (2-(4-Biphenyl)-5-(4-tert -butylphenyl)-134-oxadiazole) as an organic matrix. The use of charge transport materials in thermoelectric applications has been extremely limited; with this study we aim to fill a gap in research.

The nano and microparticles used in this work are synthesized using microwave assisted synthesis. Thermoelectric composite systems of nanoparticles dispensed in an organic matrix are made using the drop-cast method for simple film preparation and hydraulic press is used to prepare pellet samples. For the samples, electrical resistance and Seebeck coefficient are measured, and the specific electrical conductivity and power factors are calculated.

Structure, microstructure and thermoelectric properties of novel thermoelectric materials based on Mg-Ag-Sb-Cu-Bi high-entropy alloys

Tadeusz Miruszewski[1], Aleksandra Mielewczyk - Gryń[1], Klaudia Wojtkiewicz[1], Bogusław Kusz[1], Marcin Łapiński[1], Maria Gazda[1], Sheng-Wei Lee[2], Cheng-Lun Hsin[3]
[1]Institute of Nanotechnology and Materials Engineering, Gdańsk University of Technology, Poland, Poland, [2]Department of Electrical Engineering, National Central University, Taiwan, [3]Institute of Materials Science & Engineering, National Central University, Taiwan
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

High-entropy alloys (HEAs) are multicomponent materials composed of five or more elements [1]. They are commonly synthesised via liquid-state methods (arc melting, induction melting) and solid-state methods (mechanical alloying, spark plasma sintering) to obtain homogeneous solid solutions [2]. However, these methods require high temperatures, complex processing, and costly precursors. As an alternative, chemical reduction of oxides or nitrates offers lower-temperature synthesis, and potential cost reduction [3].

In this work, we report results obtained using two approaches to the solid-state synthesis of Mg–Ag–Sb–Bi–Cu thermoelectric alloys. The first approach was a conventional solid-state route performed in vacuum, in which intermetallic precursors (Mg3Sb2, Ag3Sb, Mg3Bi2, Cu3Sb) were used as reagents. The second approach was a hydrogen-assisted reduction of mixed oxides and nitrates. Phase composition and crystal structure were determined by XRD, while microstructure and morphology were characterised using SEM. They showed that both methods resulted in dense pellets; however, phase separation could not be avoided since they were composed of the main alloy and a few secondary phases. Nevertheless, the presence of secondary phases can be beneficial for both thermoelectric and mechanical properties. To characterise the phase composition, the oxidation states of constituent elements were analysed using XPS. Electrical, thermal, and thermoelectric properties of materials obtained using two methods were analysed and discussed based on the following results: the temperature dependence of the Seebeck coefficient and electrical conductivity in different atmospheres (air, H2, Ar) determined using the four-wire method, as well as thermal conductivity measurements over a wide temperature range.

[1] M. Jabri et al., Materials Today Energy 32 (2023) 101257
[2] X.Wang et al., J. Mater. Chem. A, 9 (2021) 663
[3] B. Bochentyn et al., Materials Chem. and Phys. 177 (2016) 353-359

The research was financially supported by the National Centre for Research and Development in Poland within the project POLTAJ12/2024/57/ONTHERM/2025.

Selective Defects Synchronize Thermoelectric Performance in V0.9Fe0.5Co0.5Sb-Based Half-Heuslers through Local Bonding Reconstruction

Prof. Dr. Yuzuru Miyazaki[1], Ms. Xue Nan[1], Prof. Kei Hayashi[1], Dr. Chen Chen[2], Dr. Md All Amin Newton[2], Dr. Hezhang Li[3], Prof. Dr. Jing-Feng Li[2]
[1]Department of Applied Physics, Graduate School of Engineering, Tohoku University, Japan, [2]State Key Laboratory of New Ceramic Materials, School of Materials Science and Engineering, Tsinghua University, People's Republic of China, [3]Department of Precision Instrument, Tsinghua University, People's Republic of China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Balancing carrier mobility and lattice thermal conductivity (κlat) remains a central challenge in thermoelectric materials because these transport parameters are intrinsically coupled [1,2]. Here, we demonstrate a strategy for decoupling carrier and phonon transport in XYZ half-Heusler compounds through intrinsic defect engineering and compositional tuning. A nominally 18-electron compound, V0.9Fe0.5Co0.5Sb, was designed to incorporate intrinsic defects, including vacancies (Vv) and interstitials (Fei and Coi), thereby generating compositional fluctuations, strain fields, and dislocation networks.

To elucidate the structural and bonding heterogeneity, we employed a combined experimental and theoretical approach. Multiscale microstructural characterization, ranging from atomic-resolution scanning transmission electron microscopy to mesoscale electron backscatter diffraction mapping, captured the evolution of strain and defect distributions. First-principles calculations based on different defect models were performed, and bonding characteristics were analyzed using the electron localization function, deformation charge density, and crystal orbital Hamilton population methods [3]. These results reveal substantial defect-induced bonding heterogeneity, which enhances phonon scattering while preserving carrier transport. Further tuning of the Fe/Co ratio in $V_{0.9}Fe_{0.5+x}Co_{0.5-x}Sb$ half-Heuslers shows that an Fe-rich composition ($x = 0.1$) exhibits simultaneous grain refinement and enhanced weighted mobility. The increased density of low-angle grain boundaries, together with delocalization of the V–Fe electronic network, leads to reduced κlat and improved mobility, resulting in enhanced electrical conductivity despite increased structural disorder.

These results demonstrate that carrier and phonon transport can be effectively decoupled through defect-mediated bonding reconstruction and microstructural control, providing a practical route toward synchronizing thermoelectric performance.

This research was partly supported by the grant-in-aid for scientific research from the JSPS (no. 23H00230) and by the Tsinghua-Tohoku Collaborative Research Fund from Tsinghua University and Tohoku University.

References
[1] X. Zhang et al., Sci. Adv. 2020, 6(46): eabc0726.
[2] R. He et al., Energy Environ. Sci. 2020, 13(12): 5165-5176.
[3] X. Nan et al., Sci. Adv. 11, 2375-2548 (2025).

Thermoelectric Transport in Monolayer and Bilayer MoS2

Yunhao Mo[1]
[1]King's College London, United Kingdom

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Two-dimensional materials are promising thermoelectric materials due to quantum confinement effects that can enhance the power factor [1,2]. In this work, the phonon-limited thermoelectric transport properties of monolayer and bilayer MoS_2 are investigated using a combination of first-principles calculations and analytical modelling. Electronic band structures, phonon dispersions and electron–phonon coupling matrix elements on a coarse grid in the reciprocal space are obtained using density functional theory and density functional perturbation theory implemented in the QUANTUM ESPRESSO and EPW codes [3,4]. To perform calculations of electron-phonon matrix elements on dense reciprocal space grids, an analytical framework based on the deformation potential approximation is developed. Using parameters extracted from first-principles calculations, and by solving the Boltzmann transport equation in the relaxation time approximation, the electrical conductivity, Seebeck coefficient, and power factor are evaluated. The results show that bilayer MoS_2 exhibits an enhanced power factor compared with monolayer MoS_2 due to the presence of an additional conduction-band valley at the Λ point.

[1] L. D. Hicks and M. S. Dresselhaus, Physical Review B 47, 12727 (1993)
[2] K. Hippalgaonkar et al., Physical Review B 95, 115407 (2017)
[3] I. Carnimeo et al., Journal of Chemical Theory and Computation 19, 6992 (2023)
[4] H. Lee et al., npj Computational Materials 9, 156 (2023)

Module-Level Simulation and Techno-Economic Assessment of Mg-Based and Half-Heusler Thermoelectric Cooling Materials

Puria Mahmoudi Nezhad[1], Seyedmohammad Mortazavinatanzi[1], Oleksandr Horniichuk[3], Radoslaw Radoslaw[3], P. S. Ioannou[2], T. Kyratsi[2]
[1]ParsNord Thermoelectric Filial, Sweden, [2]Department of Mechanical and Manufacturing Engineering, University of Cyprus, Cyprus, [3]IMRA Europe SAS, France

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Novel thermoelectric cooling materials have been widely studied in recent years due to their potential for improved efficiency and reduced reliance on critical elements. However, translating these materials from laboratory-scale characterization to practical module-level implementation requires careful evaluation of both thermal performance and cost. In this work, multiphysics simulations were performed using COMSOL to investigate the behavior of several thermoelectric material systems within device-level configurations. Two MgSb-based materials ($Mg_3Sb_{1.99}Te_{0.01}$ and MgBiSb), two Half-Heusler compounds ($TiFe_{0.5}Co_{0.15}Ni_{0.35}Sb$ and $Nb_{0.55}Ta_{0.40}Ti_{0.05}FeSb$), and BiTe as reference p-type and n-type materials were considered. A range of module configurations was simulated by varying p–n leg combinations, and key performance metrics including cooling power and temperature difference (ΔT) were evaluated under consistent boundary conditions. In parallel, a techno-economic assessment was conducted to estimate material costs and determine the cost per unit cooling power for each configuration. The results show that selectively replacing the n-type leg with Mg-based materials leads to a favorable balance between performance and cost. This configuration achieves temperature differences comparable to those of commercial BiTe-based modules while delivering higher cooling capacity. Such characteristics are particularly relevant for applications with high heat flux, such as power electronics and LED thermal management. In addition, this approach offers a potential reduction in overall module cost of approximately 30%, highlighting its promise for practical and scalable thermoelectric cooling solutions.

Thermoelectric effect in excitonic insulators

Dr. Jernej Mravlje[1], Ana Štuhec[1], Dr. Denis Golež[1]
[1]Jozef Stefan Institute, Slovenia

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Excitonic insulators are semimetals in which electron and hole pairs spontaneously condense. Whereas excitonic insulating state has been conclusively demonstrated in heterostructures through the Coulomb drag effects, convincing demonstration of excitonic insulating state in bulk materials is lacking. One of the main bulk candidates is Ta2NiSe5. Recent measurements of Seebeck coefficient have argued that electron-hole binding causes vanishing of the Seebeck coefficients in the condensate. We performed extensive simulations of thermoelectric coefficent in excitonic insulating state, both for the simplified models as well as for realistic bandstructure of Ta2NiSe5, using time-dependent Hartree Fock methods, finite temperature-Lanzczos and dynamical mean-field theory methods. These calculations indicate that transition into the excitionic insulating state may well be accompanied by the change of the sign of the Seebeck coefficient at low temperatures but strict vanishing occurs due to the influence of the impurities only. We discuss also the influence of corrections beyond Jonson-Mahan formula and the vertex corrections.

Fabrication and Validation of a Seebeck Cell for Precise Thin-Film Thermoelectric Coefficient Measurement: An Integrated Experimental and COMSOL Simulation Study

Ms. Hadiqa Naaz[1], Ms. Misha Khalid[1], Dr. Jose Ordonez Miranda[2], Dr. Michał Pawlak[1]
[1]Institute Of Physics, Faculty Of Physics, Astronomy And Informatics, Nicolaus Copernicus University, Poland, [2]Sorbonne Université, CNRS, Institut des NanoSciences de Paris (INSP), Paris, France, France

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Abstract
Accurate thermoelectric property measurement remains challenging in conventional systems, where distributed heating architectures introduce thermal losses and limit precise temperature gradient control. To address this a Seebeck cell was developed through a two-stage fabrication process for reliable thin-film thermoelectric characterization. In the first stage, a copper-electrode Seebeck cell was fabricated and validated against a Constantan reference sample at room temperature. The measured Seebeck coefficient of −36 μV/K showed close agreement with established literature values, confirming the validity of the measurement approach [1]. In the second stage an improved platinum-electrode Seebeck cell was designed for spatially confined point heating, exploiting platinum's superior thermal and chemical stability. Prior to fabrication, COMSOL Multiphysics simulations were conducted to model temperature distributions and thermoelectric behavior across an operating range of −10 °C to 150 °C. Simulations identified optimal conditions of 3 W heating power and 1.3 m/s forced convection yielding a stable measurement temperature of 75 °C with well-confined point heating, and predicted thermoelectric voltages reaching a maximum of 14.2 mV at 100 °C. Experimental results confirmed close quantitative agreement with COMSOL predictions, validating both the simulation framework and physical design [2]. The platform was subsequently applied to characterize pristine and antimony-doped ZnO thin films where Sb incorporation systematically enhanced thermoelectric performance relative to pristine ZnO, demonstrating the effectiveness of controlled doping for optimizing oxide-based thermoelectric materials. The approach offers a reproducible tool for microscale thermoelectric characterization in energy and sensing applications.

References
Kumar, A., Singh, A., Kumar, R., Singh, R., & Singh, R. (2019). Apparatus for Seebeck coefficient measurement of wire, thin film and bulk materials in the wide temperature range (80–650 K). arXiv preprint. arXiv:1906.08023.
Marinescu, C., Gropila, B., Leca, A., & Galca, A. C. (2024). Hot probe technique for thin films Seebeck coefficient measurement. Open Engineering, 14(1), 20220359.

Numerical Modelling of Anisotropic Nano-crystalline Materials

Keitaro Nakamura[1], Ms Liu Yaqi[1], Ms Moeka Sato[1], Dr Mitsuhiro Matsumoto[1], Mr Nobuhiko Kajinami[2], Mr Manabu Iwakawa[2], Ms Misaki Hanaoka[2]
[1]Kyoto University, Japan, [2]Mitsubishi Electric Corporation, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

We have developed a numerical simulation scheme for thermoelectric devices with nano-scale structures [1]. For the phonon transport, we adopted the Boltzmann transport equation (BTE) with the relaxation-time approximation; to treat the various types of nanostructures, the volume of fluid (VOF) scheme, which is conventionally used in multi-phase flows, was extended to properly trace the phonon fluxes near interfaces. The electron transport is evaluated with a simple electric network model since the spatial scale of our target systems (typically 10-1000 nm) is larger than the mean free path of electrons. We have successfully investigated the thermoelectric properties of silicon thin films with nano-scale holes of various shapes [2].
In this study we focus on sintered systems of typical thermoelectric materials, such as Bi2Te3 [3], in which anisotropic transport properties, such as the dispersion relation and the mode-dependent relaxation time, are enormous and should be appropriately considered. Choosing a simple model of sintered nanocrystals with needle shapes as a test target, we extended the original scheme to take the local anisotropies into account and investigated its transport properties. In this presentation, we discuss how the size and the shape distributions affect the thermoelectric efficiency.

[1] Y. Takahara et al., “Phonon transport simulation with an extended VOF scheme for nano-structured thin film,” Applied Physics Letters, 124, 172204 (2024).
[2] N. Kajinami et al., “Si thin film with nanohole structures to improve thermoelectric performance Part 1: Effects of shape and arrangement in periodic holes,” J. Heat Mass Transfer, 148, 012501 (2026).
[3] M. Hase et al., “Determining phonon transport properties of bismuth telluride thin films with extremely small grain size using nanoindentation and 3ω method,” Applied Physics Express, 16, 015004 (2023).

Co-doped Cu2SnS3 thermoelectric material synthesized by a simple and low-cost method

Shigeyuki Nakamura[1], Hideaki Araki[2], Yoji Akaki[3]
[1]National Institute of Technology, Tsuyama College, Tsuyama, Japan, [2]National Institute of Technology, Nagaoka College, Japan, [3]National Institute of Technology, Miyakonojo College, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Cu2SnS3 (CTS), which is composed of abundant and non-toxic elements, is one of the attractive candidates for low-cost and environmental-friendly thermoelectric (TE) materials. We have developed indium-doped CTS TEs by using a simple and low-cost method (1). Cobalt, which has unfilled d-orbital, is one of the most attractive dopants for CTS TEs because of a strong possibility of simultaneous enhancement of the Seebeck coefficient and electrical conductivity (2). In this presentation, we report on the TE properties of Co-doped CTS TEs fabricated with the above-mentioned method.

A vertical tube furnace with a single-ended round-sealed quartz tube is used for CTS synthesis. The detail of the method is presented elsewhere (1). The raw material with a composition of Cu:Sn:S:Co = 2.2:0.9:4.0:0.1 and additional sulfur of 1.5 g are heated continuously at 723 K and 873 K for 2 hours each. The resulting powder is plasma-sintered at 673 or 773 K, 20, 30 or 40 MPa, and 5 min to obtain the CTS TE legs.

Despite the sintering pressure, the amount of secondary phase, the crystal structure, and the density, the average ZT at 573 K of the CTS TE sintered at 773 K (0.228) is larger than that of the CTS TE at 673 K (0.126). Former is ranging from0.190 to 0.286, while later 0.084 to 0.175. Namely, these properties except the sintering temperature are found to hardly affect the thermoelectric property.

In this study, it was found that the sintering temperature is crucial for high performance CTS TE. Higher temperature sintering will be attempted in the future.

References

(1) S. Nakamura et al., ICT/ECT 2024, I-P47.
(2) H. Zhao et al., J. Mater. Chem. A, 2017, 5, 23267.

From Coffee Waste to Thermoelectric Materials: Sustainable PEDOT: PSS Composites

Şeyma ÖZKAN[1,2], Gökhan GÜRLEK[3], Bekir ÖZKAN[4], Süleyman İNAN[4], Mert ŞENER[5], Berkan ÇETİNKAYA[4], Barış Oğuz GÜRSES[3], Yoldaş SEKİ[6]
[1]Graduate School of Natural and Applied Sciences, Department of Chemistry, Dokuz Eylül University, Turkey, [2]Central Research Test and Analysis Laboratory Application and Research Center, Ege University , Türkiye, [3]Faculty of Engineering, Department of Mechanical Engineering, Ege University, Türkiye, [4]Institute of Nuclear Sciences, Ege University, Türkiye, [5]Faculty of Engineering, Department of Mechanical Engineering, Balıkesir University, Türkiye, [6]Faculty of Sciences, Department of Chemistry, Dokuz Eylul University, Türkiye

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Sustainability has become one of the key topics in material research. And this approach has grown attention in utilization of biomass waste into usable parts. Thermoelectric materials enable direct heat–electricity interconversion, supporting sustainable energy and waste heat use [1]. Although conventional inorganic thermoelectric materials exhibit high performance, they often suffer from high cost, scarcity of critical elements, and limited processability [2]. Consequently, organic and hybrid systems have emerged as promising alternatives, offering low toxicity, mechanical flexibility, and scalability [3]. However, the performance of purely organic systems remains limited, motivating the incorporation of functional fillers. In this study, waste coffee grounds were converted into functional thermoelectric components. Coffee waste was dried, cryogenically milled, and subjected to mild thermal treatment to stabilize the particles, which were then surface-functionalized using three different acids (sulfuric acid, phosphoric acid, and citric acid) at a fixed concentration. These functionalized particles were incorporated into a PEDOT: PSS matrix at different loadings, ranging from 0 to 1 wt%, and the resulting composite films were systematically characterized to investigate their effects on the Seebeck coefficient and electrical conductivity. This approach demonstrates a sustainable and scalable strategy for valorizing biomass waste while enhancing the performance of flexible organic thermoelectric materials.

[1]-Fiedler, C., Kleinhanns, T., Garcia, M., Lee, S., Calcabrini, M., & Ibanez, M. (2022). Solution-processed inorganic thermoelectric materials: Opportunities and challenges∇. Chemistry of Materials, 34(19), 8471-8489.
[2]- Zhang, Y., Heo, Y. J., Park, M., & Park, S. J. (2019). Recent advances in organic thermoelectric materials: Principle mechanisms and emerging carbon-based green energy materials. Polymers, 11(1), 167.
[3]- Zhang, Y., & Park, S. J. (2019). Flexible organic thermoelectric materials and devices for wearable green energy harvesting. Polymers, 11(5), 909.

Fabrication and Characterization of Electrospun PCLPEDOTPSSMWCNT Thermoelectric Nanofiber Composites

Umut Doğu Seçkin[1], Şeyma ÖZKAN[2,3], Elif KÜÇÜK SEÇKİN[4], Barış Oğuz GÜRSES[5], Gökhan GÜRLEK[5], Mert ŞENER[6], Aylin ŞENDEMİR[1], Yoldaş SEKİ[7]
[1]Faculty of Engineering, Department of Bioengineering, Ege University, Türkiye, [2]Graduate School of Natural and Applied Sciences, Department of Chemistry, Dokuz Eylül University, Türkiye, [3]Central Research Test and Analysis Laboratory Application and Research Center, Ege University, Türkiye, [4]Graduate School of Natural and Applied Sciences, Department of Mechanical Engineering, Ege University, Türkiye, [5]Faculty of Engineering, Department of Mechanical Engineering, Ege University, Türkiye, [6]Faculty of Engineering, Department of Mechanical Engineering, Balıkesir University, Türkiye, [7]Faculty of Sciences, Department of Chemistry, Dokuz Eylul University, Türkiye

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Materials exhibiting thermoelectric properties have emerged as a promising and environmentally sustainable approach for energy harvesting by directly converting waste heat into electrical energy. Organic thermoelectric materials have gained significant attention due to their intrinsic flexibility, low thermal conductivity, and potential biocompatibility, making them highly suitable for wearable and implantable energy harvesting systems[1]. However, their generally low electrical conductivity remains a major limitation, often requiring the incorporation of conductive nanofillers and the engineering of optimized micro/nanostructures to improve charge transport[2].

In this study, a flexible nanofibrous composite system was developed via electrospinning using Polycaprolactone (PCL), PEDOT:PSS, and multi-walled carbon nanotubes (MWCNTs). The synergistic combination of PEDOT:PSS and MWCNTs is expected to establish efficient percolated conductive networks, thereby enhancing electrical conductivity and charging carrier mobility within the insulating PCL matrix. Meanwhile, the electrospun fibrous architecture provides a high surface area, tunable porosity, and reduced thermal conductivity, all of which are beneficial for improving thermoelectric performance. The resulting composite materials are designed not only to optimize electrical transport but also to maintain mechanical flexibility and structural stability. Comprehensive characterization will be performed, including morphological analysis (SEM), thermal stability (TGA), crystallization behavior (DSC), mechanical properties, degradation behavior, in vitro cytotoxicity, electrical conductivity, and Seebeck coefficient measurements. The outcomes of this work are expected to contribute to the development of flexible, bio-compatible, and multifunctional thermoelectric materials for next-generation implantable and bio integrated devices.

1- Xiao, R., Zhou, X., Zhang, C., Liu, X., Han, S., & Che, C. (2024). Organic thermoelectric materials for wearable electronic devices. Sensors, 24(14), 4600.
2- Idir, M., Chamelot, G., He, Y., Lemieux, T., Bueley, K., Beaupré, S., ... & Leclerc, M. (2026). Organic thermoelectric films: achieving high conductivity and power factor through sulfonated-poly (3, 4-ethylenedioxythiophene) and single-walled carbon nanotube composites. Journal of Materials Chemistry C.

Design, Fabrication, and Environmental Reliability of Standardized Bi2Te3-Based Reference Thermoelectric Modules for Industrial Applications

Mr. Jongho Park[1], Ms. Jeongin Jang[1], Dr. Jaywan Chung[1], Dr. Byungki Ryu[1], Dr. SuDong Park[1]
[1]Korea Electrotechnology Research Institute (KERI), South Korea

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric (TE) technology is being adopted in a growing range of applications, such as shipboard and industrial waste-heat recovery systems. These applications often expose thermoelectric generator modules (TGMs) to harsh environmental conditions. Ensuring long-term durability, structural integrity, and electrical reliability is therefore critical for their practical deployment. In this study, we present the design, fabrication, and environmental reliability assessment of a Bi2Te3-based reference thermoelectric generator module (TGM), which was developed to reflect industrial requirements while serving as a benchmark for performance evaluation.

Representative Bi2Te3-based ternary compositions were defined for p- and n-type legs using a machine-learning model that predicts composition-dependent transport properties, targeting compositions near the zT maximum at 150 °C, where the performance is relatively insensitive to compositional deviations. These are referred to here as the reference compositions. A representative module geometry was identified based on surveys of commercial module specifications and is hereafter referred to as the reference module (Type C, 40×40 mm^2, 199 leg pairs). The designed module based on the reference compositions was fabricated and used as the module for standardized performance evaluation and reliability testing.
Comprehensive environmental reliability tests were conducted to simulate stress conditions commonly encountered in real-world applications, particularly in ship-TEG applications: salt-mist resistance, high-humidity endurance, and mechanical vibration conditions. All tests were conducted in accordance with standardized reliability protocols established by the Korea Electronics Technology Institute (KETI). After testing, the variation in the TGM internal resistance remained within ±1.5%, and no evidence of corrosion, surface degradation, or mechanical failure was observed, confirming structural integrity. Post-test characterization showed that the module maintained stable power output and conversion efficiency.
Overall, these results validate the reliability of the reference TGM and provide a standardized evaluation protocol that can serve as a solid foundation for industrial deployment.

Thermoelectric module design governed by heat exchangers

PhD Nerea Pascual[1], PhD Álvaro Martínez[1], PhD Irantzu Erro[1], PhD Patricia Alegría[1], PhD Miguel Araiz[1], PhD Leyre Catalán[1], PhD Laura Carlosena[1], Mr Adrian Ibañez[1], PhD David Astrain[1]
[1]Public University Of Navarre, Spain

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Geometric optimisation of thermoelectric modules is often treated as a module-level problem, even though performance is ultimately dictated by the thermal system in which they operate. This study challenges this assumption by developing an integrated system-level optimisation framework for thermoelectric module geometry in a geothermal passive thermoelectric generator deployed in Antarctica. The approach is based on the coupled nature of heat transfer and electrical phenomena.

A comprehensive multi-parameter, multi-objective computational model for thermoelectric module geometric optimisation is presented, incorporating temperature-dependent material properties, all thermoelectric effects, and interactions between system components. The framework simultaneously maximises electrical power output and minimises semiconductor material volume by optimising thermocouple length and cross-sectional area.
Applied to the Antarctic installation, the method predicts energy production gains of up to 12.6% compared to the commercial modules currently in use. The analysis further shows that optimal geometry is not governed by the source temperature difference, but by the thermal resistance of the heat exchangers. A 26% reduction in the thermal resistance of the heat exchangers installed in Antarctica increases optimisation potential by 60%, while reducing semiconductor volume by 18.5%.

These results demonstrate that thermoelectric modules cannot be optimised in isolation and establish a clear optimisation strategy. Heat exchangers must first be designed to minimise thermal resistance, after which module geometry should be tuned by increasing thermocouple cross-sectional area within manufacturing constraints and subsequently adjusting leg length to achieve the optimal thermal resistance determined by the heat exchangers.

Optical based thermal anisotropy methods for thin films.

Prof Michal Pawlak[1]
[1]Nicolaus Copernicus University, Poland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

This paper presents methods for measuring thermal anisotropy (in plna thermal conductivity, and cross plane thermal conductivity) in nanostructures in different temperatures. The measurement methods are based on two techniques: infrared radiometry [1] and thermal reflectance [2]. The advantages and disadvantages of these methods will be discussed. Theoretical models and the results obtained for AlGa/AlAs, ZnO, and PEDOT:PSS will be presented.

[1] M Pawlak, N Jukam, T Kruck, D Dziczek, A Ludwig, AD Wieck Measurement of thermal transport properties of selected superlattice and thin films using frequency-domain photothermal infrared radiometry, Measurement 166, 108226

[2] M Pawlak, T Kruck, N Spitzer, D Dziczek, A Ludwig, AD Wieck
Experimental validation of formula for calculation thermal diffusivity in superlattices performed using a combination of two frequency-domain methods: Photothermal infrared ...Applied Sciences 11 (13), 6125

Thermoelectric Device Integration for Sustainable Energy Optimization in aerial Systems

Pedro Silva[1,2], Dr. António Gonçalves[1], Mr. Marcelo Soares[2]
[1]Instituto Superior Técnico - Universidade de Lisboa, Portugal, [2]TEKEVER UAS, S.A., Portugal
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The pursuit of improved energy efficiency in established systems, using non-toxic, non-critical and low-cost materials, has significantly increased interest in thermoelectrics. Thermoelectric devices enable energy conversion for power generation and refrigeration without noise or moving parts. Magnesium-based thermoelectric materials, particularly Mg2Si- and MgAgSb-based compounds, are promising for applications from room temperature to medium temperatures (~300ºC), exhibiting average figures of merit, zT, of 0.9 and 1.1 in that range, respectively.

Aerial systems such as Unmanned Aerial Systems (UASs) and Fixed-Wing Ultralights (FWU) are small flying platforms, either unmanned or crewed, with applications in critical areas including traffic monitoring, agriculture, surveillance, and defense. Their main challenges include flight autonomy, power efficiency, and material durability. In this work, we propose a hybrid approach that converts waste heat from combustion engines into electrical power using magnesium-based thermoelectric generators (TEGs) to improve performance. These materials are stable under operating conditions (of 230 ºC), while also offering high availability and low density. We present different configurations of thermoelectric modules based on Mg materials. One configuration employs a flexible silicone resin substrate to reduce vibrations, combined with a commercial thermal paste. The developed modules are compared with a commercial TEG. Key design parameters, including the number of thermoelectric legs and the thickness of the copper electrodes, were evaluated. An increase in the number of legs led to higher voltage output, while increasing the electrode thickness from 0.05 to 0.1 mm resulted in a more stable performance. The influence of pellets dimensions and module integration within a combustion engine was also evaluated through simulations and compared with the voltage output of a commercial module. The results indicate that optimizing TEG design could potentially eliminate the need for alternators, reduce fuel consumption, and improve aerial systems autonomy.

Rational Co-dopant Design in Thermoelectrics via Electronegativity-Guided Alloy Scattering Potentials: A Descriptor-Driven Framework Illustrated by MnTe

Mr. Srivathsan Prakasam[1], Mr. Sri Sai Samhitha Gadhavajhala[1], Dr. Veera Prabu Kannan[1], Dr. Gang Bahadur Acharya[1], Prof. Bhuvanesh Srinivasan[1]
[1]Thermal Energy Materials Group, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

MnTe is a promising thermoelectric material owing to its intrinsically high Seebeck coefficient and unique antiferromagnetic ordering; however, its efficiency is hindered by low electrical conductivity resulting from poor carrier dynamics. Co-doping has emerged as an effective strategy to enhance performance through band convergence, carrier concentration tuning, and phonon suppression, yet the absence of systematic guidelines for co-dopant selection has limited progress. In this work, a rational co-dopant selection framework has been developed that integrates two key descriptors - alloy scattering potential and electronegativity difference - alongside strain and mass fluctuation analysis. The alloy scattering potential quantifies carrier scattering from local potential fluctuations (electrostatic perturbations), while electronegativity difference governs bond polarity. Together, these parameters determine the extent to which reduction in mobility has been mitigated in the presence of dopants, while strain and mass fluctuations serve as powerful phonon-scattering centres that reduce lattice thermal conductivity. Within this MnTe framework, a progression from Ag-Sn to Ag-Ge to Ag-Sb co-doping demonstrates improved carrier concentration and mobility, attributed to modified defect thermodynamics and reduced bond polarity. The Ag-Sb co-doped system achieves a low alloy scattering potential of ~ 0.6 eV and a minimal electronegativity mismatch with Te, effectively minimizing potential fluctuations and electrostatic perturbations, thus mitigating the reduction in mobility. Simultaneously, size and mass fluctuations efficiently scatter phonons, yielding an optimized balance between electrical and thermal transport. This electronegativity-guided alloy scattering potential framework establishes a universal and predictive strategy for co-dopant design in thermoelectrics, extending beyond MnTe to next-generation high-performance energy materials.

This presentation is based on our article published in Acta Materialia:
S. Prakasam, S.S.S. Gadhavajhala, V.P. Kannan, G.B. Acharya, B. Srinivasan, Rational co-dopant design in thermoelectrics via electronegativity-guided alloy scattering potentials: A descriptor-driven framework illustrated by MnTe, Acta Mater. (2026) 122221. https://doi.org/10.1016/j.actamat.2026.122221.

Characterization of novel nitride thin films prepared by magnetron sputtering for enhanced thermoelectricity

Dejan Prokop[1,2], Joris More-Chevalier[2], Petr Hruška[1,2], Michal Novotný[2], Stanislav Cichoň[2], Esther de Prado[2], Petr Levinský[2], Ursula Danuta Wdowik[3], Jiří Martan[4], Ján Lančok[1], Dominik Legut[3]
[1]Faculty of Mathematics and Physics, Charles University, Czech Republic, [2]FZU - Institute of Physics of the Czech Academy of Sciences, Czech Republic, [3]VSB Technical University of Ostrava, Czech Republic, [4]NTC University of West Bohemia, Czech Republic

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Nitride thin films represent a broad class of materials with favourable electronic, optical and mechanical properties. Their ability to form solid solutions and accommodate doping within their common crystalline structures makes them promising candidates for future thermoelectric energy conversion devices. Among these, ScN, HfN and CrN thin films have shown significant potential, particularly for high-temperature applications. To further improve their thermoelectric efficiency, we recently prepared semimetallic ScN-, HfN- and semiconducting CrN-based thin films on MgO(100) substrates by reactive DC magnetron sputtering. By systematically tailoring their microstructure and stoichiometry through variation of deposition parameters, controlled doping and the fabrication of multilayered heterostructures, we achieved an enhancement of the thermoelectric figure of merit. The microstructure was characterised using AFM, SEM and XRD measurements, while the chemical composition was determined by WDS/EDX and XPS. Furthermore, these properties were correlated with the presence of open-volume defects, such as vacancies and nanoscopic pores, investigated by variable energy positron annihilation spectroscopy, a unique non-destructive technique well suited to this purpose. This approach enabled optimization of the deposition process and the fabrication of films with improved performance. These experimental results are supported by ab initio DFT calculations.

MOVPE-Grown InAlGaN/GaN/Al2O3 Heterostructures for Thermoelectric Applications

Ramesh Raju[1]
[1]Aalto University, Finland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The thermoelectric (TE) properties of binary and ternary III-nitrides such as AlGaN and InGaN have been widely investigated. However, the quaternary alloy InAlGaN remains unexplored for its TE potential. In this work, we aim to investigate InAlGaN with low indium and aluminum content grown by metalorganic vapor phase epitaxy (MOVPE) on GaN/sapphire substrates. This alloy exhibits promising TE properties for high-temperature applications. The work demonstrates that the compositional fluctuations in InAlGaN critically influence carrier transport and phonon scattering by systematically varying the growth temperature (800–1000 ◦C). Despite its lower electrical conductivity, the 800 ◦C grown sample achieves the highest Seebeck coefficient (−700 μVK−1) and power factor of 2.32 × 10−3 Wm−1K−2 due to energy filtering effects in the In/Al doped nanodomains. In contrast, the 1000 ◦C sample exhibits the highest electrical conductivity but a reduced Seebeck coefficient (−485 μVK−1), as increased Al/Ga incorporation homogenizes the alloy. Furthermore, the thermal conductivity is minimized to 19.3 W m−1K−1 at 800◦ C due to raised boundary phonon scattering from compositional disorder. Consequently, the figure of merit (zT) maximizes to 0.035 for the sample grown at 800 ◦C, highlighting the trade-off between electronic and thermal transport. These results elucidate the role of growth temperature-controlled phase separation in InAlGaN and provide design principles for optimizing nitride-based TE materials through deliberate defect and nanostructure engineering.

Strong anharmonicity guided weaker temperature-dependent phonon transport in CaSnS3: A chalcogen perovskite showing wavelike phonon tunnelling

Surbhi Ramawat[1], Ambesh Dixit[1]
[1]Indian Institute of Technology Jodhpur, India

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Environmental robustness and halide-perovskite-like performance of devices ranging from optoelectronics to thermoelectrics have sparked the scientific community's interest in chalcogen perovskites (CPs) [1]. The search for high-performance thermoelectric materials has led to the discovery of numerous promising candidates; however, materials with intrinsically low thermal conductivity are particularly desirable [2]. Comprehending lattice dynamics and thermal conductivity is crucial for energy conversion devices. Here, we investigate the lattice thermal conductivity of the chalcogenide perovskite $CaSnS_3$ by including temperature-dependent phonon renormalization, loop and bubble self-energy corrections, four-phonon scattering, and wave-like heat transport. Weak and inhomogeneous bonding produces strong anharmonicity, reflected in an average Grüneisen parameter of approximately 1.92. The predicted lattice thermal conductivity is ultralow, decreasing from approximately 0.75 W m^{-1} K^{-1} at 300 K to 0.63 W m^{-1} K^{-1} at 700 K. At 300 K, particle-like and wave-like contributions are approximately 0.40 and 0.35 W m^{-1} K^{-1}, respectively. The wave-like contribution increases from 46% at 300 K to 56% at 700 K because of coupling between closely spaced phonon branches. The interplay between higher-order anharmonicity and wave-like transport leads to a weak temperature dependence of approximately T−0.20 highlighting the need to go beyond conventional three-phonon transport models. Overall, while emphasizing lattice anharmonicity and glasslike thermal conduction, this study will help to improve the understanding of chalcogen perovskite design for multiple technological applications [3].

References

[1] G. G. Njema and J. K. Kibet, A review of chalcogenide-based perovskites as the next novel materials: Solar cell and optoelectronic applications, catalysis and future perspectives, Next Nanotechnol. 7, 100102 (2024).

[2] N. Li, G. Wang, Z. Zhou, G. Wang, G. Han, X. Lu, and X. Zhou, IV-VI/I-V-VI2 thermoelectrics: Recent progress and perspectives, Adv. Funct. Mater. 34, 2405158 (2024).
[3] Surbhi Ramawat, Sumit Kukreti and A. Dixit, "Strong anharmonicity guided weaker temperature-dependent phonon transport in CaSnS3: A chalcogen perovskite showing wavelike phonon tunneling", APS Physical Review B 113, 024310 (2026).

Experimental Investigation and Validation of Computationally Predicted Stable Double Half-Heusler Thermoelectric Materials

Mr Latif Bukari Rashid[1], Dr Muath Mohammed Al Malki[1,2]
[1]King Fahd University Of Petroleum And Minerals, Dhahran, Saudi Arabia, [2]Interdisciplinary Research Center for Sustainable Energy Systems (KFUPM), Saudi Arabia

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Double-Half Heusler (DHH) compounds have gained prominence in recent times as promising TE materials, an improvement on regular half-heuslers (HHs) with several compositions computationally predicted stable and capable of delivering competitive zT values. However, many of these candidates including Nb_2Co_2InSb have not yet been synthesized and experimentally validated, leaving a critical gap between theoretical predictions and practical TE performance. The proposed study aims to provide the first experimental investigation of unreported DHH compositions using successful synthesis techniques including high-energy ball milling, spark plasma sintering, and hot pressing (HBM, SPS, and HP respectively). This study will examine phase formation, crystal structure, and microstructure using qualitative and quantitative techniques, followed by a full assessment of TE properties. The proposed study aims to contribute reliable data for novel DHH compositions and insights to guide the development of stable, efficient, and scalable TEs for waste heat energy recovery and energy conversion purposes. This work is actively being carried out at the time of submission and results would be incorporated well ahead of the conference for presentation.

A Review of Double Half-Heusler Thermoelectrics

Mr Latif Bukari Rashid[1], Dr Muath Mohammed Al Malki[1,2]
[1]Department of Mechanical Engineering, King Fahd University of Petroleum and Minerals, Saudi Arabia, [2]Interdisciplinary Research Center for Sustainable Energy Systems, KFUPM, Saudi Arabia

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

This paper presents the first systematic and data driven review of double half-heusler (DHH) thermoelectrics (TEs) reported from 2019-2025. Over 1,000 papers across scientific databases were screened, from which 37 high-confidence DHH focused studies were selected for full analysis following the PRISMA approach. Results from this paper highlight that, the DHH research domain is dominated by computational studies (COMP), with fewer experimental (EXP) or hybrid (HYB) validations representing 54%, 32%, and 14% of papers analysed respectively. Most reported DHH systems crystallise in tetragonal (I-42d) or cubic-derived structures (F-43m, MgAgAs-type), and synthesis routes are largely centered on arc melting (AM), ball milling (BM), or spark plasma sintering (SPS). The peak experimental performance identified in this review is a figure of merit (zT) of 0.82 at 973K for the $Ti_2CoNi_{0.9}Cu_{0.1}(Sb_{0.925}Bi_{0.075})_2$ sample, and zT of 1.75 at 1000K predicted for the ordered $Ti_4Fe_2Ni_2Sb_4$ composition. Cross-property correlation analysis of DHH studies reveals consistent trends where high zT values are strongly correlated with low lattice thermal conductivity (κl), balanced electrical conductivity (σ), and moderate seebeck coefficients (S), while systems with high κl or poor carrier mobility record low zT. Despite the prediction of over 131 thermodynamically stable DHH compositions through COMP efforts, EXP realisation remains limited to a small subset of mainly Ti, Zr, and Hf-based systems, leaving much of the predicted DHH design space unexplored. Reporting inconsistencies in TE data further restrict cross-study interpretation, while emerging structural families and thin-film DHHs remain largely unstudied.

Shape-invariant thermoelectric efficiency

Byungki Ryu[1,2], S Oh[1,3], J Chung[1], S Park[1], M Lee[3], E Mueller[4]
[1]Korea Electrotechnology Research Institute (KERI), South Korea, [2]University of Science and Technology, South Korea, [3]Kyungpook National University, South Korea, [4]German Aerospace Cener (DLR), Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric (TE) effects, such as Seebeck and Peltier effects, enable applications in power generation, solid-state cooling, and thermal management. Thermoelectric conversion efficiency (η) is often estimated using the material figures of merit, $ZT = (\alpha^2/\rho\kappa)T$, where α, ρ, κ, and T are Seebeck coefficient, electrical resistivity, thermal conductivity, and temperature. However, device-level performance requires geometric information. Along with the complexity arising from T-dependent TE properties and geometric shapes, evaluation of η is far more challenging than the conventional wisdom based on ZT from constant-property models. Moreover, diverse thermal and electrical boundary conditions make analytical treatment of η difficult.

In this work, we report that thermoelectric conversion efficiency becomes shape-invariant when thermal and electrical boundary conditions are exactly matched. By employing the load resistance ratio γ to the internal resistance, the governing differential equation can be transformed into a first derivative of the relative heat flux, defined as $\kappa.\mathrm{grad}T/J$, that only depends only on T, α, and $\rho\kappa$. This indicates that normalized thermoelectric performance remains invariant under transformation of $\rho\kappa$ in both T and spatial domains. Starting from a special form of the differential equations in high-symmetric coordinate systems, we prove that efficiency is inherent. Finite-element analysis further confirms that a single curve of γ emerges across many geometries.

Finally, we demonstrate that in ideal situations, any 3D performance can be mapped into 1D performance, characterized by the condition $J \times \mathrm{grad}.T = 0$. However, when boundary conditions are not matched, this condition is violated leading to reduced η. We conclude by discussing the implications of shape on practical TE generator modules and the origin of dimensional energy losses, thereby providing new guiding principles for thermoelectric shape design.

Thermal Stability Limits of Cu-Based Argyrodites: Phase Evolution and Degradation in Cu8SiS3Se3

Sagarika Sharma[1], Dr. Oleksandr Cherniushok[1], Dr. Taras Parashchuk[1], Prof. Kinga Pielichowska[2], Prof. Krzysztof T. Wojciechowski[1]
[1]Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Poland, [2]Department of Glass Technology and Amorphous Coatings, Faculty of Materials Science and Ceramics, AGH University of Krakow, Poland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Cu-based argyrodites have attracted increasing attention as thermoelectric materials due to their intrinsically low thermal conductivity and promising electrical transport properties. However, their operational reliability is critically limited by insufficiently understood thermal stability, particularly under realistic environmental conditions. Here, we address this gap by introducing a quantitative framework for evaluating temperature-dependent stability and by establishing the operational limits of Cu8SiS3Se3.

We investigate phase stability, degradation pathways, and transport reversibility of Cu8SiS3Se3 up to 873 K under inert (argon) and oxidative (air) conditions. High-temperature X-ray diffraction and thermogravimetric analysis are combined with cyclic transport measurements up to 773 K to directly assess structural and functional stability. To resolve degradation mechanisms, prolonged annealing at 873 K for 48 h is performed in vacuum and air, followed by cross-sectional SEM analysis to identify compositional gradients and volatile-element loss. Centre of this work, we introduce the Temperature Reversibility Index (TRI), a metric that quantifies the reversibility of transport properties during thermal cycling.
We demonstrate that Cu8SiS3Se3 maintains structural stability and reproducible transport properties only up to 473 K. Above this threshold, rapid degradation occurs. Under inert conditions, phase decomposition leads to Cu2(S,Se) and Cu2Si(S,Se)3, while exposure to air further accelerates degradation through oxidation, forming CuSO4, Cu2SO5, and SiO2. In both environments, selenium evaporation is the primary cause for degradation. TRI analysis provides a direct, quantitative measure of the collapse of transport reversibility and clearly shows the material's operational stability window.

These results establish 473 K as the practical upper limit for reliable operation of Cu8SiS3Se3 and identify the coupled effects of phase instability, oxidation, and volatile-element loss as the governing degradation mechanisms. More broadly, the TRI framework offers a generalizable tool for assessing stability limits in thermoelectric materials and enables more rational design of Cu-based argyrodites with improved thermal durability.

Design and Fabrication of Cobalt-Oxide-based Thermoelectric Uni-leg Modules

Mrs Yoshimi Shimizu[1], Dr Kei Hayashi[1], Prof Yuzuru Miyazaki[1]
[1]Tohoku University, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Funahashi et al. successfully developed thermoelectric (TE) modules composed entirely of oxide materials†. However, the performance of the n-type oxide legs remained inferior to that of the p-type legs. Misfit-layered cobaltate $[Ca_2(Co_{0.65}Cu_{0.35})_2O_4]pCoO_2$ ((Co, Cu)-221) is a promising p-type oxide TE material because of its crystallographic anisotropy and high power factor of 2.2×10^-4 W/mK^2 at 900 K. In our previous study, simulations predicted that the surface power density (Pd) of a (Co, Cu)-221-based module would be 78 % higher than that reported by Funahashi et al. However, the experimentally obtained output was only about 1/50 of the predicted value because of high internal resistance.

In this study, we designed and fabricated uni-leg modules operable at high temperature in air. To reduce internal resistance, metallisation layers were introduced, and the contact interfaces between the uni-leg element and the electrodes were systematically optimised.
The power-generation characteristics of the module were simulated using ANSYS. Ni was used for the electrodes, and contact resistance was neglected. An alumina layer was inserted between the p-type leg and the electrode as an electrical insulator. The (Co, Cu)-221 samples were prepared by a conventional solid-state reaction method, sandwiched between metal plates, and sintered by spark plasma sintering (SPS).

Based on previous optimisation studies, the module dimensions were fixed at 3.1 × 3.1 × 6.4 mm^3. The maximum output power (Pmax) was evaluated at a temperature difference (ΔT) of 500 K for modules with Ni and Cu-metallised layers. The simulated Pmax was 16.8 mW and was almost independent of the metallisation material, although Cu gave a slightly higher value than Ni. In this presentation, we will report the measured Pmax and Pd values of fabricated uni-leg modules with Ni and Cu metallisation.

References
† R. Funahashi et al.: J. Appl. Phys., 99 (2006) 066117.

Investigation of the effect of systematic Nb-addition on the Grain Boundaries of Te-doped Mg3(Sb,Bi)2

Mr. Vishak Sivasubramaniyan Sudandiradevi[1], Prof. Dr. Kornelius Nielsch[1], Dr. Ran He[1]
[1]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric materials are significant facilitators of energy conversion, power generation and refrigeration, via the direct interconversion of heat (temperature gradient) and electricity. In pursuit of tellurium-free sustainable thermoelectrics for the low-mid temperature range, Mg3(Sb,Bi)2 based Zintl compounds are now evolving as a suitable n-type substitute. The challenge within the system to achieve high efficiencies, thereby via high figure of merit (zT), arises out of the low electrical conductivity, especially at the room temperature to mid temperature range, originating primarily due to the domination of grain boundary scattering (GBS) of carriers. Amongst the various mitigation techniques, in this study we investigated the systematic addition of a metallic inclusion, Niobium (Nb), aiming to enhance the carrier mobility combatting the GBS. We observe the inclusion of metallic Nb, which has been studied to preferentially deposit at the grain boundaries due to greater wetting at the same, to result in the modification of the grain boundary by possibly facilitating a high-mobility pathway for the carriers across the boundary potential barrier, despite the reduction of average grain size. We hypothesize these dual antagonistic mechanisms to result in the observation of an optimal Nb addition concentration, to obtain enhancement of zT, especially in the lower temperature range. This study thus systematically analyzes the varying concentration of metallic Nb addition in this series of compounds to benefit the carrier mobility enhancement thereby overcome GBS to obtain Mg3(Sb,Bi)2-based materials with better efficiencies at the room-mid temperature regime.

Enhanced Thermoelectric Performance and Phase Stability of $AgSbTe_2$ via Cation Vacancy Engineering

Hyoju Son[1], Ms. Suhyeon Woo[1], Mr. Jihwan Im[1], Dr. Samuel Kimani Kihoi[1], Dr. Joseph Ngugi Kahiu[1], Prof. Ho Seong Lee[1]
[1]Department of Materials Science and Metallurgical Engineering, Kyungpook National University, South Korea

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

$AgSbTe_2$ has attracted significant attention as a mid-temperature thermoelectric material due to its inherently low thermal conductivity. However, the conventional stoichiometric composition forms secondary phases due to thermal instability, which deteriorate both performance and reliability. In this study, we aimed to enhance the thermoelectric performance of $AgSbTe_2$ by modulating the Ag-content to suppress phase separation and control electronic transport properties.

High-density bulk samples were fabricated using a combination of melting/quenching and hot-pressing processes. The phases and microstructures were characterized via XRD and SEM, followed by a comprehensive evaluation of temperature-dependent thermoelectric properties. Our findings confirm that a controlled reduction in Ag-content effectively inhibits the formation of the Ag_2Te secondary phase and contributes to the stabilization of the matrix phase. Furthermore, the cation vacancies generated by the Ag-deficiency were found to optimize the carrier concentration, thereby improving transport properties. Notably, the $Ag_{0.98}SbTe_2$ composition successfully mitigated the bipolar effect at elevated temperatures, whereas excessive non-stoichiometry, such as in $Ag_{0.9}Sb_{1.1}Te_{2.1}$, exacerbated the bipolar contribution. This phenomenon is attributed to unintended band structure modifications caused by excessive defect introduction.

As a result, the optimized $Ag_{0.98}SbTe_2$ sample achieved a power factor approximately twice that of the stoichiometric sample, leading to a peak zT of ~1.46 at 673 K. These results demonstrate that defect engineering through compositional control is an effective strategy for ensuring phase stability and suppressing detrimental bipolar effects, providing a clear pathway for the design of high-performance $AgSbTe_2$-based thermoelectric materials.

Simulation of Thermoelectric Modules for Energy Harvesting in Cryo-Fuel Applications

Dr Christian Stiewe[1], Dr. Matthias Helmich[1], Prof. Eckhard Mueller[1,3], Dr. Soma Salamon[2]
[1]German Aerospace Center (DLR), Germany, [2]University of Duisburg-Essen, Germany, [3]Justus Liebig University Giessen, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric (TE) generators are an option for waste heat recovery in a large diversity of applications, such as automotive, aerospace and industrial processes with high energy throughput.

The rapid deployment of cryogenic fuels (liquid H_2, LNG) in road and rail transport creates a new source of low-temperature waste heat at the fuel-evaporator. Harvesting this heat with thermoelectric generators (TEGs) offers a compact, solid-state solution for auxiliary power, but the extreme temperature asymmetry (cold side ≈ -190 °C to -80 °C, hot side ≈ 0 °C–500 °C) demands a dedicated module design.

We present a comprehensive 1D simulation of single-stage and segmented TE modules comprising Bi_2Te_3, Skutterudites and Mg based alloys. The model uses measured temperature-dependent material properties, geometries of the single pellets and TE module with variation of the filling factor and considers electrical and thermal contact resistances.
The boundary conditions of an experimental setup for TE module testing at cryogenic temperatures have been used as input parameters. The experimental results of module characterisation were used for the validation of the 1D model. Performance maps of modules with variation of hot and cold side temperatures were calculated and the influence of geometries and aspect-ratios have been investigated under the consideration of contact resistances. Finally the choice of different module substrates is discussed.
The simulation framework enables rapid “design-for-TEG” optimisation, guiding material selection, stack segmentation, and geometrical limitations for TE modules.

The reverse milling phenomenon and thermoelectric properties of sintered compact in PbTe

Tomoki Tamamura[1], Prof. Kazuhiro Hasezaki[1]
[1]Department of Mechanical Science, Division of Science and Technology, Graduate School of Science and Technology for Innovation, Tokushima University, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Grain refinement in sintered compacts improves thermoelectric performance by reducing phonon thermal conductivity. A fine powder particle size is generally required to obtain fine grain sizes in sintered compacts. Powder particle size does not monotonically decrease during milling, but increases beyond a critical powder size [1]. In this study, this increase beyond a critical powder size is referred to as the "reverse milling phenomenon". The reverse milling phenomenon has been reported in various materials. Its origin and material dependence have not been fully clarified. This research aims to clarify the reverse milling phenomenon in thermoelectric materials and evaluate the thermoelectric properties of sintered compacts. Lead telluride (PbTe) samples were prepared by mechanical grinding using planetary ball milling, followed by hot pressing. A two-step milling process was applied. The first step was high-energy milling at 200 rpm to obtain homogeneous powders. The second step was milling at rotational speeds of 100–200 rpm to clarify the reverse milling phenomenon.
The minimum particle size of the milled powder was obtained at a rotational speed of 160 rpm in the second step, as observed by scanning electron microscopy.

For the sintered compacts, both the minimum thermal conductivity κ and the maximum Seebeck coefficient α were obtained at a rotational speed of 160 rpm in the second step.
In addition, the Seebeck coefficient α exceeded that of a single crystal [2].
As a result, the reverse milling phenomenon was observed in thermoelectric materials. Controlling the milling condition resulted in thermoelectric materials with optimal thermoelectric properties, characterized by both minimum κ and maximum α. Controlling the milling condition is expected to be applicable to other thermoelectric materials, and further improvement in thermoelectric properties.

Reference
[1]Guzzo, P. L. et al. Powder Technology, 368, (2020), 149–159.
[2] A.Todosiciuc, CAS 2012 (International Semiconductor Conference),269–272

Thermoelectric Properties of Ultrathin MoS2 Layers

Dr. Tetiana Tavrina[1,2], Prof. Dr. Stefan Linden[1], Jonas Strubich[1]
[1]Physikalisches Institut, Universität Bonn, Germany, [2]National Technical University "Kharkiv Polytechnic Institute", Ukraine

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Keywords: layered transition metal dichalcogenides, electrical conductivity, Seebeck coefficient, doping, temperature dependence

Molybdenum disulfide (MoS_2), a transition metal dichalcogenide (TMDC), exhibits significant potential for optoelectronic and thermoelectric (TE) applications [1,2]. The fabrication of ultrathin two-dimensional TMDC layers is a promising strategy to optimize their performance in TE devices [3]. Various factors, including doping level, layer thickness, contacts, substrate, and temperature, can strongly influence TE properties, leading to considerable variability in experimental results.

Here, we investigate the TE properties of pristine and Nb-doped ultrathin MoS_2 layers mechanically exfoliated from bulk materials and transferred onto SiO_2/Si wafer substrates. The morphology, microstructure, and thickness of the layers were characterized using optical microscopy, reflectance measurements, scanning electron microscopy, and atomic force microscopy. Electrical conductivity and the Seebeck coefficient were measured in the temperature range of 80-300 K using fabricated microdevices equipped with gold contacts, integrated heaters, and microthermometers. These devices were prepared via two-step electron-beam lithography followed by thermal evaporation. The obtained data are analyzed to evaluate how thickness reduction and Nb doping can be utilized to enhance the TE performance of ultrathin MoS_2 layers.

References:
[1] M.B. Askari, P. Salarizadeh, Materials for Renewable and Sustainable Energy (2025).
[2] O. Samy, A. El Moutaouakil, Energies, 14, 4586 (2021).
[3] L.D. Hicks, M.S. Dresselhaus, Phys. Rev. B, 47, 12727 (1993).

Acknowledgments:
This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under project number TA 2293/1-1.

Enhancement in the thermoelectric figure of merit of 3D-CuNi interconnected nanonetworks

Cristina Vicente Manzano[1], Olga Caballero-Calero[1], Daniele Casari[2], Amit Sharma[2], Alba Díaz-Lobo[1], Xavier Maeder[2], Marisol Martin-Gonzalez[1]
[1]Micro and Nanotechnology Institute (IMN-CSIC), Spain, [2]Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory, Switzerland

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The pursuit of efficient thermoelectric materials, particularly those composed of low-toxicity and earth-abundant elements, has intensified in recent years. This study introduces an approach to increase the thermoelectric properties of CuNi alloys through the synergistic application of two nanostructuring techniques: the incorporation of saccharine in the electrolyte to achieve a crystallite size reduction to 23-26 nm, and the utilization of three-dimensional (3D) anodic aluminum oxide (3D-AAO) templates to fabricate nanowires networks. While the electrical conductivity and Seebeck coefficient remained consistent between the nanocrystalline CuNi films and the 3D-nanonetworks, a significant reduction in thermal conductivity was observed, decreasing from 29 W/m·K for the bulk material to 4.9 ± 0.6 W/m·K for free-standing 3D CuNi nanonetworks. This reduction is attributed to enhanced phonon scattering within the 3D architecture together with the nanocrystalline size inside the nanowires. The figure of merit (zT) exhibited an impressive increase of more than four times (4.8) time for free-standing 3D-CuNi nanonetworks, when compared to bulk. Our findings underscore the potential of dual nanostructuring strategies to optimize the thermoelectric performance of environmentally friendly, stable, and abundant materials like CuNi, paving the way for advancements in sustainable energy technologies.

Is There Anyone Anywhere in the World Who Knows Anything At All about the Thermoelectric Behaviour of Dental Amalgams?

Mr Keith Walsh

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

It was first reported around 200 years ago that when a material which is known to consist of an inhomogeneous mixture of dissimilar electrical conductors is subjected to a temperature difference, an electromagnetic disturbance can be detected near the surfaces of the material [1]. Dental amalgams are accurately described as inhomogeneous mixtures of dissimilar electrical conductors. However, and in spite of the fact that countless millions of amalgam dental fillings have been placed in people's teeth, it appears that experimental procedures to measure the thermoelectric behaviour of dental amalgams have never been carried out. This presentation seeks to establish a rational explanation as to how the scientific community should be completely ignorant of the thermoelectric behaviour of metal dental restorations.

Conference delegates are urged to have read the following poster presentations prior to attending ECT2026.

"Frogs' Legs, Thermoelectricity, and Hans Christian Oersted" - ICT2017, Pasadena.

"Thermoelectric Eddy Current in Bio-Compatible Materials" – ICT2018, Caen.

"Thermoelectric Effect in Metal Dental Restorations" – ECT2019, Limassol.

"Establishing A Protocol for the Approval of Thermoelectric Materials Used in Biomedical Applications" – ECT2023, Prague.

Reference:
[1] "New Experiments by Dr Seebeck on Electromagnetic Effects", H. C. Oersted, 1823.

Formation Mechanism of Lamellar Microstructure in (TiCr)FeSb Double Half-Heusler derived Compounds

Suhyeon Woo[1], Prof. Ho Seong Lee[1], Ms. Hyoju Son[1], Mr. Jihwan Im[1], Dr. Joseph Ngugi kahiu[1], Dr. Samuel Kimani Kihoi[1]
[1]Department of Materials Science and Metallurgical Engineering, Kyungpook National University, South Korea

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Double half-Heusler (dHH) thermoelectric materials have been proposed as an effective strategy to reduce the intrinsically high lattice thermal conductivity of conventional half-Heusler compounds. However, the experimental realization of stable dHH phases remains challenging, often accompanied by phase separation and complex microstructural evolution.
In this study, (TiCr)FeSb alloys with a nominal double half-Heusler composition were synthesized via arc melting, followed by annealing and sintering, to investigate their phase evolution and microstructural characteristics. Phase analysis using X-ray diffraction (XRD) and energy-dispersive spectroscopy (EDS) suggests that the system does not form a single homogeneous dHH phase, but rather exhibits phase-separated structures consisting of multiple half-Heusler-related phases and/or substitutional solid solutions.
Scanning electron microscopy (SEM) analysis showed the formation of a well-defined lamellar microstructure. Further Transmission electron microscopy (TEM) investigations confirmed that the lamellar features consist of distinct phases with different crystal structures
The results suggest that the observed lamellar structure originates from a decomposition process of the metastable dHH phase into energetically favorable phases during annealing. This study provides insight into the phase stability and microstructural evolution of (TiCr)FeSb systems and highlights the critical role of processing conditions in controlling phase separation and microstructure formation in double half-Heusler compounds.

Suppressing Mg Volatilization Enables High Carrier Mobility in Mg3(Sb, Bi)2

Dr. Liangjun Xie[1], Prof. Dr. Kornelius Nielsch[1], Dr. Ran He[1]
[1]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Mg3(Bi, Sb)2-based thermoelectric materials have emerged as leading candidates for sustainable solid-state cooling and medium-temperature power generation. However, the performance of these polycrystals is fundamentally limited by intense carrier scattering at grain boundaries, originating from the electrostatic potential barriers induced by Mg deficiency. In this study, we demonstrate that Mg volatilization during conventional sintering, driven by high vapor pressure under dynamic vacuum, is the primary bottleneck for grain-boundary integrity. To address this, we implemented a quasi-closed sintering architecture to effectively suppress Mg loss, enabling precise compositional control and prolonged high-temperature isothermal dwelling. This process-engineering breakthrough triggered substantial grain growth from ~ 10 μm to ~ 50 μm, effectively eliminating the grain-boundary scattering effect. Consequently, the electrical conductivity surged from 479 S cm-1 to 773 S cm-1, leading to a room-temperature power factor enhancement from 16.5 μW cm-1 K-2 to 24.6 μW cm-1 K-2 in Mg3Sb1.5Bi0.5. The robustness of this strategy was further validated in Mg3Sb0.5Bi1.5, which is usually used in thermoelectric cooling, achieving a superior power factor of 29.8 μW cm-1 K-2. Our findings provide a scalable and efficient pathway to optimize polycrystalline thermoelectrics by decoupling microstructural evolution from compositional degradation, offering new perspectives for high-performance Mg3(Bi, Sb)2 device integration.

Machine Learning-enabled optimisation of multi-pair thermoelectric coolers under dynamic operating conditions

Haoji Yang[1]
[1]School of Electronics and Computer Science, University Of Southampton, United Kingdom
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Keywords: thermoelectric cooler, design and optimisation, artificial neural network, genetic algorithm, multi-objective genetic algorithm

The increasing power density of advanced microelectronic systems imposes stringent requirements on localised thermal management, particularly for hotspot-driven heating in highly integrated chips. Thermoelectric coolers (TECs) offer a solid-state solution with high reliability and scalability; however, their performance is strongly coupled to device architecture (e.g. number of thermoelectric pairs), operating current, and boundary conditions, making design optimisation computationally intensive when using conventional finite element methods (FEM).

In this work, we develop a machine learning (ML)-enabled optimisation framework for multi-pair TECs, enabling rapid prediction and design exploration under realistic operating scenarios. A high-fidelity dataset is first generated using COMSOL Multiphysics simulations, covering variations input current, hotspot characteristics (location and heat flux), and environmental conditions (ambient temperature and convective heat transfer coefficients). This dataset is used to train a hyperparameter-optimised artificial neural network (ANN) surrogate model, achieving >99% accuracy in predicting key performance metrics including maximum temperature reduction on both top and bottom side of TEC module. The trained ANN enables orders-of-magnitude faster evaluation compared to FEM, allowing efficient coupling with a multi-objective genetic algorithm (MOGA). The optimisation framework simultaneously considers competing objectives, such as minimising power consumption and maximising cooling performance, under application-specific constraints. By systematically exploring the design space, the model identifies optimal combinations of TEC architecture (multi-pair configuration) and operating current tailored to different hotspot distributions and environmental conditions.

Results demonstrate that the proposed framework not only captures the complex nonlinear interactions between electrical, thermal, and geometrical parameters, but also enables adaptive optimisation of TEC operation for dynamic thermal loads. This approach provides a scalable pathway for integrating thermoelectric cooling into next-generation electronics, bridging the gap between high-fidelity simulation and real-time design optimisation.

Rolling-Enabled High-Performance Free-Standing Ag2Se/PVDF Composite Films for Flexible Thermoelectric Devices

Prof. Qin Yao[1]
[1]Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The development of wearable electronics demands flexible thermoelectric (TE) materials that simultaneously possess high energy-conversion efficiency and robust mechanical compliance. Conventional strategies often rely on passive substrates or suffer from a trade-off between electrical and mechanical properties. In this work, we report a hot-rolling process to fabricate high-performance, free-standing Ag2Se/PVDF composite films, which synergistically optimizes both microstructure and functionality. By systematically tuning the Ag2Se content (80-100 wt%), we demonstrate that hot rolling not only aligns Ag2Se nanowires into a highly oriented, continuous lamellar conductive network along the rolling direction, but also induces the α→β crystal phase transition in PVDF, forming an interpenetrating network structure with Ag2Se as the rigid conductive skeleton and PVDF as the flexible toughening phase, thus significantly enhancing interfacial bonding and carrier transport. The optimized composite film with 90 wt% Ag2Se (R-90) exhibits an exceptional room temperature power factor of 1129.5 μW·m-1·K-2 and a planar TE device constructed using R-90 legs achieves a high power density of 7.0 W·m-2 under a temperature difference of 35.6 K, at the highest level of free-standing inorganic-organic composite flexible thin films and devices. Moreover, the R-90 film exhibits outstanding mechanical flexibility, retaining 96.3% of its electrical conductivity after 3000 bending cycles (3 mm radius), along with a tensile strain of 1.32% at room temperature (3.3 times that of pure Ag2Se). This study highlights rolling as a potent microstructural control strategy that concurrently enhances TE and mechanical properties in organic inorganic composites, paving a promising route toward substrate free, high performance flexible TE devices for wearable energy harvesting.

Grain recovery facilitated low-angle grain boundaries and texture for high-performance BiSbTe alloys

Yuzheng Li[1,2], **Boyang Ying**[1], Prof. Chenguang Fu[1], Prof. Tiejun Zhu[1,2]
[1]State Key Laboratory of Silicon and Advanced Semiconductor Materials, School of Materials Science and Engineering, Zhejiang University, China, [2]Institute of Wenzhou, Zhejiang University, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Low-angle grain boundaries (LAGBs) bring an effective scattering of phonons while maintaining a weak effect on charge carrier transport, which could be utilized for enhancing the thermoelectric performance of solid materials. In the Bi2Te3-based materials fabricated by hot extrusion (HE) technique, however, the formation of the LAGBs is inevitably accompanied by severe recrystallization, resulting in texture loss and hindering further zT improvement. Here, we demonstrate a feasible strategy utilizing the grain recovery to maintain dense LAGBs with high grain orientation by the optimized HE technique. As a result, a low thermal conductivity of about 1 W m-1 K-1 and a high power factor of 4.2 mW m-1 K-2 are achieved at 300 K for p-type Bi0.5Sb1.5Te3 alloys, leading to a high room-temperature zT of 1.3. Further, with a decent flexural strength of 25.3 MPa, a 23-pair TE cooling module with the dice dimensions of 0.63×0.63×1.00 mm3 is assembled, which exhibits a maximum temperature difference of 87.8 K at a hot-side temperature Th of 350 K. These results highlight the important role of grain-recovery manipulation in simultaneously optimizing the thermal and electrical properties toward high-performance Bi2Te3-based TE materials.

Topology Design of Ni-Based Thermoelectric Modules via COMSOL Simulation

Dr. Pingjun Ying[1], Karolin Amstein[1], Aayush Dobhal[1], Ran He[1], Julia Kristin Hufenbach[1], Kornelius Nielsch
[1]IFW-Dresden, Germany

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

The performance of thermoelectric (TE) modules is strongly influenced not only by material properties but also by the geometric design of thermoelectric legs. This work investigates the influence of thermoelectric leg geometry on the performance of Ni-based modules using COMSOL Multiphysics simulations. Various topologies including solid and hollow cuboids, cylinders, lattice structures, pyramids, double-pyramids, and spring-like designs are systematically analyzed under consistent operating conditions. The study focuses on how geometric variations affect key performance metrics such as electrical resistance, heat flux distribution, and overall energy conversion efficiency. Additionally, the potential of these geometries for active cooling applications is explored by evaluating temperature gradients and localized heat dissipation capabilities. This study highlights the importance of topological design as a complementary approach to material optimization, providing insights for the development of high-performance thermoelectric modules.

Compared Degenerate and Non-Degenerate Approximations with Dimensionless Figure of Merit ZT in Fine-Grained n-type Bi2Te3 Thermoelectric Materials

Jun YOSHIDA[1], Prof. Kazuhiro Hasezaki[1]
[1]Tokushima University, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Currently, the dimensionless figure of merit ZT, defined by directly measured Seebeck coefficient α, electrical conductivity σ, and thermal conductivity κ, is widely used as a standard for evaluating thermoelectric materials. ZT can also be determined using the material parameter β, scattering parameter γ, and reduced Fermi energy η, which are dimensionless quantities. Although the approach based on parameters β, γ, and η is material-independent and facilitates theoretical prediction, it lacks empirical confirmation of the theoretical model. The degenerate and non-degenerate states of the semiconductor are taken into account when determining β, γ, and η. The degenerate state is a high-level doping in which a material behaves more like a metal than a semiconductor. In contrast, the non-degenerate state is a pure and low-level doping in which a material behaves like a semiconductor. Some thermoelectric materials, such as BiTe–based materials, are degenerate semiconductor. In this study, we proposed the method to determine the dimensionless figure of merit ZT by using β, γ, and η, relying solely on α and the Lorenz number L. The β, γ, and η of fine-grained n-type Bi_2Te_3 thermoelectric materials were empirically analyzed using two methods. The first is the degenerate approximation based on Fermi–Dirac statistics and a one-electron parabolic-band model. The second is the conventional non-degenerate approximation based on Boltzmann statistics and a one-electron parabolic-band model. At all measurement points, ZT of the degenerate approximation exactly corresponded to that of the direct measurements of the Seebeck coefficient and electrical and thermal conductivities. On the other hand, the non-degenerate approximation produced partial discrepancies. Considering the degenerate state enables more accurate predictions as well as material-independent evaluation.

Three-Dimensional Ag2Se Thermoelectric Network Advances Multimodal Intelligent Perception

Fangyuan YU[1], Ping Sun[1], Jun Mao[1], Qian Zhang[1], Feng Cao[1]
[1]Harbin Institute of Technology, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Embodied artificial intelligence (Embodied AI) depends on the integration of multimodal sensing and physical interaction to achieve autonomous perception and adaptive control in complex environments. However, conventional multimodal sensing systems often rely on separate sensors for each physical stimulus, leading to integration challenges and signal interference. Here, we report a monolithic bimodal sensor based on a three-dimensional Ag2Se thermoelectric network that enables simultaneous and decoupled detection of temperature and pressure within a single device. The sensor demonstrates a high temperature sensitivity of −122.7 μV K−1 with a fast response time of ~0.14 s, and a high pressure sensitivity of −2.94% kPa−1 with a fast response time of about 0.08 s, indicating excellent signal isolation between the two sensing channels. When combined with deep learning, the sensor enables a real-time intelligent sorting system that achieves 96% recognition accuracy across nine materials, outperforming single-mode sensing approaches. This work provides an integrated multimodal sensing solution that advances the deployment of embodied AI in complex environments.

Enhancement of Power Factor in PEDOT:PSS Composites Using In- and Tl-Doped PbTe Nanopowders Synthesized by Pulsed Plasma in Liquid

Karolina Zazakowny[1], Abinaya Rengarajan[1], Marcelina Stasik[1], Taras Parashchuk[1], Oleksandr Cherniushok[1], Tsutomu Mashimo[2], Krzysztof T. Wojciechowski[1]
[1]Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Poland, [2]Institute of Industrial Nanomaterials, Kumamoto University, Japan

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Conducting polymer–inorganic composites are promising thermoelectric materials for low-grade heat recovery due to low thermal conductivity, flexibility, and solution processability. This study investigated PEDOT:PSS-based composites containing indium- or thallium-doped PbTe nanopowders, focusing on power-factor enhancement. $Pb_{1-x}In_xTe$ and $Pb_{1-x}Tl_xTe$ nanopowders were synthesized using a pulsed plasma in liquid (PPL) technique, yielding particles with characteristic sizes of 20–30 nm. Composite films were fabricated by solution processing and characterized using X-ray diffraction, Raman spectroscopy, scanning and transmission electron microscopy, elemental mapping, and temperature-dependent thermoelectric measurements. Structural analyses revealed that incorporation of PbTe-based nanoparticles induced conformational changes in PEDOT:PSS, promoting enhanced chain ordering and stronger interfacial interactions. Microscopic investigations confirmed homogeneous dispersion of the inorganic phase and the formation of extensive organic–inorganic interfaces. These interfaces facilitate energy-dependent carrier transport and contribute to enhanced thermoelectric performance. The Seebeck coefficient and electrical conductivity exhibited strong dependence on nanoparticle composition, concentration, and the presence of the surfactant Triton X-100. Thallium-doped composites displayed superior electrical conductivity, reaching approximately 325 Scm^{-1}, while surfactant-assisted formulations achieved Seebeck coefficients up to ~36 μVK^{-1}. An optimal balance between these parameters resulted in a maximum power factor of 9.7 $\mu Wm^{-1} K^{-2}$ for the PEDOT:PSS/PbTe:Tl composite containing Triton X-100.

The results demonstrate that plasma-engineered doped PbTe nanoparticles, combined with controlled interfacial engineering and surfactant-assisted dispersion, provide an effective strategy for optimizing thermoelectric performance in polymer-based composites intended for near-room-temperature energy harvesting applications.

Acknowledgments. The densified pellets were transferred into nano powder using Pulsed Plasma Liquid technique build by Prof. T. Mashimo from Kumamoto University, Japan. The authors acknowledge financial support from the Horizon Europe Framework Programme funded by the European Commission (project GHOST, grant agreement No. 101182946 (AMD-101182946-4). Project co-financed by the Polish Ministry of Science and Higher Education under the "International Co-financed Projects" program in the years 2025-2028 (grant agreement No. W103/HE/2025).

Symmetry-based orbital overlap rules for scattering in band degenerate valleys

Dr Yao Zhao[1], Dr Bhawna Sahni[1], Prof Neophytos Neophytou[1]
[1]University Of Warwick, United Kingdom

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric candidate materials, such as half-Heuslers and Zintl phases, often exhibit complex electronic band structures typically with band degeneracy or valley convergence at the extrema. Transport in these systems is controlled by the competition between inter- and intra-band/valley scattering. Yet a mechanistic understanding for these processes, governed by wave-function overlap integrals, has been missing. Here we derive general rules for predicting the overlap factors in a two-fold orbitally degenerate valley, rationalised with group theory.

Using first-principles DFT calculations on half-Heuslers [1,2], we first show that overlaps have a simple sine-cosine dependency on the angles of k-vectors of relevant Bloch states projected on the plane perpendicular to the high-symmetry line of the valley. Without the spin-orbit coupling, the average of squares of overlaps within a two-fold orbitally degenerate manifold are ≈1/2, while for a three-fold manifold they are ≈1/3, with equal overlap factor contribution that determines intra and inter band transitions near the degenerate point. However, a more complex relationship between inter and intra band transitions is found when SOC is considered. Specifically for half-Heusler compounds, intra- and inter-bands transitions can transform half-half to one-zero intra-inter band overlap relationships, depending on the strength of SOC.

We rationalise this behaviour based on the k.p Hamiltonian that incorporates the symmetry of the crystal. Within a spinless model we obtain analytic expressions for overlap factors governing intra- and inter-band scattering, but this model ceases to be valid in crystals lacking inversion symmetry, where SOC lifts spin degeneracy. These results establish a unified picture of how electronic states interact and provide rather simple criteria for identifying when intra- versus inter-band/valley channels govern transport.

[1] B. Sahni et al. Mater. Horiz. 12, 10255 (2025)
[2] R. Dutt et al. Mater. Chem. A 14, 10332 (2026).

High thermoelectricity obtained in thermoelectric alloy processed under super gravity

Min Zhou[1], Jinghao Liu[1], Ankui Lu[1], Jiawei Wang[2], Laifeng Li[1]
[1]State Key Laboratory of Cryogenic Science and Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, China, [2]Beijing Municipal Key Laboratory of New Energy Materials and Technologies, School of Materials Science and Engineering, University of Science and Technology Beijing, China

Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Thermoelectric materials allow direct conversion between heat and electricity and maybeuseful for power generation or solid-state refrigeration. However, improving thermoelectric performance is challenging because of the strong coupling between the electrical and thermal transport properties. We demonstrate a new super-gravity-field fabrication technology that synergistically optimizes the thermoelectric performance. Using a super gravity field, the thermoelectric alloy undergoes unusual plastic deformation and forms mounts of microstructure defects, such as high density of dislocations. These microstructure defects enhanced the phonon scattering, resulting in low lattice thermal conductivity and high figure of merit. The increased thermoelectric performance was realized in some thermoelectric materials, such as Bi2Te3, SnTe, Cu2SnSe3. A record-high figure of merit of>1.91 was even obtained in the BiSbTe alloy. The strong enhancement of thermoelectric properties was validated in a thermoelectric module with high conversion efficiency of 6.4% when subjected to a temperature difference of 185K. The work highlights a new super-gravity strategy to achieve a high thermoelectric performance.

Keywords: Thermoelectric cooling, Thermoelectric material, Thermoelectric application

TEGonaut: Self-Sufficient Sensor Nodes Powered by Thermoelectric Generators — Development and In-Flight Demonstration on the MAPHEUS Sounding Rocket

Mr Pawel Ziolkowski[1], Mr Karsten Karlowski[1], Mr Matthias Rossmeier[1], Mr Christoph Dreißigacker[1], Mr Christian Neumann[1], Prof. Dr. Thomas Voigtmann[1], Prof. Dr. Eckhard Müller[1,2]
[1]German Aerospace Center, Germany, [2]Justus Liebig University Gießen , Germany
Poster Session and Afternoon Break, September 16, 2026, 15:00 - 18:00

Mass, integration complexity, and maintenance overhead of wired sensor networks with hundreds of transducers in launch vehicles motivate the development of self-sufficient wireless sensor nodes offering enhanced flexibility for condition and structural health monitoring, payload instrumentation, and reusable stage applications. This work presents the development and in-flight demonstration of nodes fully powered by Bi_2Te_3-based thermoelectric generator (TEG) modules harvesting aerodynamic frictional heat from the rocket hull. DLR's MAPHEUS sounding rocket programme — operational since 2009 and spanning 16 flights from Esrange, Sweden — provides an ideal, recurrently accessible demonstration and testing platform for such technologies.

In 2024, on MAPHEUS-15, a mechanically clamped TEG module (40×40 mm²) was characterized under real flight conditions, establishing baseline thermal and electrical output parameters. In 2025, MAPHEUS-16 carried five miniaturized modules (< 10×10 mm²) exploring two thermal management concepts — PCM-based latent heat storage and dissipative cold-side coupling to the experiment housing via copper braid — with thermal coupling by epoxy adhesive. The fifth module powered an autonomous sensor node performing three-axis acceleration measurements with Bluetooth Low Energy data transmission to an onboard hub. Node power demand ranges from ~60 µW at 24 s^{-1} sampling, met by a 40×40 mm² TEG at temperature differentials as low as 1.6 K, to a few milliwatts for the 600 s^{-1} acceleration measurements with appropriate telemetry rates, supplied above 5–10 K. Recorded peak output of 434 mW (PCM) and 78 mW (coupling to housing) exceed operational requirements by 1-2 orders of magnitude. 23 seconds after launch, the node reached its operation supply voltage and transmitted ~15,000 acceleration samples over five minutes of stable operation, showing excellent agreement with reference accelerometer data from the the rocket's housekeeping system. All hardware relies exclusively on COTS components, supporting cost-efficient development and transferability to future launcher, lander, and small satellite platforms.

European Conference on Thermoelectrics

14–18 September 2026
John McIntyre Conference Centre,
Edinburgh, UK

IOP Institute of Physics

Registered Charity no. 293851 (England & Wales) and SCO40092 (Scotland).