ECT' NANCY 25

PROGRAM
BOOK OF ABSTRACT
LIST OF PARTICIPANTS

21ST EUROPEAN CONFERENCE ON THERMOELECTRICS

FROM MONDAY 8TH TO FRIDAY 12TH SEPTEMBER 2025

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- Dario Narducci, *Dept. of Material Science, University of Milano-Bicocca, Italy*
- Antonio Pereira Gonçalves, *Center for Nuclear Sciences and Technology, University of Lisbon, Portugal*
- Neophytos Neophytou, *University of Warwick, UK*
- Janusz Tobola, *Dept. of Physics, AGH University of Science and Technology, Krakow, Poland*
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ORGANIZING COMMITTEE

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ECT' NANCY 25

PART I
PROGRAM

TUESDAY, 9 SEPTEMBER | MORNING

8:30	Introduction & ETS General Assembly		
9:00 10:15	Auditorium 300 | Chair: Antonio Pereira Goncalves		
9:00	**Lone pairs as a design strategy for thermoelectric materials** Paz Vaqueiro *University of Reading, United Kingdom*		
9:45	**Emerging Thermoelectric Properties from Semimetal to Semiconductor** Susan M. Kauzlarich *UC Davis, USA*		
10:15	*Coffee Break*		
	Auditorium 300	Room 201	Room 101
10:45 12:00	Zintl phases | Chair: Johannes de Boor	Thin films 1 | Chair: Marie-Christine Record	Theory 1 | Chair: Bartlomiej Wiendlocha
10:45	**Exploring High-Temperature Thermoelectric Properties of $(Ca,Sr)_{14}(Al,Ga,In)(Sb,Bi)_{11}$ Zintl Phases** Umut Aydemir *Koç University, Istanbul, Türkiye*	**Thin Film Nanodecoration and Nanostructuring Techniques to Enhance Thermoelectric Efficiency in Silicon Micro-Thermoelectric Generators** Marc Aceituno *Institute of Microelectronics of Barcelona (IMB-CNM-CSIC), Bellaterra, Spain*	**Theoretical study of electronic structure and transport properties of halfmetallic ferromagnetic $Cu_2FeSnS_xSe_{4-x}$ with strong electron correlations** Dariusz Wieczorek *University of Krakow, Krakow, Poland*
11:00	**Grain Boundary Electrical Resistance in the High Temperature Thermoelectrics $Yb_{14}MgSb_{11}$ and La_3Te_4** Duncan Zavanelli *Northwestern University, Evanston, USA*	**Heavily Doped p-type Silicon Nanopillars Obtained by Metal-Assisted Chemical Etching for Thermoelectric Applications** Federico Giulio *University of Milano-Bicocca, Milano, Italy*	**A high-throughput framework for ab initio deformation potential extraction for thermoelectric materials** Zhao Yao *University of Warwick, Coventry, UK*
11:15	**Grain boundary engineering to enhance $Mg_2(Si,Sn)$ stability** Amandine Duparchy *German Aerospace Center, Cologne, Germany*	**Design and optimization of flexible free-standing PEDOT:PSS-based thermoelectric composites** Adrianna Lis *AGH University of Krakow, Krakow, Poland*	**Electronic properties of thermoelectric pseudo-hollandite and hollandite-like phases** Bruno Fontaine *ISC Rennes, Rennes/ Saint-Cyr, France*
11:30	**A computational study on type-I Sn clathrates with inorganic and organic guests** Nikolaos Kelaidis *National Hellenic Research Foundation, Athens, Greece*	**Energy Filtering in Heavily Boron-Doped SiGe Thin Films** Antonio Mazzacua *University of Milano Bicocca, Milan, Italy*	**When are elongated bands most effective for the power-factor?** Sahni Bhawna *University of Warwick, UK*
11:45	**Improved thermoelectric performance in very finely grained $Co_{0.91}Ni_{0.09}Sb_3$ skutterudites** Johari Kishor Kumar *Univ Paris Est Creteil, CNRS, Thiais, France*	**Thermoelectric properties of Nb doped ScN multilayer structures** Joris More-Chevalier *Institute of Physics of the Czech Academy of Sciences, Praha, Czechia*	**The use of descriptors within featurization for improved machine learning prediction of half-Heusler thermoelectric materials** Ramalingam Nirmal Kumar *University of Warwick, Coventry, UK*
12:00 13:30	*Lunch*		

TUESDAY, 9 SEPTEMBER | AFTERNOON

	Auditorium 300	Room 201	Room 101
13:30 15:00	Half-Heuslers | Chair: Eric Alleno	Organic materials | Chair: Mickaël Beaudhuin	Device 1 | Chair: Dario Narducci
13:30	**Recent developments in n-type XNiSn half-Heusler thermoelectrics using Cu dopants** Jan- Willem G. Bos *University of St Andrews, Scottland*	**Performance of thermoelectric PEDOT:PSS composite films with $Bi_{0.4}Sb_{1.6}Te_3$** Savvas Hadjipanteli *University of Cyprus, Nicosia, Cyprus*	**Coupling of a Genetic Algorithm and a Thermoelectric Network Model for Radioisotope Thermoelectric Generator (RTG) Optimisation** Kyrimis Stylianos *German Aerospace Center, Cologne, Germany*
13:45		**Polymorphism Controls Thermoelectric Properties In Oriented PBTTT Films** Said Oummouch *Institut Charles Sadron (ICS), Strasbourg, France*	**Fabrication of Thermoelectric Devices Based on Colusites** Koichiro Suekuni *Kyushu University, Kasuga, Fukuoka, Japan*
14:00	**Thermoelectric properties of single-crystalline TiCoSb-based half-Heuslers** Jun Mao *Harbin Institute of Technology, Shenzhen, P.R. China*	**Organic Thermoelectrics: Advances, Challenges, and Emerging Directions** Laure Biniek *Institut Charles Sadron (ICS), Strasbourg, France*	**Digital and scalable laser-based fabrication of reusable bismuth telluride thermoelectrics with superior performance and mechanical flexibility** Isidro Florenciano Cano *Department of Materials Engineering (MTM), KU Leuven*
14:15	**Improved thermal stability of NbCoSn Half-Heusler compounds via Sb doping-induced complementary point defect evolution** Kyuseon Jang *Max Planck Institute for Sustainable Materials, Germany*		**Planar Silicon-Based µTEG Test Platform for Evaluating Thermoelectric Materials and Optimizing Thermal Management** Alex Rodriguez-Iglesias *IMB-CNM-CSIC, Bellaterra, Spain*
14:30	**Half-Heusler thermoelectric compounds with intrinsically low thermal conductivity** Fu Chenguang *Zhejiang University*	**Graphene-based Organic semiconductor composites for low-temperature- grade energy harvesting: from cell to module** Muhammad Sajid *University of Rome Tor Vergata, Rome, Italy*	**Thermoelectricity as an energy source for the powering of industrial IoT sensors: use cases and perspectives** Dimitri Taïnoff *Institut Néel – Start-up Moïz, Grenoble, France*
14:45	**p-type Dopability in Half-Heusler Thermoelectric Semiconductors** Lirong Hu *Zhejiang University, Hangzhou, China*	**Role of Polymer Electrodes for Liquid and Gelified Thermoelectrochemical Redox Systems for waste-heat recovery applications** Mona Haq *Department of Electronic Engineering, Centre for Hybrid and Organic Solar Energy, University of Rome , Rome, Italy*	
15:00 15:30	Coffee Break		

TUESDAY, 9 SEPTEMBER | AFTERNOON

	Auditorium 300	Room 201	Room 101
15:30 17:00	Advanced materials | Chair: Jun Mao	Emerging materials 1 | Chair: Koichiro Suekuni	How to take TE to the market by academia-industry collaboration?
15:15			**Bridging Nanoscale Thermoelectrics and Triboelectrics: From Lab-Scale Innovations to Prototypes** Marisol Martín-Gonzalez *Instituto de Micro y Nanotecnología, IMN-CNM, Madrid, Spain* **Driving thermoelectric innovation through research-industry collaboration** Filipe Neves *Materials for Energy Unit, Lisbon, Portugal* **Needs and Challenges in Re-shaping TEG Supply-Chain in EU** Hao Yin *TEGnology ApS, Maskinvej 5, Søborg, Denmark* **Thermoelectric Modules and Applications: An Industrial Perspective** Ray Aniruddha *RGS Development Langedijk, Netherlands* **How to Transfer Thermoelectric Technology from Academia to Industry? The Case of Thermo Power Systems** Frederic Lani *Thermo Power SRL, Belgium* **Durable and sustainable thermoelectric devices made from zinc and magnesium-antimony alloys** Kornelius Nielsch *Leibniz Institute of Solid States and Materials Research University of Dresden* **Towards industrial production of high-temperature thermoelectric modules** Vicente Pacheco *Fraunhofer Institute for Manufacturing Technology and Advanced Materials, Dresden, Germany*
15:30	**Cation-deficient Half-Heusler Thermoelectric Materials** Tiejun Zhu *Zhejiang University, Hangzhou, P.R. China*	**Direct electron cooling at millikelvin temperatures with quantum-well heat pump** Matthew Grayson *Program in Applied Physics Northwestern University, USA*	
15:45	**New efficient thermoelectric half-Heusler compositions from Machine Learning** Philippe Jund *ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier France*	**Transverse thermoelectric effect in WSi_2 with/without magnetic field** Shoya Ohsumi *Fac. of Science and Technology, Tokyo University of Science, Japan*	
16:00	**Heavier element substitution in *p-type* Fe_2Val Heusler alloy** Moorthy Manojkumar *Univ. Paris Est. Creteil, CNRS, ICMPE, THIAIS, France*	**Thermoelectric properties of kagome metals Ni_3Sn and $Ni_{3-x}Co_xSn$** Shogo Yoshida *Department of Physics and Astronomy, Tokyo University of Science, Japan*	
16:15	**Dominance of Coulombic scattering in the power factor on half Heuslers** Rajeev Dutt *University of Warwick, Coventry, UK*	**Decoupling electrical and thermal properties in $Ca_{12}Al_{14}O_{33-\delta}$ ceramics** Jesús Prado-Gonjal *Dpto. Química Inorgánica, Universidad Complutense de Madrid, Spain*	
16:30	**Plastic deformation mechanism of single-crystal thermoelectric materials** Tianyu Zhang *School of Materials Science and Engineering, and Institute of Materials Genome & Big Data, Harbin Institute of Technology, Shenzhen, China*	**Thermoelectric Potential of Te-Free Diamond-Like $Cu_{2-x}Ag_xIn_2Se_4$ Chalcopyrites: Low Thermal Conductivity and High Carrier Mobility** Federico Serrano-Sanchez *Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, Spain*	
16:45	**Prefer-oriented Ag_2Se crystal for high-performance thermoelectric cooling** Jiang Feng *School of Materials Science and Engineering, and Institute of Materials Genome & Big Data, Harbin Institute of Technology, Shenzhen, China*	**Frustrated vacancy order in diamagnetic metal Kutinaite $Ag_6Cu_{14.4}As_7$** Pavan Kumar Ventrapati *SRM University Amravati-AP, Mangalagiri, AndhraPradesh, India* *Department of Chemistry and iNANO, Aarhus University, Aarhus, Denmark*	

WEDNESDAY, 10 SEPTEMBER | MORNING

9:00 10:15	Auditorium 300 | Chair: Janusz Tobola		
9:00	**Computational strategies for modeling transport: electron, phonon, and machine learning.** Atsushi Togo *(NIMS), Tsukuba, Japan*		
9:45	**Combining the Power of High-Throughput Ab Initio Calculations and Machine Learning towards Materials Informatics** Gian-Marco Rignanese, *Université Catholique de Louvain, Belgique*		
10:15	*Coffee Break*		
	Auditorium 300	Room 201	Room 101
10:45 12:00	Chalcogenides 1 | Chair: Eleonora Isotta	Oxides | Chair: Sylvie Hébert	Device 2 | Chair: Guillaume Savelli
10:45	**The devil is in the detail(s): How to get the synthesis of high performance MgAgSb right?** Johanned De Boor *German Aerospace Center, Cologne, Germany* *University of Duisburg-Essen, Duisburg, Germany*	**Oxide thermoelectric materials – Challenges and opportunities** Kriti Tyagi *CSIR-National Physical Laboratory, New Delhi, India AcSIR, Ghaziabad, Uttar Pradesh, India*	**Thermoelectric Metamaterials for Enhanced Power Generation Modules** Xanthippi Zianni *National and Kapodistrian University of Athens, Greece*
11:00	**Crystal structure and thermoelectric properties of $Cu_{30}Ti_6Sb_2S_{32}$ and Cu_7VSnS_8: New phases discovered with the pseudo-binary approach** Pierric Lemoine *Institut Jean Lamour, UL, CNRS, Nancy, France*	**Spark Plasma Sintering: an efficient tool for thermoelectric oxides** Fabien Giovannelli *GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, France*	**Investigation of Titanium as a Potential Diffusion Barrier in Bismuth Telluride Thermoelectric Generators** Ilayda Terzi *Institut Jean Lamour, UL, CNRS, Nancy, France*
11:15	**Defect controlled thermal and electric properties of single crystalline Bi_2O_2Se** Jiri Hejtmanek *FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic*	**Decoupling the Electrical Conductivity and Thermopower by Chemically Manipulating Ni^{2+}/Ni^0 and Ti^{4+}/Ti^{3+} Redox Pairs in Ni-doped $Sr(Ti,Nb)O_3$** Michitaka Ohtaki *Kyushu University, Kasuga, Fukuoka, Japan*	**Ultra-low Power Thermoelectric Sensor for Sweat Rate Monitoring** Ping Sun *Harbin Institute of Technology, Shenzhen, Guangdong, China*
11:30	**High thermoelectric performance in novel Cu-based chalcogenide with Cr_3Si-type structure** Oleksandr Cherniushok *AGH University of Krakow, Krakow, Poland*	**Electrochemical and thermoelectric properties of multicomponent oxides** Tadeusz Miruszewski *Gdańsk University of Technology, Gdańsk, Poland*	**Design of Oxide Thermoelecric Uni-leg Modules** Yoshimi Shimizu *Department of Applied Physics, Graduate School of Engineering, Tohoku University, Japan*
11:45	**Crystal structure and transport properties of $Cu_{2-x}Ag_xSn_{1-y}Ga_ySe_3$** Arthur Wieder *Institut Jean Lamour, UL, CNRS, Nancy, France*	**Cost-Effective Performance Enhancement: How High-Entropy Engineering Optimizes In_2O_3-Based Thermoelectric Oxides** Jia Chuang *Université Paris-Saclay, Gif sur Yvette, France*	**Smart Thermoelectric IIoT for Steam Trap Leak Detection: A Sustainable Approach** Raúl Aragonés *Alternative Energy Innovations Terrassa, Spain*
12:00 13:30	*Lunch*		

WEDNESDAY, 10 SEPTEMBER | AFTERNOON

<table>
<tr><td></td><td>Auditorium 300</td><td>Room 201</td><td>Room 101</td></tr>
<tr><td>13:30
15:00</td><td>Theory 2 | Chair: Neophytos Neophytou</td><td>Lattice dynamics 1 | Chair: Stéphane Pailhès</td><td>Device 3 | Chair: Oliver Fenwick</td></tr>
<tr><td>13:30</td><td rowspan="2">Resonant Levels in Thermoelectrics: What They Are and How They Work in Metals and Semiconductors
Bartlomiej Wiendlocha
AGH University of Krakow, Pologne</td><td>Mechanochemical Synthesis and Low-Energy Phonon Scattering in Mixed-Anion Chalcohalides $Bi_{13}S_{18}X_2$ (X = I, Br, Cl)
Tiadi Minati
Laboratoire CRISMAT, CNRS, Caen, France</td><td>Tuning ionic thermoelectric behaviour of Lignin derived hydrogels
Mario Culebras Rubio
ICMUV, Universitat de València, Paterna, Spain</td></tr>
<tr><td>13:45</td><td>Exploring Defect-Driven Phonon Dynamics in GeTe: Raman and Thermal Perspectives
Vinayak Kamble
Indian Institute of Science Education and Research Thiruvananthapuram, India</td><td>Thermoelectric Flexible Module with Anodized Aluminum Substrate
Hitoshi Kohri
Kogakuin University, Japan</td></tr>
<tr><td>14:00</td><td>Enhanced Thermoelectric Performance of PbSnTeSe High-Entropy Alloys via Magnetic Doping and Strain Engineering
Pascal Boulet
Aix-Marseille University, Marseille, France</td><td rowspan="2">Inelastic Neutron Scattering, an Experimental Tool for Understanding Phonons and Diffusion Processes in Thermoelectric Materials
Michael Marek Koza
Institut Laue Langevin (ILL), Grenoble, France</td><td>Life Cycle Assessment (LCA) as a Design Tool for Sustainable Thermoelectric Materials, Modules and Systems
Geoffrey Roy
Thermo Power SRL, Belgium Institute of Mechanics, UCLouvain, Belgium</td></tr>
<tr><td>14:15</td><td>Scattering exponent approximation for complex electronic structure thermoelectric materials from ab initio calculations
Yuji Go
University of Warwick, Coventry, UK</td><td>Elevating the thermoelectric performance in the sub-ambient temperature range for electronic refrigeration
Xiaojing Ma
School of Materials Science and Engineering, and Institute of Materials Genome & Big Data, Harbin Institute of Technology, Shenzhen, China</td></tr>
<tr><td>14:30</td><td>Quantifying the impact of band change upon alloying on the power factor
Ankit Kumar
University of Warwick, UK</td><td>Unraveling the Lattice Dynamics of Silicides: Strategies for Improved Thermoelectric Efficicency
Mickael Beaudhuin
ICGM, Univ Montpellier, CNRS, Montpellier, France</td><td rowspan="2">Perspective on thermoelectric applications of heat pump, cooling and geothermal energy
David Astrain
University of Navarre, Spain</td></tr>
<tr><td>14:45</td><td>A novel method for evaluating dimensionless thermoelectric properties of fine-grained n-type Bi_2Te_3 by scattering parameter γ, materials parameter β, and reduced Fermi energy η at room temperature
Ayumu Ijitsu
Tokushima University, Tokushima, Japan</td><td>s-d Coupling Induced Dynamic Off-centering of Cu Drives High Thermoelectric Performance in TlCuS
Animesh Bhui Animesh
New Chemistry Unit), Jakkur P.O., Bangalore, India</td></tr>
<tr><td>15:00
17:00</td><td colspan="3">Poster session</td></tr>
</table>

THURSDAY, 11 SEPTEMBER | MORNING

8:30	Welcome participant		
9:00 10:15	Auditorium 300 | Chair: Jan König		
9:00	**Driving Innovation and Empowering Wearables: Advances in Thermoelectric Generators for Automotive and Body Heat Harvesting** Olga Caballero *Instituto de Micro y Nanotecnología (IMN-CNM) of the Spanish Research Council (CSIC), Madrid, Spain*		
9:45	**Advancing Thermoelectrics to Market: An Industrial Perspective** Richard Tuley *European Thermodynamics, UK*		
10:15	*Coffee Break*		
	Auditorium 300	Room 201	Room 101
10:45 12:00	Chalcogenides 2 | Chair: Tetiana Tavrina	Emerging materials 2 | Chair: Jiri Hejtmanek	SOLAR-TEG | Chair: Peter Baláž
10:45	**Defect Engineering in Cu-Based Diamond-Like Chalcogenides for Enhanced Energy Conversion** Taras Parashchuk *AGH University of Krakow, Krakow, Poland*	**Semiconducting-to-metallic transition leading to large n-type Seebeck coefficient in a copper thiolate-based coordination polymer** Chloe Andrade *Univ Lyon 1, CNRS, Villeurbanne, France*	**Temperature-driven electrochemical separation of oxygen** Krzysztof T. Wojciechowski *AGH University of Science and Technology, Krakow, Poland*
11:00	**Manipulating Charge Carrier in Thermoelectric Sulfides** Xiaoyuan Zhou *College of Physics, Chongqing University*	**Seebeck coefficient measurement in bidimensional thickness dependant topologically insulated WSe_2** Nathan Aubergier *Université Grenoble Alpes, Grenoble, France*	**Thermoelectric-Based Energy Harvesting System with Integrated Electromagnetic Induction Unit** Mert Şener *Balikesir University, Balikesir, Türkiye*
11:15	**Process-controlled defect engineering and intrinsic low thermal conductivity in layered Cu_2ZrS_3** Carmelo Prestipino *Laboratoire CRISMAT, Caen, France*	**Towards a better understanding of the complex defect diffusivity in Mg_2Si/metal contact interfaces using Kelvin Probe Force Microscopy** Emily Beck Sarah *University of Duisburg-Essen, Duisburg, Germany*	**Personalized Thermal Management through Thermoelectric Technology and Textile-based Heat Exchange Systems** Giovanna Latronico *CNR – ICMATE, Lecco, Italy*
11:30	**Improved thermoelectric efficiency of $Sb_2Si_2Te_6$ through yttrium-induced nanocompositing** Kivanc Saglik *Technology and Research (A*STAR), Singapore*	**Thermal conduction in free-standing monolayer MoS_2 and its nanoscroll** Liu Huili *ShanghaiTech University, Shanghai, China*	**Concept of Solar Tri-generation Using Cold-Side Time-Modulated Heat Withdrawal** Dario Narducci *University of Milano Bicocca, Milan, Italy*
11:45	**Improving Thermoelectric Efficiency of Hybrid Lignin-Copper sulfide Materials** Clara Maria Gómez *Institute of Materials Science (ICMUV), Universitat de València, Paterna, Spain*	**Electrical transport and Seebeck measurements in highly disordered channels buried in diamond** Sana Salami *University Lyon 1, CNRS, Lyon, France*	**The Impact of Electrical Connections on Maximum Power Point Tracking within Hybrid Photovoltaic-Thermoelectric Devices** Mashiul Huq *Institut Jean Lamour, UL, CNRS, Nancy, France*
12:00 13:30	*Lunch*		

THURSDAY, 11 SEPTEMBER | AFTERNOON

	Auditorium 300	Room 201	Room 101
13:30 15:00	Additive manufacturing | Chair: Geoffrey Roy	Nano Materials | Chair: Marisol Martín-Gonzalez	Device 4 | Chair: Nicole Fréty
13:30	**Leveraging Additive Manufacturing to Re-envision Thermoelectric Systems** Saniya LeBlanc *George Washington University, USA*	**Scalable Solution Chemical Synthesis of Nanostructured Thermoelectric Materials** Bejan Hamawandi *KTH Royal Institute of Technology, Stockholm, Sweden*	**Development of Reliable Interfacial Barrier for Low-Cost Argyrodite Thermoelectric Module** Anilkumar Bohra *AGH University of Krakow, Krakow, Poland*
13:45		**Solution-based synthesis of inorganic metal chalcogenide particles: Methods and thermoelectric properties analysis** Mohammad Waquar Uddin Siddiqui *Univeristy of Caen Normandy, France*	**Effect of gamma radiation on Mg-based thermoelectric materials** Antonio Pereira Goncalves *Universidade de Lisboa, Bobadela, Portugal*
14:00	**Laser Sintering of Thermoelectric Chalcogenides Nanopowders** Carlo Fanciulli *CNR-ICMATE, Lecco, Italy*	**Optimizing Thermoelectric Materials: Balancing Performance, Cost, and Sustainability** Maria Ibañez *Institute of Science and Technology Austria, Klosterneuburg, Austria*	**Oxidation of skutterudites and their protective coatings: a comparative study** Arige Hodroj *Univ Rennes, CNRS, Rennes, France*
14:15	**Silicon Germanium alloys developed by additive manufacturing: influence of thermal treatments** Guillaume Savelli *Univ. Grenoble Alpes, CEA, Liten, Grenoble, France*		**Oxidation Behavior and Integration into High Power Density Thermoelectric Generators of Commercial Half-Heusler Alloys** Soufiane El Oualid *Institut Jean Lamour, UL, CNRS, Nancy, France*
14:30	**Additive screen-printed 3D thermoelectric generators for energy harvesting** Mallick Mofasser *Light Technology Institute, KIT, Karlsruhe, Germany*	**Seeking for high-performance Ag_2Se using a sustainable solution synthesis** Francesco Milillo *Institute of Science and Technology Austria, ISTA*	**Thermoelectric Measurement Methods: From Transport Properties to Generator Characterization** Pawel Ziolkowski *German Aerospace Center, Cologne, Germany*
14:45	**Tailoring the microstructure and thermoelectric properties of CuNi and NiCr by laser powder bed fusion** Karolin Amstein *IFW Dresden, Dresden, Germany*	**Enhancement of Thermoelectric and Flexibility Performance of Bi-Sb-Te Thin Films via $MAPbI_3$ Composite Strategy** Dong Yang *Univ Rennes, Rennes, France* *Shenzhen University, Shenzhen, Guangdong, China*	
15:00		**Induction melting synthesis of Mg-based thermoelectric materials** Beatriz Santos *Universidade de Lisboa, Bobadela LRS, Portugal*	**Comprehensive Insights into the Carbon Footprint and Energy Intensity of Thermoelectric Generator (TEG) Production through Life Cycle Analysis** Amir Pakdel *The University of Dublin, Dublin, Ireland*
15:15 15:45	*Coffee Break*		

THURSDAY, 11 SEPTEMBER | AFTERNOON

	Auditorium 300	Room 201	Room 101
15:45 17:00	Lattice dynamics 2 | Chair: Emmanuel Guilmeau	Thin films 2 | Chair: Latronico Giovanna	Theory 3 | Chair: Philippe Jund
15:45		**Thermoelectric Properties of $(MoO_3)_x$-*doped* C60 films** Masato Nakaya *Nagoya University, Japan*	**Amorphous-like thermal conductivity and high thermoelectric figure of merit in "n" SnS and SnSe** Min Zhang *University of Manchester, UK*
16:00	**Stability and lattice dynamics of thermoelectric type IX Clathrates** Romain Viennois *ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France*	**Tailoring Defects in ScN Thin Films via Ion Implantation** Charlotte Poterie *Université de Poitiers–ENSMA, Poitiers, France*	**Structural and stacking fault modelling of low-density $Cu_{2+y}Zn_{1-y}SnS_{4-x}Se_x$ systems for thermoelectric applications** Marcelo Malagutti *University of Trento, DICAM, Trento, Italy*
16:15	**Phonon Transport in K_3SbS_4 Solid-State Battery Incorporating an Ion Diffusion Mechanism Using Machine Learning** You Hao-Jen *Institute of Physics, Academia Sinica, Taipei, Taiwan*	**Influence of electron-phonon coupling and phonon-drag effect at interfaces on the electronic and thermoelectric transport properties of thin films** Max Marrot *CNRS and University Lyon 1, Lyon, France*	**Tuning of electronic structure and thermoelectric properties via defects engineering in $Cu_{8-x}Si(S_3Se_3)_{1-y}I_y$ argyrodites** Janusz Tobola *AGH University, Krakow, Poland*
16:30	**Decoupling Thermoelectric Parameters in $CuCrO_2$: Role of Interlamellar Porosity via Zn^{2+}, Mg^{2+}, and Ni^{2+} Multi cation-Doping** Sanam P.k Jamshina *University of Calicut, Malappuram, Kerala, India*	**Non-Contact Electrical and Thermal Characterizations of Electrodeposited SnSe Films** Axel Tahir *Institut Jean Lamour, UL, CNRS, Metz, France*	**Enhancing thermoelectric properties of n-type (Pb-Sn)Te via resonant doping** Kacper Pryga *AGH University of Krakow, Krakow, Poland*
16:45	**Electron-phonon interaction-driven phonon transport attenuation above ambient temperature** Wentian Li *Zhejiang University, Hangzhou, China*	**Relative Leg-Height Optimized Micro-Thermoelectric Devices** Bharadwaj Pulumati Nithin *TU Dresden, Dresden, Germany*	
17:30	*Departure to the Gala Dinner at the Abbaye*		

FRIDAY, 12 SEPTEMBER | MORNING

8:30	Welcome participant		
9:00 9:45	Auditorium 300 | Chair: Eckhard Müller		
9:00	**Radioisotope Thermoelectric Generators for US Space Missions: Past, Present, and Future** Thierry Caillat *Jet Propulsion Laboratory (JPL), NASA, Pasadena, USA*		
9:45	*Coffee Break*		
	Auditorium 300	Room 201	Room 101
10:15 11:15	Device 5 | Chair: Eckhard Müller	Chalcogenides 3 | Chair: Taras Parashchuk	Emerging materials 3 | Chair: Carlo Fanciulli
10:15	**Transuranium Thermoelectrics Properties: a support for Space Exploration** Jean-Christophe Griveau *European Commission, JRC, Karlsruhe, Germany*	**Multinary sulphides for thermoelectrics: Mechanochemical synthesis via industrial milling** Peter Balaz *Slovak Academy of Sciences, Košice, Slovakia*	**Halide perovskites as thermoelectric materials** Oliver Fenwick *Queen Mary University of London, UK*
10:30	**Silicide thermoelectric modules based on high purity Si and recycled Si-kerf** Panagiotis S. Ioannou *University of Cyprus, Nicosia, Cyprus*	**Magneto-thermoelectric properties of selected sulfides** Sylvie Hebert *Normandie Université, CNRS, Caen, France*	**The Potential of High-Entropy Oxides: Insights from Perovskite Structures** Adrien Moll *ICMMO, University Paris-Saclay, Orsay, France*
10:45	**Primary and Secondary Properties of Amorphous TiNiSn for Flexible Thermoelectric Devices** Sana Khayyamifar *Malmö University, Malmö, Sweden*	**Solid solution alloying strategy to enhance thermoelectric efficiency of layered metal chalcogenides; $(Bi,Sb)_2Te_3$, $Bi_2(Se,Te)_3$ and beyond** Sang-Il Kim *University of Seoul, South Korea*	**Optimization of Copper Iodide nanoparticle based composite thermoelectric material** Oskars Bitmets *Institute of Solid State Physics, University of Latvia*
11:00	**Thermal Wave Dynamics and Thermoelectric Transport in InGaAs/GaAs Superlattices** Ankur Chatterjee *Nicolaus Copernicus University, Torun, Poland*	**Thermal conductivity imaging to advance microstructure engineering in thermoelectrics** Eleonora Isotta *Max-Planck-Institute for Sustainable Materials, Düsseldorf, Germany*	**V_2Se_2O and Janus V_2SeTeO: Monolayer altermagnets for thermoelectric applications** Shubham Singh *Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia*
11:15 12:15	*Aryan Sankhlar (ETS thesis award) + Poster awards + announcement ECT2026*		
12:15 13:30	*Lunch*		
Farewell - Departure			

PART II
PLENARY TALKS

Lone pairs as a design strategy for thermoelectric materials

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Keywords: structural distortion; low lattice thermal conductivity; electronic transport properties.

The heavier elements from groups 13, 14 and 15 of the periodic table exhibit stable oxidation states that are two lower (e.g. Tl^{+}, Sn^{2+}, Pb^{2+}, Sb^{3+}, Bi^{3+}) than the expected oxidation state for their respective groups. This is due to the inert pair effect, which can be described as the reluctance of the two electrons in the outermost *s* orbital (ns^2) to participate in bonding. Many of the best performing thermoelectric materials (e.g. Bi_2Te_3, PbTe, GeTe, SnSe…) contain cations with lone pairs, and this presentation will explore the impact of lone pairs on the structure as well as the electronic and thermal transport properties of thermoelectric materials.[1] The presence of a ns^2 lone pair leads to off-centering of the cation, and hence distorted cation coordination geometries, which can be correlated over long length scales (hence lowering the symmetry of the crystal structure) or uncorrelated. Cation off-centering causes variations in bond lengths (and therefore bond strengths), as exemplified by the typical distorted octahedral coordination geometry of Bi^{3+} cations, consisting of three short and three long bonds. Materials containing cations with lone pairs can exhibit strong anharmonicity, which is reflected in large values of the Grüneisen parameter, and lowers the lattice thermal conductivity. Moreover, the presence of ns^2 lone pairs can also change the character of the bands near the Fermi level, leading to increases in the band degeneracy and highly-desirable multi-valley Fermi surfaces. Concepts such as emphanisis, resonant bonding and metavalent bonding will be discussed.

Computational strategies for modeling transport: electron, phonon, and machine learning

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Keywords: phonons, first-principles calculation, machine learning potentials

First-principles electronic structure calculations now enable accurate prediction of phonon states in crystals. Before these computational advances, determining phonon band structures was extremely challenging, and their importance may have been underestimated simply because we lacked the tools to study them properly. With current computational power and advances in first-principles methods and codes, computing harmonic phonons for many crystals has become routine.

Phonon-mediated heat transport is largely governed by phonon-phonon scattering, which first-principles methods can also predict well[1]. From a materials science perspective, calculating lattice thermal conductivity remains computationally intensive even for pristine crystals without defects, requiring several orders of magnitude more computational resources than harmonic phonon calculations. Recent progress in machine learning potentials (MLPs) offers a solution by efficiently compressing atomic interaction information[2, 3].

For thermoelectric materials, electron-phonon scattering information is crucial and can also be obtained from first-principles calculations[4, 5]. Thus, we can now compute electrons, phonons, phonon-phonon interactions, and electron-phonon interactions all from first principles. Yet non-specialists in computational science may reasonably ask: how can we actually benefit from these state-of-the-art calculations?

While the underlying computational techniques are complex, well-designed, user-friendly implementations can make these powerful tools accessible to many researchers. Looking ahead, computational simulation codes must be designed not only for human users but also for automated systems. In the near future, most computer simulations will likely run automatically, with researchers controlling these calculations through natural language interfaces.

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Driving Innovation and Empowering Wearables: Advances in Thermoelectric Generators for Automotive and Body Heat Harvesting

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Keywords: Thermoelectric generators (TEGs), Waste heat, Energy harvesting, Device efficiency, Integration challenges

Thermoelectric generators (TEGs) have garnered significant attention for their potential to convert waste heat into electrical energy, particularly in automotive and wearable technologies. This presentation will discuss recent progress in TEG materials and device architectures, emphasizing practical considerations such as material selection, device efficiency, and integration challenges. These findings contribute to a better understanding of the opportunities and limitations of thermoelectric energy harvesting in real-world conditions.

Radioisotope Thermoelectric Generators for US Space Missions: Past, Present, and Future

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Keywords: RTGs, space power, thermoelectric

Radioisotope Thermoelectric Generators (RTGs) used in past U.S. space missions have predominantly employed SiGe or PbTe/TAGS thermoelectric materials, which were developed in the 1950s and 1960s. This paper compares key performance metrics of these legacy RTGs.Since the 1990s, in an effort to improve RTG efficiency, the Jet Propulsion Laboratory (JPL) has spearheaded the development of advanced thermoelectric materials. These include skutterudites, La_3Te_4, Yb_4MnSb_{11} Zintl-related phases, and nanostructured SiGe. In 2013, the concept of a skutterudite-based Multi-Mission Radioisotope Thermoelectric Generator (SKD-MMRTG) was proposed. This new design retrofits the flight-proven MMRTG, which uses PbTe/TAGS thermoelectric couples, with higher-efficiency skutterudite-based thermoelectric couples developed at JPL. The goal is to improve performance while maintaining the system's balance. A multi-organization team, including Teledyne Energy Systems (TESI), Aerojet Rocketdyne, and JPL, has been working to develop and refine the SKD-based thermoelectric converter technology. The objective is for the SKD-MMRTG to provide a minimum of 77 watts of power after 17 years of operation (3 years in storage and 14 years in use), representing at least a 30% increase in power over the original MMRTG at the same operating conditions. The skutterudite-based couple design was finalized in 2020 following extensive verification testing. Manufacturing has also been demonstrated through the fabrication of couples and a 48-couple module. Life testing at TESI and JPL has accumulated over 4 years of data to date. This paper briefly outlines the SKD-MMRTG concept, presents the results from life performance tests, and discusses the associated performance predictions. The SKD-MMRTG is expected to deliver at least 38% more power than the legacy MMRTG under equivalent conditions. Additionally, the paper provides a brief development status update on La_3Te_4, Yb_4MnSb_{11} Zintl-related phases, and nanostructured SiGe-based converters, comparing their projected performance when integrated into advanced RTGs with that of heritage RTGs.

Acknowledgment
This work was supported by NASA's Radioisotope Power Systems Program.

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PART III
INVITED TALKS

Emerging Thermoelectric Properties from Semimetal to Semiconductor

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Keywords: polar intermetallic, Zintl phase, low thermal conductivity

The structure of a new intermetallic, $Eu_5Al_3Sb_6$, which crystallizes in the pseudo rock-salt structure of (Eu/Al)Sb, will be presented. Its surprisingly complex structure results in low thermal conductivity. The thermoelectric properties are investigated as a function of composition. The rock-salt structure results in high valley degeneracy and n-type conduction, leading to a high Seebeck coefficient and low electrical resistivity. The evolution of the thermoelectric properties with composition, and for the solid solution of $Sr_{5-x}Eu_xAl_3Sb_6$, will be presented and discussed.

Acknowledgments
This work was supported by the National Science Foundation.

Recent developments in n-type XNiSn half-Heusler thermoelectrics using Cu dopants

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Keywords: Half-Heusler materials, Thermoelectric performance, Copper doping (Cu dopant), Lattice thermal conductivity, In-situ neutron diffraction

Half-Heusler materials are leading contenders for thermoelectric power generation due to their favourable combination of good performance, mechanical properties, easy contacting and stability. We have explored the use of Cu as a dopant in the n-type XNiSn materials. However, beyond simple carrier doping, introduction of Cu leads to a plethora of favourable effects. These include an enhanced Seebeck effect and improved power factors due to formation of a dopant band, strong reductions of the lattice thermal conductivity and coherent layers and wetting layers at grain boundaries. During synthesis Cu promotes homogenisation of the X-site metals, Ti, Zr and Hf, overcoming kinetic barriers that lead to multiphase behavior. In-situ neutron powder diffraction has been used to obtain new insights in the formation of XNiSn materials from elemental precursors.

Organic Thermoelectrics: Advances, Challenges, and Emerging Directions

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Keywords: Organic thermoelectrics, macromolecular engineering, structural engineering, material thermoelectric efficiency, flexible devices

Organic thermoelectric materials have emerged as promising candidates for low-cost, lightweight, and flexible energy harvesting technologies, particularly for applications in wearable electronics and low-grade heat recovery. In recent years, significant progress has been made in improving their performance, largely driven by advances in π-conjugated polymer design, doping efficiency, and structural control.
This talk will present an overview of the current state of the art in organic thermoelectrics, highlighting key achievements in materials development. It will explore recent strategies for optimizing charge carrier mobility, enhancing the Seebeck coefficient, and reducing lattice thermal conductivity. The talk will also address persistent challenges, including doping stability and device integration, as well as open opportunities for advancing the field toward practical applications.

Acknowledgments
This work was supported by ANR (grant number ANR- 19-CE06-0004). This work of the Interdisciplinary Thematic Institute HiFunMat, as part of the ITI 2021-2028 program of the University of Strasbourg, CNRS and Inserm, was also supported by IdEx Unistra (ANR-10-IDEX-0002) and SFRI (STRAT'US project, ANR-20-SFRI-0012) under the framework of the French Investments for the Future Program.

Thermoelectricity as an energy source for the powering of industrial IoT sensors: use cases and perspectives

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Keywords: industry 4.0, Decarbonization, Thermal energy harvesting, Autonomous sensors, Industrial IoT

As industry faces 4.0 revolution and the issue of decarbonization, the need for affordable and easy industrial measurements has never been more crucial. In this context, MOÏZ start-up offers a range of self powered Industrial IoT nodes thank to patented thermal energy harvesting architecture. In this talk, we will first address our vision of thermoelectric applications for autonomous sensors. Then, we will review some concrete industrial applications that are being addressed within MOIZ start-up, from process monitoring to railway maintenance. To conclude, we will give some perspectives on our future development in collaboration with academic research.

Combining the Power of High-Throughput Ab Initio Calculations and Machine Learning towards Materials Informatics

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Keywords: High-throughput ab initio methods, Materials discovery, Machine learning, OPTIMADE API, MODNet framework

In this talk, I will address the influence of high-throughput ab initio methods on materials discovery via online databases. While investigating complex properties remains challenging, the integration of machine learning has emerged as a viable solution. The talk will cover recent advancements in materials informatics, focusing on the use of the OPTIMADE API and the MODNet framework for predicting materials properties.

Resonant Levels in Thermoelectrics: What They Are and How They Work in Metals and Semiconductors

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Keywords: resonant levels, thermopower, electronic structure, resonant scattering, DFT

Resonant levels (RLs) are a special type of electronic states that are formed due to presence of impurity atoms in metallic or semiconducting materials. They were first described in 1950. in diluted metallic alloys by Korringa and Gerritsen [1] and Friedel [2] as "virtual bound states", being a "hybrid" of a localized (atomic-like) and delocalized (band-like) electronic state. The interest in RLs and associated resonance scattering, primarily appearing on a 3d shell of transition metal impurity, was related to their unusual transport properties, mainly the electrical resistivity. Decades later, RLs were observed in thermoelectric semiconductors containing transition-metal impurities (like PbTe:Ti [3]), but also doped with p-like elements, with the best-known example of PbTe:Tl [4,5], where, counter-intuitively, resonance is formed on 6s (usually free-electron-like) states. Since the publication of [5], RLs have become widely studied in thermoelectric community as a way to increase the thermopower and power factor of the material via non-rigid-band-like resonant doping.

In my presentation, I will provide a general overview of resonant levels (RLs) in thermoelectric materials in view of density-functional calculations. I will focus on the modifications of the electronic structure, conductivity, and charge carrier scattering induced by RLs to explain how to detect them, how they function, and what the controversies or misunderstandings were that have led to claims that RLs cannot improve thermoelectric properties. Additionally, I will highlight the similarities and differences in how RLs operate in metallic alloys and semiconducting thermoelectrics. While RLs can enhance thermoelectric properties in both cases, they do so in distinctly different ways, leading to opposite signs of thermopower despite a similar positioning of RLs relative to the Fermi level. Finally, I will discuss how RLs interact with other strategies for improving thermoelectric performance, such as multiple doping and band convergence.

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Acknowledgements

This work was supported by the program "Excellence Initiative - Research University" for the AGH University of Krakow.

Inelastic Neutron Scattering, an Experimental Tool for Understanding Phonons and Diffusion Processes in Thermoelectric Materials

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Keywords: Thermoelectric materials, Lattice thermal conductivity, Phonon engineering, Inelastic neutron scattering, Heat transport mechanisms

The optimisation of thermoelectric materials (TEM) is associated with the reduction of their lattice thermal conductivity, which is taken into account in the denominator of the dimensionless figure of merit. Phonons as the main carriers of thermal energy in TEMs are of central interest in this optimisation process because a targeted design of phonons, e.g. through the material composition and structuration, leads directly to reduced thermal conductivity and because dynamic interactions, such as phonon-phonon, electron-phonon and solid state diffusion, leave their mark on the phonon properties.
A thorough insight into phonon dispersion, spectral density and lifetime as well as mass transport is therefore important for understanding of the processes that mitigate heat transport. Inelastic neutron scattering (INS) is a powerful experimental tool to successfully approach this task. We will discuss essential INS techniques to explore different phonon aspects in detail and present examples from recent studies on promising thermoelectric compounds.

Perspective on thermoelectric applications of heat pump, cooling and geothermal energy

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Keywords: Thermoelectric applications, Heat pumps, Hybrid cooling systems, Geothermal generators, Experimental results

In this talk, different thermoelectric applications, developed by ITF from Spain, will be presented, including doble-stage heat pumps for building and thermal process, hybrid cooling systems and geothermal generators. The most important experimental results will be shown, and the critical points of these applications will be analyzed, as well as their advantages and disadvantages compared to compressor- and turbine-based technologies.

Advancing Thermoelectrics to Market: An Industrial Perspective

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Keywords: Thermoelectric generation, Commercial barriers, Market scalability, Niche applications, Thermoelectric coolers

The thermoelectric research community has made significant scientific advances over the years, consistently showing strong potential. However, commercial success has been far more limited. Most devices on the market still rely on materials and architectures developed over 50 years ago, and numerous companies that have attempted to push beyond these established technologies have ultimately gone out of business.

In this talk we consider some of the strengths, challenges and opportunities for thermoelectrics, alongside the barriers to getting to market. Thermoelectric generation offers the potential for very high growth, but it also faces the largest barriers, with a difficult balance between cost and scalability, performance, and reliability. Higher value niche markets need to be exploited to enable creation of a commercial foothold to enable a true understanding of costs, and allow more gradual scale up and cost reduction.

Thermoelectric coolers have a more established market presence, with modest predicted growth, enabling easier introduction of new innovations. However, achieving step changes in development is more challenging in this area, though there may be promising opportunities in human-orientated thermoelectrics, exemplified by a case we present.

Leveraging Additive Manufacturing to Re-envision Thermoelectric Systems

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Keywords: Additive manufacturing, Thermoelectric materials, Geometry design, Multi-scale structuring, System integration

Traditional thermoelectric device manufacturing uses steps that lead to material waste and performance limitations and offer little flexibility in designing the geometry of thermoelectric modules. Additive manufacturing offers the potential to structure thermoelectric materials and devices at multiple length scales, thus improving both intrinsic properties, overall system performance, and application integration. This talk will explore progress in additive manufacturing of thermoelectric materials, including the link between multi-scale materials, manufacturing, and system-level considerations for thermoelectric generators.

Optimizing Thermoelectric Materials: Balancing Performance, Cost, and Sustainability

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Keywords: Colloidal chemistry, 3D printing, Ink formulation, Porous microstructures, Thermoelectric integration

Advancing thermoelectric technology requires more than chasing ever-higher zT values; it demands a rethink of how we design, synthesize, and manufacture materials. Colloidal chemistry and extrusion-based 3D printing offer a powerful combination: the former enables precise control over material composition and microstructure through solution-based routes, while the latter provides a flexible platform for shaping materials into device-ready architectures with minimal waste and energy input. Together, they open a new space for engineering thermoelectric materials that are not only high-performing but also scalable and sustainable.

In this talk, I will discuss how interfacial chemistry, ink formulation, and porous microstructures can be harnessed to create functional materials with excellent charge and phonon transport, challenging the assumption that high performance requires high density or high-temperature processing. This approach can be broadly applicable, and I will highlight how it can be adapted beyond traditional systems to inspire new strategies for thermoelectric integration and fabrication.

Thermoelectric Measurement Methods: From Transport Properties to Generator Characterization

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Keywords: Transport properties, Measurement methods, Seebeck coefficient, Generator characterization, Performance optimization

Thermoelectric materials play a crucial role in energy conversion by directly transforming heat into electric energy. Accurate measurement of their transport properties - such as electrical conductivity, Seebeck coefficient, and thermal conductivity - is essential for assessing their performance. This talk provides an overview of key thermoelectric measurement methods, from fundamental transport property evaluation to the characterization of complete thermoelectric generators. We will discuss experimental techniques, challenges in measurement accuracy, and their impact on material and device optimization. By combining different measurement methods at both the material and module levels, we gain deeper insights into performance-limiting factors and optimization strategies, ultimately supporting the development of more efficient thermoelectric generators

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PART IV
CONTRIBUTED TALKS

-

2ND SESSION
ZINTL PHASES AND SKUTTERUDITES

Exploring High-Temperature Thermoelectric Properties of $(Ca,Sr)_{14}(Al,Ga,In)(Sb,Bi)_{11}$ Zintl Phases

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Keywords: Zintl phases, 14-1-11 compounds, thermoelectric properties

Zintl phases, particularly those within the 14-1-11 structural family, are of significant interest in thermoelectrics due to their intrinsically low lattice thermal conductivity and tunable electronic transport characteristics. Their intricate crystal structures effectively scatter phonons while preserving favorable semiconducting properties, making them particularly well-suited for high-temperature power generation. Among these, $Yb_{14}MnSb_{11}$ sets a benchmark with *zT* exceeding 1 at 1200 K, positioning this structural family at the forefront of thermoelectric research [1]. While 14-1-11 antimonides have been extensively investigated, their bismuth-based counterparts, despite offering greater suppression of lattice thermal conductivity due to the heavy-atom effect of Bi, remain comparatively underexplored. In this context, Tan *et al.* synthesized $A_{14}MgBi_{11}$ (*A* = Ca, Sr, Eu) compounds and demonstrated that, even without compositional or structural optimization, these materials exhibit substantial potential as promising thermoelectric candidates [2]. A particularly notable advancement supporting this shift toward Bi-based analogs is the successful synthesis and structural characterization of $Ca_{14}AlBi_{11}$ by Baranets and Bobev, achieved via both solid-state and Pb-flux synthesis routes. However, despite this progress, the comprehensive thermoelectric performance of $Ca_{14}AlBi_{11}$ remains largely unexplored and merits further investigation [3]. In this work, we report the successful solid-state synthesis of high-purity $Ca_{14}AlBi_{11}$ in Ta ampoules without detectable secondary phases, as confirmed by X-ray diffraction. We also present a systematic investigation of its thermoelectric transport properties, including electrical resistivity, Seebeck coefficient, and thermal conductivity, measured across a wide temperature range. In addition, we extend our investigation to a broader $(Ca,Sr)_{14}(Al,Ga,In)(Sb,Bi)_{11}$ compositional space to understand structure–property correlations and the role of chemical substitution in enhancing thermoelectric performance. This study not only deepens insight into the thermoelectric behavior of 14-1-11 Zintl phases but also provides a robust and scalable route for advancing their integration into thermoelectric modules for high temperature applications.

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Grain Boundary Electrical Resistance in the High Temperature Thermoelectrics $Yb_{14}MgSb_{11}$ and La_3Te_4

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Keywords: Grain boundary engineering, conductivity, microstructure, Zintl

Detrimental electrical resistance from grain boundaries in polycrystalline materials has been a major obstacle to achieving good performance in several low and mid temperature thermoelectric materials such as Mg_3Sb_2. Recent attempts to mitigate this detrimental resistance through increasing grain size or changing the boundary chemical composition have resulted in improved zTs for many materials. As added electrical resistance from grain boundaries is temperature activated, most of this work has focused on improving low temperature electrical conductivity. Even when applied to higher temperature materials, such as half Heuslers, the focus has been on improving low temperature performance to boost average zT. Thus there has been little work on investigating grain boundary resistance in very high temperature thermoelectrics.

In this work, the importance of mitigating grain boundary resistance even at extremely high temperatures is highlighted by analyzing two materials, $Yb_{14}MgSb_{11}$ and La_3Te_4. In the case of $Yb_{14}Mg_{Sb11}$, increasing grain size by controlling hot pressing conditions leads to the expected large improvement in low temperature conductivity and zT. However, this improvement is not negligible at high temperatures, with the peak zT at 1000°C increasing from 0.86 in the smallest grain sample to 1.07 in the largest despite constant Seebeck and thermal conductivity. In La_3Te_4, grain boundary resistance is present, but increases with temperature and is most significant at higher temperatures. By showcasing these two examples, this presentation will demonstrate the importance of mitigating grain boundary resistance at all temperatures.

Acknowledgments
This work was supported by a National Aeronautics and Space Administration (NASA) Space Technology Graduate Research Opportunity.

Grain boundary engineering to enhance $Mg_2(Si,Sn)$ stability

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Keywords: $Mg_2(Si,Sn)$, thermoelectric material, stability, microstructural analysis, grain boundaries

Performance and stability of thermoelectric (TE) materials are essential for scaling up TE devices to industrial applications, ensuring long-term durability and reliability. While many TE materials show high performance, stability remains a challenge, particularly for Mg-based materials such as $Mg_2(Si,Sn)$. Loosely bound dissolved magnesium has been identified as a key factor in the material degradation. By adjusting the magnesium composition and synthesizing Mg-poor n-type $Mg_2(Si,Sn)$ material, we demonstrate that we can reach similar TE properties as the state-of-the-art Mg-rich $Mg_2(Si,Sn)$. However, the stability of the composition requires further investigation.

In this study, we investigate the stability of doped and undoped n-type Mg-poor $Mg_2(Si,Sn)$ through high-temperature annealing (450-500°C) over several days. Our findings indicate that undoped Mg-poor samples remain stable, whereas those doped with Sb or Bi exhibit degradation. By combining microstructural analysis, transport property measurements, and first-principles calculations, we investigate the degradation mechanism, which differs from the behaviour previously observed in Mg-rich $Mg_2(Si,Sn)$. Although the degradation is slower in Mg-poor samples than in Mg-rich ones, they remain unstable. Our results reveal that the observed instability in Mg-poor samples is not related to Mg loss but rather to dopant effects, likely caused by formation of cluster defects and dopant segregation. To address this instability, we applied grain boundary decoration to block the grain boundaries and hinder dopant or Mg diffusion, significantly enhancing the stability of the material. Samples without grain boundary decoration show loss in carrier concentration down to 12-15% of the starting amount, while those with grain boundary engineering exhibit only 3% variations. This represents a substantial step forward in achieving stability, offering promising potential for practical application of the $Mg_2(Si,Sn)$ material system.

Acknowledgments
This work was supported by the German Academix Exchange Service, fellowship 57622551 and the government of North Rhine Westphalia for the funds received to finance the LUNA project.

A computational study on type-I Sn clathrates with inorganic and organic guests

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Keywords: Clathrates, Zintl phases, DFT calculations, Hirshfeld analysis, thermoelectrics

Semiconducting clathrates that feature a Sn host framework and encapsulate guest species such as Cs^+ and I^- hold great promise for thermoelectric applications. Using density functional theory (DFT), we investigate a series of existing and hypothetical type-I Sn-based clathrates with a diverse range of cationic (Rb^+, Cs^+, NH_4^+, NH_3Me^+, $NH_2Me_2^+$, $NHMe_3^+$, NMe_4^+, $(NH_2)_2CH^+$, Me_3S^+) and anionic (F^-, Cl^-, Br^-, I^-, NO_3^-, BF_4^-, SCN^-, $HCOO^-$, $CF_3SO_3^-$) guests, expanding upon previous work [1]. We examine the feasibility and properties of these structures by exploring their stability, formation energies, and electronic characteristics, identifying key trends in guest-framework interactions. Hirshfeld surface analysis provides further insights into the influence of guest size, charge, and framework vacancies on stability and structural distortions. Our results show that electron-counting and stereochemical constraints govern the formation of A_8Sn_{46-x} clathrates, where x denotes the number of framework vacancies per unit cell. In particular, cationic guests such as Rb^+, Cs^+, and NH_4^+ stabilize the framework with two vacancies per unit cell ($x = 2$), while larger cations and most anionic guests prefer a fully occupied framework ($x = 0$) [2]. An exception is found in halide anions, which, despite favoring the Sn_{44} composition, induce strong lattice distortions that ultimately disrupt the clathrate structure. Finally, we assess the thermoelectric properties of the most promising candidates, providing insights into their potential for practical applications.

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Acknowledgments

The research project is implemented in the framework of H.F.R.I call "Basic research Financing (Horizontal support of all Sciences)" under the National Recovery and Resilience Plan "Greece 2.0" funded by the European Union–NextGenerationEU (H.F.R.I. Project Number: 14730). This work was supported by computational time granted from the National Infrastructures for Research and Technology S.A. (GRNET S.A.) in the National HPC facility ARIS-under project ID pr017021.

Improved thermoelectric performance in very finely grained $Co_{0.91}Ni_{0.09}Sb_3$ skutterudites

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Keywords: Skutterudites, nanostructuring, sintering

Filled *n*-type skutterudites have shown a high thermoelectric figure of merit, $ZT \geq 1.5$. [1] Rare earth fillers increase the cost and reduce the stability, making them unsuitable for commercial applications. Making an ultra finely grained densified polycrystal is a potential strategy for reducing thermal conductivity that leads to an increased *ZT*. The key challenge here is to minimize the grain growth during sintering for achieving low phonon thermal conductivity.

The grain growth inhibitor such as nano-CeO_2 (~ 8 nm) was utilized to limit the grain growth during sintering of nanostructured Ni-doped $CoSb_3$ skutterudites ($Co_{0.91}Ni_{0.09}Sb_3$). By varying the sintering temperature between 340 and 630°C under 75 MPa, the grain size and relative mass density ranged in the interval 35 nm – 212 nm and 80% – 98%, respectively. A sintering map, grain size vs mass density was created for the first time. We found a good compromise between a grain size equal to 101 nm and a mass density of 94% for the sample sintered at 500°C. This compromise was found reproducible, even by changing the sintering conditions (450 – 500°C under 75 – 135 MPa for 0 – 30 min). Finally, *ZT* was improved by ~ 30% and reached a value equal to 0.9 at 800 K.

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Acknowledgments

We acknowledge the funding provided by DIM MaTerRE and Region Ile de France.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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3RD SESSION
THIN FILMS I

Thin Film Nanodecoration and Nanostructuring Techniques to Enhance Thermoelectric Efficiency in Silicon Micro-Thermoelectric Generators

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Keywords: Nanoparticle decoration, block copolymer, silicon, hydrodynamic phonon transport, hydrodynamic phonon

Thermoelectric (TE) materials enable direct heat-to-electricity conversion for cooling, power generation, and sensing [1]. Their efficiency is governed by the figure of merit (zT), which depends on the Seebeck coefficient, electrical conductivity, and thermal conductivity. Conventional TE materials, such as chalcogenides, achieve $zT \approx 1$ at room temperature but rely on scarce, toxic elements (Bi, Te, Sb), limiting their integration with semiconductor technology. In contrast, bulk silicon is a poor TE material, but nanoparticle decoration or nanostructuring significantly enhance its performance by reducing phononic thermal conductivity [2, 3, 4]. The approaches used in these work is based on thin films that offer a viable alternative to silicon nanowires as thin films are easier to integrate into micro thermoelectric generators (μTEGs). These μTEGs are a sustainable replacement for batteries used in IoT devices, addressing battery disposal concerns. Our strategy includes the fabrication of low-pressure chemical vapor deposition (LPCVD) SiNx membranes and characterizing their thermal conductivity (κ) using the 3ω Völklein method. This measurement is made in operando while evaporating metal nanoparticles that decorate the membrane. Results confirm a κ reduction due to an increased phonon scattering with the nanoparticles at the initial stages of the evaporation, consistent with hydrodynamic phonon transport model predictions. Alternatively, we have also patterned silicon ultra-thin films via block copolymer lithography, a scalable and cost-effective method. Our measurements on nanopatterned silicon membranes on Silicon-on-Insulator (SOI) wafers exhibit a 25-fold zT enhancement due to a two-order-of-magnitude reduction in thermal conductivity compared to bulk silicon. These advancements in silicon-based TE materials and μTEG architectures pave the way for efficient energy harvesting in self-powered electronics.

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Grant TED2021-129612B-C21 (MICIU/AEI/10.13039/501100011033 and by European Union NextGenerationEU/PRTR), by ESF+ through grants RYC2022-038370-I and RYC2022-037016-I, and grant 2021-SGR 00497 funded by AGAUR (Generalitat de Catalunya), JAE Intro-ICU-CSIC fellowship and ICTS Network MICRONANOFABS partially supported by Spanish Ministry of Economy and Competitiveness.

Heavily Doped p-type Silicon Nanopillars Obtained by Metal-Assisted Chemical Etching for Thermoelectric Applications

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Keywords: Silicon nanopillars, Metal-Assisted Chemical Etching, heavily doped silicon nanowires

Silicon nanowires (SiNW) display a reduced thermal conductivity compared to bulk Si, leading to a figure of merit of ≈ 0.8 at room temperature [1-2]. Among the ways to fabricate SiNWs, Metal-Assisted Chemical Etching (MACE), a facile, low-cost, and scalable technique, provides a way to obtain high-density forests of Si nanopillars (SiNPs), i.e. NWs oriented normally to the Si substrate [3]. However, MACE has enabled the production of p- and n-type single-crystalline SiNPs only up to to 10^{19} cm^{-3} [4]. In the high doping range ($\geq 10^{20}$ cm^{-3}), only n-type SiNPs could be obtained [5]. We report here about a strategy that enabled for the first time the making of p-type SiNPs doped above 10^{20} cm^{-3}. The approach we followed assumed that two factors hindered MACE on heavily doped p-type Si. On one side, when Ag is used as a catalyst, its reoxidation by H_2O_2 enables its secondary nucleation at SiNP sides and tips, causing undesidered SiNP etching. Additionally, non-localized etching unavoidably occurs by direct hole injection from the solution at Si bare surface, more effectively competing with MACE at high doping levels. On these bases, we designed an experiment where a discontinuous Au layer replaced Ag as the catalyst while $Na_2S_2O_8$ was used as the oxidizing agent. SiNPs could be successfully fabricated. TEM and Raman spectroscopy confirmed the formation of dense, high-aspect ratio porous SiNPs with a diameter of ≈ 150 nm, lower than Si phonon mean free path – then enabling the reduction of thermal conducivity. Electrical conductivity and Seebeck coefficient were found in line with literature data for porous Si NWs while the fill factor was estimated to exceed 20%. Thus, our results habilitate the prospective use of SiNPs in the making of thermoelectric devices with ouput power densities and cooling loads fully comparable to those attainable with telluride-based devices [6].

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Acknowledgments

This work was supported by the Ministry of University and Research in the frame of the PON Program "Research & Innovation" 2014-2020, Axis IV, Action IV.5, Grant DOT 13C6492 and by the European Union - Next Generation EU, Mission 4 Component 1, CUP H53D23003770006.

Design and optimization of flexible free-standing PEDOT:PSS-based thermoelectric composites

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Keywords: Composites, PEDOT:PSS, $Cu_{12+x}Sb_4S_{13}$

Flexible thermoelectric composites based on conducting polymers such as PEDOT:PSS are gaining increasing attention as alternatives to conventional inorganic TE materials, owing to their unique advantages, including low weight, processability, and mechanical flexibility. In this study, we focused on a detailed investigation of the impact of synthesis parameters and the content of inorganic nanoparticles on the physicochemical and thermoelectric properties of PEDOT:PSS-based composites.

Composites incorporating environmentally friendly nanoparticles such as $Cu_{12+x}Sb_4S_{13}$ (tetrahedrites, TH), multiwalled carbon nanotubes (MWCNT), and graphene were fabricated via a simple drop-casting method into flexible, free-standing films. Tetrahedrites, synthesized via a novel solvothermal synthesis, exhibit ultra-low thermal conductivity (0.25 $W \cdot m^{-1} \cdot K^{-1}$ at 300 K) and a tunable Seebeck coefficient ranging from 150 to 400 $\mu V \cdot K^{-1}$ by adjusting the Cu content. Both binary and ternary composites were prepared and analyzed. PEDOT:PSS underwent pre- and post-treatment with DMSO and EG to enhance its electrical conductivity. We systematically examined the influence of various factors, such as surfactant content, drying time and temperature, and the order of component addition, on the microstructure and thermoelectric performance of the composites. Material characterization was conducted using XPS, FTIR, SEM, and Scanning Thermal Microscopy (SThM), the latter of which enabled assessment of Seebeck coefficient homogeneity across the film surface. The results revealed that even subtle changes in processing conditions significantly influence the structural and functional properties of the composites. For a ternary composite containing 20% TH and 5% MWCNT, a fivefold increase in power factor (PF) was achieved compared to the optimized PEDOT:PSS.

These findings offer valuable insights into the complex relationship between composition, microstructure, and thermoelectric performance, providing a framework for the rational design of efficient, flexible thermoelectric materials.

Energy Filtering in Heavily Boron-Doped SiGe Thin Films

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Keywords: Thin Films, Sputtering, SiGe, Boron doping, energy filtering

SiGe alloys hold a significant role in high-temperature thermoelectric applications. Instead, their room-temperature (RT) applications are not yet competitive. In this contribution, we will discuss the possibility of inducing energy filtering (EF) in the SiGe system [1], following the approach pursued with boron hyper-doped Si thin films [2]. Activation of EF could lead to even higher figures of merit than in Si due to the intrinsic lower thermal conductivity of SiGe alloys. Samples were prepared in an UHV system, to ensure hydrogen-free conditions [3], on quartz substrates by co-sputtering SiGe and B for in-situ doping [4]. Films were then annealed using rapid thermal process, followed by treatments at 1000 °C for 120 minutes to enable boron migration and precipitation at grain boundaries. Deposition conditions were optimized by testing different temperatures and targets powers. X-ray diffraction and SEM analyses confirmed the formation of a crystalline SiGe phase at deposition temperature $\geq$ 550°C. Moreover, cross-section SEM images suggest a columnar shape of the grains, with an in-plane diameter of $\approx$ 50 nm, as required by EF. Finally, through Raman spectroscopy we were able to determine the composition of the films and a possible correlation between Raman peaks and electrical conductivity of samples. Factors affecting the activation of EF will be presented and discussed.

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This work was partially supported by the European Union - Next Generation EU, Mission 4 Component 1, CUP H53D23003770006 and ERC Advanced Grant POWERbyU (ERC-2021-ADG-101052603).

Thermoelectric properties of Nb doped ScN multilayer structures

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Keywords: Scandium Nitrides, Thermoelectric, thin films, multilayer structures

In recent decades, thermoelectric research has garnered significant attention due to growing awareness of the energy crisis, the pursuit of sustainable clean energy, and the miniaturisation of sensors and electronic circuits. Scandium nitride (ScN) exhibits promising thermoelectric properties. As a group III(B) transition metal nitride, ScN can overcome certain limitations of group III(A) nitride semiconductors for various applications. [1-2-3]. In this study, ScN/$Sc_{1-x}Nb_xN$ multilayers were deposited on MgO (001) substrates using DC magnetron sputtering in an ultra-high vacuum (UHV) system. The Nb dopant concentration varied from x = 0.004 to 0.05. Quantum-mechanical calculations, using density functional theory, simulated the effect of Sc substitution by Nb on thermoelectric properties, showing good agreement with experimental results. Material characterisation, including X-ray diffraction, X-ray spectroscopy, and Raman spectroscopy as a function of temperature from room temperature to 800K, was performed to understand doping-induced changes. A clear improvement in the Seebeck coefficient (S) was observed with Nb doping across this temperature range. The ScN layer showed an S value of -60 µV/K at 800K, which increased to -110/-115 µV/K at 800K for $Sc_{1-x}Nb_xN$ layers with x varying from 0.004 to 0.02. However, the electrical resistivity increased with Nb doping, indicating a slight decrease in conductivity. Electrical resistivity showed semimetal behavior with temperature variation for all layers. Specifically, the electrical resistivity increased 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. This conductivity reduction is compensated by a decrease in thermal conductivity from approximately 10 W/m·K to approximately 4 W/m·K at room temperature with Nb doping. This reduction leads to an overall improvement in the thermoelectric properties when comparing ScN and $Sc_{1-x}Nb_xN$ layers.

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Acknowledgments

The authors acknowledge the support from Czech Science Foundation (GAČR) Project No. 23-07228S.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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4TH SESSION
THEORY I

Theoretical study of electronic structure and transport properties of halfmetallic ferromagnetic $Cu_2FeSnS_xSe_{4-x}$ with strong electron correlations

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Keywords: Electronic structure, transport properties, DFT, strong correlations

The purpose of this study was to perform theoretical calculations of the electronic structure and transport properties for low-cost and eco-friendly thermoelectric materials $Cu_2FeSnS_xSe_{4-x}$. These materials are semiconductors with diamond-like tetragonal structure. Calculations were carried out based on density functional theory. For the electronic structure, the WIEN2k package [1] was used, which is based on the APW+lo method. The modified Becke-Johnson semi local exchange-correlation potential was used [2]. It appeared that 3*d* orbitals of Fe exhibit strong electronic correlations [3] since to obtain the semiconducting ground state the Hubbard U term was necessary (LDA+U method). Based on the obtained electronic structure, the transport properties of $Cu_2FeSnS_xSe_{4-x}$ were determined using BoltzTraP2 [4]. Results for electronic structure indicated that all studied materials are intriguing halfmetallic ferromagnetic semiconductors (E_F penetrates only spin-majority channel) with total magnetic moment of 4 μ_B. That opens the possibility for a spin-dependent thermoelectric phenomena. The obtained energy gaps for majority spin were about 0.5 eV in all compounds, while for the minority spin band gap was larger of about 0.8 eV. These gaps were two times smaller than reported in Song et al. paper [3] for $Cu_2FeSnSe_4$. Including spin-orbit coupling into the calculations caused disappearance of degeneracy in band structure and 'anti-crossing' effect. Because of difference between energy gaps for spin up and down, the main contribution to Seebeck coefficient for *p*-type material came only from one of the spins.

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Acknowledgments

This work was partially supported by the National Science Centre (Poland), project No. 2023/51/B/ST11/00329 and the program "Excellence Initiative – Research University" forthe AGH University of Krakow.

A high-throughput framework for ab initio deformation potential extraction for thermoelectric materials

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Keywords: First-principles, high-throughput calculation, deformation potential, electron-phonon interactions

The deformation potential theory offers an efficient and accurate framework for computing electron-phonon scattering rates. Several protocols have been established to extract deformation potentials from first-principles calculations, including fitting volume-dependent band-edge energies or phonon q-dependent electron–phonon matrix elements [1, 2].

In this work, we present a high-throughput protocol for calculating deformation potentials using density functional perturbation theory (DFPT), starting directly from crystal structure inputs. By first identifying the participating phonons relevant to the relevant electron scattering processes, we extract a finite but highly relevant subset of matrix elements near the electronic energy and k-space region of interest. This approach reduces the number of required matrix element evaluations from approximately 100,000 (in fully *ab initio* methods) to around 100, drastically lowering computational cost.

Our protocol also incorporates symmetry considerations of momentum space to minimise computational effort and is benchmarked against conventional volume- (or stress-) variation approaches. Moreover, it not only distinguishes between intra- and inter-valley scattering events and quantifies their respective strengths, but also differentiates acoustic and optical deformation potentials. We demonstrate the effectiveness of our approach by computing deformation potentials for a selection of materials including half-Heusler compounds, which are afterwards used within Boltzmann transport simulations for evaluation of electronic transport beyond the constant relaxation time approximation.

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Acknowledgments

This work is supported by the European Research Council (ERC) [grant number 678763]; and the Engineering and Physical Sciences Research Council [grant number EP/X02346X/1].

Electronic properties of thermoelectric pseudo-hollandite and hollandite-like phases

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Keywords: Electronic properties, hollandite-like, pseudo-hollandite, thermoelectrics

The syntheses, structural and thermoelectric properties of the hollandite-like cesium-inserted chromium telluride $Cs_xCr_5Te_8$ (x = 0.73, 0.91, and 0.97) and pseudo-hollandite $Rb_{0.2}Ba_{0.4}Cr_5Se_8$ selenide were investigated [1,2]. Thermal conductivity measurements indicated low values for both compounds in the 300 – 900 K range. Decorrelated transport properties observed in the later are beneficial for their relatively good thermoelectric performance. For the former, periodic density functional theory (DFT) calculations indicate that the $Cs_{0.73}Cr_5Te_8$ composition is the most stable one with a weak metallic conductive behavior. For the latter, DFT calculations showed that the density of states of $Rb_{0.2}Ba_{0.4}Cr_5Se_8$ is more polarized than that of $Ba_{0.5}Cr_5Se_8$, resulting in a higher Seebeck coefficient.

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Acknowledgments

This work was supported by the French National Research Agency (ANR_Project HIGHTHERM_ref ANR-18-CE05-0037), the Japan Society for the Promotion of Science (JSPS_PE21708 and 19H05819), and the JST Mirai Program JPMJMI19A1.

When are elongated bands most effective for the power-factor?

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Keywords: Elongated bands, band anisotropy, materials screening

Recently there has been a large interest for materials that exhibit elongated/low dimensional tube-like bands in their 3D Brillouin zone. The high anisotropy of these bands and possibly their low dimensional like features are believed to be beneficial for the power factor [1]. In fact, for a certain density of states, an elongated ellipsoidal band allows for even up to 50% higher power factor compared to a spherical one. In this work, we examine the potential of such electronic structures for power factor improvements by examining a series of materials that exhibit such bands. Utilizing the Boltzmann Transport as implemented in the ElecTra code [2], we incorporate the complete energy/momentum/band dependencies of all significant electronic scattering rates, including those from acoustic phonons, non-polar optical phonons (both intra- and inter-valley), polar optical phonons (POP), and ionized impurity scattering (IIS) [3], where we account fully for intra-/inter valley/band transitions, screening from both electrons and holes, and bipolar transport effects. We show that indeed some moderate improvements can be achieved using flat bands as we have noticed that in all these materials, the polarity that includes flat bands i.e. p-type can significantly provide high power factor compared to the opposite other polarity (n-type) which doesn't have flat bands, despite the variations in other parameters that control transport. However, the most significant improvements are obtained in materials in which elongated bands begin from one high symmetry point other than the Γ-point, and are directed towards another high symmetry point again other than the Γ-point. This allows for a large degeneracy of elongated bands, which increases power factor substantially. We have identified a case where excessive strain in NbFeSb can lead to such possibility, where the power factor increases by three-fold. Although in that case the strain is unrealistically excessive, (thus this example remains as a thought experiment), it still points towards the optimal direction of full utilization of such band features. We also found high power-factors in materials beyond cubic, for example, KAsCd and KMgBi which have elongated bands and have quasi-2D transport. On the other hand, we also examine cases where elongated bands lead to the opposite, i.e. power factor reductions. Overall, our results can set a benchmark for the optimal elongated band material features, which would effectively drive material screening studies and experimental efforts.

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Acknowledgments

This work has received funding from the UK Research and Innovation fund (project reference EP/X02346X/1).

The use of descriptors within featurization for improved machine learning prediction of half-Heusler thermoelectric materials

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Keywords: Scattering rates, descriptors, matminer, machine learning

In this work, we design a new descriptor to assist machine learning-based prediction of thermoelectric (TE) power factors in Half-Heusler (HH) materials. The TE power factors (PFs) for 12 HH compounds (both n-type and p-type) were calculated using the ElecTra code, fully accounting for essential scattering mechanisms such as ionized impurity scattering (IIS), polar optical phonon (POP), and non-polar acoustic and optical phonon (ADP and ODP) scattering [1]. Based on these results, we developed a novel descriptor that incorporates key physical parameters such as dielectric constants (ε_o and ε_∞), conductivity and density of states effective masses (m_{cond} and m_{DOS}) extracted as in the method implemented in our EMAF code [2], and valley degeneracy. Our new descriptor has ~0.8 correlation with the fully computed PF. Turning to machine learning, using *matminer* features alone, the model achieves a moderate to weak correlation (-0.2 to 0.7) with the computed power factor due to very sample size [3]. However, when our descriptor was combined with *matminer* features in a Random Forest model, the correlation improved significantly, reaching R^2 scores of 0.931 for n-type and 0.933 for p-type [4]. Feature importance analysis confirmed that the descriptor is the most dominant feature for n-type prediction and among the top contributors for p-type, demonstrating its strong physical relevance and predictive capability [4]. Afterwards, additional HH compositions are be considered. These will be used to train the model, which will then predict power factors for a larger number of similar and novel materials. The goal is for promising candidates to undergo DFT-based validation and be added to the training set, forming a loop that incrementally improves model accuracy. Key descriptor components—such as valley degeneracy, m_{DOS}, m_{cond}, ε_o, and ε_∞ - are extracted from DFT outputs. These scripts interface with tools like Quantum ESPRESSO, EMAF [2], and other post-processing utilities to analyze the band structure and dielectric responses, enabling a high-throughput and scalable approach to thermoelectric materials discovery, capable of screening large number of materials with ab initio electronic transport-informed calculations.

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This work has received funding from the UK Research and Innovation fund (EP/X02346X/1).

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PART IV
CONTRIBUTED TALKS

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5TH SESSION
HALF-HEUSLERS

Thermoelectric properties of single-crystalline TiCoSb-based half-Heuslers

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Keywords: Half-Heusler, single crystal, electron mobility

Half-Heuslers emerged as promising candidates for medium- and high-temperature thermoelectric power generation. However, polycrystalline half-Heuslers inevitably suffer from the defect-dominated scattering of electrons that greatly limits the optimization of their electronic properties. Herein, high-quality TiCoSb-based single-crystals with a dimension above 1 cm have been obtained. Benefitting from the improved electron mobility, an average power factor of ~ 37 μW cm^{-1} K^{-2} in the temperature range between 307 and 973 K has been realized in the n-type single-crystalline $Ti_{1-x}Nb_xCoSb$. In addition, Hf alloying results in the expansion of the weighted scattering phase space and enhances the anharmonic scattering rate, thereby effectively suppressing the lattice thermal conductivity. Eventually, co-doping of Nb/Ta and alloying of Hf effectively elevate the thermoelectric performance of TiCoSb single crystal, and a peak *zT* above 1.0 has been realized, which outperforms the previously reported polycrystalline (Ti, Zr, Hf)CoSb-based and ZrCoBi-based materials. Importantly, a single leg of TiCoSb-based single crystals exhibits a heat-to-electricity energy conversive efficiency of ~10.2% at a temperature difference of 700 K. Here, our findings reveal the promise of TiCoSb-based single crystals for thermoelectric power generation, and can potentially guide the future explorations of other single-crystalline half-Heuslers.

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This work was supported by the National Natural Science Foundation of China for Distinguished Young Scholars (52425108), National Key Research and Development Program of China (2023YFB3809400), and the GuangDong Basic and Applied Basic Research Foundation (2024B1515040022). J.M. acknowledges the financial support from the National Natural Science Foundation of China (52473298), Shenzhen Science and Technology Program (RCJC20221008092725020). Q.Z. acknowledges the financial support from the the National Natural Science Foundation of China (52172194, 52425108), and the Shenzhen Science and Technology Program (RCJC20210609103733073, JCYJ20241202123659001). F.C. acknowledges the financial support from the National Natural Science Foundation of China (52472196). Y.F. acknowledges the financial support from the National Natural Science Foundation of China (62474081 and 22090044).

Improved thermal stability of NbCoSn Half-Heusler compounds via Sb doping-induced complementary point defect evolution

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Keywords: Thermal stability, half-Heusler, point defect evolution, transmission electron microscopy, neutron diffraction

The high thermal stability of a thermoelectric material, which maintains a stable conversion efficiency under prolonged heat exposure, is essential for sustainable thermoelectric applications. Despite the well-known relationship between thermal degradation and microstructural evolution, their underlying interplay remains unclear, with contradictory findings reported in the literature owing to the complex dependence of microstructural changes on the material composition. Herein, the beneficial effect of Sb doping on the thermal stability of NbCoSn half-Heusler compounds is investigated by comprehensively analyzing their microstructural evolution. Advanced techniques, including atom probe tomography, scanning transmission electron microscopy, and neutron diffraction, show that the evolution of Sb-induced complementary point defects drives this improvement. Although heat exposure significantly reduces lattice disorder in intrinsic NbCoSn, $NbCoSn_{0.9}Sb_{0.1}$ retains its lattice disorder by forming alternative point defects, thereby maintaining its lattice thermal conductivity. This detailed experimental work, corroborated by ab initio calculations, highlights the pivotal role of the point defect dynamics in achieving robust thermoelectric performances in half-Heusler compounds for high-temperature applications

Acknowledgments
This work was supported by the Global Joint Research Program funded by Pukyong National University and the Deutsche Forschungsgemeinschaft (DFG).

Half-Heusler thermoelectric compounds with intrinsically low thermal conductivity

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Keywords: Thermoelectric, half-Heusler, lattice thermal conductivity, anharmonicity

Half-Heusler compounds are very promising thermoelectric materials but generally have intrinsically high lattice thermal conductivity (e.g., 10-30 W m^{-1} K^{-1} at 300 K), a major obstacle for achieving the high TE figure of merit *zT*. In this work, we report a series of new half-Heusler compounds that exhibit significantly lower intrinsic lattice thermal conductivity. The combined experimental analysis and first-principles calculations reveal that the existence of localized weak bonding coupled with the heavy atom induces strong phonon anharmonicity in these half-Heusler compounds, resulting in intrinsically low lattice thermal conductivity. These half-Heusler compounds with intrinsically low thermal conductivity provide new opportunities for exploiting promising candidates for thermoelectric applications.

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This work was supported by the National Natural Science Foundation of China.

p-type Dopability in Half-Heusler Thermoelectric Semiconductors

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Keywords: p-type dopability, half-Heusler, defect formation energy, complex

Half-Heusler (HH) semiconductors with high valence band degeneracy are promising p-type thermoelectric materials. However, effective p-type dopability in HH semiconductors remains a significant challenge, hindering the further development of high-performance p-type HH thermoelectrics. In this work, we investigate p-type dopability in NbFeSb, NbCoSn, and ZrNiSn through comprehensive first-principles defect calculations. We identify that interstitials (B_i) and vacancies (V_A) primarily limit dopability by setting the maximum achievable doping level. Using dopability limits and pinned Fermi levels as indicators, we systematically evaluate the doping feasibility of p-type dopants at three different Wyckoff positions. Moreover, by taking NbCoSn as an example, p-type dopability was experimentally scrutinized, validating the calculation results. This work offers valuable insights into the challenges associated with p-type doping in HH compounds and provides practical guidance for the experimental selection of suitable host materials and dopants, which can help facilitate the realization of effective p-type doping.

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PART IV
CONTRIBUTED TALKS

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6TH SESSION
ORGANIC MATRERIALS

Performance of thermoelectric PEDOT:PSS composite films with $Bi_{0.4}Sb_{1.6}Te_3$

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Keywords: Conductive polymer, low temperature thermoelectrics, PEDOT:PSS, thermoelectric composite films

An emerging interest in alternative low-temperature thermoelectric applications has appeared in the form of organic-based thermoelectric materials instead of the classic well-known inorganic thermoelectric materials. This stems from the intrinsic properties of organic conductive polymers such as low thermal conductivity, ease of processability, abundance, low-toxicity, cost-effectiveness and tunable electrical properties via various additives and processing methods. Simultaneously, the inherent flexibility of polymers supports the development of novel thermoelectric device designs that can help expand the low temperature thermoelectric applications field. One such promising conducting polymer is PEDOT:PSS due to its high electrical conductivity compared to other polymers, that is easily tunable with various doping methods that modulate its morphology. Furthermore, its comparatively high Seebeck coefficient due to the bipolaron network with asymmetric density of states at Fermi level and its low thermal conductivity deriving from weak lattice vibrations, makes it a suitable candidate for low temperature thermoelectric applications.

This work studies the thermoelectric performance of PEDOT:PSS and its composite films deposited on glass substrates via drop-casting. The effects on performance of various additives, such as DMSO, $Bi_{0.4}Sb_{1.6}Te_3$ along with HCl in organic-inorganic PEDOT:PSS composite films, are investigated. This is done by means of Seebeck coefficient and electrical conductivity measurements to obtain the material power factor across a temperature range, demonstrating significant improvements depending on the additive and its concentration.

Polymorphism Controls Thermoelectric Properties In Oriented PBTTT Films

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Keywords: Thermoelectricity, Polythiophenes, Polymorphism

Polymorphism is a common feature of polymer semiconductors such as polythiophenes and determines their optical and electronic properties. Controlling polymorphism is thus an elegant means to probe structure-property correlations in doped polymer semiconductors. In this contribution, we focus on PBTTT bearing single-ether side chains, namely PBTTT-8O.1-3 This polymer forms two distinct polymorphs under controlled growth conditions: form 1 and form 2 are prepared by thermal annealing and solvent treatment in n-hexane, respectively. Polarized UV-vis-NIR spectroscopy demonstrates that backbone planarization is reduced in form 2, whereas regular π-stacking and extended planarization is present in form 1. Upon doping with the strong acceptor F6TCNNQ, the aligned polymorphs show substantially different charge transport and thermoelectric properties. The best thermoelectric properties are observed for the doped form 1 with a very high power factor of 1380 ± 240 µW/m.K² versus 240+50 µW/m.K² for the doped films of form 2.

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This work was financially supported by the European Commission through the Marie Sklodowska-Curie project HORATES (GA-955837). S.O. thanks the French national research agency (ANR) for funding through contract Thermopolys (ANR-22-CE50-0020) as well as University of Strasbourg.

Graphene-based Organic semiconductor composites for low-temperature- grade energy harvesting: from cell to module

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Keywords: Seebeck coefficient, thermoelectrics, organic semiconductor, composites

Thermoelectric (TE) materials, in the context of recent technological advancements, are regarded as the foremost choice for converting waste heat into electrical energy [1]. Nonetheless, their industrial application is constrained by factors such as high-temperature fabrication processes, the high cost of inorganic TE materials, and their inherent toxicity. Additionally, the depletion of raw materials, such as petroleum and metals, further restricts their utilization. Organic materials have thus garnered significant interest due to their promising potential across various domains, including supercapacitors, biosensors, and optoelectronics. In the past decade, composites of organic polymers with carbon-based nanostructures, such as graphene nanoplatelets or carbon nanotubes, have attracted considerable attention as TE materials suitable for energy harvesting applications. Yet, the high thermal conductivity and adhesive properties of graphene nanoplatelets present challenges that necessitate resolution. Consequently, TiO_2 emerges as a viable option to enhance thermal conductivity and facilitate improved composite dispersion [2]. Here we will present a printable TE paste with graphene nanoplatelets (GNPs) and poly(3-hexylthiophene) (P3HT), using various filler-to-semiconductor ratios (2:1, 1:1, 1:2). The impact of the dopant Lithium bis (trifluoromethane sulfonic) imide (LiTFSI) and Tributyl phosphate (TBP), together with the ceramic spacer comprising Titanium oxide nanoparticles (TiO_2 NPs), has been investigated on films, pellets, and a module. Doping has led to a significant enhancement in the electrical conductivity and Seebeck coefficient (S) for the films of G:P3HT composite, which increased from 40 S/m to 140 S/m, and from 35 μV/K to 85 μV/K, respectively, in the 1:2 ratio. Similarly, the power factor (PF) for thin films demonstrated a significant increase from 35 nW/mK² to 1022 nW/mK² following doping. The Seebeck coefficient (S) of the composite with a TiO_2 spacer rose to 160 μV/K, while the electrical conductivity remained stable. Additionally, the development of a three-dimensional structure, identified as a cylindrical pellet, effectively altered the dopant, filler, and spacer. A refined G:P3HT (LiTFSI) pellet was employed to construct a thermoelectric (TE) module for practical performance evaluation, achieving a maximum power output (P_{max}) of approximately 0.40 μW/cm². This methodology may serve as a guide for producing efficient, cost-effective TE materials.

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Acknowledgments

This work was partially supported by PTR25-27 Ricerca di Sistema - WP3 – LA3.5 Moduli termoelettrici e termoelettrogalvanici per il recupero di energia negli edifici orientati ad applicazioni flessibili, and Progetto 4S – MIMIT.

Role of Polymer Electrodes for Liquid and Gelified Thermoelectrochemical Redox Systems for waste-heat recovery applications

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Keywords: Seebeck coefficient, thermogalvanic cell, Co(II)/Co(III) electrolyte, energy harvesting

Thermogalvanic cells (TGCs) have emerged as a promising technology for converting lowgrade thermal energy into electricity. Cobalt-based electrolytes are known for their stability and tunable redox properties, promising for enhancing thermogalvanic cells. Recent research focuses on optimizing electrode materials, electrolyte composition, and device architecture, with organic semiconductors like poly(3,4-ethylenedioxythiophene) (PEDOT) gaining attention due to their mechanical flexibility, ease of fabrication, and cost-effectiveness [1]. Additionally, Liquid electrolytes are no doubt effective in terms of ionic conductivity but often struggle with leakage and rigidity issues that restrict their use in flexible and wearable applications. Gel electrolytes have emerged as an ideal solution, especially when ionic liquids are incorporated into the gel matrix.

We present a TGC device using various PEDOT-based electrodes and Co(II)/Co(III) electrolytes. Our reference liquid TGC based on PEDOT PH1000(10% DMSO)/ITO electrode compositions on both Glass and PET have shown Seebeck coefficient ranging from -700 μV/K to -1700 μV/K across different electrode materials, with 100 mM Co(II)/Co(III) along with PEDOT PH1000(10% DMSO)/ITO/PET showing the highest value. We verified that the electrochemical Seebeck coefficient depends on electrode distances. In the range from 100 μm to 600 μm Seebeck rose from -300 μV/K to -1100 μV/K. Electrical conductivity reached up to 0.37 mS/cm, and the power factor peaked at 4.0 μW/mK². The power density exceeded 40 μW/cm² at $\Delta T = 25°C$, highlighting the material's potential for high-performance thermoelectric applications. We investigate the role of different solvent systems, considering Acetonitrile and Propylene Carbonate as low and high viscosity systems, and we show the scale up from single TGC cells to full TGC module. Further we aim to explore the formulation of gelified electrolyte, considering different strategies like by adding an additive like mineral clay as its being using in gelifying the electrolyte in the literature recently or by using other approaches i.e radiation induced in-situ polymerization to with the focus on creating flexible, high-efficiency energy harvesting systems [2].

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ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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7TH SESSION
DEVICE I

Coupling of a Genetic Algorithm and a Thermoelectric Network Model for Radioisotope Thermoelectric Generator (RTG) Optimisation

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Keywords Radioisotope Thermoelectric Generator (RTG), Thermoelectric Network Model, Genetic Algorithm (GA), lunar exploration, deep space exploration

Lunar exploration requires a continuous supply of electrical power, independent of solar irradiation availability, which can be provided by radioisotope thermoelectric generators (RTG). RTG contain a radioisotope heating unit, enclosed in an aeroshell core and coupled with thermoelectric modules (TEM). TEM utilizes the temperature difference developed between their hot side, adjacent to the RTG core, and their cold side, connected to radiation fins attached to the outer RTG surface, to convert part of the released heat into electricity through the Seebeck effect. Design and operation of RTG is a complex multi-disciplinary challenge, as they are comprised of multiple components that affect performance. The surfaces of the aeroshell not connected to TEM are covered by thermal insulation, driving most of the source heat through the TEM. Excessive insulation however, could undersibaly increase the system mass which should be minimized. The materials and geometry of the TEM affect the heat-to-electricity conversion efficiency as well as the temperature at its hot side which should not exceed the TEM's safe operating temperature to prevent device failure. To address these challenges and optimize the RTG for lunar operation, we developed a multi- physics and multi-parametric thermoelectric (TE) network model, which represents the RTG as a series of thermal resistors and TE elements. By solving the heat transfer equation, the temperature difference on all resistors can be calculated, while the TE heat transfer equations on the TEM provide an estimate of the RTG's performance. We then coupled this model with a Genetic Algorithm for rapid design investigations to identify the RTG design which maximizes the RTG's specific power, i.e. electrical power output over system mass, while maintaining safe operating temperatures on the TEM. The optimized RTG design, which utilizes a Bi_2Te_3 TEM, achieves a specific power of 1.42 W/kg, with an electrical power of 13.9 W and a conversion efficiency of 6.9 %. This is a significant improvement over the pre- defined specifications of the European Space Agency (ESA), i.e. power of 10 W with a 5 % conversion efficiency [1]. Our model can further adapt the RTG to incorporate TEM which can operate at higher temperatures, such as Skutterudites or Half-Heusler materials, thus allowing for higher performances.

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This work was supported by the DLR-ESA co-developed LUNA project.

Fabrication of Thermoelectric Devices Based on Colusites

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Keywords: Sulfides, colusites, diffusion barrier, device, thermoelectric conversion efficiency

Copper-based multicomponent sulfides have emerged as promising candidates of p-type thermoelectric (TE) materials, and have been studied extensively over the past decade. However, less effort has been devoted to search interface materials (e.g., diffusion barrier materials) and to fabricate TE devices for the sulfides. Colusites with the general formula $Cu_{26}T_2M_6S_{32}$ (T = Ti, V, Nb, Ta, Cr, Mo, W; M = Ge, Sn, Sb) have attracted attention due to their high TE performances. [1] We have explored interface materials from metals and reported that a single-leg device of $Cu_{26}Nb_2Ge_6S_{32}$ with Au diffusion barrier layers showed low contact resistance at the Au/colusite interface, leading to the TE conversion efficiency of 3.3 % under the temperature difference of $\Delta T \sim 270$ K. [2] In order to reduce the overall cost of TE devices, alternative materials to Au are required. In this study, we examined the potential of Ni-Sb based compounds as interface materials for a sulfur-deficient colusite, $Cu_{26}Ti_2Sb_4Ge_2S_{31.5}$.The powders of $Cu_{26}Ti_2Sb_4Ge_2S_{31.5}$, Ni-Sb based compounds ($NiSb_2$, NiSb, $Ni_{0.9}Co_{0.1}Sb$), and Ni were carefully placed in a WC die to form 5 layers in the order of Ni/Ni-Sb/$Cu_{26}Ti_2Sb_4Ge_2S_{31.5}$/Ni-Sb/Ni, and hot-pressed to fabricate TE devices. The device with $NiSb_2$ was broken while being removed from the die after the sintering, whereas the devices with NiSb and $Ni_{0.9}Co_{0.1}Sb$ were successfully fabricated. The coefficient of volumetric thermal expansion of NiSb is close to that of the colusite, whereas that for $NiSb_2$ is smaller. The well-matched thermal expansion coefficients would have led to the crack-free NiSb/colusite interface. The contact resistivity was ~ 13 mΩ mm² for the NiSb/colusite interface, which was reduced to ~9 mΩ mm² for the $Ni_{0.9}Co_{0.1}Sb$/colusite interface. The latter contact resistivity remained unchanged after a heat treatment at 573 K for 50 h. The device with $Ni_{0.9}Co_{0.1}Sb$ showed a maximum conversion efficiency of 3.2 % under $\Delta T \sim 270$ K.

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This work was financially supported by JSPS KAKENHI (grant no. JP24H00415, JP25K01503) and Thermal and Electric Energy Technology Foundation, and a grant from Research and Development Program for Promoting Innovative Clean Energy Technologies through International Collaboration (grant no. JPNP20005) funded by NEDO.

Digital and scalable laser-based fabrication of reusable bismuth telluride thermoelectrics with superior performance and mechanical flexibility

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Keywords: LPBF, Printing, Bi_2Te_3, Flexible

Thermoelectrics (TEs) are highly promising for powering and managing the thermal demands of wearable electronics and Internet of Things (IoT) devices. However, conventional TEs are limited by their rigid form factors and complex fabrication processes.

In this work, we present a simple, scalable, and recyclable thermoelectric platform using laser powder bed fusion (LPBF) combined with hot-press lamination to produce flexiblemodules. These modules are fabricated by directly printing Bi_2Te_3-based materials onto plastic substrates. We have optimized both p-type and n-type materials to achieve power factors exceeding 1200 $\mu W \cdot m^{-1} \cdot K^{-2}$ and a figure of merit (zT) greater than 0.2.

The resulting devices deliver up to 70 μW of output power at a temperature difference (ΔT) of 40 K for an 8.3 cm^2 footprint and demonstrate active cooling of approximately 3 °C below ambient temperature. Designed for durability and sustainability, the modules can be fully reconditioned after damage from extreme bending or disassembled for reuse.

This work underscores the potential of digitally manufactured, multifunctional flexible TEs for next-generation energy harvesting and thermal management in IoT nodes and wearable electronics.

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This work was supported by the Internal Funds KU Leuven, C1 project C14/21/078 and the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program: grant agreement 948922 – 3DALIGN

Planar Silicon-Based µTEG Test Platform for Evaluating Thermoelectric Materials and Optimizing Thermal Management

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Keywords: Silicide, perovskite, thin film, micro-thermoelectric generator (µTEG)

Waste heat can be converted into useful energy, but mechanical heat engines face miniaturization challenges. Thermoelectric materials offer a solid-state alternative, ideal for self-powered devices in harsh environments, with recent advancements focusing on sustainable, low-toxicity materials [1]. µTEG performance is influenced not only by material properties (zT) but also by device architecture and thermal engineering, which are key to maximizing efficiency by optimizing the temperature difference between hot and cold regions [2,3]. Most efforts in thermoelectrics focus on optimizing material zT, with fewer addressing thermal management at the device and system levels to improve ZT. In this work, we develop a planar silicon-based micro-thermoelectric generator (µTEG) test platform to evaluate various thermoelectric materials in thin-film form under real operating conditions. By integrating a multiscale approach, the platform explores three design scales: material, geometry, and thermal management. The platform features different designs to evaluate the µTEG performance with different geometries. The measurements are made in test mode, where temperature gradients are applied externally through integrated heaters, and in harvesting mode, where realistic operating conditions are applied placing the µTEG on a hotplate and cooling through ambient air. To improve the thermal management and enhance the µTEG performance, we also integrate a heat dissipator on top of the chip to maximize the thermal gradient seen by the µTEG under natural convection and forced convection conditions, resulting in a 100-fold enhancement compared to the bare chip exposed to air. In order to validate the µTEG platform, in this work we have successfully integrated two different materials in thin film form, namely $CrSi_2$ and 6 mol% Nb:STO [4], demonstrating the platform's flexibility for different materials and deposition techniques.

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Acknowledgments

H2020 Programme under Grant Agreement no 824072 (HARVESTORE), Grant PID2022-142003OB-C22 (MCIN /AEI /10.13039/501100011033 / FEDER, UE), the ESF+ through grants RYC2022-038370-I and RYC2022-037016-I, grant 2021 SGR 00497 funded by AGAUR (Generalitat de Catalunya) and ICTS Network MICRO-NANOFABS, partially funded by FEDER funds through MINATEC-PLUS-2 project FICTS2019-02-40.

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PART IV
CONTRIBUTED TALKS

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8TH SESSION
ADVANCED MATERIALS

Cation-deficient Half-Heusler Thermoelectric Materials

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Keywords: Half-Heusler compounds, defects, vacancy order, physical properties

Semiconducting half-Heusler compounds with the valence electron count of 18 have been identified as a class of promising high-temperature thermoelectric materials. Recently, nominal 19-electron half-Heusler compounds, possessing massive intrinsic vacancies at the cation site and intrinsically low lattice thermal conductivity, have gained reacquaintance and popularity due to their unexpected high thermoelectric performance and fascinating defective structure. In this talk, we introduce the current progress of half-Heusler thermoelectric materials and focus on the discovery and challenge of new cation-deficent half-Heusler compounds with the vacancy-related short-range order. The insightful understanding of the defect-tailored thermoelectric and other physical properties are offered.

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This work was supported by the National Key Research and Development Program of China (no. 2024YFA1409200), and the National Natural Science Foundation of China (nos.92163203, U23A20553, 52471239).

New efficient thermoelectric half-Heusler compositions from Machine Learning

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Keywords: Machine learning, DFT, datasets, half-Heuslers

Machine learning (ML) can facilitate the accelerated discovery of efficient thermoelectric (TE) materials from the enormous configurational space of a given structural family. Nevertheless the scarcity of experimental TE datasets limits the application of several conventional ML techniques. Moreover, the lack of data curation in the available datasets poses further challenges in accurate training of ML models. In this work, merging the data from literature and existing datasets, we propose a systematic approach of TE materials dataset creation and curation for a promising class of TE materials (half-Heuslers) as an example. We further show that how using a novel symbolic regression-based ML technique, SISSO (Sure Independent Screening – Sparsifying Operator) physically interpretable descriptors for predicting the TE figure-of-merit, zT can be determined from a small dataset. Lastly, we discuss the performance and high-throughput predictions, for new efficient half-Heusler compositions, of SISSO model with other conventional ML techniques (neural networks, RF, and XGBoost).

Acknowledgments
This work was supported by the French National Research Agency through the ANR-DFG project CombiHeusler.

Heavier element substitution in *p*-type Fe_2VAl Heusler alloy

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Keywords: Full-heusler alloy, mass fluctuation phonon scattering, high power factor

Sensors in industries operate around room temperature and typically require only microwatts of power that can indeed be supplied by a thermoelectric (TE) generator [1,2]. These self-powered sensors are one of the essential building blocks of the Industrial Internet of Things (IOT).[1] Until now, researchers have relied on Bi_2Te_3; however, the costlier and toxic nature of "Te" in Bi_2Te_3 limits mass production and commercialization. In this context, the Fe_2VAl Heusler alloy has attracted attention, due to its cheaper and less toxic chemical elements. On the one hand, the TE properties of *n*-type Fe_2VAl alloy have already been optimized since its power factor ($S^2\sigma$) reaches impressive values larger than 8 mW/mK^2 with a maximum figure of merit (zT) of 0.3 at 300 – 400 K. On the other hand, *p*-type Fe_2VAl is not yet optimized with a lower value of power factor $S^2\sigma$ = 3 mW/mK^2 and a larger lattice thermal conductivity (κ_{lattice}) of 12 W/mK at 300 K, leading to zT = 0.1 [3-6]. We hence strategized to optimize the thermoelectric performance of *p*-type $Fe_{2.04}V_{0.91}(Al_{1-x}Ga_x)_{1.05}$ ($0 \leq x \leq 1$) compositions, by substituting Al by Ga, a heavier and isoelectronic element expected to decrease κ_{lattice} by the mass fluctuation effect. Our synchrotron diffraction study shows for the first time that all the samples of this series crystallize in the fully ordered cubic $L2_1$ structure. Ga substitution has minimal influence on the hole concentration and mobility until x = 0.75 is reached, where the first quantity significantly increases. Additionally, the Seebeck coefficient (S) shows a monotonic decrease with increase in Ga concentration, leading to a $S^2\sigma$ value of 2.8 mW/mK^2 at 300 K for x = 0.5. Interestingly, the κ_{lattice} systematically decreases upon Ga-substitution, from 18.3 W/mK for x = 0 to 6.9 W/mK for x = 0.5 at 300 K. Currently, a maximum zT of 0.1 at 300 K is achieved in *p*-type $Fe_{2.04}V_{0.91}Al_{0.525}Ga_{0.525}$ (x = 0.5), revealing that it can further be optimized for room temperature heat recovery.

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Acknowledgments

This work was supported by Agence Nationale de la Recherche through contract IoTEGH.

Dominance of Coulombic scattering in the power factor on half Heuslers

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Keywords: Scattering rates, Heusler alloys

The electronic and thermoelectric (TE) transport properties of materials are determined by the underlying scattering mechanisms, such as electron-phonon (non-polar and polar) and electron-ionized impurity scattering (IIS). Their strength has implications in understanding a materials' transport properties and in the optimization of its TE properties [1,2,3].
We examine the TE transport properties of 12 half Heusler alloys (HH) for both n-type and p-type. We use an advanced Boltzmann transport solver as implemented in ElecTra [4], which accounts fully for electronic scattering due to all relevant phonon interactions and ionized impurities. We find that the Coulombic interactions POP and IIS, dominate electronic transport, with significantly higher scattering rates than the non-polar interactions (ADP and ODP).
Our analysis reveals that the valence band, characterized by multiple degenerate bands with valleys of different masses at the same high-symmetry point and flattened bands deeper inside the valence band, renders holes more susceptible to POP scattering. We demonstrate that the combined effects of POP and IIS determine the power factor (PF) of the HHs examined, accounting for approximately 67% of the PF for electrons and over 80% for holes. Consequently, we show that n-type materials would outperform their p-type counterparts by around 30%, with average room-temperature power factors peaking at 6.28 mW/mK^2 for n-type carriers and 4.45 mW/mK^2 for p-type carriers for the 12 HHs we examined.
This study highlights the crucial role of Coulombic scattering processes in shaping the TE properties of HHs and provides valuable insights into electronic transport, applicable to other materials with complex band structures. Our results suggest that the relatively inexpensive calculations of POP and IIS scattering can offer a reliable first-order estimate of the power factor, while the more computationally demanding non-polar contributions, (which require ab initio density dunctional perturbation theory treatment), may be of secondary importance.

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Acknowledgments

This work has received funding from the UK Research and Innovation fund (EP/X02346X/1).

Plastic deformation mechanism of single-crystal thermoelectric materials

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Keywords: Thermoelectric materials, Single crystal, Plastic deformation mechanism

Elucidating the fundamental microscopic mechanisms governing plastic deformation is crucial for the rational design of functional materials with desired mechanical properties. Such understanding not only can provide new insights into the interplay between chemical bonding and dislocation dynamics in non-metallic materials but also establish a material design paradigm for discovering novel functional materials with tailored mechanical-electronic properties. Herein, we have investigated the deformation process of common single-crystal thermoelectric materials at different scales and identified the types of slip systems and dislocations that significantly improve plasticity. In addition, the underlying atomistic origin of the plastic behavior of this class of compounds is further revealed through molecular dynamics simulations.

Acknowledgments
This work was supported by the National Natural Science Foundation of China for Distinguished Young Scholars (52425108). J.M. acknowledges the financial support from the National Natural Science Foundation of China (52473298), and the Shenzhen Science and Technology Program (RCJC20221008092725020). Q.Z. acknowledges the financial support from the National Natural Science Foundation of China (52172194), and the Shenzhen Science and Technology Program (RCJC20210609103733073, JCYJ20241202123659001). Y.H.F. acknowledges the financial support from the National Natural Science Foundation of China (62474081, 22090044). F.C. acknowledges the financial support from the National Natural Science Foundation of China (52472196). The authors are sincerely grateful to Guisen Chen for his assistance in the TEM characterization and analysis.

Prefer-oriented Ag_2Se crystal for high-performance thermoelectric cooling

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Keywords: Ag_2Se thermoelectrics, Room-temperature performance, Phase transition challenge, High carrier mobility, Cooling device integration

Ag_2Se-based materials with promising room-temperature thermoelectric performance have been known for decades. However, thermoelectric cooling devices based on bulk Ag_2Se have seldom been reported, mainly due to the phase transition around 400 K poses a grand challenge for leg design and module integration. Herein, Ag_2Se crystals with the preferred orientation have been prepared. A high carrier mobility of ~1846 $cm^2V^{-1}s^{-1}$ and a power factor of ~31.2 $\mu W\ cm^{-1}\ K^{-2}$ at room temperature has been realized, and results in a zT of ~0.95 at 300 K. Importantly, by applying Ag as the contact layer, the $Ag/Ag_2Se/Ag$ joint has been prepared by one-step sintering. By maintaining the pressure of ~10 MPa after sintering and during the reflow soldering, the deleterious effect of the large thermal expansion can be alleviated. The contact resistance of the Ag/Ag_2Se interface is as low as ~2.9 $\mu\Omega\ cm^2$, indicating negligible electrical parasitic loss. The thermoelectric device with 7 pairs of Ag_2Se and $(Bi,Sb)_2Te_3$ has been fabricated and it can achieve a maximum cooling power of ~2.90 W and a cooling temperature difference of ~70.4 K at the hot-side temperature of 350 K, demonstrating the great potential of Ag_2Se for cooling applications.

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PART IV
CONTRIBUTED TALKS

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9TH SESSION
EMERGING MATERIALS I

Direct electron cooling at millikelvin temperatures with quantum-well heat pump

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Keywords: Cryogenic heat pump, electron refrigeration, quantum well

To extend the performance of dilution refrigerators below millikelvin temperatures, a cryogenic solid-state heat pump is proposed [1] that expands the phase space of a two-dimensional electron system (2DES) from one to multiple subbands to generate cooling power in the sub-Kelvin range. By electrostatically "expanding" electrons to higher subband degeneracy and "compressesing" to lower degeneracy in an Otto cycle, we propose that a stack of ultra-wide 150 nm GaAs quantum wells filling a 1 cm^3 volume can be operated as a cryogenic heat pump with $T_H = T_C = 100$ mK, to actively pump $\dot{Q} = 100$ μW of heat out of the electrons into the bath. Piggy-backed onto dilution refrigerators, it could cool from base temperature on the hot side $T_H = T_{base}$ to $T_C = T_{base}/4$ to cool quantum computers and infrared detectors. The T^3 suppression of phonon specific heat is exploited to suppress phonon thermal conductivity at cryogenic temperatures until the T-linear electron heat capacity dominates. In this low-temperature limit, electrons in a quantum well can serve a working fluid. A central wide quantum well biased *asymmetrically* to low single-subband degeneracy $g_1 = 1$, can then be biased *symmetrically* to a high multi-subband degeneracy $g_2 = 4$. Each adiabatic cooling cycle can therefore reduce the electron temperature by as much as a factor of $g_1/g_4 = 1/4$. This central reservoir is isolated laterally via narrow electrostatic heat-switch depletion gates.To achieve efficient cooling, the Otto cycle is chosen, comprised of adiabatic expansion and compression cycles alternating with isochoric heat transfer from the cold and hot leads, respectively, via the heat-switch gates. Whereas a single-shot mechanism for electron cooling had been previously proposed [2], here, a continuous cyclic operation is studied. Potential heat loss mechanisms are considered, including heat loss through the electrical leads, ohmic heating of electron currents under heat-switch depletion, phonon backflow, and electron-phonon coupling. The quantum-well heat pump would operate at sub-millikelvin temperatures with 20 MHz – 1 GHz pump frequencies. The resulting heat pumped is 1 μW/cm^2 per quantum well area, or, assuming 100 layers of 0.1 mm thick substrate, 100 μW/cm^3 of stacked quantum wells. This refrigeration mechanism overcomes a significant thermal bottleneck by cooling the electrons, themselves, which in a standard dilution refrigerator would otherwise couple through phonons, with coupling suppressed as T^5. Initial experimental characterization of subband degeneracy in GaAs quantum wells will be shown.

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Acknowledgments

US DoE, SQMS Center, contract No. DE-AC02-07CH11359 and NSF DMR-1720139.

Transverse thermoelectric effect in WSi_2 with/without magnetic field

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Keywords: Transverse thermoelectric effect, axis-dependent conduction polarity, semimetal

Transverse thermoelectric (TTE) effect, which generates an electromotive force perpendicular to a temperature gradient, has attracted much attention as an application to the flexible thermoelectric devices [1]. To realize efficient TTE conversion in single crystals, it is essential to enhance the off-diagonal component of Seebeck tensor.

WSi_2 is a compensated semimetal characterized by anisotropic Fermi surfaces and large carrier mobility. Owing to its unique electronic structure, this material exhibits axis-dependent conduction polarity (ADCP) of thermopower and extremely large magnetoresistance [2,3]. In this presentation, we will introduce TTE conversion based on this material under two different mechanisms.

In the absence of a magnetic field, thermopower along the *a*-axis is positive, whereas it is negative along *c*-axis [2,4]. By applying the temperature gradient between *a*- and *c*-axis directions, we directly measured a transverse thermopower of $S_{yx} = 6$ μV/K [4]. On the other hand, WSi_2 exhibits large Nernst effect under an magnetic field, which two order of magnitude larger than transverse thermopower observed due to the ADCP. To elucidate the origin of the TTE conversion via these distinct mechanisms, we also conducted first-principles calculations and found that the Fermi velocities of hole and electron bands are highly anisotropic due to the dimensional characteristics of the Fermi surfaces. We will discuss band-resolved carrier concentration, mobility, and thermopower to better understand the semimetallic characteristics of this material.

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Acknowledgments

This work was supported by the Japan Society for the Promotion of Science (JSPS) KAKENHI via Grants No. 22K20360, No. 22H01166, and No. 24K06945, and the Research Foundation for the Electrotechnology of Chubu (REFEC) via Grant No. R-04102.

Thermoelectric properties of kagome metals Ni_3Sn and $Ni_{3-x}Co_xSn$

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Keywords: Kagome lattice, flat band, strong electronic correlation

In the kagome lattice with geometrical frustration, fermions are allowed only nearest-neighbor hopping, resulting in perfect destructive quantum interference and thus forming flat bands that do not exhibit dispersion in momentum space [1]. Recently, the existence of flat bands in kagome lattices has been experimentally confirmed, and the high density of states and strong electronic correlations of flat bands have attracted much attention as they are expected to represent novel physical properties [2,3]. In systems where the Fermi surface reaches the band edge, large Seebeck coefficients are expected and await experimental verification [4]. Ni_3In belongs to the space group $P6_3/mmc$, where the Ni kagome network surrounds the In atoms in hexagonal voids [5]. Density functional theory calculations suggest the existence of a flat band with a bandwidth of ~60 meV and a high density of states in the Γ-M-K-Γ plane at the Fermi energy, as well as a highly dispersive Dirac-like bands near the Fermi energy [6,7]. The isostructural Ni_3Sn is predicted to shift to approximately 0.25 eV higher energy with a similar electronic structure. However, the detailed transport phenomena in these system have not yet been clarified. In order to clarify the transport phenomena in the system with both flat and Dirac bands, we performed transport measurements on Ni_3Sn and its Co-substituted system. Polycrystalline samples were successfully prepared by the solid-state reaction method. Ni_3Sn exhibits a negative Seebeck coefficient and a metallic behavior at low temperatures. In $Ni_{3-x}Co_xSn$, the negative Seebeck coefficient shows an expansion with the amount of substitution. To analyze based on the band structure, we have calculated the band structure and also the transport coefficients based on the Boltzmann equation with the relaxation time approximation. The detailed results and analyses will be shown in the presentation.

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This work was supported by the Japan Society for the Promotion of Science (JSPS) KAKENHI Grants No. 24K06945.

Decoupling electrical and thermal properties in $Ca_{12}Al_{14}O_{33-\delta}$ ceramics

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Keywords: Electride, mayenite, ceramics, decoupling properties, neutron diffraction

The mineral and Earth-abundant oxide, "mayenite," characterized by the chemical composition $Ca_{12}Al_{14}O_{33}$, traditionally finds application as a component in commercial cement and has more recently gained attention as an electronic material under specific processing conditions [1]. The crystal structure features a positively charged framework represented by $[Ca_{24}Al_{28}O_{64}]^{4+}$, with cages accommodating O^{2-} oxygen ions. The structure adopts a cubic arrangement within the space group I4-3d, with 12 cages per unit cell, two of which randomly host oxide ions to charge balance the positive framework. This unique clathrate-like structure permits the substitution of extra-framework oxide ions with electrons, resulting in reduction and the formation of a mayenite electride, $Ca_{12}Al_{14}O_{33-\delta}$ ($\delta \leq 1.0$), transforming the material from insulating into a metallic or semiconducting state [2]. Furthermore, mayenite exhibits a 'glass-like' lattice thermal conductivity [3].

In this work, we explore two approaches for tuning the electrical properties of mayenite: (1) graphene compositing and (2) Spark Plasma Sintering (SPS) sintering. Neutron powder diffraction data confirm the formation of mayenite electride, with a maximum reduction level identified as $Ca_{12}Al_{14}O_{32.40(5)}$ ($\delta = 0.6$) for the composite with 2.0 wt.% graphene. EPR and Raman spectroscopy reveal the presence of a fraction of superoxide (O^{2-}) anions within the mayenite cages that persist in the reduced phases. The introduction of graphene leads to a change in dominant charge carriers, from p-type to n-type behavior. The composite material demonstrates an impressive reduction of up to 13 orders of magnitude in electrical resistivity decreasing from 1011 Ω m for thermally sintered $Ca_{12}Al_{14}O_{33}$ to 10-2 Ω m for the $Ca_{12}Al_{14}O_{32.40(5)}$ + 3.0 wt.% graphene composite at room temperature. Meanwhile, the already low thermal conductivity undergoes minimal change, ranging from 2.5 to 4.0 W m^{-1} K^{-1} at the same temperature. Compositing of mayenite with graphene leads to effective decoupling of electrical and thermal transport properties. Such a strategy may find applicability in other functional ceramics, particularly high-efficiency thermoelectric materials.

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This work was supported by the Spanish MICINU/AEI/10.13039/501100011033, by "European Union Next Generation EU/PRTR" (R+D+i projects TED2021-129569A-I00 and CNS2022-135302).

Thermoelectric Potential of Te-Free Diamond-Like $Cu_{2-x}Ag_xIn_2Se_4$ Chalcopyrites: Low Thermal Conductivity and High Carrier Mobility

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Keywords: Thermoelectric, diamond-like, synchrotron XRD, high-carrier mobility

Diamond-like ternary I-III-VI_2 chalcopyrite materials are wide gap semiconductors exhibiting high Seebeck coefficients and carrier mobilities [1,2]. $Cu_{2-x}Ag_xIn_2Se_4$ (x = 0.0-0.3) derivatives are investigated as promising Te-free thermoelectric materials, combining low thermal conductivity with enhanced tunable electronic transport. Structural analysis *via* synchrotron X-ray diffraction reveals the unit cell expansion and lattice disorder at Cu/Ag crystallographic position by atomic displacement parameter analysis. This behavior is attributed to tetrahedral off-centering distortions that promote strong phonon scattering upon Ag alloying. Thermoelectric characterization shows a significant increase in Seebeck coefficient and high carrier mobilities (up to 400 $cm^2\ V^{-1}\ s^{-1}$), and decreasing carrier concentrations due to the hole introduction by Ag substitution of Cu atoms. In addition, this substitution promotes a reduction of the lattice thermal conductivity, yielding values as low as 1.3 $W\ m^{-1}\ K^{-1}$ at 748 K.

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This work is partially financed by the MCIN/AEI/10.13039/501100011033/ and by the "European Union NextGenerationEU/PRTR".

Frustrated vacancy order in diamagnetic metal Kutinaite $Ag_6Cu_{14.4}As_7$

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Keywords: Kutinaite, frustrated vacancy ordering, Cu sublattice, diamagnetic metal

Ideal crystals are fully ordered, but real-world crystals always contain defects breaking translational symmetry. Random defects are essential e.g. for the properties of semiconductor devices, but defects may also be structurally correlated thereby creating novel materials with emergent properties. The additional level of complexity induced by correlated disorder on the chemistry and physics of solids has initiated new frontiers in solid-state science. Here, we discovered that the defect structure of the mineral Kutinaite, $Ag_6Cu_{14.4}As_7$, exhibits unprecedented metallic diamagnetism, a hallmark of non-trivial electronic states that require delicate symmetrical protection. Using a combination of X-ray scattering methodologies, simulations, and physical property measurements, we deduced and verified subtle frustrated vacancy ordering beginning at the 5th nearest vacancy-neighbor of the Cu2 sublattice when cooling crystals below ~300 K. The defect structure of Kutinaite has unique properties, and our study calls for a reconsideration of the role of vacancies as quasi-chemical species in crystals.

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Acknowledgments

This work was supported by the Villum Foundation (25861) and the Danish Center for Synchrotron and Neutron Research (Danscatt).

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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10TH SESSION

HOW TO TAKE TE TO THE MARKET BY ACADEMIA-INDUSTRY COLLABORATION?

Bridging Nanoscale Thermoelectrics and Triboelectrics: From Lab-Scale Innovations to Prototypes

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Keywords: Thermoelectrics, nanoscale, devices, IoT

Our research at the FINDER group advances nanostructured thermoelectric materials and devices to harness low-grade heat for energy recovery, while exploring emerging triboelectric systems to harvest also mechanical energy. By tailoring nanoscale architectures in bismuth telluride-based composites and alumina-based or Cu-Ni metamaterials we have been able to excel the values of the bulk materials. While, we have achieved record thermoelectric figures of merit ($zT > 1.2$ at 300 K) in flexible AgSe unileg thin film devices or $SnSe/Sn_2Se$ p/n junction devices, enabling efficient heat-to-electricity conversion in wearable medical sensors and IoT nodes. Prototypes developed in collaboration with automotive partners demonstrate an average efficiency in recovering waste heat from exhaust systems, validated through field trials under dynamic thermal gradients.
Our fabrication methods always rely on scalable to industry techniques, such as electrochemical deposition or a pre-industrial sputtering system to facilitate the transition from lab-scale thermoelectric modules (e.g., few cm^2 devices generating ~10 mW) to industrial production.
By aligning fundamental research with industry-driven design criteria, we aim to deliver scalable solutions for energy autonomy in sectors ranging from smart manufacturing to personalized healthcare.

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Acknowledgments

This work was supported by ERC Adv. Grant POWERbyU.

Driving thermoelectric innovation through research-industry collaboration

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Keywords: Mineral-based TE materials, sustainable materials development

The urgent need for sustainable energy solutions has intensified interest in thermoelectric (TE) technologies, which can convert waste heat into electricity and contribute to decarbonization across multiple sectors. Despite significant scientific advancements, the commercialization of TE systems remains limited, hindered by material costs, supply chain issues, and a gap between research outputs and industrial needs. The START project (https://www.start-heproject.com/) addresses these challenges by bringing together a multidisciplinary consortium of research institutions and industrial partners to collaboratively drive innovation in sustainable TE materials and systems.

START focuses on the development of cost-effective and environmentally friendly TE materials derived from mine waste, specifically the tetrahedrite mineral series. By targeting materials that are abundant, non-toxic, and compatible with circular economy principles, START provides an alternative to conventional TE materials that rely on scarce and geopolitically sensitive elements such as tellurium. Additionally, the project engages with European policy frameworks related to raw materials independence and green innovation, underscoring the broader societal and regulatory relevance of the work.

This presentation will outline the project's key activities and outcomes, highlighting the methodologies employed, challenges addressed, and tangible benefits achieved. A strong focus has been placed on aligning scientific development with the practical requirements of industry partners, ensuring that the resulting technologies are not only innovative but scalable, economically viable, and policy-aligned. The presentation aims to inform and connect stakeholders from both research and industry, fostering a shared vision for the future of TE technology.

Acknowledgments
This work was funded by the Horizon Europe START project (project number: 101058632), co-funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Health and Digital Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

Needs and Challenges in Re-shaping TEG Supply-Chain in EU

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Keywords: Resillient Supply-chain, robust manufacturing, critical materials

The commericalization of thermoelectrics, especially for thermoelectric power generation (TEG), has staggered for decades. Despite the efforts on searching new materials, optimizing production precedures and exploring noval applications, TEG modules remain alomst unchanged, since NASA has firstly exploited them in the deep space probes (Voyagers 1 and 2) in the 1970s [1]. Moreover, the recent geopolitical confilects and reshaping in the global supply chain has led to an astonishing 3-fold increase on the market price of the TEG modules in Europe [2]. It will undoubtedly bring more challenge and uncertainty on the future development of TEG.

Fortunately, EU has made strategic decisions on improving its resilience on critical raw materials and on strengthening its manufacturing capabilities [3]. It has also set ambitious goals in accelerating green manufacturing and forstering sovereignty and competitiveness of European manufacturing sectors [4]. The author want to make an appeal to the thermoelectric society to re-think thermoelectrics applications and re-shape its supply chain together.

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Acknowledgments

This work was supported by the Horizion Europe project START (101058632, HORIZON-IA HORIZON-CL4-2021-RESILIENCE-01), M-ear.net project THERMOS (9225) and Horizon 2020 project iClimabuilt (210659194, DT-NMBP-05-2020). The author also ackowledge the financial support from Innovationfund Denmark (IFD).

Thermoelectric Modules and Applications: An Industrial Perspective

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Keywords: Thermoelectric modules, generators, combined heat and power, RTG

Since 2014, RGS Development has specialized in silicon-germanium (SiGe) production, employing scalable techniques like ribbon growth, ingot casting, and ball milling. Proficient in simulating heat interfaces, RGS customizes thermoelectric generator (TEG) devices for optimal power generation. The company introduced a modular Thermagy architecture, all-SiGe based, with patented interconnection technology, subjected to rigorous testing, including over 10.000 hours of continuous heat flow and thermal cycling up to 1000°C. Through development and prototyping, RGS has honed expertise in COMSOL simulations, thermo-mechanical and interface engineering, device aging, and testing. This positions the company to provide TEG solutions for both single-stage and cascaded device architectures, tailored to various source temperatures and heat flux densities. Recent estimates reveal that industrial processes contribute to 26% of European primary energy consumption and 48% of final CO_2 emissions, with nearly 300 TWh/year deemed recoverable. Additionally, heating and cooling constitute half of the EU's energy supply, primarily from collective infrastructure or solid/liquid fuels like biomass. Analyzing trends from 1990 to 2015, biomass's primary energy supply has doubled to approximately 570 TWh. Capitalizing on this market demand, RGS has embarked on significant projects, focusing on power generation through waste heat recovery in heavy industries (Tata Steel, Elkem, ArcelorMittal) and combined heat and power (CHP) generation for homes. These experiences emphasize the necessity for thermoelectric generator (TEG) devices capable of handling various temperature zones. In response, RGS is developing advanced nanostructured SiGe materials with high ZT values [1] for high-temperature applications and telluride-free thermoelectric modules for the low to mid-temperature ranges. [2] Furthermore, with cascading these modules RGS aims to develop a hybrid TEG-TIG solution to solve the intermittency problem of renewable energy via thermal batteries. [3] RGS's expertise in SiGe is also proving to be invaluable for the development of radioisotope power systems (RPS) in outer space. NASA's current flight-qualified system, the Multi-Mission Radioisotope Thermoelectric Generator (MMRTG), outputs around 120 watts. The upcoming Next Generation Radioisotope Thermoelectric Generator (NGRTG) is anticipated to produce 250-270 watts. Recognizing a need for low-power generators below 100 watts, RGS Development and UDRI conducted a concept study exploring the feasibility of a low-power RPS using a single General Purpose Heat Source (GPHS) and the modular Thermagy TEG. [4]

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How to Transfer Thermoelectric Technology from Academia to Industry? The Case of Thermo Power Systems

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Keywords: Sustainable thermoelectrics, technology transfer, tndustrialisation

The European scientific community focused on thermoelectrics is highly active, driving key advancements in knowledge. However, the transition from academic research to industrial applications remains limited. Most private companies in this field are start-ups or SMEs that face significant challenges not only in scaling up thermoelectric technology but also in bridging the gap between academia and industry - a crucial yet complex step in a niche sector that demands substantial production infrastructure.

Recently, Thermo Power Systems has begun industrializing a sustainable thermoelectric technology developed at UCLouvain (Belgium) over the past decade [1-4]. This contribution highlights the key factors enabling a successful technology transfer: (i) an innovative funding strategy involving collaboration with a climate-tech start-up studio, (ii) a strong partnership with academia through licensing and lab access agreements, (iii) vertical integration from raw material processing to thermoelectric system manufacturing, and (iv) a technology designed from the outset for sustainability, scalability, and cost efficiency. These elements have enabled thermoelectric technology to move beyond the lab.

Finally, we present several prototypes of thermoelectric waste heat recovery systems successfully installed and operating in real industrial environments.

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Durable and sustainable thermoelectric devices made from zinc and magnesium-antimony alloys

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Keywords: Sustainable TE materials, thermoelectric modules, atomic layer deposition, solid state cooling, metal oxide encapsulation

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 $Mg_3(Sb,Bi)_2$ 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 HfO_2, 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 Bi_2Te_3. 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]. In a further attempt, we have coated the grains of BiSb and ZnSb powders with ALD of metal oxides. This powder based ALD coatings lead to a significant enhancement of the thermal stability of these materials and for device applications and suppresses in the case of ZnSb die formation of Zn whiskers.

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Acknowledgments

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

Towards industrial production of high-temperature thermoelectric modules

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Keywords: thermoelectric module, module production, up scaling thermoelectrics

Spite the progress in the field of thermoelectrics (TE), the market is still dominated by the traditional Bi_2Te_3-based TE modules which are produced by small number of companies located mainly in Asia or in the USA. Several companies tried to produce TE modules based in new materials, bulk nanostructured materials, or with new designs. Unfourtnately, most of the new companies have not succeed in entering to the market and disappeared or are struggling to survive. One reason for such unsuccesfull development are the high risks innerents in a new complex and multidisciplinary production line. In this contribution we present the progress of a running project ProTEM, where we develop an automated chain for the production of TE Modules. We took Mg- and Mn-silicides as materials for the production line but it could be easily adapted for other type of bulk TE-Materials. The consortium is formed by six industrial partners and two research institutions. In order to minimize the risks of the industrial partners, the production chain was divided in five fields: productions of starting powder mixtures, synthesis and compaction, dicing into wafers and TE-legs, coating with diffusion barriers, brazing and assembling of components. Involving specialized industrial partners in each step enables the production of TE-Modules in large scale. We succeed in producing 1 Kg of starting powder materials per batch, in sintering TE-blocks of diameter of 6 – 8 cm with a heigh of 3 cm, we raised the productivity of processing the blocks into TE legs in a factor 100 by using industrial multi-wire dicing and avoiding slow and low-productivity lapping process. Moreover, we develop diffusion barriers which can be applied fast and in large scale to the wafers by PVD. The assembling of TEM takes place by using pick-and-place systems.

Acknowledgments
This project is founded by the German Federal Ministry for Economic Affairs and Climate Action under the grant 03EN4040A.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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11TH SESSION
CHALCOGENIDES I

The devil is in the detail(s): How to get the synthesis of high performance MgAgSb right?

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Keywords: MgAgSb, thermoelectric material, composition-processing-microstructure-property relationship, phase purity, sensitivity analysis, nanostructure, transport analysis

A thorough understanding and optimization of microstructure are key to enhancing transport properties in thermoelectric (TE) materials. By combining high-resolution microstructural analysis with local and integral transport property measurements of a set of ~50 samples with varying composition and synthesis conditions, we establish an interrelation between the phase constitution and the thermoelectric properties of MgAgSb, a promising p-type TE material near and above room temperature. The samples were synthesized by a combination of ball milling and high-temperature pressure-assisted annealing steps, with MgAg as a precursor for the MgAgSb synthesis. Scanning transmission electron microscopy with energy-dispersive X-ray spectroscopy combined with Selected Area Electron Diffraction was employed for unambigious identification of secondary phases and revealed that those form not only according to the global off-stoichiometry with respect to the MgAgSb single phase but also due to local fluctuations in compositional balance. We deduce several reaction chains that are competing with the intended MgAgSb formation. These reactions may be initiated by remnants of the constituent elements of the initial synthesis steps or local compositional variations in the precursor MgAg, which has a wide homogeneity range. Further analysis using spatially resolved Seebeck microprobe measurements combined with correlating secondary phase type and amount with effective weighted mobility of composite samples containing secondary phases showed that a decrease in weighted mobility can be understood as an overlay of a classical mixing effect and a grain boundary phase effect. Equipped with an understanding on how the secondary phases in MgAgSb are formed and a quantitative assessment of their respective impact on the thermoelectric performance of MgAgSb, we show that fine-tuning the composition of MgAg and its homogenization before the final reaction step with Sb are crucial to reduce the secondary phase content in MgAgSb and with this reproducibly achieve its performance at $zT_{max} \geq 1.3$.

Acknowledgments
This work is supported by the LUNA project, Spaceship EAC and inspired by the Wieder line.

Crystal structure and thermoelectric properties of $Cu_{30}Ti_6Sb_2S_{32}$ and Cu_7VSnS_8: New phases discovered with the pseudo-binary approach

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Keywords: Sulfide, crystal structure, X-ray diffraction, DFT calculations

Copper-based sulfides with sphalerite-derivative structures have received attention due to their potential as thermoelectric materials [1-4]. Recently, we proposed a strategy to design Cu-S-based quaternary compounds, "the pseudo-binary approach" [5]. This new approach led us to discover $Cu_{30}Ti_6Sb_2S_{32}$ [5] within the "Cu_3SbS_4"-"Cu_4TiS_4" system (i.e. $Cu_{3+x}Sb_{1-x}Ti_xS_4$, x = 0.75) and Cu_7VSnS_8 [6] within the "Cu_3SnS_4"-"Cu_4VS_4" system (i.e. $Cu_{3+x}Sn_{1-x}V_xS_4$, x = 0.5). $Cu_{30}Ti_6Sb_2S_{32}$ crystallizes in a colusite-like cubic structure of space group characterized by "interstitial" Ti atoms forming tetrahedral-octahedral $[TiS_4]Cu_6$ complexes linearly arranged in an original way within the Cu-S corner-sharing matrix [5]. Cu_7VSnS_8 crystallizes in a tetragonal sphalerite derivative structure with space group , where the tetrahedral-octahedral $[VS_4]Cu_6$ complexes also form one-dimensional chains within the Cu-S corner-sharing matrix but oriented only along the c-axis [6]. Despite different crystal structures, both phases are characterized by a semiconducting behavior and low thermal conductivity. In this presentation, I will discuss on the crystal structures and the relationships with the electronic structure and vibrational properties of these new quaternary copper-based sulfides, investigated by the combination of experiments and first-principles calculations. These results demonstrate that the pseudo-binary approach is a fruitful direction for the discovery of new copper-based sulfides with tunable transport properties.

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Defect controlled thermal and electric properties of single crystalline Bi_2O_2Se

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Keywords: Bi_2O_2Se, thermal transport, charge carrier mobility, native defects

Bismuth oxyselenide Bi_2O_2Se represents a typical example of a material demonstrating that defect chemistry represents one of the key factors determining its thermoelectric potential [1]. Native defects based on growth conditions are projected both to crystalochemical crystal perfection, material morphology and define its electrical properties. To address this issue, we present a complex experimental and theoretical study of single crystalline Bi_2O_2Se including thermal, magnetotransport and magneto-spectroscopic data down to cryogenic temperatures. Here, namely, the thermal and thermoelectric properties of our crystal exhibiting the low temperature maximum of thermal conductivity at 8 K of 57 $Wm^{-1}K^{-1}$ and thermoelectric phonon-drag peak of -220 μVK^{-1} confirm independently its high quality [2]. Cyclotron resonance probed with circularly polarized THz radiation revealed an effective mass of electron-like charge carriers of ~0.1 m_e which corroborates ~0.13 m_e determined by SdH oscillations. The thermal properties are analysed and explained using phonon spectra calculated from first principles, the respective roles of stacking faults/dislocations in low temperature thermal conductivity and anharmonicity influencing heat capacity are also evidenced. Electric and magnetoelectric transport data are supported by theoretical calculations of electronic structure and, importantly, by calculations of native defect formation energy. In this respect it seems evident that as the least energy-demanding form of native defect represent the oxygen atoms in Se positions (O_{Se}) and selenium-vacancies (V_{Se}), both creating the important perturbation of 2D selenium layer, most likely highly mobile electrons in the Bi_2O_2 double layers are responsible for extremely large mobilities achieved at low temperatures in this phase. Finally, another plausible point defect represented by selenium atoms in Bi positions (Se_{Bi} antisites) is probably reflected in a more pronounced change in the electronic structure and is characterized by the phenomenon called "midgaps" states.

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Authors would like to 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).

High thermoelectric performance in novel Cu-based chalcogenide with Cr_3Si-type structure

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Keywords: Copper chalcogenides, crystal structure, phase transitions, ultralow thermal conductivity, energy conversion efficiency

Copper-based chalcogenides are promising thermoelectric materials due to their cost-effectiveness, environmental friendliness, and excellent transport properties. However, conventional binary Cu_2X (X = S, Se, Te) chalcogenides undergo superionic phase transitions above room temperature, leading to microstructural evolution and unstable transport properties, which hinder their practical application. In this work, we report a new γ-phase $Cu_{6+\delta}Te_{3-x}S_{1+x}$ with a Cr_3Si-type structure (space group *I-43d*), which exhibits remarkable thermal stability and does not undergo phase transitions over a broad temperature range. Unlike most Cu-based chalcogenides, the γ-phase demonstrates also excellent repeatability of transport properties. By introducing an appropriate excess of Cu, an optimal carrier concentration is achieved, and by adjusting the Te/S ratio, a favourable energy bandgap (E_g) is obtained in $Cu_{6+\delta}Te_{3-x}S_{1+x}$ ($0 \leq x \leq 1$, $0 \leq \delta \leq 0.7$) narrow bandgap semiconductor. The simultaneous use of both factors enhances charge carrier mobility in comparison to the reported metallic Cu_6Te_3S leading to the improved thermoelectric power factors (PFs). The discovered $Cu_{6+\delta}Te_{3-x}S_{1+x}$ materials possess one of the lowest lattice thermal conductivity ($\kappa_L \approx 0.2$-0.25 $Wm^{-1}K^{-1}$ at 300 K), due to the strong bonding inhomogeneity accommodated in large unit cells. Due to the enhanced PFs and ultralow κ_L, $Cu_{6+\delta}Te_{3-x}S_{1+x}$ materials achieve very high $zT > 1.3$ at 500 K, making it a new candidate for the development of medium-temperature thermoelectric converters. With further carrier concentration tuning, these materials could also be explored for cooling applications, expanding their potential in thermoelectric energy conversion.

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The research was funded by the PRELUDIUM-21/2022/45/N/ST5/02070 and “OPUS-26” UMO-2023/51/B/ST11/00329 grants financed by the National Science Center (Poland). O.C. also acknowledges support from the program "Excellence Initiative - Research University" for the AGH University of Krakow, Action 4, ID 12491.

Crystal structure and transport properties of $Cu_{2-x}Ag_xSn_{1-y}Ga_ySe_3$

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Keywords: Chalcogenide, Cu_2SnSe_3, chemical potential, effective mass, lattice symmetry

Cu_2SnSe_3 is theoretically and experimentally investigated as potentially promising thermoelectric material due to its intrinsic low lattice thermal conductivity, complex crystal structure, and tunable transport properties [1]. Optimizing the charge carrier concentration by shifting the lightly-doped p-type semiconducting behavior of Cu_2SnSe_3 towards a more heavily-doped character is an obvious route for enhancing the thermoelectric properties of this compound. An evident candidate for a p-type dopant is Ga, since it has one fewer valence electron than Sn [2,3]. While acting as an acceptor impurity, Ga could also lead to lattice symmetry enhancement and to improved power factor values through enhanced density of states effective masses, likely due to a greater number of valleys [3]. In this presentation, we will discuss how the interplay between crystal structure and transport behavior through Ga alloying can influence the electronic properties of Cu_2SnSe_3. The use of Ag for further optimization of the thermoelectric performance by reducing the lattice thermal conductivity through mass and strain field fluctuation effects will also be investigated.

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PART IV
CONTRIBUTED TALKS

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12TH SESSION
OXIDES

Oxide thermoelectric materials – Challenges and opportunities

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Keywords: Oxide thermoelectrics, synthesis, Seebeck coefficient, thermal conductivity

BiCuSeO oxy-chalcogenides are considered promising thermoelectric materials due to high Seebeck coefficient values combined with intrinsically low thermal conductivity. BiCuSeO showcases properties of a semiconductor and possess low electrical conductivity values. The present work determines the optimal synthesis route for synthesizing pristine BiCuSeO. To analyze the effectiveness of chosen route, further exploration of BiCuSeO based materials for optimum thermoelectric performance was carried out. The phase analysis of the samples were carried out using XRD and morphology was studied using FESEM. The samples were then characterised for their transport properties. The mechanical properties were determined to ensure that enhanced thermoelectric performance is not adversely affecting the mechanical robustness.

Acknowledgments
K.T. thanks funding support from Indo-German Technology Centre WISER Grant (IGSTC/WISER2023/KT/34/2023-24) and ASEAN grant (CRD/2022/000565). Additional funding from Science and Engineering Research Board (SERB) SIRE fellowship grant (SIR/2022/000958) is also acknowledged by K.T. CSIR – National Physical Laboratory for research facilities. R.Y. acknowledges the fellowship support from CSIR.

Spark Plasma Sintering: an efficient tool for thermoelectric oxides

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Keywords: Oxides, SPS, n-type thermoelectrics

The carbon die and punches of Spark Plasma Sintering (SPS) impose the use of a reducing atmosphere during the synthesis, which affects the material's functional properties. This reducing atmosphere could be an opportunity for thermoelectric oxides. Indeed, only a handful of studies are focused on ferroelectrics because they are electrically insulating. However, their reduced form can be promising thermoelectric oxides [1]. In the case of $K_{0.5}Na_{0.5}NbO_3$, SPS sintering induces the appearance of oxygen vacancies and carbon contamination, leading to an electrical conductivity of the order of 10 S/m at room temperature and a ZT of 0.01 at 1000 K [2]. The SPS sintering of $Sr_xBa_{1-x}Nb_2O_6$ (x = 0.25, 0.5 and 0.6) a well-known ferroelectric tungsten bronze, allows to avoid anomalous grain growth during sintering and an electrical conductivity of 4000 S/m is reached at 400 K and a ZT close to 0.15 at 1000 K [3]. Insulators are often doped in order to become semiconducting as La-substituted $SrTiO_3$. However the thermoelectric properties require long term annealing at 1400°C under Ar/H_2 after sintering. SPS sintering of this material directly achieves relative densities of 99% at 1200°C, with a power factor of 0.2 mW/mK² at 50°C. Increasing the maximum temperature of the SPS thermal cycle to 1500°C increases the reduction of the material and the power factor is multiplied by 10 to reach 2 mW/mK² at 50°C [4]. The same effect is observed for the fully lanthanum-substituted compound $La_{0.66}TiO_3$, which exhibits greatly reduced thermal conductivity due to vacancies on the A-site of the perovskite. Moreover the material quenched during SPS leads to domains ten nanometers in length due to a structural transition from cubic to tetragonal structure at high temperature. SPS reduction allows to synthesize reduced ceramics from oxidized powder. Indeed, SPS sintering of the the low thermal conductivity oxide, $La_2Mo_2O_9$, leads to its in-situ transformation into the reduced phase $La_7Mo_7O_{30}$, enabling the thermoelectric properties of this compound to be measured for the first time and showing a low thermal conductivity of 0.7 $Wm^{-1}K^{-1}$ [5].

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Decoupling the Electrical Conductivity and Thermopower by Chemically Manipulating Ni^{2+}/Ni^{0} and Ti^{4+}/Ti^{3+} Redox Pairs in Ni-doped $Sr(Ti,Nb)O_3$

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Keywords: Oxide thermoelectric material, strontium titanate, metal exolution, conduction path

Strontium titanate $SrTiO_3$ (STO) has been known to show a fairly good thermoelectric performance as an oxide upon n-type doping under reducing conditions. Our previous studies on Cu- and Ni-containing oxides exsolving metallic Cu and Ni nanoparticles, respectively, under strongly reducing conditions [1,2] inspired us to explore a possibility to form nanosized conduction paths and phonon scattering centers at the same time. Here we report exsolution of Ni nanoparticles from Ni-doped STO and an improved thermoelectric performance of the oxide via decoupling the electrical conductivity and the thermopower. We synthesized $Sr_{1-x}(Ti_{0.8}Nb_{0.2})_{1-y}Ni_yO_3$ (x, y = 0, 0.05, 0.10) by solid state reaction of starting materials of $SrCO_3$, TiO_2, Nb_2O_5 and NiO at the prescribed molar ratios. After sintering in air at 1420 °C, the samples were reduced under 20% H_2/N_2 or 100% H_2 at 1350 °C. Whereas the electrical conductivity σ of the samples showed metallic behavior and significantly varied from 200 to 1900 S/cm at room temperature, the Seebeck coefficient S at the same temperature was within a narrow range of –50 to –80 μV/K, being unexpected from a fundamental theoretical relation between σ and S as a function of the carrier concentration. The molar fractions of Ni^0, $f(Ni^0)$, out of total Ni amounts in the samples were obtained by the XPS spectra from the ratios of $Ni^{2+/3+}$ and Ni^0 $2p_{3/2}$ peak areas. The molar fractions of Ti^{3+}, $f(Ti^{3+})$, out of total Ti were determined from the changes in the lattice parameters taking the difference in the ionic radii of Ti^{3+} and Ti^{4+} into account. Although $f(Ni^0)$ widely varies from 0.5 to 55% depending on the reducing conditions such as the H_2 concentrations in the reaction atmosphere, $f(Ti^{3+})$ stays within 16 – 18% for all the samples. This analysis clearly explains the discrepant behaviour of σ and S, the former being tuned by the amount of the metallic Ni particles having formed conduction paths, while the latter being governed by the carrier concentrations in the STO matrix. A highest ZT of 0.37 at 800 °C was achieved by the sample with the largest amount of Ni^0. These results strongly suggest that the different chemical tendency of the Ni^{2+}/Ni^0 and Ti^{4+}/Ti^{3+} redox pairs in Ni-doped $SrTiO_3$ against reduction by hydrogen can manipulate σ and S independently.

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Acknowledgments

This work was financially supported by JSPS KAKENHI JP22H01779.

Electrochemical and thermoelectric properties of multicomponent oxides

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Keywords: Multicomponent oxides, mixed ionic-electronic conductivity, barium cerate-zirconate, protonic defects

Multicomponent oxides (MOs) represent an interesting class of materials known for their exceptional thermal stability, adjustable electronic structures, and broad chemical adaptability. These characteristics make them promising candidates for applications in electrochemical or thermoelectric devices. When various elements occupy one site in a crystal structure, the neighbourhood of each cation is different. This leads to an intense lattice strain that distorts the atom's positions. The lattice distortions influence multicomponent oxides' mechanical and transport properties [1,2]. Triple-conducting oxides (TCOs) belong to mixed ion-electron conductors, which may contain three mobile charge carriers - electrons, protons, and oxygen ions. Combining the multiple cations in one sublattice and mixed oxygen ionic- electronic conductivity (MOs-TCOs) may render interesting thermoelectrical and electrochemical materials [3,4].

This work is related to the understanding of the thermoelectrical and electrochemical properties of different multicomponent oxides based on (Sr, Ba)(Ce, Zr, Hf, Y, Bi, Ti, Sn, Fe, Co, Mn)$O_{3-\delta}$, being protonic, oxygen ionic and electronic conductors. Structure and microstructure were analyzed using X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The thermoelectric properties were assessed by measuring the temperature dependency of the Seebeck coefficient using the four-wire (4W) technique in atmospheres with varying water vapour content. The temperature dependency of the total electrical conductivity was further analyzed via DC-4W and Electrochemical Impedance Spectroscopy (EIS) as functions of partial oxygen (pO_2) and water vapour (pH_2O) pressures. A key aspect of this work was the investigation of protonic defects in multicomponent oxides, as these defects can significantly influence transport properties and enhance thermoelectric and electrochemical performance.

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Cost-Effective Performance Enhancement: How High-Entropy Engineering Optimizes In_2O_3-Based Thermoelectric Oxides

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Keywords: High-entropy, In_2O_3, thermoelectricity

High-entropy engineering has emerged as a promising strategy to expand the functional properties, demonstrating effectiveness in various domains including thermoelectricity. Indeed, it can enable a partial decoupling of carriers and phonons transport [1]. In this study, we introduced entropy engineering into In_2O_3 through a combination of +II/+IV cation substitutions at In sites, $In_{2-2x}(Cu_x/_3Ni_x/_3Zn_x/_3)Sn_xO_3$ single-phase compounds via a standard solid-state reaction at 1300°C for 48 hours. Structural characterization confirms the formation of a bixbyite-type phase with space group Ia3 up to x=0.5. The results show that the electrical resistivity is significantly reduced from 23.0 mΩ·cm to 3.0 mΩ·cm at 1000 K compared to undoped In_2O_3, while the thermal conductivity is concurrently suppressed due to strong phonon scattering because of the short-range disorder inherent to high-entropy materials. Although the Seebeck coefficient decreases from 220 to 150 $\mu V \cdot K^{-1}$ due to increased carrier concentration, the partial decoupling of electrical and thermal transport properties leads to an enhanced thermoelectric figure of merit (zT) of ~0.4 at 1173 K in $In_{1.0}(Cu_1/_6Ni_1/_6Zn_1/_6)Sn_1/_2O_3$. Furthermore, multi-element substitution at In sites reduces the reliance on expensive In_2O_3, thereby improving cost efficiency. Overall, this work underscores the potential of entropy engineering as a viable approach for optimizing thermoelectric performance in oxide materials.

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This project was funded by French Agence Nationale de la Recherche, Grant/No. ANR 21-CE08-0006-01 and by the France 2030 programme "ANR-11-IDEX-0003" via Integrative Institute of Materials from Paris-Saclay University - 2IM@UPSaclay. Chuang Jia also acknowledges the Chinese Scholarship Council for PhD funding.

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PART IV
CONTRIBUTED TALKS

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13TH SESSION
DEVICE II

Thermoelectric Metamaterials for Enhanced Power Generation Modules

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Keywords: Geometry modulation, metamaterials, thermoelectric efficiency, heat transfer, thermoelectric modules

Thermoelectric metamaterials have been proposed as a means to enhance thermoelectric efficiency through geometric design [1,2]. Theoretical predictions suggest that width modulation, involving constrictions and openings, can enhance the figure of merit (ZT) by altering electron and phonon energy states, as well as their transmission probabilities, within the quantum confinement regime. Additionally, width modulation remains effective beyond the quantum confinement regime due to distinct physical mechanisms, such as enhanced phonon scattering and reduced thermal transmissivity [3-5]. Recent experimental evidence supports these predictions, validating our models.

In this study, we apply our modeling approach to investigate the potential of geometry-modulated metamaterials for thermoelectric modules. Our findings demonstrate that width modulation can be strategically designed to regulate heat transfer in devices operating under realistic conditions. We also examine the possibilities and limitations of improving the output power of thermoelectric generators. This analysis is applicable to a wide range of thermoelectric materials, spanning scales from the nano- to the macro- scale.

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Investigation of Titanium as a Potential Diffusion Barrier in Bismuth Telluride Thermoelectric Generators

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Keywords: Bismuth telluride, titanium diffusion barrier, intermetallic layer, thermal stability, tomography.

The long-term performance and operational lifetime of bismuth telluride-based thermoelectric devices is strongly influenced by interfacial stability and contact resistance at metal junctions. While diffusion barriers have been explored to mitigate these effects, the choice of barrier material remains a key factor in ensuring reliability. Among potential barrier materials, titanium (Ti) has attracted attention due to its lower Young's modulus which helps minimize interfacial stress, and its strong adhesion to both metal electrodes and thermoelectric materials [1, 2]. In this work, we investigate the role of Ti as a diffusion barrier for both p-type $Bi_{0.4}Sb_{1.6}Te_3$ and n-type $Bi_2Te_{2.76}Se_{0.24}$ thermoelectric legs which are attached to Cu electrodes via a thin Ni metallization layer and Sn-Ag solder. Contact resistivity measurements confirm the formation of efficient ohmic contact, with $TiTe_2$ intermetallic layers yielding values in the range of 3 to 7 $\mu\Omega$ cm². Comparative aging studies reveal that Ti exhibits superior thermal stability over commonly-used Ni diffusion barrier due to its lower diffusion coefficients in both p-type and n-type bismuth telluride. To further elucidate interfacial evolution, advanced tomography techniques provide high-resolution three-dimensional imaging and mechanical insights into the structural integrity of thermocouple legs. The findings highlight the importance of tailored interfacial engineering in thermoelectric legs and contribute to the ongoing optimization of metal contacts for high-performance thermoelectric generators.

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Acknowledgments

This work was supported by the French National Research Agency (ANR) in the frame of the project HYDRES (project identifier ANR-21-CE50-0003).

Ultra-low Power Thermoelectric Sensor for Sweat Rate Monitoring

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Keywords: Thermoelectric materials, sweat sensor, energy-efficient, bioelectronic

Real-time sweat rate monitoring is essential for health diagnostics, athletic performance optimization, and personalized healthcare. However, current techniques, such as the whole-body wash method, wearable conductivity sensors, and microfluidic systems, suffer from critical limitations, including trade-offs between real-time capability and energy efficiency, as well as challenges in reliability and adaptability to demanding environments. To address these challenges, we developed a wireless sweat sensor based on a coupled thermal-fluid-thermoelectric multiphysics system, enabling simultaneous real-time measurement of sweat rate, sweat loss, and skin temperature. This sensor features an innovative design that leverages high-performance thermoelectric materials to serve both as thermal actuators and sensors, thereby drastically reducing power consumption while eliminating the need for complex circuitry. This unique approach not only demonstrates the versatility of thermoelectric materials in wearable sensing applications but also opens new possibilities for their use in next-generation, energy- efficient bioelectronic devices.

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Acknowledgments

This work was funded by the National Natural Science Foundation of China (52425108), the Guangdong Basic and Applied Basic Research Foundation (2024B1515040022), the Shenzhen Science and Technology Program (JCYJ20241202123659001, RCJC20210609103733073, KQTD20200820113045081).

Design of Oxide Thermoelecric Uni-leg Modules

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Keywords: Calcium cobaltate, (Co, Cu)-221, misfit-layered, Uni-leg Module

Fuhanashi *et al*. successfully developed thermoelectric (TE) modules composed of oxide materials [1]. However, the *n*-leg oxide materials exhibited poorer TE properties than the *p*-leg materials. Misfit-layered cobaltate $[Ca_2(Co_{0.65}Cu_{0.35})_2O_4]_pCoO_2$ ((Co, Cu)-221) has anisotropic properties due to its crystal structure [2] and exhibits a high power factor (PF = $S^2\rho^{-1}$, S: Seebeck coefficient, ρ: electrical resistivity) 2.2×10^{-4} $Wm^{-1}K^{-2}$ at 900 K in the *ab*-plane [3]. In this study, we design Uni-leg modules capable of generating at high temperature in the air. The Uni-leg modules, composed of (Co, Cu)-221, are simulated and fabricated to evaluate their power generation characteristics.

The power generation characteristics of the Uni-leg module were simulated by ANSYS. The electrodes were composed of Ni, and contact resistance was ignored. An alumina layer was placed between the *p*-leg and the electrode as an insulator. (Co, Cu)-221 samples for modules were prepared using the standard solid-state reaction method and sintered via Spark plasma sintering (SPS). The samples were cut parallel to the *ab*-plane (//*ab*) or *c*-axis (//*c*).

The cross-sectional area of the Uni-leg module was optimized using the reduced current approach (RCA) [4] and determined to be 3.1×3.1 mm^2. The power generation characteristics were evaluated at a temperature difference (ΔT) of 600 K. The maximum output power P_{MAX} and the surface power density P_d of the module //*ab* were higher than the module //*c*. Compared to Fuhanashi *et al*., P_{MAX} was approximately 40 % lower, while P_d was about 75% higher. In the presentation, we will report P_{MAX} and P_d of fabricated Uni-leg modules.

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Acknowledgments

This work was supported by the KAKENHI grant (No. 23K04903) from the Ministry of Education, Culture, Sports, Science, and Technology (MEXT).

Smart Thermoelectric IIoT for Steam Trap Leak Detection: A Sustainable Approach

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Keywords: LoRaWAN, steam trap, NETZERO, TEG, ultrasound

Industrial processes generate vast amounts of waste heat, much of which remains useless, contributing to both energy inefficiencies and increased greenhouse gas emissions [1]. A particularly critical issue in steam systems is the undetected failure of steam traps, leading to energy losses and excess CO_2 emissions. This paper presents a novel thermoelectric-powered Industrial IoT (IIoT) [2] solution that leverages temperature and ultrasound sensing to detect steam trap leaks in steam pipelines and steam traps with a high accuracy approach [3]. Our system employs thermoelectric generators (TEGs) [4] o harvest waste heat and power autonomous IoT sensors, eliminating the need for lithium batteries, reducing maintenance costs, and enhancing deployment feasibility in hazardous environments. The integration of LoRaWAN connectivity ensures long-range, low-power data transmission, enabling continuous monitoring of steam trap performance in large-scale industrial facilities.
Key features of this system include:

- Self-Powered Operation: Thermoelectric energy harvesting removes reliance on conventional batteries, offering a truly sustainable solution.
- Multimodal Sensing: A combination of temperature and ultrasonic measurements provides enhanced leak-detection capabilities.
- Remote Monitoring & Predictive Maintenance: Real-time data transmission via LoRaWAN enables proactive maintenance strategies, minimizing steam losses and operational costs.
- Environmental Benefits: Reducing steam trap failures directly translates into lower fuel consumption and a significant reduction in CO_2 emissions.

Preliminary results from industrial deployments indicate that our approach effectively detects faulty steam traps, achieving substantial energy savings and operational efficiency improvements. By addressing steam losses at their source, this technology offers a scalable, cost-effective, and environmentally friendly solution for industrial energy management. Future work will focus on further optimizing signal processing algorithms and expanding field tests.

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Acknowledgments

This work was supported by the European Commission HORIZON-EIC-2023-TRANSITION OPEN-01. GRANT AGREEMENT: 101158721 Project OxyBatt

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PART IV
CONTRIBUTED TALKS

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14TH SESSION
THEORY II

Enhanced Thermoelectric Performance of PbSnTeSe High-Entropy Alloys via Magnetic Doping and Strain Engineering

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Keywords: Thermoelectric materials, high-entropy alloys, magnetic doping, strain engineering, Density Functional Theory

Improving the thermoelectric efficiency of materials remains a critical challenge, with various strategies being explored. Among them, magnetic doping has proven effective [1-3], as well as strain engineering [4,5]. In this work, we investigate the impact of incorporating magnetic elements, specifically Cr and Fe, into the PbSnTeSe high-entropy alloy (HEA) and analyze their influence on thermoelectric performance. Our results show that Cr doping significantly enhances the thermoelectric figure of merit (ZT), whereas Fe doping has a more limited effect. Furthermore, we investigate the effect of magnetic interactions between the two dopant atoms on the thermoelectric properties, considering both ferromagnetic and antiferromagnetic coupling. We also assess the role of biaxial and isotropic strain on thermoelectric properties, independently from magnetic doping. Both types of strain contribute to optimizing the maximum ZT, depending on the doping type, strain magnitude, and temperature. These findings highlight the potential of magnetic doping and strain engineering as effective yet distinct strategies for enhancing HEA thermoelectric performance. A detailed discussion of these results will be provided in this presentation.

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This work has been carried out under the allocation A0150806881 granted by the “Grand Equipement National de Calcul Intensif” (HPC resources of GENCI−France). The “Centre de Calcul Intensif d’Aix-Marseille” is acknowledged for granting access to its high-performance computing resources. The China Scholarship Council is acknowledged for supporting M. Xia PhD thesis.

Scattering exponent approximation for complex electronic structure thermoelectric materials from ab initio calculations

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Keywords: Scattering exponents, electronic transport modelling

Knowing the dominant electronic transport mechanism in a material provides insight into its properties and directions to improve its performance. A typical way to infer the dominant mechanism is to fit experimental data into transport models where the scattering times are approximated by an exponential energy dependence as $\tau = \tau_0 (E/E_0)^r$. Here, *r*, is a characteristic exponent which depends on the dominant scattering mechanism. For example, charge transport that is dominated by acoustic deformation potential (ADP), optical (ODP), polar optical phonon (POP) and ionized impurity scattering (IIS), are thought of to follow r = - 0.5, -0.5, 0.5, and 1.5, respectively [1,2]. These values, often used without justification, are based on single, parabolic band considerations. Modern thermoelectric (TE) materials, however, have complex multi-band, multi-valley electronic structures, with complex electronic transport and scattering dynamics. To better and more confidently characterize transport measurements, this simplified approach needs to be re-examined, validated, and corrected. Here we use Boltzmann Transport theory and start with re-evaluating the exponent approximation for a single parabolic band material. We then evaluate a two-band system, where the effect of the band mass ratio and energy separation are explored. Finally, we investigate the validity of the exponent for various real materials from the half-Heusler group using ab-initio DFT electronic structures and Boltzmann transport solvers with full energy/momentum/band dependent scattering, as implemented in the code ElecTra [3]. For a single band, we find that the standard literature scattering exponent values show good agreement for ADP, only at high energies for ODP and POP, and only at low carrier densities for IIS. In the case of a two-band material, significant deviations are seen for all scattering mechanisms, which increase with band mass ratio and band energy separation. In the case of half-Heusler materials at high carrier densities, where carrier screening is significant, the scattering exponents vary at such a degree, that it is nearly impossible to link transport trends (i.e. mobility) to a specific scattering mechanism. From a statistical analysis for 11 different half-Heusler materials, we find that the scattering exponents follow a Gaussian distribution with μ = - 0.102 and σ = 0.175, which does not fit any of the standard exponents. In conclusion, our study will help improve the characterization of TE measurements, leading to better understanding and optimization.

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Acknowledgments

This work has received funding from the EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems (HetSys), and from the UK Research and Innovation fund (project reference EP/X02346X/1).

Quantifying the impact of band change upon alloying on the power factor

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Keywords: Thermoelectric, transport, half-Heusler alloys

In this study, we perform ab initio transport calculations to quantify the effect of the changes in the bandstructure as a result of alloying on the thermoelectric (TE) power factor (PF). The purpose is to initiate a direction towards simulation alloyed TE materials beyond the constant relaxation time approximation. This introduces significant challenges, because of the folded electronic structure and the changes in the band structure and band splittings upon alloying. As a first attempt we examine how the alterations in the bands alone, affect the PF. We employ the Boltzmann transport code ElecTra [1], which considers the full energy/momentum/ band dependence of the bands and of the scattering rates. We account for all relevant scattering processes, i.e. acoustic, non-polar optical and polar optical phonons (POP), and ionized impurity scattering (IIS), all described using first-principles extracted parameters.
We use two material examples to quantify how the changes in the electronic structure upon alloying change the PF. One of them has valley at the G-point, which by symmetry is not expected to change much after alloying: XNiSn ($Ti_{1-x}Zr_xNiSn$, $Zr_{1-x}Hf_xNiSn$, $Hf_{1-x}Ti_xNiSn$). The other one has L & X valleys, for which we expect larger band changes: $Ta_{1-x}Nb_xNiSn$. Upon alloying, in both cases, the electronic structure changes in terms of the density of state effective mass (m_{DOS}) and conductivity effective mass (m_{Cond}). In the first case, we find that this electronic structure modification is benefitial, with alloying 25% of Hf in TiNiSn leading to 24% enhancement in the PF due to electronic structure changes alone. In the second case, we observe an additional significant band splitting of the degenerate X bands. Here we do not observe significant band mass changes, however, the valley splitting results up to 40% PF reduction (upon alloying 50% Ta with Nb). Calculation of the low field mobility in this case demonstrated the well-known U-type shape of mobility upon alloying. This is pronounced much less in the first case where splitting is not observed and the m_{Cond} change is monotonically decreasing. We also demonstrate, alloying with different types of elements changes the band and splitting differently (i.e. doping Ti/Zr/Hf in TaFeSb).

These findings are a step forward in understanding the role of alloying on the PF by examining how changes in the band structure alone determine its amplitude, which would be extremely useful in leading experimental effords towards high power factor materials.

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Acknowledgments

The work received funding from the EPSRC under grant no EP/Y015916/1.

A novel method for evaluating dimensionless thermoelectric properties of fine-grained n-type Bi_2Te_3 by scattering parameter γ, materials parameter β, and reduced Fermi energy η at room temperature

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Keywords: Powder metallurgy, materials parameter, Lorenz number, scattering parameter, reduced Fermi energy

The dimensionless figure of merit ZT can be determined using the material parameter β, scattering parameter γ, and reduced Fermi energy η, which are dimensionless quantities. The γ is defined as $\mu \propto T^{\gamma-3/2}$ where μ is the mobility. Hall effect measurements analysis cannot be performed in the range where the γ is below - 0.3 due to the uncertainty in carrier concentration, since the Hall factor can no longer be regarded as 1 [1]. This research aims to evaluate the fundamental properties of thermoelectric materials in detail and provide guidelines for designing high-performance thermoelectric materials. In the present study, the variables β, γ, and η, in fine-grained n-type Bi_2Te_3, produced by mechanical grinding followed by hot pressing, were evaluated using Fermi-Dirac statistics and a one-electron parabolic model at room temperature. The thermal conductivity κ was assumed to be a quadratic function of σ, under a constant phonon thermal conductivity κ_{ph}. The γ and η were estimated using the Lorenz number and the measured Seebeck coefficient α, composed of γ and η [2,3]. The analytical $ZT_{\beta\gamma\eta}$, composed of β, γ, and η, obtained based on the relationship between the ZT and η, is consistent with the measured $ZT_{\alpha\sigma\kappa}$ composed of α, σ, and κ. The obtained β, γ, and η indicate fundamental physical properties of thermoelectric materials alongside α, σ, and κ. If the correct Seebeck coefficient, electrical and thermal conductivities, and Lorenz number can be determined, this approach can be widely applied across various fabrication methods, thermoelectric materials, and structures.

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PART IV
CONTRIBUTED TALKS

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15TH SESSION
LATTICE DYNAMICS I

Mechanochemical Synthesis and Low-Energy Phonon Scattering in Mixed-Anion Chalcohalides $Bi_{13}S_{18}X_2$ (X = I, Br, Cl)

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Keywords: Anharmonic lattice vibrations, Raman spectroscopy, phonon lifetime, thermal transport, rattling motion

Mixed-anion compounds, which incorporate multiple types of anions into materials, display tailored crystal structures and physical/chemical properties, garnering immense interests in various applications such as batteries, catalysis, photovoltaics, and thermoelectrics. We first present the ultrafast and mechanochemical synthesis of nanocrystalline ternary mixed-anion chalcohalide $Bi_{13}S_{18}X_2$ (X = I, Br, Cl) via high-energy planetary milling. This scalable and solvent-free process enables the rapid formation of this complex chalcohalide within 30 minutes, and futher densification and grain growth by Spark Plasma Sintering, offering a promising route for the elaboration of bulk chalcohalide materials. In a second part, we will discuss the thermoelectric properties of the mixed-anion chalcohalides $Bi_{13}S_{18}X_2$ (X = I, Br, Cl), with a more detailed focus on $Bi_{13}S_{18}I_2$. We analyze the lattice thermal conductivity using temperature-dependent Raman spectroscopy and identify a high-intensity acoustic phonon mode at 37 cm^{-1}. This mode significantly lowers the sound velocity (1734 m/s), leading to strong phonon scattering. The calculated phonon lifetime, determined from fitted Raman modes by using energy-time uncertainty relation, provides insights into phonon scattering behavior as a function of temperature. Our study highlights how the rattling motion of Bi and I atoms induces strong phonon anharmonicity, effectively reducing lattice thermal conductivity [1,2]. By analyzing the phonon lifetime derived from low-temperature lattice thermal conductivity measurements and Raman spectra of the phonon modes, we establish a direct correlation between anharmonic lattice vibrations and heat transport. This provides deeper insights into the underlying physics governing phonon scattering in such complex chalcohalide compounds.

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Acknowledgments

This work was supported by CNRS, France.

Exploring Defect-Driven Phonon Dynamics in GeTe: Raman and Thermal Perspectives

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Keywords: GeTe, defects, phonon dynamics, crystals, transport

Softer lattice dynamics, characterized by low-frequency phonon modes and reduced bonding rigidity, significantly influence the thermal, electronic, and vibrational properties of materials [1]. Among group IV-VI monochalcogenides, GeTe is an octahedrally coordinated compound with a high density of Ge vacancies [2]. The impact of defects, such as vacancies or disorder, on lattice dynamics becomes particularly pronounced at temperatures below the Debye temperature ($T < \theta_D$). Using low-temperature Raman spectroscopy, we have investigated the mode dynamics of two off-stoichiometric GeTe crystals ($Ge_{0.88}Te$ and $Ge_{0.80}Te$), revealing contrasting features in the doubly degenerate E mode and the A_1^T mode, which are vibrations perpendicular and parallel to the three-fold symmetry c-axis [3]. Klemen's model successfully describes the linewidth of the E mode, highlighting the role of higher-order phonon scatterings in the defective system. Raman shifts for the A_1^T mode also show heightened sensitivity to defective environments. Specific heat measurements further support these findings, confirming lattice softening in the more defective crystal, which aligns with the lowering of the effective-phonon frequency calculated from low-temperature conductivity measurements.

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Acknowledgments

The authors are thankful to ANRF, GoI for the funding that supported this work. (EEQ/2022/001016) and the UGC CSR Indore for the access to advance measurement facilities (09/2023/5517 and 07/2023/5134).

Unraveling the Lattice Dynamics of Silicides: Strategies for Improved Thermoelectric Efficicency

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Keywords: Lattice dynamics, nanostructuring, silicide

Silicides such as $CrSi_2$, $FeSi_2$, and $SrSi_2$ have garnered attention due to their Earth-abundant composition and promising thermoelectric properties. However, their thermal conductivity remains a major limiting factor in optimizing their thermoelectric performance, as quantified by the dimensionless figure of merit ZT. In this work, we investigate the lattice dynamics and thermoelectric properties of these silicide alloys, with particular emphasis on the impact of nanostructuring on phonon transport. For $CrSi_2$ and $FeSi_2$, we explore the effects of size reduction and strain on their phonon dispersion and lattice thermal conductivity through a combination of experimental techniques and first-principles density functional theory (DFT) calculations. We report the phonon density of states for bulk and nanostructured $CrSi_2$ and $FeSi_2$, demonstrating a spectral weight transfer at low energy in nanostructured samples. This shift is associated with a decrease in the Debye temperature and sound velocity, contributing to enhanced phonon scattering and a significant reduction in lattice thermal conductivity. For $SrSi_2$, we present a detailed study combining Raman spectroscopy, neutron inelastic scattering, and ab initio calculations to describe its lattice dynamics. The phonon spectra reveal the presence of low-energy optical modes with high Grüneisen parameters, which interact with acoustic phonons to decrease the lattice thermal conductivity. The measured phonon dispersion and density of states show excellent agreement with theoretical predictions, confirming that $SrSi_2$ exhibits relatively low lattice thermal conductivity compared to other silicides, driven by its unique phonon interactions and localized vibrational modes. Overall, our findings highlight the critical role of nanostructuring in tuning the lattice dynamics and thermoelectric performance of silicide materials. By leveraging experimental and computational insights, we provide a pathway for optimizing these materials for future thermoelectric applications.

Acknowledgments
This project is supported by the French National Research Agency through the funding 16 CARN 0008-01 and ANR-19-CE05-0001. We would also like to thank the ILL for providing beam-time and the Carnot Institute ICCBC for its support.

s-d Coupling Induced Dynamic Off-centering of Cu Drives High Thermoelectric Performance in TlCuS

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Keywords: Local off-centering, *s-d* coupling, pair distribution function analysis, low thermal conductivity, sulfide thermoelectrics

Seeking new and efficient thermoelectric materials requires a detailed comprehension of chemical bonding and structure in solids at microscopic levels, which dictates their intriguing physical and chemical properties. In this work, we investigated the influence of local structural distortion on the thermoelectric properties of TlCuS, a layered metal sulfide featuring edge-shared Cu-S tetrahedra within Cu_2S_2 layers. While powder X-ray diffraction suggests average crystallographic symmetry with no distortion in CuS_4 tetrahedra, the synchrotron X-ray pair distribution function experiment exposes concealed local symmetry breaking, with dynamic off-centering distortions of the CuS_4 tetrahedra. The Cu off-centering is driven by the on-site coupling of filled 3*d* and unoccupied 4*s* orbitals (*s-d*) of Cu through a second-order Jahn-Teller mechanism. Bond softening by the *p-d** (S-*3p* and Cu-*3d*) antibonding interaction coupled with dynamic off-centering distortions, causes quartic anharmonicity in the lattice, which acts as a phonon-blocking mechanism conducive to ultra-low lattice thermal conductivity (k_{lat}) (~0.35-0.23 W m^{-1} K^{-1} in the ~ 296-573 K temperature range) in TlCuS. The synergy between low k_{lat} and multiband electronic structure leads to thermoelectric figure-of-merits (zT) of ~1 and ~1.3 at 573 K for pristine TlCuS and $TlCu_{0.98}S$, respectively, underscoring the potential of metal sulfides as promising high-performance thermoelectrics. In my presentation, I will highlight the relationship between chemical bonding, lattice dynamics, and thermal transport which is crucial for thermoelectrics.

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PART IV
CONTRIBUTED TALKS

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16TH SESSION
DEVICE III

Tuning ionic thermoelectric behaviour of Lignin derived hydrogels

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Keywords: Ionic thermoelectrics, lignin, hydrogels

With increasing global demand for renewable energy solutions, thermoelectric technologies that convert low-grade waste heat into electricity are gaining traction. Ionic thermoelectric materials (i-TEs), which exploit ion transport and thermodiffusion rather than traditional electronic conduction, offer an eco-friendly and efficient pathway for sustainable energy harvesting. These materials boast high Seebeck coefficients, low thermal conductivity, and excellent ionic conductivity, making them compelling alternatives to conventional thermoelectrics [1]. This study focuses on the synthesis, functionalization, and characterization of lignin-derived hydrogels as i-TE platforms. Lignin's aromatic, highly branched structure and abundance of reactive groups provide a robust framework for hydrogel development. Two approaches were explored: (1) optimization of lignin concentration, crosslinkers, and electrolyte composition, and (2) crosslinking followed by amine functionalization using 2-chloroethylamine hydrochloride (CEH) via a green NaOH–water system. The functionalized hydrogels infiltrated with 1 M KCl exhibit n-type i-TE behavior, showing a negative Seebeck coefficient (-7.48 mV/K), ionic conductivity of 39.9 mS/cm, and a power factor of 223.52 μW/mK², leading to a figure of merit (ZTi) of 0.145 [2,3]. In contrast, crosslinked hydrogels infiltrated with 6 M KOH demonstrate p-type behavior with exceptionally high performance Seebeck coefficient of 13 mV/K, ionic conductivity of 226.5 mS/cm, a power factor of 3831 μW/mK², and a ZTi of 3.75 representing one of the highest reported values for sustainable p-type i-TEs [3,4]. These complementary n- and p-type materials enable the formation of efficient i-TE junctions for applications in temperature sensing, wearable electronics, and energy harvesting. This work paves the way for advanced, biodegradable thermoelectric devices through the valorization of lignin, contributing to circular economy goals and green energy transitions.

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We gratefully acknowledge the Generalitat Valenciana for the Santiago Grisolia research grant (CIGRIS/2022/132). This research was also supported by Grant PID2021-124845OA-I00 funded by MCIN/AEI/10.13039/501100011033 and co-financed by "European Union NextGenerationEU/PRTR".

Thermoelectric Flexible Module with Anodized Aluminum Substrate

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Keywords: Bismuth telluride, Thermoelectric generating module, Flexible module, Anodized Al substrate

Conventional thermoelectric generators have no deformation ability, so even if they are installed on a tubular exhaust heat source, the heat recovery efficiency is poor. Therefore, in order to improve the power generation efficiency, Al substrates are attracting attention because of their high thermal conductivity, ease of plastic processing, and the ability to form an insulating film on the surface by anodizing to prevent leakage to the heat source. In this study, the anodization conditions for Al that achieve both flexibility and insulation were investigated. In addition, a TEG module was fabricated using Bi2Te3 as the thermoelectric material and an anodized Al plate as the insulating substrate, and the power generation characteristics of the module were evaluated using a curved heat source. An Al plate with dimensions of 0.50 x 25 x 25 mm was anodized using 0.3 mol/L oxalic acid as the electrolyte, the Al plate as the anode, and the graphite plate as the cathode. The solution temperature was 303 K, 50 V was applied from a DC stabilized power supply, and the current time was changed from 10 to 60 minutes. High melting point solder or In was soldered onto the anodized film as the electrode material. The thickness of the anodized Al film was obtained from the results of SEM observation. The three-point bending test was performed using an AUTOGRAPH AG-I with a curvature radius of the indenter of 10 mm. The flexibility of the anodized film was evaluated from the peeling state of the insulating film from the results of SEM surface observation. Bi_2Te_3 was used as the thermoelectric material, and the bottom surface perpendicular to the cleavage plane was processed to a height of 5 x 5 mm, and the parallel surface was processed to a height of 10 mm. It was confirmed that the thickness of the oxide film also increased with the increase in the anodization time. Comparing the surface observation results after the three-point bending test of substrates with anodization times of 1800 s and 3600 s, cracks were confirmed in both samples, but peeling was not confirmed. It was also found that the insulation of the film was broken down in the case of anodization time of 1440 s or less, while the insulation was maintained in the case of anodization time of 1500 s or more. The film thickness at 1500 s was 15.95 μm, and it was revealed that the insulation of the film was maintained above this. When the substrate side of the fabricated module was heated with hot water in a vacuum, the Al_2O_3 substrate temperature deviated from the hot water temperature by more than 10 K. In contrast, the temperature difference between the hot water and the anodized Al substrate was about 1 to 2 K. It became clear that the anodized Al substrate was very effective in terms of thermal conductivity and thermal contact.

Acknowledgments
The author is grateful to Mr. K. Matsumura, Mr. H. Izumoya and Mr. H. Chiba of Kogakuin University for their great help in achieving the experiment.

Life Cycle Assessment (LCA) as a Design Tool for Sustainable Thermoelectric Materials, Modules and Systems

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Keywords: Life Cycle Assessment, sustainable thermoelectrics, optimisation method

Thermoelectrics are often cited as a sustainable technology for the energy transition. However, this claim is rarely quantified and there is a lack of tools designed for such quantification that could also be used to optimise sustainability.

In this study, Life Cycle Assessment (LCA) is used to evaluate the environmental impact of a thermoelectric system for industrial waste heat recovery based on full Heusler thermoelectric modules. The method proves effective in enhancing sustainability at different levels: (i) doping strategies to improve thermoelectric material performance, (ii) module manufacturing, including waste management and end-of-life consideration, and (iii) the impact of heat exchangers at the system level.

Comprehensive optimisation is shown to reduce most environmental impact indicators by a factor of 3 to 16 compared with the baseline scenario. The environmental impact per kilowatt-hour of electricity generated by the optimised thermoelectric system is significantly lower than the impact of the Belgian electric mix and even lower than Belgian wind power generation

Finally, the proposed method is compared with established techno-economic analysis [1] to highlight similarities and differences between cost impacts and environmental impacts on thermoelectric generator design.

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Acknowledgments

This work was supported by Wallonia through the Proof of Circularity Programme.

Elevating the thermoelectric performance in the sub-ambient temperature range for electronic refrigeration

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Keywords: Single-crystalline, Mg_3Bi_2-based materials, double-stage cooler, cooling performance

The solid-state thermoelectric coolers, which can directly pump the heat by utilizing electricity, play an essential role in electronic refrigeration. Since thermoelectric devices usually cool down to the sub-ambient temperature range, the performance of the coolers critically hinges on the properties of the material below 300 K. Therefore, it is of great significance to promote the materials' properties below room temperature. Herein, the single-crystalline Mg_3Bi_2-based material has been prepared and ensured a high electron mobility. As a result, thermoelectric figure-of-merit values of ~1.05 at 300 K and ~0.87 at 250 K (along the ab plane) have been achieved, which are superior to the commercial n-type $Bi_2(Te, Se)_3$-based alloys. Thermoelectric coolers (single- and double-stage devices) based on the n-type single-crystalline $Mg_3Bi_{1.497}Sb_{0.5}Te_{0.003}$ and p-type $(Bi, Sb)_2Te_3$ have been fabricated. The maximum cooling temperature difference of the double-stage device is ~106.8 K at the hot-side temperature of 350 K, which outperforms the commercial Bi_2Te_3-based device. After ~2000 cycles between the input electrical currents of 1 A and 3 A, the Mg_3Bi_2-based double-stage device does not show any degradation in the cooling temperature differences. Our results show that the single-crystalline Mg_3Bi_2 alloys hold great promise for thermoelectric cooling applications.

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Acknowledgments

This work was supported by the the National Natural Science Foundation of China, the Shenzhen Science and Technology Program, the China Postdoctoral Science Foundation, and the Key-Area Research and Development of Guangdong Province

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PART IV
CONTRIBUTED TALKS

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17TH SESSION
CHALCOGENIDES II

Defect Engineering in Cu-Based Diamond-Like Chalcogenides for Enhanced Energy Conversion

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Keywords: Copper chalcogenides, crystal structure, lattice thermal conductivity, electronic localization function, Debye-Callaway analysis

Thermoelectric materials with diamond-like structure (DLS) have garnered significant attention due to their potential for efficient energy conversion, cost-effectiveness, and environmental sustainability. However, their performance is often hindered by high lattice thermal conductivity and relatively low carrier mobility. In this study, we investigate the role of native defects and anion substitution in tuning the electronic and thermal transport properties of Cu-based DLS thermoelectrics, focusing on Cu_2XYQ_4 (X = Fe, Co; Y = Ge, Sn; Q = S, Se). Through powder X-ray diffraction and Rietveld refinement, we elucidate the point defect scheme in these materials, revealing mixed cation occupancy and substitutional defects that significantly influence carrier concentration and lattice thermal conductivity. Our findings show that increased selenium content enhances crystal symmetry by approaching the ideal tetrahedral bond angle (109.5°), which in turn improves carrier mobility. Simultaneously, bonding inhomogeneity between anions and cations induces strong lattice anharmonicity, effectively reducing lattice thermal conductivity. As a result, $Cu_2CoSnSe_4$ exhibits a remarkably low thermal conductivity of below 0.6 $Wm^{-1}K^{-1}$ at 773 K and achieves a high thermoelectric figure of merit ZT of 0.75. These results highlight the importance of crystal symmetry optimization and defect engineering in enhancing the thermoelectric properties of lightweight DLS materials.

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Acknowledgments

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

Manipulating Charge Carrier in Thermoelectric Sulfides

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Keywords: Charge carrier, Mobility, Doping, Power factor, Thermoelectric performance

Thermoelectric effect primarily originates from the movement of charge carrier driven by temperature gradient. Therefore, the proper manipulation of charge carrier is of great importance to thermoelectric performance. Here, we give three examples of how to realize the carrier transport behavior control in thermoelectric sulfides to boost their electrical performance. (1)
A novel doping strategy is proposed, where a small trace of alien atoms is used to stabilize cation vacancies in Cu_3SbSe_4 and Cu_3SbS_4 by compositing with $CuAlSe_2$ and $CuAlS_2$, in which the cation vacancies rather than the alien atoms provide a high density of holes. Consequently, the hole concentration enlarges by six times but the carrier mobility is well maintained. Both the average power factor and zT values are significantly promoted in a series of sulfide composites designed by the new strategy.(2)
A phase-dependent mobility edge in $(Cu_2Sn_{1-y}S_3)_{0.85}(CuGaS_2)_{0.15}$ solid solutions is demonstrated. By control over the mobility edge in these solid solutions by increasing the ratio of tetragonal phase with less disorder, a weakened localization of electronic states and promoted carrier mobility are realized. Finally, a high zT value associated with decent power factor is achieved in the optimized solid solution.

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Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant Nos. 52125103 and 12274044).

Process-controlled defect engineering and intrinsic low thermal conductivity in layered Cu_2ZrS_3

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Keywords: sulphides, stacking-faults, triangular copper

Controlling lattice thermal conductivity (κ_L) is pivotal in designing materials for thermoelectric and thermal management applications. Sulfide-based compounds offer an eco-friendly, earth-abundant alternative to tellurides and selenides but generally suffer from high κ_L. Here, we investigate Cu_2ZrS_3, a layered metal sulfide recently reported to exhibit intrinsically low κ_L (~0.35 $W \cdot m^{-1} \cdot K^{-1}$ at 683 K), attributed to its unique Cu-based trigonal coordination and strong lattice anharmonicity [1].

Through a combined approach of controlled synthesis, advanced diffraction techniques, and first-principles modeling, we uncover the existence of two novel structural polytypes of Cu_2ZrS_3, resulting from different thermal histories. These polytypes display distinct stacking sequences (ABCB and ABC), variations in atomic displacement, and levels of structural disorder, all of which critically impact phonon transport. Notably, diffuse scattering and mixed-site occupancy indicate the presence of stacking faults that has been simulated and quantitatively evaluated.

Heat capacity measurements, Raman spectroscopy, and phonon calculations confirm the presence of low-energy optical phonons associated with Cu, facilitating strong optical-acoustic phonon interactions that intrinsically suppress κ_L. These findings establish a clear correlation between structural polytypism and thermal transport in Cu-rich sulfides, offering new pathways toward sustainable, cost-effective materials with tailored thermal properties.

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Improved thermoelectric efficiency of $Sb_2Si_2Te_6$ through yttrium-induced nanocompositing

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Keywords: thermoelectricity, tellurides, $Sb_2Si_2Te_6$, Y-nanocompositing; carrier concentration

Thermoelectric 2D materials are highly attractive due to their inherently low thermal conductivity. $Sb_2Si_2Te_6$ is a promising candidate for medium temperature applications: however, its potential is limited by its low power factor. In this study, we successfully enhanced the performance of $Sb_2Si_2Te_6$ by incorporating Yttrium nanoparticles. The reduced carrier concentration and enhanced seebeck coefficient led to a power factor of 946 μWK^{-1} at 570 K. Jonker plot analysis confirmed that the intrinsic electrical properties remained unchanged. SEM, TEM and Debye Callaway model revealed that Y nano-compositing effectively reduced the lattice thermal conductivity to near the amorphous limit. As a result, $Sb_{1.98}Y_{0.02}Si_2Te_6$ achieved a peak *zT* of 1.49 at 773 K due to the ultralow lattice thermal conductivity of 0.29 $Wm^{-1}K^{-1}$. The single parabolic band model (SPB) suggests that further optimization of the effective mass and lattice thermal conductivity could push *zT* to 1.55. These findings highlight the potential of Y nanocompositing for enhancing $Sb_2Si_2Te_6$ as a high-performance thermoelectric material for medium-temperature applications.

Acknowledgments
Q. Yan acknowledges the financial support from the Ministry of Education (MOE) Academic Research Fund (AcRF) Tier 1 (RG128/21 and RG78/23), and MOE Tier 2 (MOE-T2EP50223-0003). J. Cao acknowledges the financial support from e-ASIA project R22I1IR053 and LCER Phase 2 Programme U2411D4011. K. Saglik acknowledges the support from A*STAR's SINGA scholarship. The authors acknowledge Dr Zhang Mingsheng for his help with the XPS analysis. The authors would like to acknowledge the facility for analysis, characterization, testing and simulation (FACTS), Nanyang Technological University (NTU), Singapore.

Improving Thermoelectric Efficiency of Hybrid Lignin-Copper sulfide Materials

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Keywords: lignin, thermoelectric materials, copper sulfide

The limitation of energy resources such as coal and fossil fuels results in the global energy crisis. Furthermore, 60% of the global energy is lost as heat. Hence, developing a more sustainable energy-harvesting solution has been a huge topic in the research field for the past decades. An effective way to maximize energy recovery efficiency is by converting waste heat into electrical energy. This can be achieved by using thermoelectric materials. The technology of thermoelectric materials provides an alternative solution to generate clean and eco-friendly energy.Lignin is a biopolymer that is abundant in nature. As the world is getting more attention in green chemistry, scientists bring attention to lignin which can be obtained from renewable raw materials. A great number of research is done to understand the chemical and physical properties and to explore its possible applications in the technologies to achieve a more sustainable development. Lignin waste is also considered as an environmental issue as the waste is commonly thrown away as unwanted residue or used as low-grade fuel. Considering that there is an approximately 30% of lignin in the biomass source, dumping it or just simply burning it is indeed a great wastage of natural resource.

In this work, the possibilities of the integration of copper sulfide, $Cu_{2-x}S$, in lignin matrices for thermoelectric applications are explored. The objective is to develop hybrid based thermoelectric materials based on lignocellulose fractions. Synthesis of Cu2-xS using different precursors is investigated to determine the most suitable method that provides the desired product. [2,3] The Cu2-xS samples synthesized using different precursors are characterized by Powder X-ray diffraction, SEM, TEM and by measuring their thermoelectric properties. These Cu2-xS samples are further studied by mixing them with lignin at different ratios to form a Cu2-xS/Lignin composites. The thermoelectric properties measurement after heating at different temperatures, DSC, TGA, SEM and TEM are used to study these composites. Values of power factors around 3000 $\mu W/m \cdot K^2$ position these lignin-copper sulfide thermoelectric materials as strong candidates for next-generation sustainable energy solutions.

Acknowledgments
This work has been developed under the Grant PID2023-1523470B-I00 funded by the Ministerio de Ciencia, Innovación y Universidades (MCIU) and by the Agencia Estatal de Investigación (AEI)/ 10.13039/501100011033/ FEDER, UE.).

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PART IV
CONTRIBUTED TALKS

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18TH SESSION
EMERGING MATERIALS II

Semiconducting-to-metallic transition leading to large n-type Seebeck coefficient in a copper thiolate-based coordination polymer

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Keywords: 2D metal-organic frameworks ; electronic transport properties ; thermoelectricity ; semiconductor-to-metal transition

The exploration of metallicity in metal-organic frameworks (MOFs) and coordination polymers (CPs) remains challenging but crucial for their development toward various applications in electronics[1] and thermoelectrics. MOFs and CPs are crystalline extended networks consisting of metal ions and multidentate ligands, where metal ions act as nodes between the bridging ligands. In this vein, we have reported a new p-type semiconducting 2D CP, copper(I)-1,3-benzenedithiolate, $[Cu_2(1,3\text{-BDT})]_n$, made of thiolate-based ligand and Cu(+I) metal ion, which shows a remarkable Seebeck coefficient of approximately 420 $\mu V.K^{-1}$ and an electrical conductivity of 10^{-5} $S.cm^{-1}$ at room temperature. The structure, crystallizing in the monoclinic $P2_1/c$ space group, features tubular chains of distorted Cu_3S_3 hexagons along the b-axis. These Cu-S chains are interconnected by 1,3-BDT ligands, forming a 2D network in the (a,c) plane.[2] Here, the low-temperature structural properties, electronic transport properties, and magnetic susceptibility will be first presented, followed by an interpretation of the results based on a band-like conduction model. While no structural change is detected by powder X-ray diffraction, a semiconductor-to-metal transition in electrical resistivity is observed below 150 K. This transition is reflected in the temperature-dependent resistivity, which exhibits an exponential increase upon cooling down to 150 K, followed by a plateau at lower temperatures. This transition is accompanied by a sign change and the emergence of large negative Seebeck coefficient values, along with a shift from diamagnetic to paramagnetic behavior in magnetic susceptibility. Based on first-principles calculations, we analyzed the dominant nature of the conducting electronic states and proposed an interpretation of the overall temperature-dependent behavior of resistivity, the Seebeck coefficient, and magnetic susceptibility.[3]

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Seebeck coefficient measurement in bidimensional thickness dependant topologically insulated WSe_2

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Keywords: Thermoelectricity, 2D materials, Seebeck coefficient, WSe_2, Lab-on-chip

Fabrication and characterization progress of new bidimensional material leads the way to a promising generation of thermoelectric generator (TEG). Indeed, while energy harvesting can arise from the MW to the µW, an effort is made to develop scalable TEG nanometer sized (nanoTEG) for large-markets applications at the µW scale (e.g. IoTs)[1]. For that, TEG based on 2D topological insulators (TIs) are promising due to the particular band structure of such materials that could give rise to a remarkably high TE conversion efficiency thanks to an important Sebeeck coefficient and a reduced thermal conductivity induced by the sample size. In fact, performance of TEG scales with the value of figure of merit ZT; ZT is equal to $S^2\sigma T/\kappa$, where S is the Seebeck coefficient, $\sigma(\kappa)$ the electrical (thermal) conductivity, and T the absolute temperature. Characterisation of 2D TE materials candidate for energy harvesting can then be challenging considering that the temperature accros the material of interest must be precisely controlled. For that we developed a lab-on-chip based measurement method to probe locally and in a well controlled environment the Seebeck coefficient[2] as well as the electrical conductivity. In this work, we used this novel measurement method to characterize thermoelectrics properties of thin (2D) and thick (bulk) WSe_2 grown on sapphire substrate, and observe the effect of thickness on TE performances.

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Acknowledgments

This work was supported by the French National Research Agency from the ANR NEXTOP Grant No. ANR-22-CE09-0035

Towards a better understanding of the complex defect diffusivity in Mg_2Si/metal contact interfaces using Kelvin Probe Force Microscopy

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Keywords: Mg_2Si, Kelvin Probe Force Microscopy, Transient Potential Seebeck Microprobe

Magnesium silicide (Mg_2Si) and its solid solutions exhibit excellent thermoelectric properties. Being non-toxic and composed of readily available elements, it is a promising candidate for the development of highly efficient, environmentally friendly thermoelectric (TE) generators. [1] While for p-type Mg2Si the implementation of Ag contacts was shown to exhibit exceptionally low contact resistance and good adhesion, the suitability of Ag as an electrode for n-type Mg_2Si is significantly worse, presumably due to a poisoning of the Mg_2Si by Ag ions. Although energy dispersive X-ray spectroscopy (EDX) has verified the diffusion of Ag into Mg_2Si and Transient Potential & Seebeck Microprobe (TPSM) measurements reveal a change in the Seebeck coefficient in the TE material close to the interconnection zone (IZ) [1], a full understanding of the complex local diffusion mechanisms at the IZ requires a nano-scale analysis.

Here we use Kelvin Probe Force Microscopy (KPFM) to evaluate the complex evolution of diffusion gradients at the TE/metall interface by mapping the contact potential difference (CPD) on a nanometer scale [2, 3]. We found that in highly Bi-doped Mg_2Si the Ag poisoning is clearly apparent in the KPFM measurements by a continuous decrease in the CPD within the Mg_2Si towards the interface (Fig. 1). Suprisingly, the CPD reveals a pronounced local maximum near the IZ, indicating the complexity of overlaying interdiffusion mecha- nisms. Higher resolution images of the IZ show characteristic dif- fusion patterns between the various distinct phases formed at the IZ.

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This work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - 520487260.

Thermal conduction in free-standing monolayer MoS_2 and its nanoscroll

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Keywords: Thermal conduction; Flexural phonons; MoS2; Monolayer; Nanoscroll.

In two-dimensional (2D) materials, flexural phonons of out-of-plane lattice vibration in monolayer are of interest for heat conduction in thermal management and thermoelectrics. Typically, above Debye temperature, thermal conductivity κ_L) in solids is governed by phonon-phonon interaction (Umklapp process) with high density of phonons, resulting in κ_L has a relationship of $\sim T^{-1}$. Here we reported the thermal conductivity measurement for atomic-scale free-standing monolayer molybdenum disulfide (MoS_2) using suspended thermal bridge method, based on a micro-electro-mechanical system (MEMS) for steady-state heat conduction. It is found that the monolayer MoS_2 has a nearly temperature-independent κ_L above 200 K, governed by the out-of-plane flexural lattice vibrations in monolayer. As a comparison, κ_L of MoS_2 nanoscroll, rolled up from the monolayer, is more intensively decreased with elevated temperature, due to strong phonon-phonon interaction. The findings offer a platform to control heat flow in monolayer 2D materials, and shed light on potential exploration of atomic-level thermoelectrics.

Acknowledgments
This work was sponsored by Shanghai Pujiang Program (No.20PJ1411100) and ShanghaiTech University Starting Fund.

Electrical transport and Seebeck measurements in highly disordered channels buried in diamond

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Keywords: implanted diamond, buried conductive channel, electronic conductance, Seebeck coefficient, electron-phonon interaction, phonon-drag, thermoelectricity

An important parameter in thermoelectricity is the Seebeck coefficient, which plays a significant role in the figure of merit and must be enhanced to improve thermoelectric efficiency (zT=Seebeck²·electrical conductivity/thermal conductivity). Known effects that enhance the Seebeck coefficient include drag interactions between electrons and phonons, known as the "phonon-drag" effect, under the influence of an electric current (Peltier effect) or a temperature gradient (Seebeck effect). However, the enhancement of the Seebeck coefficient due to the phonon-drag effect typically occurs within the temperature range where lattice thermal conductivity is at its maximum. A fundamental challenge would be to explore new concepts for disentangling phonon-drag effects from the high values of lattice thermal conductivity and to determine whether a large phonon-drag effect can coexist with low lattice thermal conductivity. In our work, we investigate the phonon-drag effect at an interface where the electron and phonon gases belong to different media. The model system under study consists of an implanted diamond structure, where a conductive channel is buried beneath the diamond surface through ion implantation. We examined the temperature dependent electrical conductivity and Seebeck coefficient in samples implanted under varying conditions and subjected to different annealing temperatures. The results revealed different conduction mechanisms influenced by implantation and annealing conditions, which directly impact the microstructure of the conductive channel. In a recent publication [1], we demonstrated that the low temperature electronic transport properties of the conductive channel, graphitized through high temperature annealing, exhibit behavior very similar to bulk graphite. We also investigated the surface acoustic waves that propagate in the diamond layer at the top of the conducting channel [2]. In this presentation, after introducing the system and recalling our initial findings, I will present our latest measurements obtained as a function of annealing temperature, which highlight an original electronic transition followed by an intriguing behavior of the Seebeck coefficient [3].

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ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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19TH SESSION
SOLAR -TEG

Temperature-driven electrochemical separation of oxygen

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Keywords: thermoelectric unicouples, oxygen transport membranes

The separation of oxygen from air is of significant interest for the production of high- purity oxygen and has potential applications in reducing carbon dioxide emissions. However, the high energy demand of conventional separation processes remains a major drawback. In this study, we propose a novel method for oxygen separation from air by exploiting the synergy between thermoelectric phenomena and oxygen transport membranes (OTMs). To this end, a theoretical model was developed to identify the most promising thermoelectric materials capable of enhancing oxygen production through OTMs. Based on the modeling results, two series of materials were synthesized and characterized: p-type $Ce_{0.8}Gd_{0.2}O_2$-based oxygen transport membranes and n-type ZnO-based thermoelectric materials. For experimental validation, the p-type membranes and n-type thermoelectric materials were connected in series to form thermoelectric unicouples. The measured oxygen flux density ranged from 0.17 to 0.25 mL s^{-1} m^{-2} under a temperature gradient of 100 °C (with cold and hot sides at 600 °C and 700 °C, respectively), confirming the feasibility of oxygen production via the proposed thermally driven electrochemical system. This proof-of-concept demonstrates a self-powered approach to oxygen generation, which holds considerable promise for applications in sustainable energy systems and environmental protection.

Acknowledgments
This work was supported by the Foundation for Polish Science (TEAM-TECH/2016-2/14 Grant "*New approach for the development of efficient materials for direct conversion of heat into electricity*", co-financed by the European Union under the European Regional Development Fund.

Thermoelectric-Based Energy Harvesting System with Integrated Electromagnetic Induction Unit

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Keywords: thermoelectric module, magnetic induction, Seebeck coefficient

Thermoelectric generators produce electrical energy when hot temperature is applied to one side and cold to the other. This temperature gradient can be provided directly by direct heat transfer, but it can also be provided indirectly from the outside. One of these effects is achieved by applying a changing magnetic field to the generator from the outside with the magnetic induction method. If ferromagnetic particles are placed on one side of the thermoelectric material during the change of the magnetic field, heat energy will be generated by the Eddy Currents that will form inside these particles. This heat produced on one side of the thermoelectric material causes a temperature increase in the part where the ferromagnetic particles are located. Electrical energy will be generated by the temperature difference between the high-temperature side and the low-temperature side [1]. Previously, on these subject experiments were conducted on a single thin film. In this study, the same effect was created on thermoelectric pairs and energy was obtained.

The value of the voltage to be obtained can be increased by using p and n type thermoelectric materials together. In fact, this application is increased sequentially to form thermoelectric pairs and allows the voltage obtained to be increased in proportion to the number of pairs. In this study, 1% PEDOT:PSS was used for the p-type leg and 1% PEDOT:PSS + 30% Ag_2Se mixture was used to obtain the n-type leg. PEDOT:PSS based thermoelectric pairs were printed on PDMS using an injector. The thermoelectric module was produced with a thermoelectric pair by magnetic induction effect. As a result, the generated voltage between the legs is measured. In this way, applications that will provide contactless energy acquisition, especially for wearable and implantable applications, will be developed.

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Personalized Thermal Management through Thermoelectric Technology and Textile-based Heat Exchange Systems

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Keywords: Personal Cooling; Integrated Thermoelectrics; Thermoelectric Cooling Applications; Wearable Thermoelectrics

Recent complications of the energy crisis as well as climate change have sparked a growing interest for the development of cutting-edge, energy-saving systems for individual thermoregulation. Traditional methods for indoor climatic management, such as heating, ventilation, and air conditioning, require large amounts of energy. As a result, the direction is focusing on personal thermoregulation solution alternatives that meet the particular requirements of individuals since thermal comfort levels may be extremely varied. Personal cooling systems can potentially lower the energy requirements of the air conditioning system by a large amount, with the added bonus of being mobile, providing also relief for people involved in outdoor work or activities.

This work presents a solution developed in the context of the INAIL-BRIC ID39_2022 SMART-SHIRT project (SMART materials and technologies for thermal-stress & physio-monitoring SHIRT) for improving thermal regulation for workers in high-temperature working environments. The system captures biometric information in real time using sensors embedded in a t-shirt. The thermoelectric heating and cooling system responds to this information input, helping to stabilize the thermal stress of the worker.

The design of the thermoelectric system is determined by several factors, including the efficiency of heat exchangers made from 3D textiles and the need for the device to be wearable without restricting the user's mobility. The current stage of the project is concerned with overcoming challenges related to the integration of the system into clothing, ensuring it is lightweight and not obtrusive, while being effective. In addition, a benchmark system is being developed to test the thermal management of the device. The present work shows the preliminary results on the project development focusing on the different issues faced during the designing of the system.

Acknowledgments
This work was supported by the INAIL-BRIC ID39_2022 SMART-SHIRT project.

Concept of Solar Tri-generation Using Cold-Side Time-Modulated Heat Withdrawal

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Keywords: Solar harvesting, co-generation, time-modulated thermoelectric generators

Hybrid solar generation has been the subject of several investigations [1], including co-generation pairing photovoltaic cells and thermoelectric generators [2]. Tri-generation, using low-enthalpy heat released by the thermoelectric stage, has been considered only in high-concentration solar plants, mostly addressing heat toward Stirling engines [3]. No attempt was reported considering the use of low-temperature heat in roof-top solar generators, where solar concentration is typically ≤ 5 suns. In a recent paper [4], we showed how heat flux modulation may largely increase TEG efficiency at maximum power. In this communication we discuss the concept of a roof-top hybrid tri-generation solar converter using PV cells paired to a TEG stage, with TEG cold side cooled by a heat exchanger whose transfer coefficient is time-modulated. This significantly enhances TEG power generation, up to 50 %. Low-temperature heat released by the TEG is finally used to produce sanitary (hot) water. System efficiency will be reported, considering PV cells based either on conventional polycrystalline silicon or perovskites while using commercial-grade bismuth telluride TEGs.

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Acknowledgments

We acknowledge the financial support by the Italian Ministry of Environment & Energy Security (MASE) through the Program Agreement between ENEA and MASE, Three–Year Realization Plan of the Electrical System Research 2022–2024, Project 1.4, 'Frontier materials for energy uses' (contract number I53C22003040001).

The Impact of Electrical Connections on Maximum Power Point Tracking within Hybrid Photovoltaic-Thermoelectric Devices

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Keywords: Thermoelectric generator, photovoltaic, photovoltaic-thermoelectric hybridization, electrical connection, electronic interface

The thermoelectric generator (TEG) converts heat energy to electrical energy through the Seebeck effect. This abilty is especially useful in the valorization of waste heat, and is already being applied in several applications [1]. In the case of photovoltaic (PV) cells, the heat energy produced through the interactions with photons can be valorized. Indeed, the PV and TEG can be thermally coupled forming a hybridized photovoltaic-thermoelectric device (PV-TE). This way, the PV can generate electrical energy normally and the waste heat it generates can be converted by the TEG. To use this PV-TE device in practice, it requires an electronic interface which is responsible for maximum power point tracking (MPPT). The design of this electronic interface is dependant on the electrical connection between the PV and TEG sources. The three possible connections are the parallel, series, and electrically isolated. Each connection has their merits and disadvantages [2]. The parallel connection has the constraint of requiring each electrical branch to have the same voltage. The series connection has a similar constaint but in this case, the current through the TEG and PV sources is the same. There is also a common problem with both the series and parallel connection. Since the TEG and PV sources have such different natural electrical power versus voltage characteristics, both sources can never operate at their maximum power points simultaneously (considering the sources are of a similar size in the hybrid PV-TE device). This is not the case for the electrically isolated connection where MPPT can occur separately for both sources at the same time. There are several ways to optimize each electronic interface for each corresponding electrical connection to improve their performances. In the presentation, the impact of the electrical connections on the electronic interface design will be discussed and more detailed, with an emphasis on the advantages and drawbacks for each one.

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Acknowledgments

This work was supported by the French National Research Agency (ANR-21-CE50-0003).

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PART IV
CONTRIBUTED TALKS

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20TH SESSION
ADDITIVE MANUFACTURING

Laser Sintering of Thermoelectric Chalcogenides Nanopowders

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Keywords: Laser sintering, Thermoelectric chalcogenides, Thermoelectric powder processing.

With the introduction of additive technologies based on the growth of 3D structures by locally melting a material wire or powder, the interest in the development of solutions for the processing of materials confined volumes has increased. Lasers, with their unique characteristics of high-energy density, well-defined beam shape and size and precise scanning control are perfect soluitions for the development of such technology. In recent years, different systems based on a laser heat source have been developed for the material processing following a predefined design to produce highly complex objects. The solutions developed are mainly associated to a fast melting of materials powders to promote the direct building of 3D structures obtained by consecutive layers sintering or soldering. The versatility of laser sources enables the capability to process not only low melting materials, like polymers, but in general most of the available materials including metals and alloys Usually, the main issue for the laser processing is related to the constraints on the characteristics of the material to be processed. Such limits critically affect, to date, the capability of processing thermoelectric powders so, only few research groups reported successful results on laser processing of thermoelectrics.

In this work, the results achieved on the processing of thermoelectric chalcogenide nano-powders are reported. A setup equipped with an automated position controller has been developed to process a bed of powders with a low power laser source following a specific pattern. The system is designed for the processing of a single layer of nano-powders preventing oxidation and evaporation of the material. Different processing parameters have been explored to understand the dynamics of the sintering process in the material.

Silicon Germanium alloys developed by additive manufacturing: influence of thermal treatments

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Keywords: SiGe; additive manufacturing; power bed laser fusion; thermal treatment.

For 10 years, the development of Additive Manufacturing (AM) technologies has considerably increased, mainly due to optimized tools and processes. AM technologies are mainly focused on metals and polymers materials development. Among the various AM methods, Laser Powder Bed Fusion (L-PBF) stands out as a prominent approach for printing complex metal parts in small to medium series. Recent advancements in L-PBF processing have paved the way for the fabrication of novel materials, including thermoelectric (TE) materials such as bismuth telluride [1], Half-Heusler [2] or SiGe [3]. Moreover, this technique offers 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., despite tools processes are not fully adapted to these materials. Nevertheless, such techniques for these TE materials usually induce mechanical cracking occuring during L-PBF processing due to material induced stresses, and impacting highly TE properties.

Our work presents the development of silicon germanium alloys TE material, tailored for high temperatures applications. We will present here that thermal treatments can limit the presence of cracks inside SiGe and increase their TE properties.

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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).

Additive screen-printed 3D thermoelectric generators for energy harvesting

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Keywords: Printed thermoelectrics, energy harvesting, IoTs, Ag_2Se, Bi-Sb-Te

The demand for renewable energy, propelled by growing use of electronic equipment, and rapid industrialization is increasing significantly. Electronic devices and systems forming the backbone of digitalization such as wearable devices, Internet of Things (IoT), and Industry 4.0 systems, consume a growing portion of the global primary energy, with largely relying on lithium-ion batteries [1]. To enable a sustainable alternative, we explores cost effective fully printed, shape-conformable thermoelectric generators (print-TEGs), which can convert low grade heat into electrical energy and be an alternative to batteries in low-power electronics, thereby lowering electronic waste and reliance on battery production [2]. Conventional bulk TEGs, while capable of waste heat conversion, have seen limited customization and scalability for such applications, challenges that can be addressed through low-cost printing process [3]. We here report a promising additive screen-printing method together with low-temperature processing and interface engineering to fabricate two 3D TEGs with a different number of thermocouples, overcoming high contact resistance and thickness limitation. As a result, our fully printed 3D print-TEGs yield a milliwatt-scale power at low thermal gradient. The print-TEGs are prepared via layer-by-layer printing of bottom electrodes, carbon interlayers, TE legs, carbon interlayers, and top electrodes with different layouts. Here, printed Ag_2Se n-type legs and $Bi_{0.5}Sb_{1.5}Te_3$ p-type legs have been used for TEG fabrication. To attain the desired thickness, the p- and n-type legs were printed multiple times via an additive screen-printing process. The 3D print-TEG II with 50 thermocouples generates a power of 1.21 mW for ΔT = 43 K, rendering this device suitable for powering sensor systems. Compared with the existing fully printed TE devices, the print-TEGs with just a fill factor of 0.36, shows the highest-ever normalized power densities of 40 $nWcm^{-2}K^{-2}$ for a fully printed planar TEG. The print- TEGs can be employed to facilitate a steadfast power source for remote areas where access is limited, eradicating the necessity for frequent battery replacements and guaranteeing nonstop operation of electronic devices in challenging environments.

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Acknowledgments

The authors acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) and we acknowledge funding by the European Research Council, grant 101097876 - ORTHOGONAL.

Tailoring the microstructure and thermoelectric properties of CuNi and NiCr by laser powder bed fusion

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Keywords: additive manufacturing, microstructure, laser powder bed fusion, CuNi, NiCr

Thermoelectric devices provide a promising approach for energy harvesting and active cooling by converting thermal into electrical energy and vice versa. However, conventional manufacturing methods limit their integration as well as design, and alternative methods need to be explored to extend their field of application. One potential solution is offered by additive manufacturing technologies like laser powder bed fusion (PBF-LB/M), which enables the direct and rapid fabrication of complex and customized metallic structures in a layer-by-layer process. These methods significantly minimize material waste and production time compared to conventional manufacturing of legs for thermoelectric applications.
In the present contribution, we present the additive manufacturing of thermoelectric legs utilizing laser powder bed fusion. To address the demands for non-toxic and environmentally friendly thermoelectric modules, this work focuses on the earth-abundant metallic alloys CuNi as n-type and NiCr as p-type. We directly fabricated bulk samples from powders of both alloys based on process parameter optimization. The investigations show that thermoelectric properties such as electrical and thermal conductivity and the Seebeck coefficient can be tailored by adjusting the process parameters. Furthermore, employing different build strategies results in microstructural changes and an enhancement of the thermoelectric performance. For analyzing the microstructural characteristics, various techniques, including optical microscopy, scanning electron microscopy, electron backscatter diffraction and X-ray diffraction, were combined.
Concluding, this work demonstrates the highly effective application of laser powder bed fusion as a manufacturing method for thermoelectric materials. It offers the opportunity to customize material properties and meet the demands of advanced applications.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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21ST SESSION
NANO-MATERIALS

Scalable Solution Chemical Synthesis of Nanostructured Thermoelectric Materials

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Keywords: Thermoelectric materials, Microwave-assisted heating, Solution chemical synthesis, Nanostructuring.

Thermoelectric (TE) materials, which enable the direct conversion of thermal energy into electricity, hold significant potential for sustainable energy applications. Despite their promise, challenges persist in the form of costly routes, synthetic processes, and batch-to- batch variations in performance. The pursuit of high-performance thermoelectric materials has driven researchers to investigate a range of fabrication methods. The development of scalable synthesis methods capable of producing high-quality nanostructured TE materials on a large scale with consistent performance is crucial for advancing TE technologies and TE devices. To address these challenges, this study introduces simple, high-throughput solution-based synthesis approaches, employing a microwave-assisted heating process, which leverages energy-efficient volumetric heating providing high-yield and reproducibility.

Solution synthesis is considered a bottom-up synthetic method that promotes maximum yields and minimal waste and is an effective method to control the morphology and surface chemistry of the synthesized nanostructured materials. Hydrothermal, polyol, and thermolysis are the main approaches used for synthesis in this work, as each solvent and precursors impact characteristic morphology, crystallinity, and surface chemistry of the particles formed [1,2]. The synthesis and characterization of n- and p-type TE materials are presented, with evaluation of their structural, morphological, and thermoelectric transport properties.

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Acknowledgments

This work was supported by the Latvian Council of Science project No.1.1.1.9/LZP/1/24/043.

Solution-based synthesis of inorganic metal chalcogenide particles: Methods and thermoelectric properties analysis

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Keywords: Bismuth telluride, Nanostructured thermoelectrics, Kirkendall diffusion, Glucose-mediated synthesis

Solution synthesized thermoelectric materials have gathered significant attention over their bulk counterparts due to their ability to precisely control the morphology, crystal structure and surface chemistry of the particles which in turn enhances the thermoelectric figure of merit, defined by $ZT = S^2\sigma T/(\kappa_e+\kappa_l)$, where, S indicates seebeck's coefficient, σ is the electrical conductivity, κ is the thermal conductivity (κ_e is the electronic and κ_l is the lattice contributions) and T is average absolute temperature.[1] Nevertheless, several solution-based methods suffered constraints owing to utilization of either harsh reducing agents[2], expensive instrumentation[3] or elevated reaction temperatures[4]. Thus, hindering the reproducibility and scalability.

Given the exceptional thermoelectric properties and widespread commercial use of Bismuth telluride and its derivatives, in our current endeavor, we have narrowed-down our efforts on development of mild, simple, scalable and cost-effective solution-based synthesis strategies to modify the nanostructures of bismuth telluride and its derivatives. Binary Bi_2Te_3 nanotubes were synthesized via an aqueous method[5] employing 1-dodecanethiol as both reducing and capping agent. While ternary $Bi_2Te_{3-x}Se_x$ and $Bi_{2-x}Sb_xTe_3$ nanodiscs were prepared by polyol method[6] using D-glucose as both reducing as well as capping agent. This study demonstrates an improvement in thermoelectric efficiency at room temperature, highlighting the potential of solution-processed thermoelectric materials.

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Acknowledgments

This work is supported by the Labex EMC3.

Seeking for high-performance Ag_2Se using a sustainable solution synthesis

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Keywords: Thermoelectric materials, solution processing, silver selenide, recycling, sustainability

Silver selenide (Ag_2Se) has been explored as one of the most promising candidates for room-temperature thermoelectric applications. Among the different synthetic methods available, a solution-based approach based on an amine-thiol solvent system has provided unique opportunities to control material stoichiometry and microstructure, yielding to zT around 1.2 from RT to 100 °C [1,2].

Despite the effectiveness of this synthetic strategy, the use of amine-thiol solvents represents a significant drawback in terms of environmental sustainability and feasibility for large scale production. The consumption of large volumes during synthesis and purification is concerning, considering both the costs and the difficulty in handling these solvents. In fact, the amine-thiol mixture is very malodourous, corrosive, inflammable, dangerous for the environment, and characterized for both acute and chronic toxicity, in case of repeated exposure.

Herein, we'll present the investigation regarding the precursors' chemistry and the developed strategy that dramatically reduces the consumption of the amine-thiol mixture - replaced with more sustainable solvents - yielding a material with a comparable figure of merit.

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Acknowledgments

This work was financially supported by ISTA and the Werner Siemens Foundation.

Enhancement of Thermoelectric and Flexibility Performance of Bi-Sb-Te Thin Films via $MAPbI_3$ Composite Strategy

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Keywords: Bi-Sb-Te thin films; $MAPbI_3$, Organic-inorganic hybrid composites, Thermoelectric, Devices.

Achieving high thermoelectric (TE) performance and flexibility is essential for wearable electronics. Here, an organic-inorganic hybrid strategy incorporating methylammonium lead iodide ($MAPbI_3$) into Bi-Sb-Te thin films enhances both TE and mechanical properties. The incorporation of $MAPbI_3$ into Bi-Sb-Te thin films introduces micro strain, which effectively tunes the crystallographic orientation by increasing the proportion of (00*l*) planes, thereby enhancing carrier mobility. Simultaneously, interfacial doping effects contribute to the modulation of carrier concentration. These combined effects lead to significant improvements in the electrical transport properties of the films. In addition, the introduced defects, such as large angle grain boundaries and dopant atoms, serve as strong phonon scattering centers, resulting in suppressed thermal conductivity. These synergistic effects contribute to the optimization of the zT from 0.08 to 0.94 in Bi_2Te_3 and 0.20 to 0.47 in Sb_2Te_3 at 250 °C. Moreover, the $MAPbI_3$ composite strategy reduces the Young's modulus of Bi-Sb-Te films, thereby enhancing their mechanical flexibility. Flexible devices fabricated from the composite films exhibit output performance consistent with the finite element simulations, demonstrating their potential for flexible thermoelectric applications.

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Acknowledgments

This work was partially supported by the European Union through the European Regional Development Fund (ERDF), the Ministry of Higher Education and Research, the 147rench region of Brittany and Rennes Métropole, through the CPER Verre and CPER Photbreizh.

Induction melting synthesis of Mg-based thermoelectric materials

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Keywords: Magnesium-based, Induction-melting, Optimization

Magnesium-based thermoelectric materials have gained a new interest in recent years due to the search for more sustainable, cheap and reliable materials for near-room temperature applications. Despite being promising materials for thermoelectrics, magnesium is a tricky element, requiring fine tuning and careful handling, being highly reactive.

In this work, induction melting synthesis, followed by a uniaxial hot-pressing, was used as a new route for producing p-type MgAgSb and n-type $Mg_2(Si,Sn)$, to obtain a fast, efficient and easily scaled-up production method, to meet industrial demands. By optimizing it, this novel pathway allows to obtain robust thermoelectrics with good performance, which could unravel and take a step forward to increase commercial thermoelectric-based modules availability.
Hitherto, the synthesis has been optimized to require less than six minutes from the raw elements to an ingot of the desired material. The following hot-press sintering varies according to the composition, taking one hour for n-type and two hours for p-type. All theses stages were made under argon atmosphere.

The n-type $Mg_2Si_{0.385}Sn_{0.6}Bi_{0.015}$ sample exhibited a remarkable performance, with an average PF_{avg}=36.3 $\mu W.cm^{-1}K^{-2}$ and zT_{avg}=0.92 from 315 K and 525 K, the best thus far.
The p-type samples sintering step still requires further tuning to achieve similar results, the best sample being $MgAg_{0.955}Sb_{0.985}$, with an average PF_{avg}=13.0 $\mu W.cm^{-1}K^{-2}$ and zT_{avg}=0.34 for the same temperature range. This lower performance can be attributed to an excess of secondary phases, such as Ag_5Sb, that increases lattice thermal conductivity and leads to an excess of charge carrier concentration. Furthermore, poor grain aggregation was observed, which increased electron scattering around the grain boundaries ergo diminishing carriers mobility.
Further strategies to reduce secondary phase formation and increase material homogeneity will be discussed and analyzed.

Acknowledgments
This work was funded by Portuguese funds through the FCT—Fundação para a Ciência e a Tecnologia, I.P. under the projects PRT/BD/153039/2021 and UID/Multi/04349/2019.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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22ND SESSION
DEVICE IV

Development of Reliable Interfacial Barrier for Low-Cost Argyrodite Thermoelectric Module

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Keywords: Diffusion barrier, Cu-based argyrodite, thermoelectric module, material integrity

Thermoelectric (TE) materials offer a promising prospect for sustainable energy conversion [1]. Cu-based argyrodite materials are gaining significant attention for their high thermoelectric performance [2]. However, their commercial viability is limited by issues such as material degradation, interface instability, and diffusion at elevated temperatures. Diffusion barriers play a critical role in ensuring the stability of TE modules under operating conditions [3]. An ideal barrier material should exhibit low contact resistance, strong adhesion, and thermal stability to improve both efficiency and reliability. Despite their potential, research on argyrodite-based thermoelectric modules remains relatively unexplored and underdeveloped.This study focuses on developing low-resistance, reliable diffusion barriers to overcome these challenges. Specifically, it investigates the interdiffusion behavior at the barrier material/argyrodite TE interfaces using materials like Fe, Nb, and steel. The goal is to identify the most effective barrier for Cu-based argyrodite compounds such as $Cu_8SiS_xSe_{6-x}$ and $Cu_7P(S_xSe_{1-x})_6$. The diffusion barrier materials were analyzed in argyrodite samples with the structure M/ML/$Cu_7P(S_{0.55}Se_{0.45})_6$/M (Where M represent Fe.Nb and steel and ML denotes a mixed layer of barrier materials with p-$Cu_7P(S_{0.55}Se_{0.45})_6$ in 50:50 volume ratio). The TE joints were fabricated by sintering the barrier materials, mixed layer, and argyrodite powder in a graphite die via one-step pulsed electric current sintering (PECS) at 983 K for 30 minutes under 60 MPa longitudinal pressure. The joints were then sectioned to the required dimensions using a wire-saw for subsequent characterization. The interface microstructures of the fabricated samples, contact resistance along with their Seebeck mapping, were examined and compared.This study unveils the potential of cost-effective argyrodite-based thermoelectric modules through the development of efficient diffusion barriers.

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Acknowledgments

This research work supported by the program "Excellence Initiative - Research University" (IDUB) for the AGH University of Krakow, Action 4, ID 12493 and the National Science Centre (NCN) within the framework of the research projects “WEAVE-UNISONO” UMO-2022/04/Y/ST5/00139.

Effect of gamma radiation on Mg-based thermoelectric materials

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Keywords: Magnesium-based thermoelectrics, Gamma radiation effects

Thermoelectric materials can directly convert heat into electricity and vice versa, making them a promising solution for power generation and thermal management in a variety of applications. A possible use is in environments with high doses of ionizing radiation, such as Space or nuclear reactors. In fact, conventional thermoelectric materials, like Si-Ge solid solutions, have been used since the 1960s in radioisotope thermoelectric generators (where heat is generated by the decay of a radioactive isotope), and are relatively insensitive to radiation damage [1].

Good thermoelectric materials for near room temperature applications are still scarce and require further studies. Recently, new thermoelectric materials based on magnesium, like $Mg_2(Si,Sn)$ and MgAgSb, have gained major attention due to their high performance, good sustainability, low toxicity, and reduced cost, being promising candidates for such applications. However, no studies were made on how ionizing radiation affects their properties.

This work presents a preliminary investigation on the effects of γ radiation on Mg-based thermoelectric materials. Samples of n-type $Mg_2(Si,Sn)$ and p-type MgAgSb-based were synthesized and exposed to different doses of γ radiation. Structural characterization, by X-ray diffraction (XRD), and scanning electron microscopy (SEM), coupled with energy dispersive X-ray spectroscopy (EDS), were performed before and after irradiation. Results indicated changes in the surface microstructure of the samples irradiated in air, while in vacuum no visible modifications were seen. Thermoelectric properties (Seebeck coefficient, electrical and thermal conductivity) measurements were also performed from 315 K to 525 K and their impact on the thermoelectric performance under such environments was evaluated.

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Acknowledgments

This work was funded by Portuguese funds through the FCT—Fundação para a Ciência e a Tecnologia, I.P. under the projects PTDC/EAM-PEC/29905/2017 and UID/Multi/04349/2019.

Oxidation of skutterudites and their protective coatings: a comparative study

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Keywords: Skutterudites, Thermoelectric performance, Oxidation resistance, Synthesis methods, Protective coatings

Skutterudites based on $CoSb_3$ show a great potential for mid-temperature applications due to high thermoelectric performances, with ZT values nearing 2 in optimized compositions [1]. The various possible substitutions/insertions in their crystal structure not only enables the creation of both n-type and p-type materials but also facilitates precise adjustments of their transport properties. This versatility makes skutterudites particularly interesting for the manufacturing of modules, as they can be engineered from a common base material. For example, their unique properties have led to consideration for use in RTGs, which are pivotal for space exploration and remote power generation. However, a significant drawback to their widespread industrial application is their vulnerability to oxidation at their operational temperatures when exposed to air. This susceptibility poses challenges for long-term performance and reliability, necessitating further research and development to improve their stability in practical applications.

In this presentation, n-type skutterudites $In_xCo_4Sb_{12}$ synthesized via two distinct methods, melting/annealing and magnesiothermy [2,3], will be compared to elucidate how differences in synthesis process affect their oxidation behavior. Then we will show how we used commercially available protective layers, deposited by dip coating, for shielding skutterudites from oxidation. Aging results obtained at 650 K in air for both n-type and p-type skutterudites will be presented, benchmarking these findings against state-of-the-art.

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Oxidation Behavior and Integration into High Power Density Thermoelectric Generators of Commercial Half-Heusler Alloys

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Keywords: Thermoelectric materials; Half-Heusler alloys; High-temperature oxidation; Thermoelectric generators; Power density; Thermal stability.

Half-Heusler (HH) alloys are among the most promising thermoelectric materials for high-temperature applications, capable of stable operation beyond 700 °C. Their robustness, mechanical strength, and thermoelectric performance make them ideal candidates for power generation in harsh environments. In this study, we investigate the oxidation behavior of two commercial HH alloys: an n-type $Hf_{0.6}Zr_{0.4}NiSn_{0.98}Sb_{0.02}$ and a p-type $Hf_{0.2}Zr_{0.75}Ti_{0.05}CoSb_{0.8}Sn_{0.2}$. Using thermogravimetric/differential scanning calorimetry (TG/DSC), scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM/EDXS), and powder X-ray diffraction (PXRD), we examine their thermal stability and oxidation mechanisms under air exposure.

Our findings show that the n-type alloy undergoes a two-stage oxidation: a slow increase in mass up to 350 °C, followed by rapid antimony oxide (Sb_4O_6) volatilization, which leads to the formation of a hollow core-shell microstructure. In contrast, the p-type alloy forms a stable surface oxide layer, with minimal mass loss and no significant structural degradation.
To assess real-world performance, we fabricated a two-couple thermoelectric generator (TEG) using these materials, with a leg height of 2.0 mm. The assembled device demonstrated an impressive power density of 7.5 $W \cdot cm^{-2}$ at a temperature gradient of $\Delta T = 575$ K, confirming the potential of these HH alloys for high-power-density energy harvesting in oxidizing atmospheres.

Comprehensive Insights into the Carbon Footprint and Energy Intensity of Thermoelectric Generator (TEG) Production through Life Cycle Analysis

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Keywords: Sustainability, life cycle analysis, TEG, advanced thermoelectric materials

This study evaluates the sustainability of thermoelectric generators (TEGs) through a life cycle assessment of BiTe, PbTe, and SiGe-based TEGs operating at different temperature ranges. Environmental impacts were analyzed by modeling elemental extraction, synthesis, and manufacturing processes, but excluding end-of-life considerations due to the long lifespan of TEGs and lack of data on recycling processes. The energy required for manufacturing ranged from 100-800 MJ, leading to CO_2 emissions of 4-90 kg, depending on material composition. Energy-intensive processes were identified, and the resulting energy payback time varied accordingly [1]. PbTe-based TEGs at mid-range temperatures showed the most promise due to lower energy demand and emissions. However, payback times exceeded 20 years in most cases, with variations from 19 to over 200 years depending on usage and temperature differences. Increasing the temperature gradient could reduce this to as low as two years [2]. These findings highlight the need to consider both material selection and operational conditions when assessing TEG sustainability. The optimal operating range of 200-300 °C aligns with limited application cases in industry, meaning that either a different purpose for TEGs with short energy payback can be sought, or anticipated long-term functioning of several decades should be planned for [3].

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Acknowledgments

This work was supported by Science Foundation Irland (SFI) and Trinity College Dublin (Ireland).

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PART IV
CONTRIBUTED TALKS

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23RD SESSION
LATTICE DYNAMICS II

Stability and lattice dynamics of thermoelectric type IX Clathrates

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Keywords: clathrates, lattice dynamics, ab initio, neutrons, pressure

Structural complexity of the unit cell is recognized as an efficient route for reducing the thermal conductivity without impacting on the electronic conduction of crystals.This is precisely the reason for which the so-called clathrate structures, guest-host structures, have been widely investigated in the field of thermoelectricity. The type I clathrates are well-known for their very good thermoelectric properties with a a maximum ZT as large as 1.35 at 900 K for n-type $Ba_8Ga_{16}Ge_{30}$ [1]. It contains two types of cages and has a thermal conductivity of less than 2 $W.m^{-1}.K^{-1}$.The type IX clathrates such as $Ba_{24}Ge_{100}$ and $Ba_{24}Si_{100}$ have three different cages in which Ba guest atoms are intercalated. $Ba_{24}Ge_{100-x}Ga_x$ is the clathrate compound with the lowest lattice thermal conductivity (about 0.3 W/m.K) and has ZT reaching 1.25 at 950 K [2]. In $Ba_{24}Ge_{100}$ there is a structural transition involving significant changes in the charge density of the guest Ba atoms whose microscopic mechanism is not understand yet. All these physical properties are driven or take influence on the lattice dynamics of $Ba_{24}Ge_{100}$.Thus, the phonon properties require a better understanding, especially the dynamics of the guest Ba atoms.

In the present work, we report a combined experimental and theoretical study of the stability and the lattice dynamics properties of $Ba_{24}X_{100}$ (X = Si, Ge). $Ba_{24}Si_{100}$ can be obtained under high pressure-high temperature (HP-HT) conditions or by mechanical alloying and its formation mechanism is studied with in-situ synchrotron HP-HT X-ray diffraction experiments as well as its P-T stability domain and how it decomposes at room pressure. The stability of both clathrates is studied with DFT calculations which show that not only pressure but also vibrational and electronic entropies are needed to stabilize Ba24Si100. We investigate the effect of the host cage structure on the low energy vibrational dynamics in both type IX clathrates by combining inelastic neutron scattering and ab initio simulations. We evidence the existence of guest vibrational modes at about 3 meV in both compounds, but with some finer structures in the Si clathrate. We show a strong anisotropy of the vibrations of Ba guests in the open and very asymmetric X20 cages, which is a general behavior in the type IX clathrates. In $Ba_{24}Ge_{100}$, there is a strong change in the spectral weight of these modes when the compound undergoes a temperature-induced structural transformation at about 190230 K.

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Phonon Transport in K_3SbS_4 Solid-State Battery Incorporating an Ion Diffusion Mechanism Using Machine Learning

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Keywords: Phonon Transport; K3SbS4; Machine Learning

Understanding the mechanisms behind potassium-ion transport is essential for designing rational strategies for advancing the field of solid-state batteries. Although phonon transport is at play in the exceptionally low thermal conductivity of solid-state batteries, the relationship between ionic transport and thermal properties has remained elusive. Here, we discuss ion diffusion and lattice dynamics in K3SbS4 using molecular dynamics simulations powered by a machine-learning interatomic potential with DFT level accuracy. Our analysis reveals that the contribution of coherence terms to thermal conductivity increases substantially because of the liquid-like movement of potassium atoms. Our study provides insight into the intricate atomic dynamics that governs transport in superionic conductors.

Acknowledgments
HL acknowledges the support by the National Science and Technology Council (NSTC) in Taiwan under grant number MOST111-2112-M-001-057-MY3. The work at Northeastern University was supported by the National Science Foundation through NSFExpandQISE award NSF-OMA-2329067 and benefited from the resources of Northeastern University's Advanced Scientific Computation Center, the Discovery Cluster, and the Massachusetts Technology Collaborative award MTC-22032.

Decoupling Thermoelectric Parameters in $CuCrO_2$: Role of Interlamellar Porosity via Zn^{2+}, Mg^{2+}, and Ni^{2+} Multi cation-Doping

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Keywords: Interlamellar porosity, Kirkendall effect, thermal conductivity

Introducing interlamellar porosity is of significant importance as it effectively influences the modulation of both the Seebeck coefficient and thermal conductivity. The layered structure and interlamellarpores emerge as a result of the diffusion of doping cations (Zn^{2+}, Ni^{2+}, and Mg^{2+}), which leads to the repositioning of Cr^{3+} in $CuCrO_2$ crystallites. The intricate structural evolution mechanism is elucidated through the Kirkendall effect and the presence of nanopores, as depicted in FESEM images, with sizes around 100 nm, hinders the movement of phonons, resulting in a minimal conductivity of 1.7 W/mKat 973 K.The achieved electrical conductivity of 4796 S/m at 973 K and the filtering effect of nanopores, along with spin alteration and resulting spin entropy, induced higher Seebeck coefficients of 400 µW/mK at 973 K. The highest power factor obtained here is 588 $\mu W/mK^2$, and the maximum achieved ZT, obtained by optimizing all thermoelectric parameters, is 0.33 at 973 K. We have successfully addressed the primary challenge of the interdependency between various thermoelectric factors and improved efficiency, achieving the highest value among Cu-based delafossites.

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Acknowledgments

Department of Science and Technology, Government of India for financial support vide reference no DST/WISE-PhD/PM/2023/17(G)- under the ‘WISE Fellowship for Ph.D’

Electron-phonon interaction-driven phonon transport attenuation above ambient temperature

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Keywords: electron-phonon interactions, phonon transport, lattice thermal conductivity, heavily doped semiconductor

While the electron-phonon interactions (EPIs) have been predicted to strongly suppress phonon transport and lattice thermal conductivity (κ_L) above room temperature, direct experimental validation remains challenging because the observed reduction of κ_L in the doped materials is commonly a result of concurrent enhancement of EPIs and point-defect-induced phonon scattering (PDPS). Here, we circumvent this ambiguity through strategically designed aliovalent-alloying semiconductors, where the compositional deviations from the parent compound amplify EPIs while weakening PDPS. Experimentally, we observed a pronounced EPI-driven κ_L reduction of ~50% at room temperature and ~40% even at 1000 K as carrier concentration approaches 1×10^{22} cm^{-3}. The carrier-induced phonon softening and the enhanced electron-phonon scattering rates collectively lead to this remarkable phonon transport attenuation. Our findings establish a quantitative framework for disentangling EPI effects on phonon transport in heavily doped semiconductors or metals, and provide insights into phonon engineering strategies for advanced thermal management materials design.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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24TH SESSION
THIN FILMS II

Thermoelectric Properties of $(MoO_3)_x$-doped C_{60} films

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Keywords: C60 film, MoO3 doping, thermoelectric properties, energy harvesting

Thermoelectric (TE) materials have been much attractive as a power generator for various wearable devices such as healthcare sensors and smart glasses. To harvest a waste-heat from human body, requriements of the TE materials are flexible and wearable in addition to high TE conversion. Molecule-based TE materials have advantages such as an ease for constructing flexible devices and a low thermal conductivity (κ) on the order of 10^{-1} W m^{-1} K^{-1}. Recently, some organic semiconductors were reported to emerge an extremely large Seebeck coefficient (α = 10−250 mV K^{-1}) when compared to that of conventional TE materials such as Bi2Te3 (α = 0.27 mV K^{-1}), which have been called as "Giant Seebeck Effect (GSE)" [1]. However, in spite of such the giant α and low κ, dimensionless figure-of-merit ($ZT = \alpha^2\sigma T/\kappa$, T: absolute temperature, σ: electrical conductivity) of those organic semiconductors was less than 10^{-4} owing to their extremely small σ of less than 10^{-7} S cm^{-1} at room temperature (RT). Although a typical way to increase the σ of molecular films is kown to be chemical doping of carriers, α values of less than 1 mV K^{-1} were reported for the doped-organic films.[1] This suggests that increasing the σ of organic semiconductor films while keeping the GSE is not so easy.

In this talk, we present high-performance properties of C60 films doped with trioxide (MoO3) nanoclusters. Although pristine C60 films exhibit an exceptionally large N-type α value (–121 mV K^{-1}), their power factor ($PF = \alpha^2\sigma$ = 2.3 × 10^{-6} W K^{-2} m^{-1}) is smaller by three orders of magnitude than that for practical use owing to a very low σ of 1.6 × 10^{-6} S cm^{-1} (see the green circle in Fig. 1). On the other hand, C60(MoO3)x films achieved a remarkable large PF (1.8 × 10^{-4} W K^{-2} m^{-1}) by increasing σ while maintaining the GSE, as shown in the red circles of Fig. 1. In addition, the C60(MoO3)x films exhibited P-type TE properties arising from the hole injection into C60 from MoO3 nanoclusters.[2] The $|\alpha|$–σ relationship of C60(MoO3)x films cannot be explained both quantitatively and qualitatively using the convention the present C60(MoO3)x nanocomposite films.

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Tailoring Defects in ScN Thin Films via Ion Implantation

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Keywords: Ion implantation, Defects, Scandium nitride

The ion implantation process creates non-equilibrium defects that can significantly impact the transport properties of materials, which is particularly important in thermoelectrics. It was shown on scandium nitride (ScN) thin films that the defects generated through ion implantation of noble gases were decreasing the thermal conductivity and increasing the Seebeck coefficient, thus increasing the zT [1,2]. In order to fully demonstrate the benefits of ion implantation for thermoelectric applications, it is of high importance to better understand and control the defects formation. The interest in ScN is Its power factor and its n-type degenerate state, caused by oxygen incorporated during deposition [3]. To deepen the understanding of defects, the films were implanted using oxygen ions as oxygen is the cause for the degenerate state of the as-implanted films [3]. We have shown on ScN films implanted at a high damage level (9 displacement per atoms (dpa)) and progressively annealed that two types of defects were produced, both acting as acceptor-type defects and as scattering centers [4]. We have demonstrated that the first type of defects modifies the conduction mechanisms, and the second type affect the density of states. To track defect formation and evolution, we employed a cumulative ion implantation process, allowing us to observe how defects accumulate and transform with increasing level of damage. In addition to electrical properties, the optical and structural properties were also characterized. In this study, we observed that even at the lowest ion implantation doses, the introduced defects act as scattering centers for charge carriers. Around 0.5dpa, a change in the conduction mode is observed from metallic-like to semiconductor. This is due to the accumulation of point-like defects, inducing localized states near the Fermi level up to a certain concentration. Finally, we see significant structural modification starting to appear at 1dpa. The aim is to link, as a function of the damage level, the defects generated with the doping and structural modification induced and their effect on the electrical properties.

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This work was supported by the French government program "Investissements d'Avenir" (EUR INTREE—Reference No. ANR-18- EURE-0010, LABEX INTERACTIFS—Reference No. ANR-11-LABEX- 0017-01, and UP-SQUARED—Reference No. ANR-21-EXES-0013).

Influence of electron-phonon coupling and phonon-drag effect at interfaces on the electronic and thermoelectric transport properties of thin films

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Keywords: Electron-phonon interaction, Seebeck, thin films, Molecular Beam Epitaxy, implantation

The Seebeck coefficient holds a central role for thermoelectric materials, mostly by its quadratic contribution to the figure of merit zT. Therefore significant efforts are made to increase its value, either by researching new materials or exploiting various physical effects. Among them a strong coupling between out-of-equilibrium phonons and electrons, known as the phonon-drag effect, leads to a considerable increase of the Seebeck coefficient in certain materials. However, this increase appears to occur in the same temperature range as the peak of the lattice thermal conductivity, therefore hindering its utilization in thermoelectricity. However, in recent years, a theoretical approach [1] applied to bulk Si has shown that the phonons responsible for thermal transport and those contributing to the phonon-drag effect are distinct in both energy and momentum, thereby allowing for the coexistence of the phonon-drag effect with low thermal conductivity. In our research we aim at addressing this question deeper, particularly to determine whether it is possible to couple an external "phonon-bath" to a thin conducting channel where the thermoelectric transport occurs. We are studying various systems. The first is an implanted conducting channel inside an insulating diamond structure [3]. By changing the implantation conditions and the annealing temperature very different behaviors have been observed, embedding a rich physics. The second system studied consist of thin films of thermoelectric $SrTiO_{3-\delta}$ (STO) grown by molecular beam epitaxy (MBE) on an undoped diamond substrate. In the poster, after a brief description of the underlying theory and experimental methods, I will present the obtained experimental results, ranging from the structural properties to the transport properties of both systems. The impact of various parameters will be shown, such as the annealing temperature of the diamond channel (system 1) or the doping of the STO thin films (system 2).

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This work was supported by the French National Research Agency through the project ANR DragHunt (ANR-24-CE50-3505) and the grant of ENS Lyon for the PhD of MM.

Non-Contact Electrical and Thermal Characterizations of Electrodeposited SnSe Films

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Keywords : FDTR, IR-SE, electrodeposition, SnSe films

Polycrystalline SnSe have become more and more popular for thermoelectric (TE) applications at high temperature (900 K). One of the main reasons is that SnSe is less toxic (no tellurium or lead), its compounds are abundant, and presents itself as a competitive alternative to common compounds such as Bi_2Te_3. However, since the controversial work of Zhao et al. [1], which reported a bulk thermal conductivity lower than 1 $W.m^{-1}.K^{-1}$ and a TE figure of merit ZT of 2.6 at 923 K, various researches have been carried out on this family of SnSe-based compounds. At room temperature, SnSe has poor thermoelectric performances mainly because of reduced electronic conductivity. However, this behavior can be counterbalanced by further diminishing the lattice part of the thermal conductivity through nanostructuration. A promising way, demonstrated numerically by Al-Alam et al. [2], is the reduction of the TE layer below 1 µm, which may lead to a thermal conductivity lower than 0.5 $W.m^{-1}.K^{-1}$. The aim of this work is to experimentally verify this trend in measuring the thermal conductivity for low thicknesses.
To this purpose, we have carried out electroplating synthesis, which has the advantage of adjusting the microstructure and the chemical compositions of the films. However, this method requires an electronic conductive layer. As a consequence, direct measurements of thermoelectric performances are biased [3]. In this work, we used original contactless methods such as Infrared spectroscopic ellipsometer (IRSE) to indirectly determine the electrical conductivity, and Frequency Domain Thermoreflectance (FDTR) to evaluate the thermal conductivity. We will present microstructure analysis made with XRD and TEM images of oriented electrodeposited SnSe films. Finally, we will present the electrical conductivity measurements carried out by IRSE by determining the dielectric constants. Moreover, we evaluated the thermal conductivity studied by FDTR around 0.4 $W.m^{-1}.K^{-1}$ for several films.

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Acknowledgments

This work has received financial support from Lorraine Université d'Excellence (LUE). The authors wish to thank Madame Sylvie Migot, Madame Mélanie Emo, Dr. Jaafar Ghanbaja and Dr. Gwladys Steciuk for FIB-SEM lamellas preparation and TEM analysis.

Relative Leg-Height Optimized Micro-Thermoelectric Devices

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Keywords: Micro thermoelectric coolers (uTECs), Micro thermoelectric generators (uTEGs), Electrochemistry

Micro thermoelectric devices (uTEDs) offer a promising solution for localized hot spot cooling and energy-autonomous sensor applications. To optimized their performance, the device geometry must be tailored to match electrical and thermal properties of thermoelectric materials, typically involves adjusting the cross-sectional areas which limits the maximum packing-density. Here, we introduce a new design approach that optimizes the relative heights of p- and n-legs, enabling higher packing-densities, resulting in enhanced cooling power density, output power, and reduced the material usage, which are often toxic and expensive.

The uTEDs are fabricated using photolithography in combination with electrochemical deposition of $Bi_2(Te_xSe_{1-x})_3$ and Te as n-type and p-type materials [1-3]. The optimized uTECs demonstrates a maximum cooling of 10.5 K at room temperature and 21 K at 343 K. Simulations using finite element method indicate that cooling power densities of hundreds of watts per square centimeter are attainable, representing a 35% improvement over unoptimized device, all while using less Te than cross-section optimized devices [2]. Moreover, as a generator, the height optimized uTEGs exhibit high open-circuit voltages and power densities 55% higher than unoptimized devices, even at small temperature differences, while using 80% less Tellurium.

Our results highlight the exceptional potential of uTEDs for hot-spot cooling applications, enabling increased integration density in circuits and supporting energy-autonomous sensors for IoTs.

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Acknowledgement

The authors acknowledge funding from the DFG (Deutsche Forschungsgemeinschaft) within grant no. RE3973/1–1.

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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25TH SESSION
THEORY III

Amorphous-like thermal conductivity and high thermoelectric figure of merit in "π" SnS and SnSe

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Keywords: Thermoelectric; π-cubic phase; SnS; SnSe; ab initio modelling

The tin chalcogenides SnS and SnSe are an important family of optoelectronic materials with applications to clean-energy technologies including photovoltaics (PV) and thermoelectric (TE) generators. In particular, SnS has been widely studied as a potential PV material, and orthorhombic *Pnma* SnSe is one of the current flagship high-performance TEs.[1,2] The recently-discovered π-cubic phases of SnS and SnSe have similar local structures to the *Pnma* phases, have been shown to be both dynamically stable and close to the convex hull, and have been identified as potential high-performance TEs.[3] However, the physical properties required to determine the TE figure of merit, *ZT*, have yet to be measured.

We have applied a fully ab initio modelling approach to determine the TE properties and *ZT* of π-cubic SnS and SnSe as a function of temperature and carrier concentration with both p- and n-type doping. The complex structures push the "particle-like" contribution to the lattice thermal conductivity, κ_{latt}, below the amorphous limit, resulting in an ultra-low κ_{latt} from room temperature upwards. The π-cubic symmetry supports larger Seebeck coefficients than the *Pnma* phases, but higher carrier effective masses and stronger electron scattering require high doping levels to optimise the conductivity and power factors. For π SnSe, we predict a low-temperature n-type *ZT* comparable to Bi_2Te_3,[4] and a high-temperature *ZT* competitive with the flagship *Pnma* SnSe. These results demonstrate the exceptional promise of these systems as high-performance thermoelectrics, and highlight structural complexity as a route to optimising low-temperature *ZT* by minimising the κ_{latt}.

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Acknowledgments

MZ is supported by a CSC studentship (202006700004). JMS and JMF are supported by a UKRI Future Leaders Fellowship (MR/T043121/1), and JMS previously held a University of Manchester Presidential Fellowship. This work used the ARCHER2 UK National Supercomputing Service via the UK MCC (EPSRC EP/R029431 and EP/X035859).

Structural and stacking fault modelling of low-density $Cu_{2+y}Zn_{1-y}SnS_{4-x}Se_x$ systems for thermoelectric applications

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Keywords: kesterite, stacking faults, low-density, cation doping, anion substitution

The $Cu_{2+y}Zn_{1-y}SnS_{4-x}Se_x$ (CZTSSe) system has emerged as a promising candidate for thermoelectric (TE) applications owing to its structural disorder phase mechanisms [1]. Via ball-milling (BM) approach, CZTSSe forms as a metastable sphalerite cubic phase (F-*43m, 225*) at room temperature, with full cation disorder, subsequently transforming into a tetragonal I-*42m (space group 121)* phase upon annealing, resulting in a Cu and Zn positional disorder in the *4a* Wyckoff sites. While the lack of point symmetry of the disordered cations acts as a phonon scattering source in the structure, the Zn-blend structural symmetry of CZTSSe preserves its conducting pathways [1]. In the present work, we showcase the BM synthesis and characterization of low-density $Cu_{2+y}Zn_{1-y}SnS_{4-x}Se_x$ compounds for different x and y compositions, investigating their stacking faults mechanism, phase transition, and their impact on the TE properties. The stability and transport properties of CZTSSe were also computed by density functional theory (DFT) calculations. Conductivity properties peaked for y = 0.125 Cu-Zn self-substitutions since more conductive Cu_2Se/S_4 layers replaced the $SnZnSe/S_4$ insulating layers in the I-*42m* structure. In addition, BM proved to induce a high degree of stacking faults in the Sphalerite phase, which were healed by sintering, promoting partial ordering of the Cu- Sn cations in the I-*42m* structures around 550 K [2]. Among all compositions, those with y = 0.125 and x = 1 or 2 exhibited the highest thermoelectric figure of merit (*zT*) above 500 K, achieving *zT* = 0.55 at 720 K. This performance boost is attributed to reduced thermal conductivity driven by enhanced phonon scattering from the randomly occupied anion position. Furthermore, both compositions qualify as high-entropy alloys, demonstrating increased configurational entropy and enhanced thermal stability. These findings highlight the potential for partial substitution of Se with S in the kesterite structure at elevated temperatures—an approach that lowers material costs while improving TE performance, promoting the feasibility of low-density CZTSSe kesterite compounds as mid-temperature thermoelectrics.

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Acknowledgments

The support of the Italian Ministry of Universities and Research (MUR), in the framework of the project DICAM-EXC (Departments of Excellence 2023-2027, grant L232/2016).

Tuning of electronic structure and thermoelectric properties via defects engineering in $Cu_{8-x}Si(S_3Se_3)_{1-y}I_y$ argyrodites

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Keywords: argyrodites, electronic structure, vacancy defects, electron transport, entropy

Argyrodites are intensively studied in terms of thermoelectric properties due to their very low thermal conductivity, but also due to the particular role of chemical disorder affecting the configurational entropy, but also giving rise to complex topology of electronic valence bands near the Fermi energy [1,2]. Ag-based argyrodites can exhibit both *n*- and *p*-type conductivity, while the electronic transport of the Cu-based argyrodites is predominantly driven by the *p*-type carriers [3]. Very recent investigations have shown that even isovalent substitution of Se by S in Cu-based argyrodites enhances the configurational entropy and drives a crystal structure transformation, shifting a phase transition below room temperature, which greatly modifies electronic transport [4]. In this work, the results of some trials to get *n*-type thermoelectric properties by substituting the Se and S positions with richer in electrons I. The effect of the aliovalent iodine dopant on the electronic and thermal transport of the Cubased argyrodites was investigated from the Hall effect, Seebeck coefficient, electrical conductivity, and diffusivity experiments, supported by the *ab initio* electronic structure calculations. The disordered crystal structure (γ-$Cu_8Si(S,Se)_6$, *F*-43*m*) containing vacancy defects on inequivalent Cu positions as well as its ordered approximant (α-Cu_8SiSe_6, $Pmn2_1$), offer an excellent playground to consider I dopant located on various Se and S positions. We performed the accurate KKR-CPA calculations, which accounted for complex disorder (vacancies on inequivalent Cu positions, substitution of I on Se and/or S positions), in parallel with the total energy analysis of configurations. This allowed to indicate the preferential occupation of Se/S positions by I (acting as an electron donor) as well as its correlation with the appearance of vacancies on selected Cu positions (acting as a hole donor). Our theoretical results well support the measured *p*-type conductivity, but also show how the interplay of defects at Cu positions and substitutions at Se/S positions in general affect the thermoelectric properties of the Cu-based argyrodites and what are electronic and energetic reasons for that.

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Acknowledgments

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

Enhancing thermoelectric properties of n-type (Pb-Sn)Te via resonant doping

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Keywords: SnTe, resonant level, Zn impurity, electronic structure, DFT

Obtaining n-type SnTe has always been a challenging task because of its intrinsic high amount of Sn vacancies leading to a marked p-type degenerate behavior. However, this is problematic for practical applications, as both p- and n-type legs made from the same system must be coupled in thermoelectric devices. So far, n-type SnTe has been only achieved through alloying with Pb, which prevents the formation of Sn vacancies, followed by I [1] and Br [2] doping. However, this area of research remains fairly unexplored, leaving room for improvement. In this work, we present a theoretical side-by-side study of the SnTe and SnTe-PbTe alloy and the influence of Zn on electronic structure and transport properties. In the case of pure SnTe, Zn has been suggested to be a p-type resonant dopant [3]. Calculations of electronic structure were performed using two complementary methods based on Density Functional Theory, that is, the KKR-CPA (Korringa-Kohn-Rostoker with coherent potential approximation) and pseudopotential method. The energy dependent transport function was obtained within the Kubo-Greenwood formalism and the Seebeck coefficient was calculated using full Fermi integrals. In unalloyed SnTe, the introduction of Zn impurity not only distorts the conduction band due to resonant level formation, but also significantly modifies the valence band through reduction offset of the band maxima and increase in carrier effective mass. Transport calculations show an increase in the Seebeck coefficient in both n-type and p-type SnTe. We show that the Zn impurity also introduces a non-trivial electronic state in SnTe-PbTe which may enhance the thermopower in n-type samples.

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Acknowledgments

This work was supported by the program "Excellence Initiative - Research University" for the AGH University of Krakow, Action 4, ID 10732 and in part by the PL-Grid infrastructure. I.T., C.C., and B.L. acknowledge the financial support from the French National Agency (ANR) in the frame of the project HYDRES (project identifier ANR-21-CE50-0003).

ECT' NANCY 25

PART IV
CONTRIBUTED TALKS

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26TH SESSION
DEVICE V

Transuranium Thermoelectrics Properties: a support for Space Exploration

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Keywords: Transuranium, low temperature, plutonium, americium

Deep space exploration far from the Sun- typically beyond Jupiter- requires energy production needed for electronics (scientific instrumentation, telecommunication, etc.) where conventional energy conversion such as solar panel is not applicable anymore. Self-heating due to the nuclear decay of nuclear materials is a very robust and reliable heat sources used more than 70 years for energy production through thermoelectric in long distance probes (Voyagers, Cassini-Huygens, New Horizon, etc.).

During the last decades, an increase of interest of thermoelectricity and heat-to-electricity conversion in a broad range of materials, techniques and processes for industrial applications, research in extreme conditions but also from a theoretical point of view. Recent breakthroughs have taken place on "designed" materials - textured or nanostructured materials - tuning the ZT figure of merit by on purpose electrical or thermal transport properties modifications.

Some of these compounds present interesting anisotropic structures with controlled inserted elements in the crystallographic cell with specific electronic features and/or semiconducting behavior (chalcogenides, half Heusler, clathrates, silicides). Here we report studies on actinides based compounds presenting the aspect of itinerancy and localization in the 5f series which acts as an interesting way to control DOS at Fermi level, replacing at once doping effect. Few data are reported on thermopower of uranium materials and even less on transuranium based compounds where 5f electronic features are playing a definitive role in ground state and drastically tune electronic and thermal transport properties and thermopower.

Accessing these properties (electrical resistivity, thermal conductivity and thermopower) requires devoted apparatus to handle actinides (Th, Pa, U, Np, Pu, Am, Cm) materials specifically in the case of radioactive transuranium compounds. We will present versatile homemade Seebeck set-ups adapted to a standard PPMS Quantum Design equipment in the 2-300 K range under magnetic field up to 14 T and results obtained recently with them.

Silicide thermoelectric modules based on high purity Si and recycled Si-kerf

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Keywords: Thermoelectric modules, silicides, waste-heat, contact resistance, silicon-kerf

Thermoelectric energy conversion devices based on non-toxic, sustainable and low-cost silicide compounds presents great potential in the green-transition era. This potenitial can be enhanced through the utilization of recycled Si-kerf waste material, and the implementation of circular economy approach.

This work describes the development of thermoelectric modules based on *n*-type magnesium silicide and *p*-type manganese silicide synthesized from high purity Si (commercially available) and recycled Si-kerf from the PV industry. Metallization based on sputtered Ni/Cu bilayers and specific contact resistance analysis is conducted to evaluate the aptness of the metallization and bonding methodologies, through the transfer length- and the scanning probe- methods respectively. Deposition conditions are optimized, and reduction of the metallization-related contact resistance is achieved. Improvement of silver sintering bonding is enabled through the increase of the thermoelectric legs surface roughness, which is accompanied by lower cumulative specific contact resistance values. Fabrication of 4-leg thermoelectric modules, serving as proof-of-concept prototypes for the recycling of Si-kerf, is showcased. Good agreement between experimental and simulated (COMSOL Multiphysics®) performance is shown. Upscaling from 4-leg proof-of-concept prototypes to larger 16-leg Si-kerf based modules is also achieved, with high power densities being demonstrated as well.

Development and upscaling of high-performance silicide TEMs based on high purity- and recycled Si is achieved and signals the potential in upcycling of Si-kerf waste material. Although high performance has been achieved, both simulations and experimental evaluation suggest that there is still room for improvement. Developing the next generation of silicides, coating and bonding materials, holds great promise for these emerging technologies.

Acknowledgments
This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 958365 (ICARUS Project).

Primary and Secondary Properties of Amorphous TiNiSn for Flexible Thermoelectric Devices

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Keywords: Amorphous, Titanium nickel tin, Flexible thermoelectric devices

Thermoelectric devices offer a sustainable solution for wearable devices and implants. However, utilizing the specific material is demanding for such applications to ensure they are compatible with surfaces such as human skin [1]. Primary properties (Seebeck coefficient, electrical and thermal conductivity) and secondary properties (mechanical flexibility) must be tuned for sustainable applications. We have shown that amorphous TiNiSn is a promising material for wearable thermoelectric devices because of its ductility (a Cauchy pressure of 30 GPa), as well as its good adhesion to flexible substrates such as Kapton (polyimide), silk, and printer paper. Bending tests up to 154 degrees reveal minimal crack formation, indicating high flexibility [2]. To further enhance the thermoelectric efficiency of these devices, density functional theory, and Boltzmann transport theory were employed to tune the electronic structure and identify suitable doping elements among 3d and 4d transition metals. Experiments were carried out to validate these predictions, yielding an order of magnitude increase in performance at room temperature [3].

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Acknowledgments

The financial support from the Olle Engkvist Foundation (project number 217-0023) is acknowledged. The computations were enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) at the National Supercomputer Centre (NSC) in Linköping partially funded by the Swedish Research Council through grant agreement no. 2022-06725.

Thermal Wave Dynamics and Thermoelectric Transport in InGaAs/GaAs Superlattices

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Keywords: Semiconductor Superlattice, Molecular Beam Epitaxy (MBE)

Optimizing the thermoelectric performance of devices requires a deep understanding of the in-plane and cross-plane transport mechanisms driven by phonons and electrons. In this work, we grow superlattice samples of InGaAs/GaAs using MBE and optimize their thermoelectric response for different carrier concentrations and period thicknesses. This is achieved by measuring the in-plane and cross-plane Figure of Merit (ZT) through our advanced experimental setups for quantifying the Seebeck coefficient, as well as the electrical and thermal conductivities [1,3]. Analytical modelling powered by machine learning algorithms is used to distinguish between ballistic and diffusive heat flows. The diffusive and ballisitic parts are respectively described by the Cattaneo and Guyer-Krumhansl equations that are rooted in the second law of thermodynamics. integrates these components into the variable space, offering a more rigorous framework for thermoelectric transport in superlattices [2]. The obtained insights can drive advancements in the design of thermoelectric materials and enhances the efficiency of heat-to-electricity energy conversion.

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PART IV
CONTRIBUTED TALKS

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27TH SESSION
CHALCOGENIDES III

Multinary sulphides for thermoelectrics: Mechanochemical synthesis via industrial milling

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Keywords: Sulphide, thermoelectricity, mechanochemistry

Discovering sustainable, low-cost and clean energy sources represents one of the most important challenges for materials science. Thermoelectric materials offer a viable way to generate electricity from waste heat 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 under operating conditions. Several new compounds with high thermoelectric performance have recently emerged. Among them, metal chalcogenides have attracted considerable attention as potential Te-free alternatives. In this work we describe the properties and thermoelectric performance of several copper-based multinary sulphides, namely chalcopyrite $CuFeS_2$, tetrahedrite $Cu_{12}Sb_4S_{13}$, mawsonite $Cu_6Fe_2SnS_8$ and colusite $Cu_{26}V_2Sn_6S_{32}$. All of them were prepared via mechanochemical synthesis in an industrial mill. Using this procedure all benefits of mechanochemistry can be utilized [1-4]. As for thermoelectrical parameters, the Seebeck coefficient, electrical conductivity and thermal conductivity were measured and confronted with energy supplied during milling. The obtained values were used to calculate the figure-of-merit (zT). zT values are comparable or even higher than the values obtained using laboratory mills. The presented results illustrate the possibility of a large-scale deployment of mechanochemistry to prepare energy-related materials.

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Acknowledgments

This work was supported by the Slovak Grant Agency (projects 2/0112/22 and 2/0036/23).

Magneto-thermoelectric properties of selected sulfides

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Keywords: thiospinels, magnetism

The magneto-thermoelectric properties have been investigated in different families of materials, such as metals [1- 2], chalcogenides or oxides [3]. They are now extensively investigated in the field of topological materials [4], due to the large Seebeck (or Nernst) effects obtained in these materials leading to enhanced ZT.

In the case of sulfides, we will present here several examples of thiospinels with different magnetic and electronic properties, to show how the power factor can be tuned by a magnetic field. The transport properties will be discussed with respect to the Mott's formula or to the spin entropy effects [5].

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Acknowledgments

The authors acknowledge the financial support from LabEx EMC3 (Excellence Laboratory, Grant No. 10-LABX-0009) of the French National Research Agency (ANR) through the SPINTEP project, and of the French National Agency under Grant ANR-21-CE50-0033.

Solid solution alloying strategy to enhance thermoelectric efficiency of layered metal chalcogenides; $(Bi,Sb)_2Te_3$, $Bi_2(Se,Te)_3$ and beyond

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Keywords: solid solution alloying; $(Bi,Sb)_2Te_3$; $Bi_2(Se,Te)_3$; PbTe-Bi_2Te_3

Solid solution alloying (SSA) of metal chalcogenide compounds (M_xX_y) can be formed either by alloying cation or anion site. SSA by cation (i.e. $(M,N)_xX_y$) could provide a gradual change of electronic dispersions, which could optimize thermoelectric (TE) power factor by controlling band structure and band convergence. SSA by anion (i.e. $M_x(Se,Te)_y$) enables to control the band gap, which optimize level of bipolar conduction for high power factors. In addition, lattice thermal conductivity can be reduced by SSA by additional phonon scattering, which could further increase the TE figure of merit. Therefore, SSA approach can enhance TE efficiency of chalcogenides effectively.

Herein, I would like to first revisit the origin of high TE efficiency of $(Bi,Sb)_2Te_3$ and $Bi_2(Se,Te)_3$ solid solution alloys in these respects, which are the most conventional TE chalcogenides. Then, investigations to enhance TE efficiency of chalcogenides in a similar way are discussed, including simple SSA, including $(Fe,Co)Te_2$, $Co(Se,Te)_2$, and $Cr_2(Se,Te)_3$. Lastly, rather complex combinatorial SSA with (Pb,Sb)Te and $(Bi,Sb)_2Te_3$ solid-solution in layered PbTe-Bi_2Te_3 intermetallic compounds, including $PbBi_2Te_4$, $PbBi_3Te_7$, and $PbBi_4Te_{10}$.

Acknowledgments
This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean Government (MSIT) (RS-2024-00338646).

Thermal conductivity imaging to advance microstructure engineering in thermoelectrics

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Keywords: thermal conductivity imaging, microstructure engineering, grain boundaries, electron backscatter diffraction, frequency domain thermoreflectance

Engineering the microstructure of materials offers superior control over transport properties, critically impacting the thermoelectric performance. However, maximizing this performance requires a comprehensive understanding of how specific microstructural features distinctly influence phonon and electron transport. Despite its significance, the role of idividual microstructures in modulating local transport remains elusive, due to the scarcity of spatially-resolved investigations. In this talk, I will present examples demonstrating how thermal conductivity (κ) imaging can shed light on the local behavior of key microstructural features for thermoelectrics, including grain boundaries, phase segregations in alloys, and local variations in crystal orientation. Experimental observations in several thermoelectric materials reveal a κ suppression localized in the vicinity of grain boundaries, quantified in terms of a thermal boundary resistance. Remarkably, boundaries show marked variations in behavior: misorientation angle, lattice symmetry, and interface morphology are found to strongly affect the boundary resistance[1,2]. In Mg_2Si-Mg_2Sn alloys, κ imaging can resolve microscale phase segregations, offering insights into the chemical heterogeneity within the sample, and - together with Seebeck coefficent imaging- guiding further material optimization. In Sb_2S_3, κ imaging on laser-patterned, rotating-lattice single crystals enables to investigate the effect of amorphization and crystal orientation. A pronounced κ anisotropy is found in the system: the crystal out-of-plane direction exhibits amorphous-like κ, whereas the in-plane directions show 2× and 4× higher values. This in-plane κ anisotropy emerges from soft, distorted bonds along the *b*-axis, attributed to the expression of Sb lone pairs. Extracting transport properties from microscale imaging experiments offers a powerful route to clarifying how individual microstructures behave, allowing to establish local structure-chemistry-property correlations. This can advance our understanding of phonon- defect interactions, enabling the rational engineering of interfaces and microstructures for enhanced performance in thermoelectrics.

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Acknowledgments

This work is supported by the European Research Executive Agency, under Marie Skłodowska-Curie Actions, project 101150912 — MetaSCT.

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PART IV
CONTRIBUTED TALKS

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28TH SESSION
EMERGING MATERIALS III

Halide perovskites as thermoelectric materials

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Keywords: perovskite, thermoelectric, doping, stability

Halide perovskites are well known as promising candidates for photovoltaics and light-emitting diodes. Additionally, promising thermoelectric performance has been reported [1-2] for a small number a halide perovskites, with this class of materials offering ultralow thermal conductivity, good Seebeck coefficients and potential advantages in processing and sustainability. However, there is not yet a good understanding of how thermoelectric performance of halide perovskites can be optimised. This talk will cover the origins of ultralow thermal conductivity and quanitfy both the electronic and lattice [1, 3] in polycrystalline films. Extrinsic doping and self-doping will be discussed as methods to optimise the thermoelectric figure of merit *zT*, with values of *zT* reaching 0.14 in $CsSnI_3$ [1] The case of self-doping by Sn-oxidation in $CsSnI_3$ will be examined in detail and strategies to improve performance and control the rate of oxidation by modification of deposition procedures, or by using mixed halide and mixed metal stoichiometries will be presented.[1, 3, 4] Thin-film vapour deposition, single crystal growth [4] and solid-state synthesis will be discussed, along with doping techniques to improve stability and conductivity.

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Acknowledgments

This work was supported the Royal Society through Prof. Fenwick's University Research Fellowship (UF1403

The Potential of High-Entropy Oxides: Insights from Perovskite Structures

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Keywords: High-Entropy Oxides, Perovskites, Heat and Charge Transport Decoupling

High Entropy Oxides (HEOx) are a new class of materials first introduced by Rost *et al.* in 2015 [1], extending the concept of high-entropy alloys to ionic compounds. HEOx are multicomponent, single-phase oxides containing at least 5 different cations in near-equimolar proportions randomly distributed in the cationic sublattice. This concept enables the development of new materials with tunable and unique properties. The first reported HEOx, $(Mg_{0.2}Cu_{0.2}Co_{0.2}Ni_{0.2}Zn_{0.2})O$ with rocksalt structure has shown promising properties (e.g. colossal dielectric constants [2]). Since then, various other HEOx structures were discovered with various possible applications.

The high-entropy concept is a promising new strategy for the design of thermoelectric materials. Large local structural distortions and mass fluctuations are induced by the presence of at least 5 elements at the same lattice position, which significantly reduces lattice thermal conductivity while maintaining charge carrier mobility. This results in a partial decoupling of heat and charge transport, a critical factor in improving thermoelectric performances. Additionally, the chemical versatility of high-entropy materials enables for precise control over doping with aliovalent cations for charge carrier concentration tuning, offering the potential for significant improvement in *ZT* compared to conventional materials.

In this presentation we will focus on the thermoelectric properties of the high-entropy cobaltates perovskite $(La_{0.2}Nd_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2})_{1-x}B_xCoO_3$ $(0 \leq x \leq 0.1)$ (xith *B*=alkaline earth cation) [3]. We will show that the multi-cations substitution and B^{2+} doping result in comparable power factor compared to the single cation compound $La_{0.95}Sr_{0.05}CoO_3$, but reduction of thermal conductivity by phonon scattering. As a result, a maximum *ZT* of 0.22 is measured at 350 K in $(La_{0.2}Nd_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2})_{0.95}Sr_{0.05}CoO_3$, which is one of the best *p*-type oxide materials reported at this temperature. This result shows the interest of this strategy for the design of new thermoelectric materials as shown in other systems [4].

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Optimization of Copper Iodide nanoparticle based composite thermoelectric material

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Keywords: Copper iodide, hybrid material, polymer, thermoelectric properties

Copper iodide (CuI) is an abundant and non-toxic p-type thermoelectric material. CuI nanoparticle synthesis is simple and the nanoparticles exhibit high Seebeck coefficient values at room temperature. CuI nanoparticle based materials exhibit a smooth and homogeneous structure, thus making them suitable for composite material preparation.

In this work various CuI hybrid materials were studied. The hybrid materials were made from various polymers, such as PVDF and PEO. Additionally, nanoparticle and solvent compatability was investigated. Scanning electron microscopy and profilometer measurements were used to characterize the materials structure and surface smoothness. Thermal stability and degradation of the hybrid material was studied. Hybrid materials with different nanoparticle concentrations were fabricated to determine optimal polymer-nanoparticle ratio for the best electrical conductivity and Seebeck coefficient values.

Results show that CuI based hybrid materials thermoelectric properties are affected by the chosen materials. Approperiately chosen polymer and solvent is necessary to obtain the highest Seebeck coefficient and electrical conductivity.

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

V_2Se_2O and Janus V_2SeTeO: Monolayer altermagnets for thermoelectric applications

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Keywords: Altermagnetism, Thermoelectricity, Lattice thermal conductivity, Monolayer

We determine the thermoelectric properties of the V_2Se_2O and Janus V_2SeTeO monolayer altermagnets with narrow direct band gaps of 0.74 and 0.26 eV, respectively. Monte Carlo simulations reveal Néel temperatures of 800 K for V_2Se_2O and 525 K for Janus V_2SeTeO. The electrical conductivity is higher for p-type charge carriers than for n-type charge carriers due to lower effective masses. The presence of heavy Te atoms in Janus V_2SeTeO results in lower phonon group velocities, higher phonon scattering rates, and higher lattice anharmonicity than in the case of V_2Se_2O, leading to an almost 19-fold reduction of the lattice thermal conductivity at 300 K. The figure of merit of V_2Se_2O reaches 0.4 (0.1) and that of Janus V_2SeTeO reaches 2.7 (1.0) just below the Néel temperature for p-type (n-type) charge carrier densities of 1×10^{13} cm^{-2}, demonstrating that altermagnets have excellent potential in the thermoelectric recovery of low-temperature waste heat.

Acknowledgments
The research reported in this publication was supported by funding from King Abdullah University of Science and Technology (KAUST). For computer time, this research used the resources of the Supercomputing Laboratory at KAUST.

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PART V
POSTERS

Thermoelectric Materials & Processing	
P01	**Emmanuel Guilmeau** *CRISMAT (France)* **Insights into the crystal chemistry of thermoelectric sulfides, halides and sulfochlorides**
P02	**Cecilia Piscino** *University of Genova (Italy)* **Tailoring thermoelectric properties in double-filled skutterudites $(La,Sm)_y(Fe_xNi_{1-x})_4Sb_{12}$: insights from bulk and thin-film studies**
P03	**Hiroaki Konishi** *Tohoku University (Japan)* **Preparation and Thermoelectric Properties of Doubly-substituted Fe-based Half-Heusler Alloys $(V_{1-x}Ti_x)(Fe_{1-y}Coy)Sb$**
P04	**Nan Luo** *Karlsruhe Institute of Technology (Germany)* **Screen-printed Ag_2Se fabric for high-performance thermoelectric energy harvesting**
P05	**Adriana Maurucaite** *University of Latvia (Latvia)* **Thermoelectric Composite Systems: Applications of Organic Low Molecular Weight Compounds with Nano and Microparticles**
P06	**Yuechu Wang** *Zhejiang University (China)* **Iterative sublattice amorphization facilitates exceptional processability in inorganic semiconductors**
P07	**Arthur Wieder** *Institut Jean Lamour (France)* **Lattice Symmetry as a Key Factor Governing the Thermoelectric Properties of Cu_2SnSe_3-based Compounds**
P08	**Sonia Sahir** *CRISMAT (France)* **Crystal Structures and Thermoelectric Properties in the Cu-Sn-S system**
P09	**Michal Szot** *Polish Academy of Sciences (Poland)* **Two-phase thermoelectric PbTe-CdTe nanocomposite**
P10	**Abdelkader Alleg** *Laghouat University (Algeria)* **Thermoelectric properties of filled skutterudites $ThFe_4P_{12}$ and $CeFe_4P_{12}$ using DFT calculations**
P11	**Ilayda Terzi** *Institut Jean Lamour (France)* **Addressing Instability in n-Type SnTe–PbTe Thermoelectrics via Phase Equilibria Investigations**
P12	**Andrés Conca** *Instituto de Micro y Nanotecnologia (Spain)* **Thermoelectric properties of W- and Ti-doped $L2_1$ Fe_2VAl epitaxial thin films grown by magnetron sputtering**
P13	**Ketan Lohani** *Instituto de Micro y Nanotecnologia (Spain)* **Nanoporous Substrate-Driven Nanostructuring for Enhanced Thermoelectric Performance of SiGe Alloys**
P14	**Anjan Karmakar** *Institut Jean Lamour (France)* **Optimization of Contact Elements in Bismuth Telluride and Half-Heusler Based Segmented Thermoelectric Generators**
P15	**Jesús Prado-Gonjal** *Universidad Complutense de Madrid (Spain)* **Thermoelectric optimization via compositional engineering in Ag-deficient $AgSbTe_2$**
P16	**Tetiana Tavrina** *University of Bonn (Germany)* **Thermoelectric properties of few-layer transition metal dichalcogenides**
P17	**Rana Ghannam** *Institut Jean Lamour (France)* **Comparative Study of the Thermoelectric Properties of High-Entropy Semiconductor (HES) $AgMnGePbSbTe_5$**
P18	**Helmut Baumgart** *Old Dominion University (United States)* **Realization of thermoelectric Film Nanopatterning by Atomic Layer Deposition and Porous Template Replication**
P19	**Shen Han** *Zhejiang University (China)* **Filling faults and vacancy swap occupation in half-Heusler compounds**
P20	**Héloïse Martin-Victorine** *CEA (France)* **Effect of a heating plate on SiGe alloys manufacturing by Laser Powder Bed Fusion**
P21	**Kaspars Pudzs** *University of Latvia (Latvia)* **Exploring the thermoelectric characteristics of cold-pressed copper iodide composites**

P22	**Niraj Singh** *Uppsala Universitet (Sweden)* **CrN based thin films for thermoelectric applications: Experimental and DFT study**
P23	**Hyoju Son** *Kyungpook National University (South Korea)* **Effects of non-stoichiometric co-doping on the thermoelectric properties of SnTe**
P24	**Joseph Moreau** *Institut Lumière Matière (France)* **Magnetic nanoparticle doping for thermoelectricity**
P25	**Savvas Hadjipanteli** *University of Cyprus (Cyprus)* **Half-Heusler thermoelectrics based on $TiFe_{0.5}Ni_{0.5}Sb$ and (Nb,Ta,Ti)FeSb compounds synthesized via mechanical alloying**
P26	**Abayomi Lawal** *Institute of Science and Technology (Austria)* **Solution-Processed PbTe Thermoelectrics with Enhanced Performance via Post-Synthetic Modification**
P27	**Muhammad Isram** *Institute of Condensed Matter Chemistry and Technologies for Energy (Italy)* **Structure and Thermoelectric Properties of Hydrothermally Grown $Bi_2Te_{3-x}Se_x$ Nanocrystals**
P28	**Hannah Baker** *European Thermodynamics Ltd (United Kingdom)* **Production of reliable Mg_3Sb_2 material and components for use in larger scale devices**
P29	**Midhun Shah** *Farook college (India)* **Enhanced power factor in Nb doped $SrTiO_3$ thin films via strain induced band degeneracy and energy filtering**
P30	**Stefano Boldrini** *Institute of Condensed Matter Chemistry and Technologies for Energy (Italy)* **Thermoelectric and mechanical properties of $Ti_{0.25}Zr_{0.75}NiSn$ half-Heusler alloy produced by Ultrafast High-temperature Sintering**
P31	**Petr Levinský** *Institute of Physics of the Czech Academy of Sciences (Czech Republic)* **Thermoelectric properties of thin ScN layers doped with W**
P32	**Tongwei Zhu** *Matériaux Fonctionnels et Nanostructures (France)* **Towards *p-type* thermoelectric $LaCoO_3$–based epitaxial thin films**
P33	**Baopeng Ma** *Harbin Institute of Technology (China)* **Phase diagram Engineering Advances the Thermoelectric Performance of Zintl Phase $EuZn_2Sb_2$**
P34	**Shizhen Zhi** *Harbin Institute of Technology (China)* **Significant anharmonic scattering in single-crystalline $Mg_{4.8}Ag_{1.4}Sb_4$ with site-occupation disorder**
P35	**Lars Hälldahl** *Kagaku Analys AB (Sweden)* **Hard-to-Sinter materials in Easy-to-Sinter wave-forms**
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Insights into the crystal chemistry of thermoelectric sulfides, halides and sulfochlorides

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During the last decade, numerous studies have demonstrated the potential of sulfide materials for thermoelectric applications over the temperature range 300 – 700 K. Although most materials have high thermal conductivities, recent works demonstrated that extremely low thermal conductivities could be achieved in sulfides through order/disorder phenomena, rattling dynamics, and lattice anharmonicity.

During this presentation, recent advances in synthetic sulfide minerals, halides and sulfochlorides, will be shown. Some peculiar structural features in connection with materials processing, chemical bonds, lattice vibrations and atomic and nanoscale order/disorder phenomena were carefully examined to establish rules and correlations between the crystal structures, nano-microstructures, electronic structures, vibrational and thermoelectric properties. [1-5].

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Tailoring thermoelectric properties in double-filled skutterudites $(La,Sm)_y(Fe_xNi_{1-x})_4Sb_{12}$: insights from bulk and thin-film studies

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Keywords: Filled skutterudites, crystal structure, thermal conductivity

Double-filled skutterudites have emerged as promising thermoelectric materials due to their ability to combine high electrical performance with significantly reduced lattice thermal conductivity. They have the general formula $RE_yM_4X_{12}$ (where RE are rare earth elements, M is a transition metal, and X is a pnicogen) and crystallize in a body-centered cubic structure ($Im\bar{3}$) space group) with Sb_{12} icosahedral cages centred at the 2*a* (0,0,0) site. By incorporating two different filler atoms into the cavities of the crystal structure, these materials take advantage of the rattling effect of guest atoms to scatter phonons more effectively, thereby minimizing thermal conductivity while preserving favorable electronic transport properties.

This synergistic effect enhances the thermoelectric figure of merit (ZT), making them attractive for energy conversion applications, including waste heat recovery and power generation [1]. The main objectives entail investigating the thermoelectric features of bulk $(La,Sm)_y(Fe_xNi_{1-x})_4Sb_{12}$ and developing and characterizing thin-film materials from the same system to assess the influence of interfaces on thermoelectric performance. The findings are compared with those obtained for other Fe/Ni-based materials, both as bulk materials [2,3,4] and as thin films [5], to identify potential enhancements.

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Preparation and Thermoelectric Properties of Doubly-substituted Fe-based Half-Heusler Alloys $(V_{1-x}Ti_x)(Fe_{1-y}Co_y)Sb$

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Keywords: Half-Heusler, phonon scattering, thermal conductivity

Iron-based half-Heusler alloys (Fe-HHs) have gained considerable attention as potential thermoelectric (TE) materials at room temperature, owing to their high TE power factor and excellent mechanical strength. However, one limitation is their relatively high lattice thermal conductivity (κ_L), which should ideally be reduced to 1-2 W/mK for practical applications. In this study, Huang *et al*. investigated the detailed crystal structure of one of the parent Fe-HHs, VFeSb, and found that the compound exhibits approximately 10% V deficiency, along with about 10% of Fe occupying typically vacant 4*d* sites.[1] This structural deficiency helps explain the compound's negative (n-type) Seebeck coefficient, even though a perfect half-Heusler structure (i.e., no deficiencies or anti-site defects) would typically display a positive (p-type) Seebeck coefficient [1]. Previous studies have shown that partial substitution of V with Ti effectively reduces κ_L [2], while partial substitution of Fe with Co substantially enhances the power factor (PF) [3].

In this study, we aimed to optimize the TE properties of Fe-HHs by preparing doubly-substituted samples of the form $(V_{1-x}Ti_x)(Fe_{1-y}Co_y)Sb$. Polycrystalline samples were prepared by arc-melting followed by an annealing process. The resulting ingots were finely pulverized and sintered using a spark plasma sintering (SPS) apparatus. To characterize the samples, we performed Rietveld analysis using X-ray diffraction (XRD) data. The Seebeck coefficient and electrical conductivity were measured using an Ulvac-Riko ZEM-3, while the thermal conductivity was determined via the laser flash method using a Netzsch LFA467HT. By separately controlling the *x* and *y* parameters, we achieved promising TE performance near room temperature.

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Acknowledgments

This work was partly supported by JSPS KAKENHI (No. 23H00230).

Screen-printed Ag2Se fabric for high-performance thermoelectric energy harvesting

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Keywords: Wearable, printed thermoelectrics, Seebeck coefficient, fabric, energy harvesting

Thermoelectric generators (TEGs) on fabric substrates are increasingly appealing due to their breathability and the seamless integration with clothing, which is advantageous for wearable electronics.[1] However, achieving both high performance and scalable manufacturing of such TEGs remains a challenge. Here, we report a sulphur-doped optimized screen-printable Ag_2Se ink, enabling low-cost wearable TEGs fabrication. The upscaling capability is achieved through screen printing, while the TE performance is enhanced by tuning transport parameters via 'S' doping. We have investigated doping amount of 2 at.%, 5 at.% and 10at.%, and identified $Ag_2Se_{0.95}S_{0.05}$ as the optimal compound. The Seebeck coefficient (α) of the optimized printed Ag2Se fabric with 5 at.% 'S' doping reaches 145 μVK^{-1} at room temperature (RT), while the electrical conductivity (σ) increases by 25 % due to 'Se' substitution by 'S', reaching 500 Scm^{-1} at RT. Consequently, a power factor of 10 $\mu Wcm^{-1}K^{-2}$ is achieved, which is 60 % higher than that of a pure Ag_2Se fabric. These results underscore the potential for scalable TEG manufacturing and integration into wearable electronics for powering low-energy devices.

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Acknowledgments

The authors acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) for financial support. This project has received funding from the European Research Council, grant 101097876 - ORTHOGONAL. The aulthors also acknowledge support from the Karlsruhe School of Optics & Photonics (KSOP).

Thermoelectric Composite Systems: Applications of Organic Low Molecular Weight Compounds with Nano and Microparticles

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Keywords: Low molecular weight compounds, microwave assisted synthesis, thermoelectric composite systems

For many thermoelectric applications, elastic and bendable devices are required, such as for thermoelectric generators (TEG) that generate electricity from the heat of the human body (wearable thermoelectrics). While the use of organic materials offer some advantages – elastic films and low thermal conductivity, organic materials lack the thermoelectric effectiveness of inorganic materials, which are mostly used in TEGs. To utilize the best properties of both types of materials, thermoelectric composite systems can be made.

In this work, thermoelectric composite systems of nano and microparticles dispensed in an organic matrix were made using the drop-cast method. For the organic matrix, low molecular weight compounds, that are frequently used in organic light-emitting diodes as charge transport layers, were used. The nano and microparticles used in this work were synthesized using microwave assisted synthesis.

For the films, electrical resistance and Seebeck coefficient were measured, and the specific electrical conductivity and power factors were calculated. The results and analysis for p-type and n-type materials will be presented.

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

Iterative sublattice amorphization facilitates exceptional processability in inorganic semiconductors

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Keywords: Plasticity, inorganic semiconductors, $Ag_2(Te,S)$, deformation mechanism, flexible devices

Cold-forming processing is a crucial means for the cost-effective production of metal and alloy products. However, this process often results in catastrophic fracture when applied to most inorganic semiconductors owing to their inherent brittleness. Here, we report on the unique room-temperature plastic deformation mechanism involving sublattice amorphization coupled with Ag ion diffusion in the inorganic semiconductors $Ag_2Te_{1-x}S_x$ ($0.3 \leq x \leq 0.6$), and an ultrahigh extensibility of up to 10150%. Once subject to external stress, the crystalline Te/S sublattice undergoes a uniform transformation into an amorphous state, while the Ag cations continuously bond with Te/S anions, endowing bulk $Ag_2Te_{1-x}S_x$ with exceptional plastic deformability. Remarkably, even slight polishing can induce sublattice amorphization in surface layers. Furthermore, this sublattice amorphization can be reversed to crystals through simple annealing, enlightening the iterative sublattice amorphization strategy, with which metal-like wire drawing, curving, forging, and ultrahigh ductility, have been obtained in bulk $Ag_2Te_{1-x}S_x$ at room temperature. These results highlight the sublattice amorphization as a critical plastic deformation mechanism in silver chalcogenide inorganic semiconductors, which will facilitate their applications in flexible electronics and drive further exploration of more plastic inorganic semiconductors.

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Lattice Symmetry as a Key Factor Governing the Thermoelectric Properties of Cu_2SnSe_3-based Compounds

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Keywords: Chalcogenide; Cu_2SnSe_3; lattice symmetry; Synchrotron X-ray diffraction; defects

$A_2^{I}B^{IV}C_3^{VI}$-based chalcogenides are promising thermoelectric materials with unusual crystallographic features.[1] Cu_2SnSe_3-based compounds exhibit transport properties that strongly depend on lattice symmetry, which, in turn, is highly sensitive to synthesis conditions. Depending on annealing temperature and chemical composition, these materials adopt monoclinic, cubic, or tetragonal phase, resulting in either metallic or semiconducting transport properties.[2-3] This study explores these aspects by examining a broad composition range and annealing conditions. Detailed chemical and structural characterizations are performed using synchrotron X-ray diffraction, Mössbauer spectroscopy, and transmission electron microscopy. Additionally, electronic band structure calculations, combined with transport measurements from 5 to 673 K, provide further insights into structure-property relationships. This work resolves conflicting results in the literature, emphasizing the influence of crystal structure and point defects on thermoelectric performance while identifying pathways for optimization.

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Crystal Structures and Thermoelectric Properties in the Cu-Sn-S system

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Keywords: Thermoelectric, sulfides, crystal structure, coordination, doping

Cu-Sn-S compounds, composed of earth-abundant and non-toxic elements, have emerged as promising candidates due to their tunable electrical and thermal properties, making them ideal materials for thermoelectric applications. Varying the Cu/Sn ratio leads to a variety of crystal structures derived from the sphalerite-type structure, with different transport properties [1].

In this work, we investigate the crystal chemistry and thermoelectric properties of Cu-Sn-S compounds, focusing on their structural evolution, defect chemistry, and electronic band structure modifications induced by Cu/Sn substitution. Additionally, we explore the effects of doping strategies to optimize the carrier concentration and to enhance thermoelectric performance. Using a combination of synthesis, structure analyses, and transport measurements, we analyze the interplay between crystal structures, structural disorder, electrical properties, and lattice thermal conductivity. Our findings especially highlight the fondamental role of Cu vacancies and Cu coordination for optimizing the power factor and reducing thermal conductivity. This study provides new insights into the design of high-performance thermoelectric materials in the Cu-Sn-S system and underscores the potential of heterovalent substitutions and doping in tailoring thermoelectric properties.

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Two-phase thermoelectric PbTe-CdTe nanocomposite

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Keywords: Nanostructuring, PbTe-CdTe nanocomposite

Semiconductor composites are a practical implementation of the idea of nanostructured thermoelectric materials, which is one of the promising strategies for improving the parameters of known thermoelectric materials. Thermoelectric energy conversion efficiency depends on material parameter $ZT = \sigma S^2 T/\kappa$, that can be enhanced by lowering thermal conductivity κ through increasing phonon scattering (if the electrical conductivity σ and the Seebeck coefficient S remain unaffected at given temperature T). This effect can be obtained by preparing low-dimensional structures consisting of thermoelectrics or by introducing nano- and micrograins of the same or different material phase into the material during the nanostructuring process. Here we tested the idea of nanostructuring for PbTe-CdTe thermoelectric semiconductor nanocomposite meant for thermoelectric generators operating at medium temperatures (T = 500 - 800 K). The investigated nanocomposite was obtained exploiting an extremely low mutual solubility of both semiconductors and using the patented, modified Bridgman growth method. For thermoelectric *p-n* couples we have prepared and examined PbTe-CdTe composites doped with iodine or bismuth for n-type conductivity and with sodium for p-type conductivity. The electrical and thermal conductivities, thermal diffusivity and Seebeck coefficient for composite samples containing CdTe nanoprecipitations of various sizes embedded in a PbTe thermoelectric matrix have been measured over a wide temperature range from 300 to 800 K. In particular, for PbTe - CdTe composites containing nominally 2, 5 and 10 at. % of cadmium (corresponding to CdTe precipitates with diameter ranging from ≈ 100 nm to ≈ 300 nm, respectively) we observed, that at temperatures above 650 K the thermal conductivity drops to ≈ 1 $Wm^{-1}K^{-1}$, what is half the κ of pure PbTe at room temperature and is significantly below the value observed for PbTe under these conditions i.e. ≈ 1.6 $Wm^{-1}K^{-1}$. Moreover, our PbTe-CdTe composite samples with the highest (not optimal) carrier concentrations (≈ 1×10^{19} cm^{-3}) achieve the ZT parameter up to 1.2. Finally, the dependence of the thermoelectric parameters of the composite on the cadmium content and dopant concentration will be discussed in detail.

Acknowledgments
This research was partially supported by the "MagTop" project (FENG.02.01-IP.05-0028/23) carried out within the "International Research Agendas" programme of the Foundation for Polish Science co-financed by the European Funds for Smart Economy 2021-2027 (FENG) and by the Polish National Centre for Research and Development, grants number: TechMatStrateg2/408569/5//NCBR/2019 and TechMatStrateg1/346720/8/NCBR/2017.

Thermoelectric properties of filled skutterudites $ThFe_4P_{12}$ and $CeFe_4P_{12}$ using DFT calculations

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The thermoelectric properties of the filled skutterudites $CeFe_4P_{12}$ and $ThFe_4P_{12}$ were studied using density functional theory (DFT) calculations combined with semi-classical Boltzmann transport equations. The electronic band structure analysis reveals that both materials possess semiconductor behavior, characterized by suitable band gap values that are essential for thermoelectric performance. The calculated Seebeck coefficients at room temperature demonstrate a significant potential for thermoelectric applications, with values indicating efficient charge carrier transport.

In addition to electronic properties, the thermal transport characteristics were examined, showing low lattice thermal conductivity, a crucial factor for enhancing the thermoelectric figure of merit (ZT). The power factor values, derived from electrical conductivity and Seebeck coefficient, further emphasize the efficiency of these materials under typical thermoelectric conditions.

These findings suggest that $CeFe_4P_{12}$ and $ThFe_4P_{12}$ are promising candidates for thermoelectric devices, combining favorable electronic and thermal transport properties. The study highlights the need for experimental exploration to validate and optimize these theoretical predictions for practical thermoelectric applications.

Addressing Instability in n-Type SnTe–PbTe Thermoelectrics via Phase Equilibria Investigations

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Keywords: n-type SnTe, solid solution, retrograde solubility, annealing, instability, hysteresis.

Developing n-type SnTe-based thermoelectric materials for medium to high temperature applications is gaining momentum, especially as recent progress in p-type SnTe has reached efficiencies comparable to the well-established p-type PbTe, making SnTe a viable option for thermoelectric applications. However, the presence of abundant intrinsic Sn vacancies presents a major obstacle for n-type doping, as they tend to drive the Fermi level deep into the valence band. Given the complex defect chemistry of PbTe, which allows both p-type and n-type behavior, alloying SnTe with PbTe offers a promising route to achieve n-type conduction [1]. While prior research has examined SnTe–PbTe solid solutions, including halogen doping on the Te-site to optimize n-type behavior [2], issues related to their long-term stability have yet to be fully addressed. In this study, we combine theoretical analysis and experimental measurements to explore the chemical stability and transport properties of dense polycrystalline $Sn_{0.6}Pb_{0.4}Te_{0.99}$ over a wide temperature range (5 – 700 K). We find that annealed and quenched samples exhibit thermal hysteresis during heating and cooling cycles, influenced by the annealing temperature used to prepare compositionally uniform materials. This behavior appears to be tied to the nature of the phase diagram, which suggests a narrow window of compositional tolerance around the ideal stoichiometry. By examining the projected phase diagrams of both SnTe and PbTe, our results highlight the critical role of annealing conditions in achieving stable thermoelectric performance.

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Thermoelectric properties of W- and Ti-doped $L2_1$ Fe_2VAl epitaxial thin films grown by magnetron sputtering

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Keywords: Heusler, Fe_2VAl, doping, sputtering, thin films

The Fe_2VAl family of Heusler alloys shows a large potential for thermoelectric thin films 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 in the same family, which simplifies thermoelectric device fabrication. While the undoped alloy Fe_2VAl is a p-type material, the introduction of W, Si, or Ta results in a n-type one. Improved p-type alloys are obtained with Ti and Zr. The addition of dopants can also be performed in an off-stoichiometric manner [4,5]. Sputter deposition is a well-established, inexpensive, and very versatile technique for the fabrication of a wide variety of material systems. The chemical composition and dopant content can be highly controlled by the simultaneous use of several magnetrons sources (codeposition). In this work, we present experimental thermoelectric and structural results of Fe_2VAl doping with W and Ti. $Fe_2V_{0.8}AlW_{0.2}$ thin films are grown by magnetron sputtering from nominal composition targets at deposition temperatures ranging from RT to 950ºC, on Al_2O_3 (1 1 -2 0), and on MgO (1 0 0) substrates, exhibiting (1 1 0) and (1 0 0) orientations, respectively, and varying degrees of chemical order (B2 → $L2_1$ transition) as in our previous report for Fe_2VAl, where the presence of the L21 phase is shown to be of crucial importance [6]. A Seebeck value of 6 60 μV/K and a PF of 600-700 μW/(mK²) is obtained. In addition, W-doped films prepared using co-deposition are also presented. For the Ti case, a doping optimization of $L2_1$ Fe_2VAl, in a co-deposition configuration was performed, obtaining higher values of Seebeck and power factor ($PF=S^2\sigma$) were obtained reaching the range of + 100μV/K and 2600μW/(mK²) respectively.

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Financial support by the Ministerio de Ciencia e Innovación with the ThermHeus (TED2021-131746B-I00) project and the ERC Advanced Grant POWERbyU (ERC-2021-ADG-101052603) is acknowledged. Spanish MICIU/AEI/10.13039/501100011033 and "European Union Next Generation EU/PRTR" (grants PID2022-1380630B-I00, and TED2021-130874B-I00) are also acknowledged.

Nanoporous Substrate-Driven Nanostructuring for Enhanced Thermoelectric Performance of SiGe Alloys

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Keywords: SiGe, nanostructuring, nanoporous substrate

Over the past 20 years, thermoelectric materials have experienced unprecedented advancements in enhancing their figure of merit (*zT*). Several new materials, including the families of selenides, silicides, and Heuslers, have demonstrated promising performance [1]. To improve efficiency, power factor enhancement through band engineering has been one the promising approach. Alternatively, nanostructuring has made significant progress in suppressing thermal conductivity.

Various material-based strategies have been explored in this regard. In the present work, a substrate-enabled nanostructuring approach has been investigated to enhance the thermoelectric properties of the SiGe alloy, a well-known material used in deep space missions as a high-temperature thermoelectric material [2].

This study aims to utilize nanoporous alumina substrates to enhance the thermoelectric performance of nanoporous SiGe. Previous work from our group has demonstrated a significant reduction in SiGe's thermal conductivity well below the amorphous limit [3]. Instead of deploying SiGe at high temperatures, this work proposes its use for near-room-temperature applications using this approach.

The abundance of Si and Al in Earth's crust makes them suitable for large-scale, cost-effective applications. Additionally, the widespread availability of Si-based chips would facilitate their seamless integration into modern electronics as both a solid-state generator and a cooler.

The present work presents preliminary results on this approach, which will later be complemented by computational studies on material properties and multiphysics simulations for device implementation.

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Optimization of Contact Elements in Bismuth Telluride and Half-Heusler Based Segmented Thermoelectric Generators

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Keywords: Segmented thermoelectric generators, bismuth telluride, half-Heusler alloys, contact resistance, interface optimization, energy conversion

Segmented thermoelectric generators (TEGs) offer a promising route for efficient thermal-to-electrical energy conversion across broad temperature gradients. However, their performance is often limited by contact degradation at the interfaces between segments. This study addresses this critical challenge through the development and integration of advanced contact materials specifically engineered for compatibility with both bismuth telluride (Bi_2Te_3)-based compounds and Half-Heusler alloys. These materials are designed to withstand thermal cycling and mechanical stress while minimizing interfacial resistance.

To enhance structural cohesion, we employ flash sintering as a rapid densification technique. The interfaces are thoroughly characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), thermoelectric property measurements (ZEM, LFA), and custom-built contact resistance tests. These methods provide detailed insights into microstructure, thermal and electrical behavior, and mechanical integrity under simulated operating conditions.

In parallel, multiphysics simulations conducted with COMSOL Multiphysics® model heat and current distribution across the contact regions, enabling prediction of failure modes and optimization of material combinations and interface geometries.

Our results demonstrate a significant reduction in contact resistance, along with improved thermal and mechanical stability. These enhancements translate into a measurable increase in the overall efficiency and reliability of segmented TEGs. The findings support the integration of optimized contact designs in practical energy recovery and waste heat harvesting systems, contributing to the advancement of sustainable energy technologies.

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Acknowledgments

The authors would like to thank the ORION program for its contribution to the funding of Anjan Karmakar's research internship. This work has benefited from a government grant managed by the Agence Nationale de la Recherche with the reference ANR-20-SFRI-0009.

Thermoelectric optimization via compositional engineering in Ag-deficient $AgSbTe_2$

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Keywords: $AgSbTe_2$, arc-melting, vacancy, compositional engineering, synchrotron X-ray diffraction

$AgSbTe_2$ crystallizes in a cubic *Pm-3m* structure with randomly distributed Ag and Sb atoms at the 3c Wyckoff sites, a configuration that reduces carrier mobility due to disorder-induced localization but contributes to high thermoelectric performance when doped or nanostructured. Its ultralow thermal conductivity arises from strong phonon–phonon scattering driven by anharmonic bonding - primarily due to stereochemically active lone pairs and contrasting Te–Ag and Te–Sb bond strengths - while a flat, multipeak valence band structure supports a high positive Seebeck coefficient. [1] This study explores $Ag_{0.7}Sb_{1.12}Te_2$ and $Ag_{0.7}Sb_{1.12-x}M_xTe_{1.95}Se_{0.05}$ (M = Zn, Ge) to investigate the impact of compositional engineering within the $AgSbTe_2$ thermoelectric system. The compounds were rapidly synthesized via arc-melting in just 3 minutes. Synchrotron X-ray diffraction reveals significant changes in the lattice parameters and atomic displacement parameters (ADPs) that suggest a weakening of bond order in the structure. Thermoelectric measurements demonstrate a significant enhancement in the power factor across all samples. When combined with the intrinsically low, glass-like thermal conductivity, these improvements result in figures of merit (zT) exceeding unity, with a peak value of zT = 2.1 at 750 K observed for the $Ag_{0.7}Sb_{1.07}Zn_{0.05}Te_{1.95}Se_{0.05}$ composition. [2]

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Acknowledgments

This work was supported by R+D+i projects CNS2022-135302, TED2021-129569A-I00, TED2021-129254B-C21, TED2021-129254B-C22, financed by MCIU/AEI/10.13039/501100011033/ and by the "European Union NextGenerationEU/PRTR". F.S.-S. thanks the MICIN and grant RYC2021-033518-I.

Thermoelectric properties of few-layer transition metal dichalcogenides

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Keywords: Two-dimensional (2D) materials, electrical conductivity, Seebeck coefficient, temperature dependence

In light of the growing demand for sustainable energy solutions and the challenges posed by global warming, the development of efficient thermoelectric (TE) materials has become increasingly important [1]. Recent progress in nanotechnology has enabled the exploration of low-dimensional systems, where quantum confinement and phonon scattering can lead to enhanced TE performance [2]. In particular, two-dimensional (2D) transition metal dichalcogenides (TMDCs) have attracted considerable attention due to their tunable electronic properties and potential for integration into flexible and miniaturized energy harvesting devices [3]. Although theoretical predictions and several experimental studies suggest enhanced TE performance for MoS_2 and other TMDCs with decreasing thickness [4,5], the thickness at which optimal performance is achieved remains unclear. A comprehensive experimental investigation of the impact of dimensionality on thermal transport and TE efficiency is still lacking and therefore remains highly relevant. In this study, we investigate the thermoelectric properties of mono- and few-layer MoS_2 and $MoSe_2$ flakes (up to 10 layers). The flakes were prepared via mechanical exfoliation and transferred using a dry transfer technique onto pre-patterned substrates. The morphology, microstructure, thickness, and number of layers were characterized using optical microscopy, reflectance measurements, scanning electron microscopy, and atomic force microscopy. We fabricated micro-devices equipped with gold contacts, integrated heaters, and micro-thermometers using two-step electron-beam lithography and thermal evaporation techniques. Calibration of micro-thermometers and verification of electrical contact quality were carried out using current-voltage characterization prior to TE measurements. Preliminary measurements of two- and four-probe electrical conductivity and the Seebeck coefficient were conducted in the temperature range of 15 – 295 K. The obtained data will allow us to analyze the influence of thickness and temperature on the TE performance of these 2D TMDCs.

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Acknowledgments

This work was supported by the Equal Opportunity and Diversity at the University of Bonn.

Comparative Study of the Thermoelectric Properties of High-Entropy Semiconductor (HES) $AgMnGePbSbTe_5$

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Because of their highly-disordered crystal structures, which lower the lattice thermal conductivity while maintaining advantageous electrical properties, high-entropy semiconductors (HES) have attracted significant attention for thermoelectric applications. The thermoelectric (TE) performance and thermal stability of $AgMnGePbSbTe_5$, a new HES recently studied by Luo *et al*. [1], are investigated in detail in this work. The TE properties were measured between 300 and 600 K on polycrystalline samples prepared by a solid-state reaction approach. A peak of ZT of ~1.15 was achieved at 575 K, lower than that reached in the previous study (~1.66 at 750 K). We further report differences in the transport properties measured upon heating and cooling and attribute to a phase decomposition that starts near 250°C according to high-temperature powder X-ray diffraction and differential scanning calorimetry. These results highlight the potential of HES for thermoelectric energy conversion but calls for more detailed, systematic evaluation of their thermal stability.

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Realization of thermoelectric Film Nanopatterning by Atomic Layer Deposition and Porous Template Replication

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Keywords: Thermoelectric films, nanopatterning, porous template replication, atomic layer deposition (ALD), chalcogenides

This work demonstrates the nanopatterning of thermoelectric films using porous templates combined with conformal coatings applied through Atomic Layer Deposition (ALD). To enable in-plane ZT (thermoelectric figure of merit) measurements, we introduce a silicon-based Lab-on-a-Chip platform equipped with a comprehensive set of thermoelectric test structures. By localizing and trapping phonons via nanoscale patterning, the thermal conductivity (κ) of thermoelectric films can be effectively reduced - a critical strategy for enhancing ZT.

Recent research focuses on two primary approaches: optimizing the power factor ($S^2\sigma$) and minimizing lattice thermal conductivity (κ_L). The latter is constrained by the phonons' mean free path, which can be shortened through atomic substitution and nanostructuring. Nanopatterning enables phonon scattering, particularly when dimensions approach the mean free path of phonons, leading to reduced κ and improved ZT performance. Significant advancements have been achieved through template replication, where the porous templates' configuration is tailored at the nanoscale to manipulate phonon transport effectively.

This presentation reviews recent progress in improving thermoelectric film efficiency, emphasizing phonon engineering via template replication and ALD-fabricated nanostructures. Key findings include the impact of nanolaminate architectures and porous templates on the Seebeck coefficient, electrical conductivity, and thermal conductivity, and subsequently, the ZT figure of merit. We discuss case studies involving lead chalcogenides (PbTe) and antimony telluride (Sb_2Te_3)-based films, synthesized on both planar substrates and porous templates. Additionally, hybrid organic-inorganic Surface Anchored Metal-Organic Frameworks (SURMOFs) are reviewed as a comparative approach.

Filling faults and vacancy swap occupation in half-Heusler compounds

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Keywords: half-Heusler, defect, filling fault

Defects play a vital role in understanding and elucidating the structure-property relationship in materials science. Here we report on the existence of a new kind of planar defects, filling faults, in half-Heusler (HH) compounds – a structurally and functionally diverse materials family. Ideal HH structure is composed of three occupied and one vacant sublattices. The two-dimensional filling fault layer tends to form with the originally vacant 4d sites occupied, fully or partly, which results in a vacancy swap occupation between the 4c and 4d sublattices. The unique defect configurations and the formation rule clarify the long-standing structure puzzles in HH compounds. These results deepen the understanding of precise crystallographic structures and defect-property relationships in solids, and facilitate the design of advanced materials and functional devices.

Effect of a heating plate on SiGe alloys manufacturing by Laser Powder Bed Fusion

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Keywords: Laser powder bed fusion, silicon germanium, heating plate, cracks

Laser Bed Powder Fusion (L-PBF) is an alternative to conventional metallurgy for printing complex metal parts in small and medium series. It has been incorporated into the thermoelectric (TE) materials and devices manufacturing process for semiconductors to produce the best shapes and possibly increase efficiency. Among TE materials studied by this technique, SiGe alloys are promising for high temperatures applications. Nevertheless, as it is the case for other TE materials, SiGe faces cracking issues occurring during its manufacturing, mainly due to high thermal stresses. This study introduces the effect of an heating plate during SiGe manufacturing by L-PBF on TE and structural properties, including cracks rate and relative density. Several tests have been performed at different temperatures and sets of parameters (scan speed, power, etc.). The influence of these parameters will be also presented.

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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).

Exploring the thermoelectric characteristics of cold-pressed copper iodide composites

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Keywords: copper iodide, composite, sustainable thermoelectric materials, cold-press

The quest for efficient thermoelectric materials has led to the exploration of various composites and fabrication techniques. This study investigates the thermoelectric properties of cold-pressed copper iodide (CuI) composites, focusing on their potential for energy conversion applications. Cold pressing, a cost-effective and scalable method, was employed to synthesize CuI composites with varying compositions and particle sizes.

The thermoelectric performance of these composites was evaluated through measurements of electrical conductivity, Seebeck coefficient, and thermal conductivity. The results revealed that the cold-pressed CuI composites exhibit promising thermoelectric characteristics, with enhanced electrical conductivity and Seebeck coefficient Scanning Electron Microscopy (SEM) was utilized to explore the morphology of the CuI composites, revealing a uniform distribution of particles and a well-defined microstructure. Furthermore, X-ray Photoelectron Spectroscopy (XPS) was employed to study the interface between the particles and organic compounds, providing insights into the chemical interactions and bonding mechanisms.

This study highlights the advantages of cold-pressed CuI composites in thermoelectric applications, emphasizing their potential for sustainable energy solutions. The findings pave the way for further optimization and development of CuI-based thermoelectric materials, offering a promising avenue for future research and industrial applications.

Acknowledgments

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

CrN based thin films for thermoelectric applications: Experimental and DFT study

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Keywords: Thermoelectric, sputtering, nitride thin films, phase formation, DFT, flat bands

Transition metal nitrides constitute an important class of functional materials which are mainly studied for their tribological applications but also possess promising thermoelectric properties. [1,2] Near room temperature, stoichiometric CrN shows high thermoelectric power factor (PF) of ~ 5 ×10^{-4} $Wm^{-1}K^{-2}$, however possess relatively higher thermal conductivity, κ ~ 4 $Wm^{-1}K^{-1}$. [3] Achieving stoichiometric CrN thin films is challenging and the intrinsic point defects greatly impacts their electrical behavior. Exploring the impact of intrinsic defects combined with study of phase formation as a function of doping concentration supported by DFT calculations can provide crucial insights for the design of better thermoelectric materials. We report on the growth and thermoelectric properties of epitaxial CrN and Nb incorporated CrN thin films grown by DC reactive magnetron sputtering on c-plane sapphire substrates. We observe a p-type to n-type transition of CrN films based on the N content in the film. Nb shows higher solubility in CrN as compared to other transition metals. [4] Additionally, we observe suppression of Neels temperature, as the Nb content increases in CrN. CrN shows a power factor of ~ 6.5 × 10^{-4} $Wm^{-1}K^{-2}$ however, which reduces to ~ 3.3 × 10^{-4} $Wm^{-1}K^{-2}$ due to Nb incorporation. Doping induced enhancement of σ is supported by density functional theory calculations which revealed shifting of Fermi level in the conduction band along with formation of acceptor states near the Fermi level. In conclusion, the combination of theoretical calculations along with experimental studies provides greater insights into CrN system which can help in designing better TE materials.

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Effects of non-stoichiometric co-doping on the thermoelectric properties of SnTe

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Keywords: Thermoelectric, chalcogenide, SnTe

SnTe-based thermoelectric materials have gained significant attention due to their potential for mid-temperature applications, non-toxicity, and low cost. However, their relatively low thermoelectric performance necessiates further research to enhance their properties. In this study, we proposed a non-stoichiometric doping method using Mn and Bi to improve the performance of SnTe-based thermoelectric materials, and aimed to investigate the effects of each dopant by sequentially introducing them. Manganese introduced by non-stoichiometric doping reduced the lattice thermal conductivity and enhanced the Seebeck coefficient across the entire temperature range. Furthermore, the introduction of bismuth lowered the thermal conductivity across all temperature ranges, and optimization of the carrier concentration resulted in a ZT value exceeding 1.3. This study achieved high performance in SnTe-based thermoelectric materials through a non-stoichiometric doping method. Furthermore, a mid-temperature chalcogenide thermoelectric module was fabricated using n-type PbTe and a specimen doped with 2 mol% Bi, which exhibited the highest ZT value. The fabricated module demonstrated an output performance of over 650 μW under practical operating conditions, confirming its potential for commercialization. The results of this study provide basic data for materials research for commercializing mid-temperature thermoelectric devices.

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Acknowledgments

This work was supported by grants from the National Research Foundation (NRF) of Korea, and funded by the Korean government (MSIT) (No. 2022R1A2C1006790). This study was supported by the BK21 Four project funded by the Ministry of Education, Korea (2120231314753).

Magnetic nanoparticle doping for thermoelectricity

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Keywords: Nanocomposite, thin film, magnetic nanoparticles

In this poster, I will present an investigation of the thermoelectric properties of a semiconducting medium decorated with highly size-controlled magnetic nanoparticles, each of which can be considered as a macrospin [1]. Our objective is to study the local effect of a single macrospin as well as the influence of the overall magnetic state of the macrospin ensemble on the electrical and thermal transport coefficients of the semiconductor. Recent studies provide evidence of the unusual effects of magnetic nanoparticles on electronic transport, specifically highlighting the influence of their magnetic states. [2,3]

The nano-composite system we propose is composed of a semiconducting matrix (thin film of amorphous germanium) into which nanoparticles of pure cobalt or alloys are codeposited using the Low Energy Cluster Beam Deposition method (LECBD [1]) under ultrahigh vaccum conditions. With this original set-up, we are able to synthetize with a physical route nanoparticle of well-defined sizes and controlled concentration (i.e., a controlled interparticle distance) inside the e-beam evaporated matrix. This provides an ideal platform for the in-depth study of the effects of the magnetic nano-inclusions on the transport properties.

Following the presentation of the deposition technique and structural characterization, I would like to show and discuss our preliminary thermoelectric measurements on a Ge matrix embedded with cobalt nanoparticles.

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Half-Heusler thermoelectrics based on $TiFe_{0.5}Ni_{0.5}Sb$ and (Nb,Ta,Ti)FeSb compounds synthesized via mechanical alloying

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Keywords: Half-Heusler, mechanical alloying, $TiFe_{0.5}Ni_{0.5}Sb$, NbFeSb

High power factor (PF) thermoelectric (TE) materials like half-Heuslers (hH) have been investigated for improvement strategies based on scattering processes within the material by decoupling the transport phonons and electrons to achieve better thermoelectric performance. Modifying dopant concentrations to change the carrier concentration and density of states effective mass while balancing out the scattering sources and thus the carrier mobility is one way to increase the PF of the material. Additionally, due to the suppressed electron-acoustic phonon coupling in hH alloys, therefore weaker electron scattering from phonons, defects have a higher impact in electronic transport than other TE materials and it's possible to enhance mobility by reducing scattering sources like lattice defects and get a high PF. Another effective option is to modulate the microstructure and point defects of the material via methods like annealing, aliovalent and isoelectronic substitutions, therefore improving the thermoelectric performance of the material due to the weak electron-acoustic phonon interaction by selective defect reduction. This can reduce the lattice thermal conductivity while also not greatly affecting the carrier mobility, but the point defect density and the ration of mobility over lattice thermal conductivity is important and must be regulated to achieve high PF while maintaining low thermal conductivity. One suitable candidate for investigation is the MFeSb (M = V, Nb, Ta etc.) class of hH alloys with higher valley degeneracy associated with their valance band making them a competitive p-type thermoelectric material option. More specifically for this study, one option is $TiFe_{0.5}Ni_{0.5}Sb$-based half-Heusler compounds that have an adjustable band structure and intrinsic low thermal conductivity. Another candidate for study is (Nb,Ta,Ti)FeSb with good thermoelectric properties that can be improved by manipulating the defect scattering process via microstructure and defect modulation using an Sb-pressure controlled annealing process. This work focuses on the synthesis and characterization of $Nb_{0.55}Ta_{0.40}Ti_{0.05}FeSb$ and $TiFe_{0.5}Co_{0.15}Ni_{0.35}Sb$ compounds synthesized via mechanical alloying using a ball milling process. The material characterization included thermoelectric measurements of Seebeck coefficient, electrical and thermal conductivity along with XRD, SEM and EDS analysis on samples made from hot-press sintering at various temperatures.

Solution-Processed PbTe Thermoelectrics with Enhanced Performance via Post-Synthetic Modification

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Keywords: Solution-based synthesis, thiol-amine, post-synthetic treatment

Among all thermoelectrics materials, PbTe remains one of the most widely explored, due to its demonstrated high-performance, stability and practical applications, thus nearing commercial viability. Moreover, its promising performance has led to its successful integration into thermoelectric generators powering critical systems during numerous space voyages, demonstrating its stability in extreme environments. However, energy-intensive manufacturing processes results in high production costs which currently limit its applications to these niche applications. These high costs are a consequence of conventional "top-down" approaches, where precursor materials are melted at elevated temperatures for extended periods, followed by grinding and re-densification. Herein, we apply the “bottom-up” approach, starting with nanostructures produced at room temperature that are subsequently sintered for short periods of time, providing the potential for cost-effective production. However, up to now, solution-based syntheses of PbTe have consistently yielded lower performance compared to conventional solid-state methods, largely attributed to challenges in effectively incorporating dopants into the PbTe matrix and ease of oxidation of the nanostructures. This work presents a room-temperature, solution-based synthesis of PbTe utilizing thiol-amine chemistry. We then introduce a simple post-synthetic treatment to incorporate dopants into the PbTe lattice during the sintering step. This new synthetic approach allows the production of high-performance PbTe with a figure of merit of 2.48 at 723K, comparable to that achieved using conventional solid-state techniques, but with significant reduced production cost.

Acknowledgments
This work was financially supported by ISTA and the Werner Siemens Foundation.

Structure and Thermoelectric Properties of Hydrothermally Grown $Bi_2Te_{3-x}Se_x$ Nanocrystals

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Keywords: Energy harvesting, Bi_2Te_3, nanocrystals, electrical conductivity, Seebeck coefficient, power factor

The large quantity of waste heat generated at intermediate and low temperatures by industry and automotive exhaust requires the advancement of power generation utilising thermoelectric (TE) materials. Bi- and Te-based materials are often utilised near ambient temperature. N-type bismuth telluride materials are ideal for generating TE power at low temperatures. The electrical characteristics of a semiconductor material can be precisely tuned to enhance TE functionality by doping. Doping allows to optimise the materials thermopower and electrical conductivity by modifying carrier concentration and mobility. Here we use the hydrothermal technique to synthesise nanostructured TE $Bi_2Te_{3-x}Se_x$ (x = 0, 0.4, 0.8, 1.2, and 1.6) nanocrystals. By manipulating the concentration of NaOH, which has a significant impact on the synthesis mechanism of Bi_2Te_3, the particle size and morphology can be regulated. We investigated the structures and morphologies of the synthesized materials. The crystal structure exhibits a hexagonal geometry, with a preferred growth along the (015) plane. The shift of the diffraction peaks towards lower angles as the Se concentration increase is attributed to the substitution of Te atoms by Se atoms in the crystal structure. Electron microscopy indicated that the size of the nanocrystals decreased with the increase in the Se concentration. The power factor of the best performing material, $Bi_2Te_{1.4}Se_{1.6}$, was enhanced to 156 $\mu Wm^{-1}°C^{-2}$ at 350 °C (the highest reported for $Bi_2Te_{3-x}Se_x$ nanocrystals up to now), compared to the undoped sample (23 $\mu Wm^{-1}°C^{-2}$), indicating its potential for developing novel materials and devices for TE applications.

Production of reliable Mg_3Sb_2 material and components for use in larger scale devices

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Keywords: Mg_3Sb_2, material optimisation, device scale-up

Current thermoelectric devices often utilise bismuth telluride (Bi_2Te_3) because it is well studied and highly optimal for near room temperature applications. However, Bi_2Te_3 is expensive, toxic and the raw materials, especially Tellurium has scarcity challenges, if higher scales are achieved. It also well reported that the performance of Bi_2Te_3 material and the stability of the devices declines at higher temperatures. Therefore interest has grown in replacing bismuth telluride with a more eco-friendly and abundant option, such as Mg_3Sb_2, which has also been reported to improve the performance of thermoelectric devices at higher temperatures. This work has focused on developing reliable n-type Mg_3Sb_2 to replace n-type Bi_2Te_3 as well as an emphasis on scaling up thermoelectric devices. Reproducibility testing of components throughout the production process is an important step in achieving a high final yield of devices. Therefore, as part of this work, a test method was developed to evaluate the relative electrical resistance of the metallised Mg_3Sb_2, at puck level. This rapid, non-destructive method which involves no special sample preparation is performed using an 8-point-probe system at room temperature. 29 samples were prepared and tested, with an average electrical resistance of 0.28 mOhm (acceptable range: 0.2-0.4 mOhm). Only 5 samples were rejected at this stage, due to a high resistance value, giving a yield of 83%. This test helps to remove any variation in materials and joint quality. The quality and stability of the metallisation joint was evaluated further at pellet level, by measuring the contact resistance between the thermoelectric and its metallisation at 0h, 24h and 96h aging at 300°C in air. The average contact resistance at 0h was $1.9x10^{-5}$ Ohm cm² and remained stable throughout aging: $1.3x10^{-5}$ Ohm cm² at 24h and $1.7x10^{-5}$ Ohm cm² at 96h. These results have demonstrated the consistency and promising stability of the Mg_3Sb_2 components. Further work was performed at device level, which focused on scaling up reliably. To the best of our knowledge there are more than 30 literature reports on Mg_3Sb_2 based generator devices and couples, but 97% of them used <10 couples, of which 48% are only one couple. For commercial application, higher couple numbers are typically used to enable higher voltages that can be more easily handled with the interfacing electronics. The device built successfully in this work contained 32 couples, with a leading device voltage output of 6.4 μV/K, exceeding the literature reported values of 0.12-3.2 μV/K [1, 2]. The successful scale-up and reproducibility demonstrated at both material and device level highlight the strength of Mg_3Sb_2 for higher temperature applications, and has demonstrated the ability to achieve a higher couple module, without compromising on performance.

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Enhanced power factor in Nb doped $SrTiO_3$ thin films via strain induced band degeneracy and energy filtering

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Keywords: Strain engineering, energy filtering, 2DEG, power factor

Materials with high thermoelectric power factors are critical for optimizing heat-to-electricity conversion, a key aspect in the development of efficient thermoelectric devices. In this study, we report the highest reorded power factor of 0.0185 W/mK^2 in $SrTi_{0.9}Nb_{0.1}O_{3-\delta}$ thin films, synthesized using RF magnetron sputtering in oxygen free environment. The structural, compositional, and morphological characteristics, determined through XRD, XRF, SEM, and EDS analyses, were directly correlated with the electrical and thermoelectric transport properties obtained from hall and TE measurements. The high carrier concentrations, in the range of 10^{20}-10^{21} cm^{-3}, were attributed to charge carriers introduced via Nb doping and oxygen vacancies formed through pure Ar sputtering and subsequent vacuum annealing. The conduction mechanism in all samples follows a degenerate semiconductor model, well-approximated by a parabolic band structure. Seebeck coefficients in the range of 200 to 400 μV/K were achieved, attributed to the combined effects of energy filtering, effective mass modulation, and strain-induced band degeneracy. The optimized sputtering conditions were pivotal in realizing this remarkable thermoelectric power factor.

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Thermoelectric and mechanical properties of $Ti_{0.25}Zr_{0.75}NiSn$ half-Heusler alloy produced by Ultrafast High-temperature Sintering

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Keywords: Half-Heusler, ultrafast high-temperature sintering

Half-Heusler (hH) compounds are among the most promising materials for the production of intermediate temperature Thermoelectric Generators (TEGs) for the conversion of waste heat. They possess several interesting features, like high flexibility in the composition, the possibility to avoid toxic or most critical elements, and high thermoelectric average figure of merit in the temperature range 200-700 °C, often above 0.7 [1]. For these reasons some hH compounds are among the most close-to-market intermediate temperature thermoelectric materials. Despite the numerous advantages, they generally possess high sintering temperature and for many composition hH alloys suffer from oxidation problems at high temperature. For these reasons, they are normally sinterized at the laboratory scale by employing Hot pressing under vacuum or Spark Plasma Sintering. The need for these technique results in high energy consumption and a higher TEG cost. The recently proposed Ultrafast High-temperature Sintering technique [2] generally enable the densification of a wide range of materials. Sintering could be performed with a very simple setup, exploiting up to 10^4 °C/min heating and cooling rates, with total sintering times often below 1 minute: these high process rates proved their efficacy in preventing grain coarsening and reducing total energy consumption. For thermoelectric materials it proved to be effective for Mg_2Si [3]. In this work we applied UHS a for the densification of $Ti_{0.25}Zr_{0.75}NiSn$ [1] powders synthesized by arc melting of metallic precursors. The grain coarsening suppression effect on thermal conductivity has been verified. The sintering process is described and the morphological, structural and thermoelectrical properties of the sintered pellets are compared to the as cast material.

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Acknowledgments

Authors would like to thank the project ThermoSpin financed by European Union, Next Generation EU, Mission 4, Component 1, CUP D53D23005290006 and B53D23008530006.

Thermoelectric properties of thin ScN layers doped with W

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Keywords: Nitrides, thin films, ScN, magnetron sputtering

Transition metal nitrides have seen increased focus in relation to their thermoelectric properties and potential applications. [1] Here, we investigate thin films of scandium nitride doped with tungsten. We used DC magnetron sputtering in ultra-high vacuum to prepare a series of samples on MgO(001) substrates with different levels of W doping. We measured the thermoelectric properties of the resulting films between room temperature and 800 K and confronted the results with theoretical calculations. This was complemented by X-ray diffraction, X-ray spectroscopy and Raman spectroscopy characterization. All the samples showed metallic behavior with electrical resistivity ρ rising moderately with increasing temperature and the absolute value of the Seebeck coefficient *S* rising almost linearly and doubling between room temperature and 800 K. Electrons serve as the majority carriers, as evidenced by negative values of *S*. The impact of doping is clearly seen from the monotonous decrease of |*S*| with increasing level of doping.

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Acknowledgments

This work was supported by the Czech Science Foundation (GAČR) project No. 23-07228S.

Towards *p*-type thermoelectric $LaCoO_3$–based epitaxial thin films

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Keywords: $LaCoO_3$, p-type thermoelectric, epitaxial thin films, molecular beam epitaxy, Sr-doping

Thermoelectric materials, which directly convert waste heat into electricity, have emerged as promising candidates for energy-efficient technologies. Although conventional thermoelectrics—such as Bi_2Te_3—have long proven effective in the field, thermoelectric materials based on perovskite oxides are attracting increasing attention due to their structural flexibility and properties tunability, their use of abundant and non-toxic elements [1]. In particular, epitaxial thermoelectric thin films offer enhanced tunability through strain engineering [2], precise doping control at the atomic scale [3], and provide a pathway for integrating these materials into micro- and nanoscale devices on Si [4]. However, competing *p*-type thermoelectric perovskite oxides are still lacking. $LaCoO_3$ (LCO) is a versatile perovskite oxide renowned for its tunable electronic, magnetic, and chemical properties [5]. Although pristine $LaCoO_3$ does not exhibit intrinsic thermoelectric functionality, solid solutions with aliovalent cations—especially with Sr—can induce promising *p*-type thermoelectric behavior [6].

In this communication, we report the epitaxial growth by molecular beam epitaxy (MBE) of high-quality undoped $LaCoO_3$ thin films on $SrTiO_3$ (STO) substrates. We will first present the flux monitoring by quartz crystal microbalance (QCM), prior to the growth which is *in-situ* monitored by reflection high-energy electron diffraction (RHEED). We will in particular show the impact of oxygen partial pressure $P(O_2)$ and power of oxygen plasma during growth on the structural and chemical properties, through characterizations by x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). We will show the growth conditions in order to obtain the excellent crystalline quality and stoichiometry. This work establishes a reliable synthesis route for undoped LCO, providing a basis for future Sr-doping to enhance its thermoelectric performance.

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Acknowledgments

This work was supported by CNRS-MITI through the project TEOX 2024, Ecole centrale de Lyon, and project PHC Maïmonide 2025 (TOP).

Phase diagram Engineering Advances the Thermoelectric Performance of Zintl Phase $EuZn_2Sb_2$

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Keywords: Thermoelectric, phase diagram, defect chemistry

The phase diagram has proven to be an indispensable tool in guiding the discovery and optimization of materials with superior thermoelectric properties. This work conducted the 773 K isothermal section of the Eu–Zn–Sb ternary system, unambiguously identifying the multiple chemical states of $EuZn_2Sb_2$. The defect chemistry and thermoelectric properties across chemical states were systematically elucidated. Ultimately, state III ($EuZn_2Sb_2$ + ZnSb two-phase region) achieved a reproducible zT of ~ 0.8 at 723 K. Further Yb and Cd alloying synergistically improved band degeneracy and introduced substantial mass/strain fluctuations, yielding a record-high peak zT of ~ 1.2 at 773 K and an average zT of 0.68 (323–773 K). Leveraging this breakthrough, the $EuZn_2Sb_2/Mg_3(Sb,Bi)_2$ two-pair module achieves a maximum conversion efficiency of ~ 9% under ΔT = 473 K. This work provides the foundation for designing thermoelectric materials via phase diagram engineering and underscores the potential of Zintl phases in mid-temperature energy harvesting applications.

Acknowledgments
This work was funded by the National Natural Science Foundation of China for Distinguished Young Scholars (52425108), the Guangdong Basic and Applied Basic Research Foundation (2024B1515040022), the National Natural Science Foundation of China (52172194, 52302232), the Shenzhen Science and Technology Program (JCYJ20241202123659001, RCJC20210609103733073, KQTD20200820113045081), State Key Laboratory of Precision Welding & Joining of Materials and Structures (No. 24-Z-18).

Significant anharmonic scattering in single-crystalline $Mg_{4.8}Ag_{1.4}Sb_4$ with site-occupation disorder

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Exploring new materials with low thermal conductivity is of great scientific and technological importance for applications like thermoelectrics and thermal barrier coatings. Herein, $Mg_{4.8}Ag_{1.4}Sb_4$ single crystal has been obtained and it exhibits an ultralow room-temperature thermal conductivity of ~0.6 W m^{-1} K^{-1}. Structure determination based on single-crystal X-ray diffraction analysis reveals the $Fm\bar{3}m$ crystal type and identifies the mixed occupancy of Mg atoms (~60 at.%), Ag atoms (~17.5 at.%), and vacancies (22.5 at.%) at the 8c site. Such site-occupation disorder results in significant phonon scattering and is responsible for low thermal conductivity. Theoretically, first-principles calculations confirmed the high anharmonic scattering rates and the short mean free path. In addition, molecular dynamics simulation discovers the abnormal atomic vibration of Ag atoms with a large amplitude at 300 K, which induces a low-lying acoustic phonon branch and increased phonon density of states at 0.6 THz. This can explain the enhanced anharmonic scattering rates with the increase in temperature and further reduction of the lattice thermal conductivity. Our work can shed new light on the discovery of novel materials with low thermal conductivity.

Hard-to-Sinter materials in Easy-to-Sinter wave-forms

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Keywords: SPS sintering, Hard-to-Sinter materials, wave forms

Commonly the majority of SPS sintering studies, in research, development and production, are performed with the ON/OFF pulses. After the introduction of SPS some 30-40 years ago, much attention was focussed on finding an optimal ratio between ON and OFF times. During later years this has not been so much researched, instead people tend to stay with an almost "fixed" ratio, like 12/2 or 40/10. Not much optimisation is to be expected by varying the ratio. Even though ON/OFF is the absolutely most common wave current form, some very few studies use constant DC or AC.
During recent times we have been exploring a new wave-form which can be called Full wave. The findings in general can be summarized in the following sentences:
The sintering process starts at lower temperatures, consumes less energy and reaches often higher densities. There are differences between types of materials – metals/ceramics/hard-to-Sinter materials, which we try to systematize. There are also indications that reactions between different powder components proceed with different reaction rates under different wave forms. The possibility to combine this effect with an advanced de-gassing process which cleans up the powder by removing moisture and impurities under heating at low pressure before sintering commences adds further advantages to be explored.

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Improvement of Thermoelectric Performance of Mg_2Si Compound by Removing Ag impurities in Si Extracted from Photovoltaic Waste

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Keywords: Magnesium silicide, Thermoelectric performance, Reused silicon, Waste photovoltaic module

After 2030, the annual disposal of photovoltaic (PV) modules is expected to reach 800.000 tons in Japan [1]. Since Si cells contained in these waste modules include impurities such as the Ag used for electrodes and the dopants, it is difficult to reuse them for PV modules. We have reported in ICT/ECT2024 that the thermoelectric Mg_2Si compound could be synthesized using waste Si cells and the figure-of-merits (ZT) of 0.91 was obtained at 850 K. In this study, we investigated the impact of Ag contained in the extracted Si from waste PV modules on the thermoelectric performance of Mg_2Si compounds. Three types of Si powders were prepared by (i) subjecting Si cells extracted from waste PV modules to an acid treatment (AT), (ii) un subjecting them to AT, and (iii) pulverizing nondoped Si wafers for comparison. The AT was repeated three times to remove Ag impurities from the Si powder fragments. The Si fragments or wafers were pulverized using a planetary ball mill and size classified. The pure Mg powder, AZ61 Mg alloy chips, and the Si powder were weighed and mixed. The mixture was heated above the melting point of Mg in an Ar gas flow and the Al and Zn-doped Mg_2Si compounds were synthesized by a liquid-solid phase reaction method [2]. The Mg_2Si samples were consolidated using a spark plasma sintering (SPS) method. They were evaluated by scanning electron microscopy with energy-dispersive X-ray spectroscopy, and X-ray diffraction (XRD) analysis and thermoelectric measurement. The XRD analysis revealed that the waste Si powder contained Ag as an impurity, which was almost completely removed by acid treatment (AT). A comparison of SEM-EDS images showed that in the Mg_2Si sintered body synthesized using Si without AT, Ag and Al were aggregated, and the ZT values were about 15% lower in all temperature ranges compared to that of the sample with AT. This degradation in thermoelectric performance is attributed to the formation of compounds between Ag impurities and Al, which was originally intended to be doped into Mg_2Si. This interaction prevented Al doping, leading to a decrease in carrier concentration and electrical conductivity. On the other hand, Mg_2Si synthesized using Si fragments subjected to AT showed ZT values comparable to those obtained using undoped Si wafers, confirming the improvement in thermoelectric performance due to the removal of Ag impurities.

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This research was supported by COI-NEXT (JPMJPF2204) of the Japan Science and Technology Agency (JST).

Ultralow Lattice Thermal Conductivity and Colossal Thermoelectric Figure of Merit of the Room Temperature Antiferromagnet CsMnBi

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Keywords: Thermoelectricity, antiferromagnetism, lattice thermal conductivity

We study the experimentally synthesized layered material CsMnBi using first-principles calculations and the linearized electron and phonon Boltzmann transport equations. CsMnBi is found to be a semiconductor with a narrow indirect bandgap of 220 meV and to realize C-type antiferromagnetism, which is energetically favorable by 187 meV per formula unit over ferromagnetism. Energetical overlap between the acoustic and low-frequency optical phonon modes enhances the phonon scattering. Combined with low group velocities and high lattice anharmonicity this results in an ultralow lattice thermal conductivity of 0.07 $Wm^{-1}K^{-1}$ at 300 K. A high thermoelectric figure of merit of 2.1 (1.6) is achived at 300 K at a hole (electron) density of 6 x 10^{18} cm^{-3} (1 x 10^{18} cm^{-3}), pointing to potential of CsMnBi in thermoelectricity.

Acknowledgments
The research reported in this publication was supported by funding from King Abdullah University of Science and Technology (KAUST). For computer time, this research used the resources of the Supercomputing Laboratory at KAUST.

High-efficient search for high-performance Al-O based thermoelectric materials working at high temperatures using first-principles calculations in combination with machine learning

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Keywords: Al-O based thermoelectric materials, density functional theory calculations, Boltzmann transport theory, machine learning

Thermoelectric (TE) conversion is one of the waste-heat utilization technologies. Recently, although thermoelectric devices working at room temperature have been attracting attention for plant monitoring and wearable devices, those working at high temperatures, which are essential for CO_2 reduction and energy conservation, have not been investigated extensively. We focus on aluminum oxide (Al-O) based materials, because they exhibit excellent heat-resistances and are easy to perform stable substitutional doping even against 900 K. However, since the representative database, Materials Project [1] (MP), registers as many as 3.447 Al-O based materials, it is not realistic to evaluate the thermoelectric performance for all of them using first-principles calculations themselves. Thus, we aim to employ a data-scientific method to efficiently search for high-performance Al-O based TE materials from MP database. We chose 109 structures from the MP database that include bulk modulus values required for estimating lattice thermal conductivity (κ_l) [2]. We used VASP [3] and BoltzTraP [4] to evaluate their electric conductivity (σ), Seebeck coefficient (S), and electronic thermal conductivity (κ_e). A neural network model (NNM) was trained using the figure of merit [$ZT = \sigma S^2T/(\kappa_e+\kappa_l)$] at 900 K as a target. Then we optimized and used the NNM to predict the ZT of residual 3.338 Al-O based materials in MP database, and eventually succeeded in finding four high ZT candidates working at 900 K, such as three AlPO4 polymorphs and one AlAsO4 with similar structure. Details of the NNM optimization and structure-property correlations will be discussed in this talk.

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Acknowledgments

The work was financially supported by the Electric Power Development Co., Ltd. (J-Power). First-principles calculations were performed using the Supercomputer "Flow" at Nagoya University. One of the authors (R.B.) would like to thank Prof. Eric Toberer (Colorado School of Mines) and Dr. Prashun Gorai (Rensselaer Polytechnic Institute) for their valuable discussions and technical advices.

Exploring the Synthesizability of High-Entropy Skutterudites for Thermoelectric Applications

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Keywords: High-entropy, skutterudites, synthesizability

High-entropy materials, HEMs, represent a transformative class in materials science, offering a unique approach to thermoelectric material design. These materials, containing multiple principal elements, derive their stability from high configurational entropy, potentially leading to novel properties. While rational design of HEMs is challenging due to the lack of reliable models and the limitations of current empirical descriptors, their promise in thermoelectrics lies in the potential for tunable properties, including enhanced electronic transport, reduced thermal conductivity, and improved thermal stability [1-3]. This work explores the synthesizability of high-entropy skutterudites, focusing on compositions with partial substitution of Co by Ni and Fe, as a novel approach to identify sustainable thermoelectric materials

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Acknowledgments

This work was funded by grant PID2022-138063OB-I00 funded by Spanish MICIU/AEI/ 10.13039/501100011033 and by FEDER, UE and by grant TED2021-130874B-I00 funded by Spanish MICIU/AEI/10.13039/501100011033 and by European Union Next Generation EU/PRTR.

Transmission and reflection coefficients of a nonlinear acoustic mismatch model

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Keywords: Acoustic mismatch model, nonlinear dispersion relation, transmission coefficient, critical angles, interference

The transmission and reflection coefficients of plane waves incident on a perfectly smooth plane interface are reexamined. Unlike the traditional acoustic mismatch model (AMM) which deals with linear materials, a new model applicable for materials with nonlinear dispersion relation is developed. The constitutive equation takes an implicit form of stress gradients and strain gradients [1] and the involved parameters are determined by fitting the predictions with experimental measurements. Continuity conditions for displacements and stresses at the interface are then used to determine the amplitudes of reflected and transmitted waves. Results of incident longitudinal (L), shear vertical (SV), and shear horizontal (SH) waves are all studied. For the former two waves, the polarization may change after transmission/reflection. Critical angles for full reflection are also concerned. The energy fluxes are finally calculated and so are the transmission coefficients (T) and reflection coefficients (R). In particular, we propose to merge the interference energy fluxes into the incident flux. The corresponding interfacial thermal resistance is calculated and compared with the linear counterpart.

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Acknowledgments

This work was supported by the National Science and Technology Council, Taiwan (NSTC 113-2221-E-002 -195 -MY3).

Uncertainty analysis of microscopic parameters obtained from the single parabolic band (SPB) modelling of thermoelectric materials

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Keywords: Thermoelectric transport, modelling, uncertainty analysis, electronic band structure

The single parabolic band (SPB) model is a popular, easy to use and somewhat powerful tool to describe the thermoelectric transport and often employed for material optimization and extraction of band structure parameters. While the fundamental limitations of the model are well known and usually recognized, a discussion on the uncertainty of the derived parameters when the model is valid is missing, but indispensable for a qualified comparison and analysis of reported values. In this work, we derive analytical expressions for the uncertainty in the modelling parameters – the reduced Fermi level, density of states (DOS) mass, carrier concentration (n), mobility parameter (μ_0), Lorenz number (L) and electronic thermal conductivity (κ_E) based on experimental uncertainty in the Seebeck coefficient (α), electrical conductivity (σ) and Hall coefficient (R_H). As the uncertainty in the SPB-derived parameters resulting from the Seebeck coefficient depends not only on the uncertainty of the Seebeck coefficient but also on the value itself, it is discussed in detail. The uncertainty in the most cited parameter derived from the SPB model - the DOS mass, is dominated by the uncertainty arising due to α. For a relative uncertainty of 5% in α, the uncertainty in the DOS mass ranges from 8%-17% for 50 µV/K-400 µV/K. Associated challenges to accurate and insightful modelling of TE materials are discussed and exemplified by the analysis of DOS masses for Mg_2Si from various literature sources, where the observed large scatter can be rationalized by large, but realistic uncertainties in α and R_H, thereby highlighting the need for better measurement protocols.

Possibility of large power factor in full-Heuslers with elongated bands

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Keywords: Flat bands, full-Heusler alloys, elongated tubes

Half-Heuslers are known to have large thermoelectric (TE) power factors (PF). Full-Heuslers are less studied, because most of them are metals. In this work we consider semimetal/semiconducting full-Heusler materials, which in addition include elongated, low dimensional tube-like bands in their 3D Brillouin Zone (BZ). Elongated bands are known to provide high PFs compared to spherical bands (when compared at the same density of states) [1]. Our goal is to evaluate when such bands are beneficial. We examine computationally three such materials, i.e., Fe_2YAl, where Y=V/Nb/Ta. They have elongated bands in addition to different features superimposed in their bandstructure. We show that the combination of elongated bands with the rest of those features, can have large differences in their PFs. We use Boltzmann transport calculations as implemented in the ElecTra software [2]. We incorporate the complete energy/momentum/band dependencies of all relevant electronic scattering rates, i.e., acoustic phonons, non-polar optical phonons (both intra- and inter-valley), polar optical phonons (POP), and ionized impurity scattering (IIS). All parameters that define the rates are extracted ab initio (deformation potentials) [3], while we account fully for intra-/inter valley/band transitions, screening from electrons and holes, and bipolar transport effects. Fe_2VAl is a semimetal with elongated bands appearing higher in energy. We show that it experiences a large degree of Seebeck coefficient (S) oscillations between n- and p-type polarities as a function of the Fermi level (E_F). However, since it is semimetal, the PF remains low. Fe_2NbAl is a semiconductor with elongated bands at its conduction band (CB) edge, superimposed with two other dispersive valleys. That combination degrades S fast enough as a function of E_F outpacing the gain in electrical conductivity. As a result, while it has higher PF than Fe_2VAl, it still remains within a moderate range. Fe_2TaAl also has flat bands at its CB minima, but it is superimposed with one dispersive band and in this case the elongated energy surfaces extend at higher energies, such that much larger PFs can be reached. Our results show that in the presence of elongated bands, the rest of the surrounding electronic structure details matter in realizing their full potential. We provide examples of when optimization can be achieved, and when it cannot. This could lead to more targeted materials screening and experimental efforts in taking advantage of such features more optimally.

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Acknowledgments

This work has received funding from the UK Research and Innovation fund (project reference EP/X02346X/1).

Tuning Thermoelectric Properties of PEDOT:PSS Thin Films through strategist : A First-Principles and Experimental Approach

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Keywords: Thin films, BoltzTraap, Thermoelectric Properties

In order to thune thermoelectric properties of PEDOT:PSS we introduce different methods Acid treatment, metal nanoparticle doping, and graphene insertion [1]. Obtained sample characterize the eletrical conductivity around 15000 S/cm. In plane thermal conductivity will be measured using thermoreflectance method [2].

First principles DFT calculations (Quantum ESPRESSO, BoltzTraP) and experimental analyses are combined to investigate these films. These calculations survey structural optimization, electronic band structure, phonon dispersion, thermal conductivity, and thermoelectric transport coefficients.

This combined approach offers a comprehensive understanding of effect of different treatment of PEDOT:PSS films on their thermoelectric performance.

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Effect of aliovalent/isoelectronic alloying on the power factor of half-Heuslers

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Keywords: aliovalent doping, isoelectric doping, half-Heuslers, polar optical phonon, alloy electronic structure

The alloying strategy is an important factor to achieve optimal carrier concentration in a thermoelectric material. Aliovalent doping is preferred to effectively minimize thermal conductivity while synergistically optimize the electronic properties [1]. The use of appropriate dopants in highly polar half-Heusler and Zintl compounds can result in improved thermoelectric performance due to the strong screening effect imposed by the aliovalent dopants, optical phonon softening, and reduced LO-TO splitting, which could suppress polar optical phonon scattering, as observed in recent studies [2,3]. Given the importance of aliovalent dopants in achieving high power factors, we use first-principles methods to investigate the electronic, phononic, and transport properties of aliovalent Ti, Zr, Hf, compared to isoelectronic Ta-doping in p-type NbFeSb. We used the Boltzmann transport code ElecTra for transport properties including scattering by acoustic phonons, polar optical phonons and ionized impurities [4]. Unlike the isoelectronic Ta-doped NbFeSb material, the aliovalent Ti, Zr, and Hf-doped systems exhibit significant splitting along the band edge valleys, which affects the carrier velocities and thermoelectric coefficients, as also observed experimentally for other materials[5]. Importantly, aliovalent doped materials also show a large drop in their highest optical phonon frequency as well as flatter phonon dispersions, indicating a reduction in electron-polar phonon scattering, while isoelectronic Ta-doped systems do not show such effects. Our study would be helpful in understanding the effect of different alloy species in optimizing thermoelectric materials.

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Acknowledgments

This work has received funding from the UK Research and Innovation fund (project reference EP/X02346X/1).

Processing of thermoelectric intermetallic compounds for a waste heat harvesting module

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Keywords: Intermetallic compounds, metallurgical processing, thermoelectric module

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 Zn_4Sb_3 intermetallic compounds for medium/low temperature (RT-400°C).

The aim of the work is two-fold. On the one hand, 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. On the other hand, the effect of doping and processing on the thermoelectric properties of ZnSb and Zn_4Sb_3 intermetallic compounds has been investigated, in order 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 from the structural, microstructural, thermal, mechanical and thermoelectric point of view. The effect of the process on the microstructure (grain boundaries and interphase interfaces densities), transport and mechanical properties is outlined. Materials with optimized properties were selected for assembling lab-scale thermoelectric generator prototypes.

Acknowledgments
The authors would like to thank the project ThermoSpin: “Modelling and process engineering of Heusler alloys for thermoelectric waste heat harvesting and spintronic applications” financed by European Union, Next Generation EU, Mission 4, Component 1, CUP D53D23005290006 and B53D23008530006. A. Castellero, S. Boldrini, A. Ferrario and C. Fanciulli acknowledge financial support from “Ricerca di sistema elettrico - Piano Triennale 2025-2027”. Authors from Università di Torino acknowledge support from the Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023-2027" (CUP: D13C22003520001).

A Structured, Standardized, and Accessible Data Format for Thermoelectric Materials

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Keywords: Thermoelectric materials, experimental data curation, inverse materials design, transport property modelling, multimodal data integration

The rapid evolution of Materials Acceleration Platforms is driven by the integration of high-quality, structured, and reproducible data from high-dimensional experimental and simulation spaces. These datasets provide critical input for advanced machine learning and deep learning models, particularly in complex domains such as thermoelectrics, where the simultaneous optimization of conflicting properties, like electrical conductivity, Seebeck coefficient, and thermal conductivity, makes inverse design highly nontrivial. Here, we present the work of a multidisciplinary team focused on the digital transformation of experimental data for thermoelectric materials into a structured, standardized, and AI-ready format. Our data pipeline begins with the selection of an open, flexible text format with space- or tab-delimited columns to ensure interoperability and long-term accessibility. Compositional, structural, and microstructural data derived from techniques such as X-ray diffraction, scanning electron microscopy, and energy-dispersive X-ray spectroscopy were standardized and encoded in machine-readable formats. Additionally, synthesis and sintering procedures were normalized, and key transport properties, electrical conductivity (σ), Seebeck coefficient (S), and power factor ($PF = \sigma S^2$) as a function of temperature, were systematically structured. This curated dataset lays the foundation for AI-driven design workflows using models such as graph neural networks for property prediction, variational autoencoders for latent space exploration, and reinforcement learning for inverse design under multi-objective constraints. By establishing an accessible and high-integrity dataset, this work contributes to accelerating the discovery and optimization of novel thermoelectric materials for energy conversion applications.

Acknowledgments
This communication is based upon work from COST Action EU-MACE, CA22123, supported by COST (European Cooperation in Science and Technology). The work was funded by Portuguese funds through the FCT—Fundação para a Ciência e a Tecnologia, I.P. under the projects PTDC/EAM-PEC/29905/2017 and UID/Multi/04349/2019.

Tellurium-Free Thermoelectric Modules For Waste Heat Recovery

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Keywords: Tellurium-free, thermoelectric module, nanostructuring, spark plasma sintering

In recent years, the demand for sustainable energy sources have led to the rise in the interest towards thermoelectric materials for their low maintenance, noiseless operation and reliability. Though already implemented in high temperature regime (> 600 degC) in niche industuries like space, thermoelectric materials can have interesting applications in low to mid temperature regime (< 600 degC) like waste heat recovery or sensors for internet of things (IOT). Bismuth Telluride (Bi_2Te_3) is the most commonly used thermoelectric material used in this temperature regime due to its high performace at room temperature. However the use of tellurium, which is extremely scarce and toxic, has ignited the need to move towards more sustainable choices [1]. This study details the fabrication of a low/mid-temperature thermoelectric module designed for efficient energy conversion within the 200-350°C range. The 31 pair module utilizes Tellurium-Free Tetrahedrite material as p-type and Magnesium Antimonide as the n-type material. Both leg materials are obtained by ball milling and subsequent spark plasma sintering (SPS) for obtaining nanostructuring which leads to enhanced thermoelectric performance in this temperature regime. Nanostructuring has been identified previously as a method to obtain high ZT (mostly > 1) in thermoelectric materials by lowering of thermal conductivity through phonon scattering. The nanostructured SPS discs are precisely ground to desired heights, coated with a metallization layer and segmented into specified leg dimensions. These legs are then further bonded on a direct bonded copper (DBC) patterned alumina (Al_2O_3) substrate using a nano silver sinter paste, deposited via screeprinting. A custom jig is used for the placement of the legs and assembly of the module. Subsequently pressure assisted sintering of the assembled module was achieved by exposing it to a thermal cycle. The resulting module demonstrates the feasibility of developing a thermoelectric module with Tellurium-Free materials. Further characterisation of the module is performed to measure its thermoelectric performance, internal resistance and stability at operating tempetures. This work provides a pathway for the development of reliable and high-performance low/mid-temperature thermoelectric modules for applications in waste heat recovery and industrial thermal management

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START ("Sustainable Energy Harvesting Systems Based on Innovative Mine Waste Recycling") project (project number: 101058632) is co-funded by the European Union.

Printed Thermocouple Sensor Array for Human-Machine Interaction

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Keywords: Sensor array, printed thermoelectrics, Seebeck effect, human-machine interaction

Although research on thermoelectric technology (TE) has mainly focused on energy harvesting and cooling applications [1], it is also extensively used in thermal sensing through thermocouples. Despite notable progress, bulk TE materials-based thermocouples lack flexibility and shape conformability. Furthermore, fabricating a spatially resolved sensor is challenging using bulk approaches. In this work, we screen-printed shape-conformable, flexible thermocouple using Bi-Te-based n- and p-type TE materials with a Seebeck coefficient (S) > 250 $\mu V\ K^{-1}$. Sensor arrays with ≥ 10 pixels were constructed using these printed thermocouples, enabling a human-machine interaction (HMI) system [2,3]. The standard deviation of sensitivity across pixels remains within 10% of the average value. Half the length of each thermcouple was covered by an aerosol jet-printed silver reflector. These reflectors selectively shield one half of each thermocouple from radiation, facilitating both contact and non-contact HMI sensing. The output voltage generated by each pixel, governed by Seebeck effect, arises due to the temperature difference along the thermocouple either through direct heat conduction or radiation absorption from a human finger. The pixel array can locate the precise position of interaction. Hand movements and gestures are accurately detected, enabling transmition of indications and messages from hand to a computer. This work paves the way for advanced, human-machine interaction systems.

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Acknowledgments

The authors acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) for financial support. This project has received funding from the European Research Council, grant 101097876 - ORTHOGONAL. The aulthors also acknowledge support from the Karlsruhe School of Optics & Photonics (KSOP).

Thermochromic Display Modules Using Localized Peltier Cooling

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Keywords: Localized peltier cooling, thermochromic display module, thermochromic pigments, thermoelectric application, thermoelectric device

Most commercial products utilizing thermoelectric devices are applications that leverage the Peltier cooling effect. These applications include silent and vibration-free refrigerators, automotive ventilation and climate control, telecommunications, heat dissipation in electro-optical semiconductors, precision temperature-controlled coolers for biomedical DNA amplifiers, and deep cooling systems utilizing multi-stages of thermoelectric elements. As a novel application, we have fabricated a simple information display module by controlling the temperature of a localized area through rapid temperature control, a feature of micro thermoelectric cooling devices, by altering the color of thermochromic pigments. Previous similar studies include aesthetic artworks that utilize the color-changing effect of thermochromic materials by controlling the temperature change in a specific area with Peltier cooling elements [2], and a family of camouflage products that are similarly attached to the skin to provide different camouflage colors in the visible light region and different temperature sensing in the infrared region [3]. As briefly mentioned above, the thermochromic modules fabricated in this study were evaluated for their potential as simple information display modules. Thermoelectric devices were fabricated using flexible circuit boards with thermochromic pigments applied. Thermochromic pigments that transition from white to black when cooled from room temperature to 18 ℃ were selected. After selecting the thermochromic pigment with the least change in properties among various types of organic solvents, we evaluated the concentration conditions for optimal wetting of the substrate. Each cell consists of two p-n pairs of thermoelectric material, and the cells were fabricated in a 4x4 array. The temperature of the thermoelectric elements

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This research was supported by the Energy Efficiency & Resources Core Technology Program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP), which is funded by the Korea government (MOTIE, 2021202080023D). Additionally, it was supported by a grant from the Basic Research Program of the Korea Institute of Machinery and Materials (grant number NK254A, Project Title: Development of Core Technologies for Advanced Chjplet Packaging Equipment).

3D Printed Bi_2Te_3-Based Thermoelectric Converter: Process Optimization and Performance Evaluation

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Keywords: Selective laser melting, thermoelectrics, bismuth telluride

Thermoelectric (TE) energy conversion is gaining attention for its capability to directly convert waste heat into electricity, providing a sustainable solution to reduce environmental impact [1]. Traditional TE device manufacturing methods are costly, time-consuming, and lead to significant material loss, limiting devices to cuboid shapes and restricting flexible thermal design [2]. Recently, 3D printing, especially Selective Laser Melting (SLM), has emerged as a promising method for manufacturing TE materials, enabling customization of TE legs into tailored geometries [3]. Despite the potential of the SLM method for producing highly efficient TE converters, there is limited information about the effect of this process on the mechanical and transport properties. This study investigates the impact of the SLM process parameters such as laser power, scanning speed, and energy volume density on the structural, microstructural and thermoelectric properties of the Bi_2Te_3-based legs. The *n*- and *p*-type Bi_2Te_3-based materials were synthesized by direct melting of elements under vacuum, followed by annealing. The resulting ingots were crushed into fine powders by hand grinding in an agate mortar-pestle and separated into μ-sized fractions. Then, *n*- and *p*-type Bi_2Te_3-based TE legs were printed by the SLM method under conditions including the different grain size (32-200 μm), laser power (30-35 W) and scanning speed (400-1000 mm/s). The influence of these parameters on the crystal structure (i.e. the preferred orientation) was analysed by XRD analysis, while the chemical composition and microstructure have been investigated using the SEM/EDS analysis. Scanning TE Microscope measurements (SThM) have been used to investigate the effect of the printing method on the transport properties of the TE legs. The obtained data assist in the fabrication of efficient TE converters using the SLM-3D printing method.

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Acknowledgments

Research project supported by program „Excellence initiative – research university" for the AGH University of Krakow and the National Science Centre (NCN) under the project "WEAVE-UNISONO" UMO-2022/04/Y/ST5/00139 "Entropy engineering and interface optimization in materials for highly effective TE energy conversion.

Characterization of thermoelectric single leg using high-performance Mg_2Sn-based single crystal

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Keywords: Mg_2Sn, single crystal, thermoelectric single leg

Thermoelectric (TE) devices have attracted attention due to their ability to generate electricity from waste heat. For a TE device operating at mid-temperature (500-700 K), we focused on Mg_2Sn TE materials, which are advantageous for elementary abundance and low toxicity. Recently, we prepared Mg_2Sn single crystals (SCs) with a high zT value of 0.83 at 650 K (n-type) by using Sb and B as dopants [1,2]. To fabricate a TE device using the Sb and B doped Mg_2Sn SCs, we referred to a TE single leg of a $Mg_2(Si_{0.3}Sn_{0.7})$ polycrystal, where a $MgNi_2Sn$ intermediate layer was inserted between the $Mg_2(Si_{0.3}Sn_{0.7})$ polycrystal and a Cu electrode to avoid atomic diffusion and mismatched thermal expansion coefficients [3]. In this study, we prepared TE single legs of the Sb, B co-doped Mg_2Sn SC and measured their power generation characteristics. Sb, B co-doped Mg_2Sn SCs were fabricated by a melting method [1,2]. To form an intermediate layer, a part of the single crystals was pulverized and mixed with Ni powder at the weight ratio of 1:1. A laminated material consisting of a Cu electrode, mixed powder, single crystal, mixed powder, and Cu electrode in this order was sintered using spark plasma sintering (SPS; NJS Co., Ltd., LABOX-325R). The power generation characteristics were measured using a TE conversion efficiency evaluation system (Advance-Riko, Mini-PEM). We succeeded in preparing TE single legs at the SPS temperature ranging from 450°C to 550°C. The TE single leg prepared at 500°C showed the maximum generated power. The maximum power was 215 mW at the temperature difference of 314°C. The dependence of power on the SPS temperature will be discussed from the viewpoint of the microstructure of the intermediate layer.

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Acknowledgments

This work was partly supported by the Grant-in-Aid for Scientific Research (B) from the MEXT of Japan (No. 22H02161). This work was partly based on collaborative research between Sumitomo Metal Mining Co., Ltd. And Tohoku University, which is part of the Vision Co-creation Partnership. We acknowledge Dr. Murata and Mr. Nishiate at National Institute of Advanced Industrial Science and Technology for their help for power generation measurements.

Computer Design of Multi-Stage Thermoelectric Cooler for Cryoablation

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Keywords: Design, multi-stage thermoelectric cooler, thermoelectric cooling, cryoablation

Cardiac cryoablation represents a critical therapeutic approach for treating cardiac arrhythmias, requiring precise temperature control and efficient cooling systems for effective treatment outcomes [1, 2]. This paper presents a comprehensive design and optimization methodology for a multi-stage thermoelectric cooler (TEC) specifically engineered for cardiac ablation applications. Using advanced optimal control theory methods, we developed a specialized iterative algorithm to calculate and optimize the parameters of cascade TECs, taking into account the complex interplay between thermal and electrical properties of the system. The proposed design successfully achieves the required temperature range from -50 to -70°C with ± 2°C accuracy and delivers 5-10 W cooling power with a response time under 10 seconds. Our mathematical model incorporates temperature-dependent material properties, electrical and thermal losses in the module structure, and accounts for specific densities of heat flows with detailed boundary conditions for optimal performance. The model uniquely addresses the challenges of cascade cooling by optimizing inter-cascade temperatures and specific electric current density in thermoelectric legs, leading to maximized coefficient of performance. Through extensive computational analysis, we evaluated both 3-stage and 4-stage TEC configurations, considering factors such as crystal dimensions, thermal resistance, and power consumption. Results conclusively showed that the 3-stage version provides optimal performance characteristics without the additional complexity and minimal performance gains of a fourth stage. Furthermore, we identify critical future research directions, particularly focusing on the integration challenges between the TEC and the medical working tool, establishing a comprehensive framework for developing efficient thermoelectric cooling systems in cardiac ablation procedures.

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Acknowledgments

This work was supported by the Institute of Thermoelectricity of the NAS and MES of Ukraine

Simulation and Testing of Thermoelectric Cooling Modules for IR Detectors

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Keywords: Thermoelectric cooling module, IR detector

Thermoelectric cooling modules (TECMs) are widely used to ensure the stable operating temperature of IR detectors, which are the main component of most optical electronic devices. Cooling improves such parameters of IR detectors as sensitivity, detectability, speed, range of spectral sensitivity, reliability, etc. TECMs can provide the temperature of IR detectors down to 195 K. They are compact, have no moving parts, are reliable and have a long service life, reaching up to 20 years. The main disadvantage of TECMs is their low coefficient of performance (COP) compared to mechanical cooling methods. Our research is aimed to increase the efficiency of thermoelectric modules for IR detectors. One of the ways is to optimize the module design considering the undesirable electrical and thermal resistances of the contacts, interconnectors and insulating plates in the module which essentially reduce the COP. A new numerical method is proposed for designing cooling modules in the maximum COP mode. This method is developed on the basis of optimal control theory and takes into account the undesirable resistances. The results of calculating the maximum COP prove, that reduce of electrical contact resistance to its rational value is the predominant factor for the increase in the COP. This is especially true for modules made of miniscale thermoelements. Such rational values for the Bi_2Te_3-based modules have been determined. The COP of TECMs for IR detectors increases by 1.5-2.5 times compared to commercial modules if the contact resistance is brought closer to the minimum value of 10^{-7} Ωcm^2 [1]. The use of insulating plates made of aluminum nitride provides an additional increase in COP by 20 %. It is also important to optimize the design of the TECM so that the COP will be maximal in the IR detector operating mode. To control the contact resistance, an improved probe method is proposed for it measurement. Computer simulation is applied to estimate the uncertainty of contact resistance measuring by this method. It is proven that for such an improved method, the uncertainty due to the non-isothermality of the sample will not exceed 2%. An installation has been developed and manufactured for measuring contact resistance at the boundary between a thermoelectric material and a metal using an improved probe method. A special measuring setup was developed for experimental study of module performances. Computer methods were used to estimate the uncertainty of measuring the cooling capacity and temperature drop of the module. This uncertainty is a consequence of deviation of real measurement conditions from ideal ones, which assume that the module is adiabatically isolated and heat fluxes through the module are one-dimensional.

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Acknowledgments

This work was supported by the Ministry of Education and Science of Ukraine (Project MESU-44 No. 0123U101666).

Multifactor Optimization of Permeable Thermoelectric Structures

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Keywords: Multifactor optimization, thermoelectric elements, permeabler materials, coefficient of performance

A multifactor optimization of permeable thermoelectric structures is presented in order to increase their efficiency and application in various industries, such as thermoelectric cooling and electricity generation. Optimization is carried out by studying the influence of various factors, such as coolant velocity, medium permeability, electric current density, impurity concentration in semiconductor branch materials.

Using the methods of mathematical theory of optimal control with their implementation in computer programs, multifactor optimization problems were solved to determine the structural and thermophysical parameters that deliver extreme values of the efficiency of permeable generator thermoelements and the cooling coefficient of coolers.

Theoretical studies of various variants of permeable structures (planar, channel, segmental) for thermoelements operating in the modes of electric energy generation and thermoelectric cooling were carried out.

The results of computer studies of permeable structures for thermoelectric cooling are presented, in the case of using thermoelectric materials based on Bi-Te, in optimal operating modes the cooling coefficient increases by 1.2-1.5 times. In the mode of electric energy generation, the use of permeable structures from materials based on Bi-Te, Pb-Te, Si-Ge makes it possible to obtain 1.2-1.4 times higher energy efficiency than in traditional thermoelectric elements.

The results of the research can be used to develop new highly efficient thermoelectric devices for various applications.

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Acknowledgments

This work was supported by the National Academy of Science and Ministry of Education and Science of Ukraine.

Design of Multi-Leg Flexible Thermoelectric Modules Using Polymer-Based Conductive Composites

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Keywords: PEDOT:PSS, thermoelectric module, silver selenide, MWCNT, Graphene

Thermoelectric generators are devices that can convert temperature differences directly into electrical energy. Their ability to operate continuously without requiring light (solar cells), mechanical movement (piezoelectric generators), or recharging (chemical batteries) makes them highly attractive for energy harvesting applications. Thermoelectric generators provide an effective solution for alternative energy production by overcoming the limitations of traditional energy harvesting systems. Thermoelectric materials with a polymeric structure offer advantages such as flexibility, lightweight design, and tunable properties. These features provide significant benefits, particularly in emerging applications such as flexible electronics, wearable technologies, and biocompatible energy systems. Polymer-based thermoelectric generators offer greater design and integration freedom compared to conventional inorganic materials [1]. In line with these usage purposes, unlike other studies, in this study, thermoelectric modules consisting of silver-containing conductors and PDMS matrix surfaces, semiconductor p and n type legs containing different concentrations of PEDOT:PSS, graphene, multi-walled carbon nanotubes and silver selenide were produced. The flexible modules produced were designed to have 2, 4 and 8 legs. The Seebeck coefficients and generated power values of all produced modules were examined. Among the produced modules, the 8-legged one showed the highest Seebeck coefficient value (32.4 μV/K).

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Acknowledgments

This study was funded by the Scientific and Technological Research Council of Türkiye (TÜBİTAK) ARDEB 1001 Grant No 121M532. The authors extend their sincerest appreciation to TÜBİTAK.

Phase diagram design of thermoelectric materials and devices

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Keywords: Phase diagram, CALPHAD, spinodal decomposition, contact layer

Research linking phase diagrams to thermoelectric performance optimization primarily focuses on determining doping limits in multinary alloys and microstructure design. To resolve ambiguities in 4d-site atom occupation within half-Heusler alloys (*ABX*), we constructed isothermal section phase diagrams for multiple systems via the equilibrated alloy method. This clarified *B*-site solid solubility limits (e.g., $ZrNi_{1+x}Sn$, $HfNi_{1+x}Sn$, $NbCo_{1+x}Sn$, $NbFe_{1+x}Sb$, $ZrCo_{1+x}Sb$) and systematically elucidated the impact of excess B-site atoms on microstructure and thermoelectric properties. [1] For spinodal decomposition in half-Heusler systems, phase separation boundaries in the TiNiSn-ZrNiSn-HfNiSn pseudo-ternary system were mapped, revealing the decoupling mechanism of thermoelectric performance in $Ti_{1-x-y}Zr_xHf_yNiSn$ alloys post-annealing, enabling high-efficiency and high-power ("double-high") devices. [2] We further proposed a CALPHAD-guided strategy for designing thermoelectric materials and devices. By establishing a Mg-Ni-Sb thermodynamic database, Mg_2Ni was identified as a stable contact layer for n-type Mg_3Sb_2, compatible within service temperatures. Combining with the low- temperature nanosilver sintering, we facilitated a all-Zintl-phase thermoelectric device with exceptional performance and long-term stability. [3] Our work underscores phase diagram as a pivotal tool for rational thermoelectric materials and device design.

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Acknowledgments

This work was supported by the National Natural Science Foundation of China, the GuangDong Basic and Applied Basic Research Foundation, and the Shenzhen Science and Technology Program.

Development of Colusite Based Thermoelectric Devices

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Keywords: Colusite, thermoelectric generator, diffusion barrier, contact resistivity, thermal stability

The scarcity and toxicity of elements constituting thermoelectric (TE) devices have led to the development of innovative strategies to not only find novel materials with non-toxic and earth-abundant elements but also enhance their conversion efficiency. However, the performance of TE devices is significantly influenced by the nature and reactivity of the diffusion barrier used to mitigate harmful interdiffusion between TE material and electrodes [1].

Colusite is a non-toxic, cheap sulphide-based TE material that could pave the way to the production of affordable devices performing at intermediate temperatures (below 400°C) for power generation applications [2]. In this work, we will discuss the choice of diffusion barrier materials for colusite ($Cu_{26}V_2Sn_6S_{32}$) 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 of this work will be also discussed in the context of literature data on colusites.

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Acknowledgments

This work was supported by the French National Research Agency (ANR) in the frame of the project BISCOTTES (project identifier ANR-23-CE50-0004).

Machine Learning Enabled Thermoelectric Cooler Design and Optimisation

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Keywords: Thermoelectric cooler, design and optimisation, artificial neural network, genetic algorithm

The rapid advancement of computing algorithms has driven unprecedented levels of chip integration. Modern chips, composed of billions of transistors, generate significant heat due to electron-atom collisions during operation, which severely impacts performance and necessitates efficient cooling solutions [1]. Thermoelectric coolers (TECs) have emerged as a promising option due to their compactness, reliability, and noiseless operation [2]. However, optimizing TEC designs - particularly under dynamic thermal loads - remains a critical challenge, requiring fast adaptation of operating conditions to maximize cooling efficiency.

Traditional finite element method (FEM)-based tools like COMSOL, while accurate, are computationally expensive and time-consuming for iterative TEC optimization. To address this limitation, we propose a novel machine learning (ML)-driven approach combining artificial neural networks (ANNs) and genetic algorithms (GAs) to rapidly optimize TEC geometry and operational parameters. Our method leverages COMSOL-generated datasets to train a hyperparameter-optimized ANN model, achieving over 99% prediction accuracy. A genetic algorithm then explores the design space to identify optimal configurations, while real-time current adjustments further minimize chip temperatures.

This abstract will discuss the performance of my artificial neural network model, compare its results with those of the COMSOL model under different conditions including heat flux, convection, ambient temperature, TEC leg height and width, contact electrical and thermal resistances. We will also demonstrate the superior simulation speed by predicting two million results to generate a mapping image and explain how the genetic algorithm is applied in this research to find the optimal parameters for minimizing temperature. This work bridges the gap between high-fidelity simulation and real-time optimization, offering a scalable framework for next-generation electronics cooling.

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CMOS-Compatible Cavity-Free Si-Nanowire Thermoelectric Generator

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Keywords: Cavity-free, Si-nanowire, thermoelectric generator

Thermoelectric generators (TEG) have attracted great attention as wireless power supply for the sensor nodes in the IoT society. We proposed a planar cavity-free Si-nanowire thermoelectric generator (SiNW-TEG) that could be fabricated on commercially available silicon-on-insulator (SOI) substrates by the complementary metal-oxide-semiconductor (CMOS)-compatible technology. This SiNW-TEG features the use of a steep temperature gradient generated near the heat source by shortening the TEG legs. Thus, there is no need to etch away the substrate to form suspended SiNWs that is necessary in the conventional planar nanowire TEGs, which leads to a low fabrication cost and well-protected nanowires. This SiNW-TEG is composed of several hundreds of SiNW thermoelectric elements connected electrically in series and thermally in parallel. Therefore, a thermally conductive but electrically insulative heat guide layer is necessary for the heat spreading from the heat source to the hot side of each thermoelectric element. The design of the heat guide layer helps to form a large temperature difference across the thermoelectric elements by reducing the parasitic thermal resistance.

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Acknowledgments

This work was supported by the Japan Science and Technology Agency (JST).

Computational Study of the Potential Use of Thermoelectric Generators (TEGs) for Geothermal Energy and Volcanic Monitoring in New Zealand

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Keywords: Thermoelectric generator, geothermal energy, volcanic monitoring

The development of sustainable energy systems is a key challenge in the transition toward a low-carbon future. As part of its commitment to achieving net-zero emissions by 2050, New Zealand has established an energy strategy focused on achieving modern and affordable renewable electricity production, promoting innovative technologies that complement primary electricity generation and strengthen the country's energy resilience. Geothermal energy has been a pillar of New Zealand's energy mix, contributing approximately 19 MW of baseload generation from high-temperature heat flows. However, a significant amount of low-quality residual heat (80–300°C) remains underutilized in geothermal fields— such as those in the Bay of Plenty—and in industrial processes, representing an untapped resource with great potential for distributed generation. A promising solution for harnessing this low-enthalpy geothermal energy is the use of Thermoelectric Generators (TEGs), which stand out for their robustness and low maintenance requirements. The potential of this technology has already been demonstrated in Lanzarote [1], showcasing its feasibility for geothermal energy utilization, as well as in Antarctica, where its durability and reliability have been tested in extreme environments. Given these precedents, this study aims to explore the potential of TEG technology for both distributed energy generation and volcanic monitoring in New Zealand, leveraging its abundant geothermal resources and active volcanic zones.

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Acknowledgments

The authors would like to acknowledge the support of the Spanish State Research Agency and EFEDER-UE, Spain for funding under the PID2021-124014OB-I00 research project.

Printable and Flexible Thermoelectric Generators from Organic/Inorganic Hybrid Materials

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Keywords: Thin film, TEG, composite, semiconductive polymer, additive manufacturing

Conductive polymers, particularly poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS), have attracted interest in thermoelectric research due to their flexibility, non-toxicity, processability, high electrical conductivity, and low thermal conductivity [1]. A systematic investigation was conducted to optimize the TE properties of PEDOT:PSS thin films hybridized with bismuth antimony telluride (BST) particles. Initially, the influence of BST particle size (from nm to μm) and concentration (5-60 wt%) was studies on the microstructural, morphological, and TE properties of the composite films. Then, various chemical treatments using secondary dopants (DMSO, EG, H2SO4) and a dedoping agent (NaOH) were tested to optimize the TE properties, resulting in more than 900-fold increase in the power factor at room temperature [2].

Following the materials optimization, thin-film device fabrication was performed using a spray printing technique. Printing process variables were optimized, and the printed films demonstrated excellent flexibility and mechanical/electrical stability over 1000 bending cycles, confirming their suitability for wearable electronics. Finally, a fully printed flexible thin-film TEG containing 40 thermoelectric legs was fabricated, achieving open-circuit voltages of tens of mV level at room temperature when attached to human arm [3, 4].

This research presents a complete pathway from materials optimization to device fabrication and characterization, offering valuable insights into enhancing the TE performance of organic/inorganic composites for flexible energy harvesting applications.

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Acknowledgments

This work was supported by Science Foundation Irland (SFI).

Enhanced thermoelectric properties of Zinc-Indium co-doped $Sn_{1.03}Te$

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Keywords: Alloy scattering, low thermal conductivity

The development of high-performance thermoelectric materials is pivotal for energy conversion technologies. This study presents the synthesis and characterization of Zinc Indium doped $Sn_{1.03}Te$, which exhibits excellent thermoelectric properties. The doping process involved the incorporation of varying concentrations of Zinc (Zn) and Indium (In) into the $Sn_{1.03-x-y}Zn_xIn_yTe$ (x = 0.0, 0.01; y = 0.0, 0.0025, 0.01) matrix using a solid-state reaction method, followed by hot pressing to enhance the density and homogeneity of the samples. Detailed structural analyses through X-ray diffraction (XRD) and scanning electron microscopy (SEM) revealed that Zn and In atoms were successfully incorporated into the $Sn_{1.03}Te$ lattice without forming secondary phases, leading to a refined grain structure and reduced lattice thermal conductivity. The electrical transport properties were systematically investigated from 300 K to 830 K. In $Sn_{1.03-x-y}Zn_xIn_yTe$ (x = 0.01, y = 0.01), the Seebeck coefficient, electrical conductivity, and thermal conductivity measurements indicated a significant enhancement in the power factor (PF) throughout the temperature range (i.e. 10 μW/cmK² at RT to 19 μW/cmK² at 830K) and a huge reduction in the total thermal conductivity (8.0 W/mK) compared to undoped $Sn_{1.03}Te$ (3.8 W/mK) at RT due to heavy phonon scattering. Consequently, the dimensionless figure of merit (ZT) achieved an enhanced value of 0.8 at 830 K compared to only Indium (1%) doped (ZT = 0.7). We are looking to tune the zinc-indium concentration in $Sn_{1.03}Te$ further and hope for further improvement in its thermoelectric properties.

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Acknowledgments

This work was supported and Funded by CSIR India and IISER Pune.

Various estimations of Lorenz number in fine-grained Bi_2Te_3 and their verification by dimensionless figure of merit ZT at room temperature

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Keywords: Lorenz number, materials parameter, scattering parameter, reduced Fermi energy.

The Lorentz number L is an important parameter that connects electrical conductivity σ to thermal conductivity κ. In thermoelectric semiconductors, it is used to subtract the carrier thermal conductivity κ_{el} from the thermal conductivity κ to obtain the phonon thermal conductivity κ_{ph}. L must be accurately estimated to accurately determine κ_{ph}. Various methods have been proposed to obtain L, including 1) the isothermal method [1], 2) Kim's method [2], and 3) the quadratic equation [3]. However, whether the L is accurate remains unverified. In the present study, the L and κ_{ph} were compared to these methods for fine-grained Bi_2Te_3 with consistent κ_{ph}. To verify L estimation, the measured $ZT_{\alpha\sigma\kappa}$ was compared to $ZT_{\beta\gamma\eta}$, which consists of the materials parameter β, scattering parameter γ, and reduced Fermi energy η. The γ were calculated using each method. All the η values obtained in method 3) were used. These β and $ZT_{\beta\gamma\eta}$ were estimated using σ, κ_{ph}, η, and γ. The L for the isothermal method was estimated from the linear relationship between σ and κ. The L for Kim's method was derived from the measured Seebeck coefficient α. Kim's method is also assumed to be acoustic phonon scattering ($\gamma = 0$). The L for the quadratic approximation were derived as a quadratic equation of the κ and σ. $ZT_{\beta\gamma\eta}$ derived from method 3) were consistent with $ZT_{\alpha\sigma\kappa}$. In contrast, $ZT_{\beta\gamma\eta}$ derived from methods 1) and 2) significantly diverged from $ZT_{\alpha\sigma\kappa}$. Both methods, Kim's and the isothermal in which γ is constant, do not accurately reflect the scattering state within fine-grained Bi_2Te_3 thermoelectric semiconductors, making it essential to determine the variable values of γ at each measurement point for accurate analysis. The method of employing quadratic equations was demonstrated to provide an accurate estimation of L and κ_{ph} in fine-grained Bi_2Te_3 thermoelectric semiconductors.

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Unravelling grain boundary influences on electric and lattice thermal conductivity in Mn-doped SnTe thermoelectrics

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Keywords: Thermal conductivity, SnTe, EBSD, FDTR

Amongst thermoelectric materials, Tin-Telluride (SnTe) has attracted significant scientific attention as an emerging model material for mid-temperature ranges providing an alternative to the toxic lead-based PbTe. [1,2] Recent frequency domain thermoreflectance (FDTR) measurements on SnTe indicate strong differences in the magnitude of thermal conductivity (κ) suppression at grain boundaries with varying misorientation angles. [3] However, which component of κ causes this suppression remains unclear. The present study aims to unravel to which extent these differences originate in the electric (κ_E) or the lattice portion (κ_L) of the thermal conductivity in SnTe by systematically varying the Sn-vacancy concentration. For this, binary and Mn-doped samples with varying κ_E/κ_L ratios were synthesised and analysed by scanning electron microscopy (SEM) based techniques. The grain sizes and orientations as well as the local misorientation angles between individual grains were determined by electron backscatter diffraction (EBSD) experiments. The average grain size appears to be largely independent of the Mn-content and a high tendency of the system to form single crystals is observed. Suitable grain boundaries were determined and characterised. FDTR measurements were performed to correlate the misorientation with the local thermal conductivity suppression and evaluate the relative impact on κ_E and κ_L. Generally, a rise in thermal boundary resistance with increasing Mn content is detected. Future efforts will focus on the high-resolution characterisation of grain boundary arrangements by (scanning) transmission electron microscopy ((S)TEM) and developing a framework to correlate the atomic defect structures with transport properties in SnTe.

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Acknowledgments

This work was supported by the European Research Executive Agency, under Marie Skłodowska-Curie Actions, project 101150912 — MetaSCT.

NDT-Characterization of Thermoelectric Materials and Modules by Scanning Acoustic Microscopy

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Keywords: Thermoelectric, failure analysis, process control, scanning acoustic microscopy

Bringing thermoelectricity from lab-scale into industrial applications, it is very important that their positive features, such as no moving parts, easy scalability, etc. can be fully exploited through a high long-term stability. Therefore, non-destructive (NDT) characterization methods are very important tasks in the production of TE-materials and TE-modules .

In this context scanning acoustic microscopy (SAM) is a very powerful NDT-method in the process- and product control as well as for failure analysis; e. g. to characterize the quality of interfaces, to detect hidden defects in materials and systems, such as cracks, voids and delaminations, etc.

In this work, we demonstrate the great potential of this method by means of experiments and model calculations.

The experiments were carried out by the pulse-echo (PE) method in the A-scan and C-scan modes, using transducers with center frequencies of 15 MHz and 50 MHz.

Both the experiments and the theoretical investigations showed that it is possible to detect, for example, air gaps down to the low µm-range, which is very important to investigate the bonding quality of the diffusion barrier on the TE-material.

Thin film thermal conductivity: Accounting for topography and measuring anisotropy

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Keywords: Thermal conductivity, thin film, thermoelectric

Obtaining accurate thermal conductivity measurements is challenging for any material, but particularly where the amount of material is small or its thermal conductivity is low. Thermal conductivity measurements are therefore not straightforward for thin films of organic and hybrid thermoelectric materials. Topography is also an important factor in thin film conductivity measurements as small topographic features can cause bottlenecks for thermal transport. The first part of this presentation will explore the role of thin film topography on in-plane thermal conductivity measurements. I will present computational and experimental data quantifying how topography links intrinsic thermal conductivity of the material with thermal conductivity of the thin film. I will identify regimes where intrinsic material and thin film thermal conductivity are comparable and regimes where they differ.

The second part of the presentation will explore the measurement of thermal conductivity in anisotropic thin films. This will be in the context of the pseudo-steady state in-plane 3-Ω method. We have previously measured orthogonal components of thermal conductivity in an aligned polymer film [1], and the technique itself is sensitive enough to detect phases changes [2], doping-induced morphology changes in polymers [1] and small electronic contributions to thermal conductivity [3]. This presentation will use finite element modelling to verify the accuracy of this method and how it may applied to other thermally anisotropic thin films.

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Acknowledgments

This work was supported the Royal Society through Prof. Fenwick's University Research Fellowship (UF140372 and URF/R/201013).

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