

Final report for

Symposium "Advanced Thermoelectrics: From Materials to Devices"

held at the E-MRS Spring 2013 conference, May 27-31, 2013, Strasbourg, France

Symposium organizers

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Dr. Sascha Populoh
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Empa
Ueberlandstrasse 129
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Jan D. König
Fraunhofer Institute for Physical Measurements, IPM
Heidenhofstr. 8
79110 Freiburg
Germany

Dr. Antonio Pereira Gonçalves
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Portugal

Summary

The development of advanced thermoelectric materials for efficient thermoelectric devices is a major challenge in energy conversion technologies. To overcome limitations of toxic and expensive state-of-the-art bulk semiconductors, an improved fundamental understanding of the materials properties and of the thermoelectric conversion processes is needed. The aim of the symposium was to assemble scientists from universities, research institutes and industry to discuss recent discoveries in the field, and to promote co-operations on materials and devices. This goal was fully achieved as detailed in this report.



Description of the scientific content and of discussions at the event

Introduction

The use of waste heat as energy source is an attractive and environmentally clean way to generate electrical power. With a thermoelectric (TE) device heat can be directly converted into electricity. TE devices work independently of mechanical and chemical conversion processes. Thus, they are emission free, silent, and extremely durable.

A conventional TE converter has an efficiency of 5-10%. It consists of numerous thermocouples, comprising *p*- and *n*-type thermoelements connected electrically in series and thermally in parallel. Heating one side of a thermoelectric material allows electrons and holes to thermally diffuse along the temperature gradient and to carry their charge with them. The amount of electrical power produced in this way depends on the thermoelectric conversion efficiency of the device and the heat flux. The relevant material parameters, i.e., the thermopower *S*, the electrical conductivity σ , and the thermal conductivity κ , are interrelated by the specific electronic structure of the material. This interrelation does usually not work in favour of high thermoelectric efficiencies. The dimensionless thermoelectric figure of merit

$$ZT = S^2 \sigma / \kappa T$$

would, at a given temperature *T*, be maximized for materials with large thermopower, and high electrical but low thermal conductivity. In simple semiconductors, however, *S* is large when σ is small, and the electronic contribution to κ is directly related to σ via the Wiedemann-Franz law. To disentangle these properties, innovative materials design concepts are required, - and today increasingly explored by a highly active international scientific community.

Conventional TE devices as the ones used for space applications aim at high reliability, rather than high energy conversion efficiency or low cost. These devices are based on expensive and toxic materials (e.g. tellurides) and have low temperature stability when exposed to an oxidizing atmosphere. For future large-scale use, e.g. in the automotive sector, cheaper, more durable, and environmentally benign materials have to be found. To design better materials for future applications, a better understanding of the interplay of electronic and vibrational properties of solids is required. In parallel, materials engineering and device technology need to be advanced.

Organization

The symposium was organized in 12 scientifically coherent oral sessions (chronologically listed)

- Cage compounds
- Oxides
- Superlattices and membranes
- Tellurides
- Thermoelectric theory I
- Films, particles and quantum dots
- Nanowires and nanopillars
- Chalcogenides and intermetallics
- Devices and applications
- Novel thermoelectric materials
- Half-heuslers and silicides
- Thermoelectric theory II

plus two poster sessions, each introduced by flash presentations. The topic-wise grouping, which is not always done at similar events, helped to give a very good overview of the various subfields

of current worldwide research in thermoelectricity, and fostered discussions on the various subfields.

It was very fortunate that the coffee breaks were held directly in front of the lecture hall and that lunch was served at one single place (this is not always the case at E-MRS conferences!). Thus, discussions went on during the coffee breaks. In addition, most of the symposium attendees went to lunch (that was served at tables, no cueing...) together and continued intensive discussions there. This gave the symposium in fact very much the character of a workshop, with lots of informal exchange between the attendees!

Right from the beginning of the symposium, the organizers actively engaged the participants in discussions; lively discussions kept going on during the entire symposium - in particular also during the poster sessions.

There was a high involvement of young researchers and in particular of graduate students. Two graduate students received prizes for their outstanding oral presentations. Also the two poster awards were given to excellent graduate students. The oral presentation awards were announced in the general E-MRS student award session, the poster awards (certificates plus small price money) were announced at the end of an oral session during the symposium.

Scientific content

The symposium covered the topic of thermoelectricity from a very broad perspective. Not only was the subtitle - from materials to devices - taken very literally, but also were other axes explored:

- from simple model materials to materials of extreme complexity
- from plastics to borides
- from chemical to solid state synthesis
- from electrochemical thin film deposition to molecular beam epitaxy
- from nanoparticles to nanocomposites
- from lab-scale to large-scale materials fabrication
- from steady state to time resolved measurements
- from conventional thermoelectric concepts to entirely new approaches
- from phonon to electron engineering
- from molecular dynamics simulations to strongly correlated band theory
- from degradation to encapsulation
- from micro- to macro-devices

This breadth of topics made the symposium extremely inspiring.

Many outstanding talks with exciting results were presented. This short summary aims by no means at giving a full account of all the topics addressed and all results presented - it merely wants to give a flavour...

Many different materials classes were covered. Graphene, bismuth, silicon, bismuth tellurides and antimonides, lead tellurides, half-Heusler compounds, oxides, chalcogenides, oxy-chalcogenides, borides, skutterudites, clathrates, complex Zintl compounds, Kondo insulators, topological insulators, organic conductors, glasses, phase change materials, CrN.

Most of these materials were studied as bulk single or polycrystals or as single or polycrystalline thick or thin films. Some of the materials were also investigated as nano- or microwires, nanosheets, or membranes.

While some participants focussed on the bare intrinsic materials properties, most presented optimization studies. Many different concepts (electron and phonon engineering) and techniques are explored to improve the thermoelectric efficiency of a given material, frequently leading to

interesting ZT values of the order of 1 to 1.5 in varying temperature ranges: doping/substitutions (up to pentenary compounds!), nanograin formation, phase separation, strain/shear, introduction of precipitates (including for instance C_{60}), fabrication of composites, fabrication of ordered and even aperiodic heterostructures, superlattices and quantum dots, sometimes based on different isotopes different isotopes, ...

It becomes more and more common to study also the stability of the materials and in particular of their artificial nano/microstructuring upon thermal cycling. However, real long term studies have not been presented. Instead, many different strategies are explored to stabilize the structures.

On the characterization side, the spectrum has broadened considerably. While the standard steady state techniques to measure the thermoelectric quantities of bulk samples are still broadly used, alternative techniques are getting more widespread, e.g., scanning thermal probe micro-imaging, the 3 omega technique, laser flash diffusivity measurements, time domain thermal reflectance, pump-probe techniques, Raman thermometry, ...

Many presentations also dealt with the fabrication of devices. The progress on microgenerators, frequently based on nanostructures, is impressive. Also a number of traditional thermoelectric generators, fabricated typically from compacted and sintered powders, were presented. It is unfortunate that open discussion on the science of contacting is very rare. This clearly slows down the progress of this technologically highly relevant issue. Some presentations also addressed upscaling. A number of research institutes collaborate with industry on pilot materials powder production plants. Also the integration of thermoelectric modules into automobiles and roadmaps to the targeted efficiencies and costs levels were discussed.

Finally, also entirely new approaches to explore thermoelectric effects for energy generation were discussed, e.g., pn junction thermoelectric generators, thermionic converters, spin Seebeck plus spin Hall effect generators, and liquid chemical thermocouples.

And finally, just a few highlights: A new world record in thermoelectric efficiency of clathrates over the relevant temperature range was shown. An entirely new thermoelectric device concept based on spin current plus spin Hall effect was presented and realized in a microgenerator. The simultaneous drastic enhancement of the electrical conductivity and the thermopower in half-Heusler compounds by certain additives was demonstrated.

Scientific committee

Fairbanks, John W.; DOE, USA
Grin, Juri; Dresden, Germany
Hebert, Sylvie; Caen, France (f)
Nielsch, Kornelius; Hamburg, Germany
Schierle-Arndt, Kerstin; BASF AG, Germany (f)
Tobola, Janusz; Krakow, Poland

Conference Proceedings

All participants were strongly encouraged to submit a manuscript to the journal *physica status solidi (a)* that will publish a special issue of fully peer reviewed papers as conference proceedings.

Information on the budget

As detailed in the table below, the INTELBIOMAT funding was used to partly cover the conference fees and/or travel costs and/or accommodation costs of invited speakers from Europe, one invited speaker from Korea and the conference organizers. In addition a discussion dinner to which all

invited speakers and committee members were invited was funded. Three best paper awards will be given after all referee reports of the proceedings papers (see above) are received. The selection will be done by the symposium organizers, taking the reviewer's comments into account. No price will go to the organizers' groups. Focus will be on contributions from young scientists and/or scientists from emerging countries. A lump sum of 700 EUR (< 10 % of total ESF funding) covers the administrative costs.

| | Total | Conf. fee | Price | Admin. | Meals | Accomm | Travel |
|------------------------|------------------|--------------------|---------------|---------------|--------------|------------------|-----------------|
| | | Other costs | | | | | |
| Total ESF awarded | 7800 € | | | | | | |
| Organizers | | | | | | | |
| Silke Bühler-Paschen | 999,71 € | | | | | 647,50 € | 352,21 € |
| Sascha Populoh | 472,66 € | | | | | 391,00 € | 81,66 € |
| Antonio Pereira G. | 567,29 € | | | | | 248,00 € | 319,29 € |
| Jan D. König | 391,72 € | | | | | 331,50 € | 60,22 € |
| Speakers | | | | | | | |
| Kaczorowski Dariusz | 560 € | 560 € | | | | | |
| Lechermann Frank | 640 € | 640 € | | | | | |
| Schierning Gabi | 640 € | 640 € | | | | | |
| Rogl Peter | 640 € | 640 € | | | | | |
| Wooyoung Lee | 640 € | 640 € | | | | | |
| Conference Dinner | 540 € | | | | 540 € | | |
| Best paper 1. | 500 € | | 500 € | | | | |
| Best paper 2. | 300 € | | 300 € | | | | |
| Best paper 3. | 200 € | | 200 € | | | | |
| Administrative costs | 700 € | | | 700 € | | | |
| Total ESF spent | 7791,38 € | 3120 € | 1000 € | 700 € | 540 € | 1618,00 € | 813,38 € |
| | | 4120,00 € | | | | | |
| Balance | 8,62 € | | | | | | |

Details on the budget are also given in the web-form. All receipts are available on request.

Acknowledgments during the symposium

The generous funding of INTELBIOMAT was acknowledged on a dedicated slide presented in the conference hall whenever no presentation was projected. In addition the Chair of the conference mentioned INTELBIOMAT funding in her closing comments. INTELBIOMAT will also be acknowledged in the conference proceedings.

Assessment of the results and impact of the event on the future directions of the field

The symposium was a testimony of great worldwide activity in the field of advanced thermoelectrics. A vast amount of different subtopics are addressed by a broad community. The results are getting more reliable and reproducible, application relevant issues are considered by an increasing number of scientists. Overall, there is hope in the community that thermoelectric applications in waste heat generation will not remain a dream.

The symposium participants came from 21 countries.

The large percentage of non-Europeans points to the high standing of the European thermoelectrics community, but also to the need to form stronger networks within Europe to be able to compete in this challenging field.

Annexes: Programme of the meeting and full list of speakers and participants

List of invited speakers

Felser, Claudia; Max Planck Institute for Chemical Physics of Solids, Germany (f)
Heremans, Joseph; Ohio State University, USA
Kaczorowski, Darius; Inst. Low Temp. Structure Research, Poland
Lechermann, Frank; Hamburg University, Germany
Lee, Wooyoung; Yonsei University, Korea
Meisner, Gregory, GM Motors, USA
Nolas, George; Univ. South Florida, USA
Prellier, Wilfried, Caen, France
Rogl, Peter, Vienna University, Austria
Schierning, Gabi; Duisburg-Essen University, Germany (f)
Snyder, Jeff, Caltech, USA
Zhifeng, Ren; Houston University, USA

Full list of participants

| | | |
|---------------|---------------|--|
| Peter | ROGL | University of Vienna |
| Hiroaki | ANNO | Tokyo University of Science, Yamaguchi |
| Wilfried | Prellier | CNRS/ENSICAEN |
| worawut | KHUNSIN | catalan institute of nanotechnology |
| Francois | MORINI | Institut Electronique Microelectronique Nanotechnologies |
| Matthias | SCHRADE | University of Oslo |
| Wonchul | CHOI | KAIST |
| Soizic | EON | WWU Münster |
| Markus | WINKLER | Fraunhofer Institute for Physical Measurement Techniques IPM |
| Sebastian | REPARAZ | Catalan Institute of Nanotechnology |
| Daniel | GRIMM | TU Chemnitz |
| Markus R. | Wagner | Catalan Institute of Nanotechnology (ICN) |
| Davide | BERETTA | Istituto Italiano di Tecnologia |
| Kyung Tae | KIM | Korea Institute of Materials Science |
| Xinlin | YAN | Institute of Solid State Physics |
| Viskadourakis | ZACHARIAS | FORTH |
| Danila | Ovsyannikov | TISNCM |
| | PEREIRA | |
| Antonio | GONÇALVES | IST/ITN, Instituto Superior Técnico, UTL |
| Gilgeun | LEE | Pukyong National University |
| Dimitrios | CHALIAMPALIAS | Aristotle University of Thessaloniki |
| Krzysztof | DYBKO | Polish Academy of Sciences |
| Soufiene | ILAH | université of carthage |
| Nikolaeva | ALBINA | Gitsu ILEN |
| Anderson | Dussan | Universidad Nacional de Colombia - Dpto. Física |
| Seungwoo | HAN | Korea Institute of Machinery and Materials |
| Nikolaeva | ALBINA | Gitsu ILEN |
| Gyeong Ock | PARK | Yonsei University, Korea |
| Nicola | PERANIO | University of Tuebingen |
| Jonathan | HAENEL | Vienna University of Technology |

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|---------------|--------------|---|
| Leonid | KONOPKO | Ghitu Institute of Electronic Engineering and Nanotechnologies |
| Fredy | Mesa | Universidad Libre de Colombia |
| GLORIA | VILARDELL | LEITAT TECHNOLOGICAL CENTER |
| Helmut | BAUMGART | Old Dominion University |
| Helmut | BAUMGART | Dominion University |
| George | NOLAS | University of South Florida |
| Biplab | PAUL | Linköping University (Sweden) |
| Andreas | SCHMITZ | German Aerospace Center (DLR) |
| Michal | SZOT | Polish Academy of Sciences |
| Jean-Baptiste | VANEY | Institut Jean Lamour, Nancy, France |
| Matthias | WUTTIG | RWTH Aachen |
| Joseph | P. HEREMANS | The Ohio State University |
| Roberto | DAGOSTA | Universidad del Pais Vasco |
| Rafael | Frieling | University of Münster |
| | KERDSONGPANY | |
| SIT | A | Linköping University |
| Kamil | KUTORASINSKI | Akademia Górniczo-Hutnicza im. Stanisława Staszica w Krakowie |
| Zhifeng | REN | University of Houston |
| Jayaram | DADDA | German Aerospace Center (DLR) |
| Mai | NGUYEN THANH | Japan Advanced Institute of Science and Technology |
| mohsin | SALEEMI | KTH Royal Institute of Technology |
| Hanns-Ulrich | Habermeier | MPI-FKF |
| Dario | NARDUCCI | University of Milano Bicocca |
| Hung-Wei | Tsai | National Tsing Hua University |
| Noriyuki | UCHIDA | AIST |
| etienne | DRAHI | emse/cmp |
| Anil | KUAMR | National Physical Laboratory New Delhi |
| Wooyoung | LEE | Yonsei University |
| Gabi | SCHIERNING | University of Duisburg-Essen |
| Wang | CHING-CHI | National Central University |
| Jeongmin | KIM | Yonsei University, Korea |
| Jae Yong | SONG | Korea Research Institute of Science and Technology |
| XANTHIPPI | ZIANNI | TECHNOLOGICAL EDUCATIONAL INSTITUTION OF CHALKIDA |
| Alexey | ZOZULYA | DESY |
| Claudia | FELSER | Max Planck Institute |
| Céline | BARRETEAU | Université Paris-Sud 11 |
| Michihiro | OHTA | National Institute of Advanced Industrial Science and Technology (AIST) |
| Maik | WAGNER-REETZ | Max-Planck-Institute for Chemical Physics of Solids |
| Anna | SEMENOVA | Institute of Solid State Chemistry |
| | SCHWINGENSCH | |
| Udo | LOGL | KAUST |
| Sergei | VASSEL | Rostov branch of MGUTU |
| MASAMI | MORI | Chubu Electric Power Co., Inc. |
| Soufiene | ILAH | université of carthage |
| Laurie | WINKLESS | National Physical Laboratory |
| Alex | POKROPIVNY | UPR CNRS 288 Ecole Centrale Paris |
| Shaolin | Zhang | Yonsei University |
| Igor | VEREMCHUK | Max-Planck-Institut für Chemische Physik fester Stoffe |
| Gregor | KIESLICH | Johannes Gutenberg-Universität Mainz |
| Ta-Lei | CHOU | Aalto University |

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|--------------|----------------------------------|---|
| Sascha | POPULOH | Empa |
| Gesine | Saucke | Empa |
| Leyre | SAGARNA RODRÍGUEZ- VIEJO | Empa |
| Javier | VIEJO | Universitat Autònoma de Barcelona |
| Alex | POKROPIVNY | UPR CNRS 288 Ecole Centrale Paris |
| Gregory | MEISNER | GM Global Research and Development |
| Matthias | FEINAEUGLE | University of Southampton |
| Jana | HEUER | Fraunhofer IPM |
| Seungwoo | HAN RODRÍGUEZ- VIEJO | Korea Institute of Machinery and Materials |
| Javier | VIEJO | Universitat Autònoma de Barcelona |
| Raimar | ROSTEK | University of Freiburg |
| Jeff | SNYDER | Caltech |
| Alejandro R. | GOÑI | ICMAB-CSIC |
| Masatoshi | TAKEDA | Nagaoka University of Technology |
| Francisco | RIVADULLA | Universidad de Santiago de Compostela |
| Akihiro | KIRIHARA | NEC Corporation |
| Dariusz | KACZOROWSKI | Institute of Low Temperature and Structure Research, Polish Academy of Sciences |
| Krzysztof | Galazka | University of Bern |
| WENJIE | XIE | Empa |
| Titas | DASGUPTA | German Aerospace Center |
| Philippe | BELLANGER BERNARD- GRANGER | ICMCB |
| Guillaume | GRANGER | CEA |
| Frank | LECHERMANN | University of Hamburg |
| Yong-Sung | KIM MURPHY | Korea Research Institute of Standards and Science |
| Felipe | ARMANDO | University College Cork |
| Alex | POKROPIVNY | UPR CNRS 288 Ecole Centrale Paris |
| Shiyun | XIONG | Ecole Centrale Paris |

Final programme of the meeting

The final programme of the meeting is given in the table below. Invited talks are highlighted in green. Talks/posters that were canceled and other are indicated.

| TYPE | REF | DATE | HOUR | TITLE | NAME | FIRSTNAME |
|----------------|---------|--|-------|---|---------------------|---------------------|
| | | 27-05-2013 | 09:00 | Welcome | Bühler-Paschen | Silke |
| SESSION | | Cage Compounds : Silke Bühler-Paschen | | | | |
| invited | C.I-1 | 27-05-2013 | 09:15 | Thermoelectric Functions in Intermetallic Clathrates | ROGL | Peter |
| oral | C.I-2 | 27-05-2013 | 09:45 | Thermal stability and oxidation resistance of polycrystalline Ba8Al16Si30-based clathrates | ANNO | Hiroaki |
| oral | C.I-3 | 27-05-2013 | 10:00 | Iron doping of skutterudites via chemical synthesis - Changed to poster, session C.PI | YAKHSHI TAFTI | Mohsen |
| BREAK | | 27-05-2013 | | Coffee Break | | |
| SESSION | | Oxides : Zhifeng Ren | | | | |
| invited | C.II-1 | 27-05-2013 | 10:45 | Thermoelectric materials from Bulk to thin films | Prellier | |
| oral | C.II-2 | 27-05-2013 | 11:15 | Strong thickness-dependent and large thermoelectric effect in lightly doped Nb:SrTiO3 thin films | KHUNSIN | worawut |
| oral | C.II-3 | 27-05-2013 | 11:30 | Thermoelectric properties of epitaxial LiCoO2 thin films- REMOVED | MIHAILESCU | Nicolae Cristian |
| oral | C.II-4 | 27-05-2013 | 11:45 | Low work function thin film growth for high efficiency thermionic energy converter: coupled Kelvin probe and photoemission study of potassium oxide | MORINI | Francois |
| oral | C.II-5 | 27-05-2013 | 12:00 | Effect of oxygen content on the thermoelectric properties of CaMnO3-x | SCHRADE | Matthias |
| BREAK | | 27-05-2013 | | Lunch | | |
| SESSION | | Superlattices & Membranes : Hanns-Ulrich Habermeier | | | | |
| invited | C.III-1 | 27-05-2013 | 14:00 | High-Temperature Power Generation Devices from Nanostructured Half-Heusler Materials | Ren for D'ANGELO | Jonathan |
| oral | C.III-2 | 27-05-2013 | 14:30 | Thermoelectric effect of silicide and silicon hetero-junction structured devices | CHOI | Wonchul |
| oral | C.III-3 | 27-05-2013 | 14:45 | Thermal conductivity of periodic and aperiodic silicon isotope structures | EON | Soizic |
| oral | C.III-4 | 27-05-2013 | 15:00 | New results on Bi2Te3/Sb2Te3 - related superlattices grown with molecular beam epitaxy (MBE) and nanoalloying | WINKLER | Markus |
| oral | C.III- | 27-05- | 15:15 | Determination of the thermal conductivity of Si and Ge thin membranes through | REPARAZ | Sebastian |

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|------|---------|------------|-------|---|--------|-----------|
| | 5 | 2013 | | Raman thermometry. | | |
| oral | C.III-6 | 27-05-2013 | 15:30 | Thermal conductivity in nanomembrane hybrid superlattices | GRIMM | Daniel |
| oral | C.III-7 | 27-05-2013 | 15:45 | Acoustic phonon dynamics in free-standing silicon and germanium membranes | Wagner | Markus R. |

SESSION Posters-I : Sascha Populoh

| | | | | | | |
|----------------------------|---------|------------|-------|--|-------------------|---------------|
| Flash poster presentations | | | 16:00 | | all | |
| poster | C.PI-1 | 27-05-2013 | 16:00 | Thermoelectric Properties of Organic Conductors | BERETTA | Davide |
| poster | C.PI-2 | 27-05-2013 | 16:00 | Thermoelectric Properties of p-type Bi ₂ Te ₃ Thick-Film Processed by a Screen Printing Process NOT PRESENTED | KIM | Kyung Tae |
| poster | C.PI-3 | 27-05-2013 | 16:00 | Effect of process parameters for ball milling and hot pressing on the thermoelectric properties of type I clathrates | YAN | Xinlin |
| poster | C.PI-4 | 27-05-2013 | 16:00 | Transport Properties of lightly doped La(1-x)Sr(x)CoO(3) thin films | ZACHARIAS | Viskadourakis |
| poster | C.PI-5 | 27-05-2013 | 16:00 | C60-doping of nanostructured thermoelectric. | Ovsyannikov | Danila |
| poster | C.PI-6 | 27-05-2013 | 16:00 | Recent Advances on Thermoelectric Glasses | PEREIRA GONÇALVES | Antonio |
| poster | C.PI-7 | 27-05-2013 | 16:00 | Thermoelectric properties of Bi _{0.5} Sb _{1.5} Te ₃ fabricated by mechanical milling and spark plasma sintering processes | LEE | Gilgeun |
| poster | C.PI-8 | 27-05-2013 | 16:00 | Thermoelectric properties of Bi _{0.5} Sb _{1.5} Te ₃ powder synthesized using metallic salts | LEE | Gilgeun |
| poster | C.PI-9 | 27-05-2013 | 16:00 | Thermoelectric properties of Mg ₂ Si coatings deposited by pack cementation process on heavily doped Si substrates | CHALIAMPALIAS | Dimitrios |
| poster | C.PI-10 | 27-05-2013 | 16:00 | On the Effect of Ge on the Mg ₂ Si _{1-x-y} Sn _x Gey Materials- REMOVED | KYRATSI | Theodora |
| poster | C.PI-11 | 27-05-2013 | 16:00 | Thermoelectric Properties of Hot-Pressed β,-K ₂ Bi _{8-x} Sb _x Se ₁₃ Materials- REMOVED | KYRATSI | Theodora |
| poster | C.PI-12 | 27-05-2013 | 16:00 | Thermoelectric performance of n-type and p-type Pb _(1-x) Mn _(x) Te (x=0.05) bulk crystals | DYBKO | Krzysztof |
| poster | C.PI-13 | 27-05-2013 | 16:00 | Boron effects on optical and thermal properties of BGaAs/GaAs alloys NOT PRESENTED | ILAH | Soufiene |
| poster | C.PI-14 | 27-05-2013 | 16:00 | GALVANOMAGNETIC AND THERMOELECTRIC PROPERTIES OF TE DOPED SINGLE-CRYSTAL BISMUTH WIRES AND FILMS NOT PRESENTED | ALBINA | Nikolaeva |

| | | | | | | |
|--------|---------|------------|-------|--|-----------|------------|
| poster | C.PI-15 | 27-05-2013 | 16:00 | Influence of the doping profile and trap levels in thin films Si from the evaluation of thermally stimulated current NOT PRESENTED | Dussan | Anderson |
| poster | C.PI-16 | 27-05-2013 | 16:00 | High-temperature thermoelectric properties of Zn-Sb thin films deposited by co-sputtering | HAN | Seungwoo |
| poster | C.PI-17 | 27-05-2013 | 16:00 | TEMPERATURE AND MAGNETIC DEPENDENCES THE RESISTANCE AND THERMOPOWER IN A TOPOLOGICAL INSULATOR Bi _{1-x} Sb _x WIRES | ALBINA | Nikolaeva |
| poster | C.PI-18 | 27-05-2013 | 16:00 | Novel Thermoelectric PEDOT:PSS/Ge composites | PARK | Gyeong Ock |
| poster | C.PI-19 | 27-05-2013 | 16:00 | Control of stoichiometry in Bi ₂ Te ₃ based nanomaterials | PERANIO | Nicola |
| poster | C.PI-20 | 27-05-2013 | 16:00 | Thermoelectric properties of the anisotropic Kondo insulator CeRu ₄ Sn ₆ | HAENEL | Jonathan |
| poster | C.PI-21 | 27-05-2013 | 16:00 | Thermoelectric properties of Bi ₂ Te ₃ microwires | KONOPKO | Leonid |
| poster | C.PI-22 | 27-05-2013 | 16:00 | Growth and structural characterization of Cu ₂ ZnSnSe ₄ thin films used in solar cells NOT PRESENTED | Mesa | Fredy |
| poster | C.PI-23 | 27-05-2013 | 16:00 | NANOCOMPOSITES WITH INTRINSICALLY CONDUCTING POLYMERS FOR THERMOELECTRIC APPLICATIONS NOT PRESENTED | VILARDELL | GLORIA |
| poster | C.PI-24 | 27-05-2013 | 16:00 | ALD Growth of PbTe Thin Films for Thermoelectric Applications | BAUMGART | Helmut |
| poster | C.PI-25 | 27-05-2013 | 16:00 | TEM Investigation of Bi ₂ Te ₃ /Sb ₂ Te ₃ Nanolaminate Structures Synthesized by Atomic Layer Deposition | BAUMGART | Helmut |

SESSION **Tellurides : Peter Rogl**

| | | | | | | |
|---------|--------|------------|-------|---|---------|---------------|
| invited | C.IV-1 | 28-05-2013 | 08:30 | Thermoelectric research for automobile applications: An experimental and computational approach to materials and interfaces. | NOLAS | George |
| oral | C.IV-2 | 28-05-2013 | 09:00 | Compensation of excess carrier concentration by impurity levels: an alternative approach for higher thermoelectric efficiency | PAUL | Biplab |
| oral | C.IV-3 | 28-05-2013 | 09:15 | Increasing the mechanical stability of lead telluride by alloying with non-doping elements | SCHMITZ | Andreas |
| oral | C.IV-4 | 28-05-2013 | 09:30 | Thermal and thermoelectric properties of Pb _{1-x} Cd _x Te (x=0-0.11) solid solutions | SZOT | Michal |
| oral | C.IV-5 | 28-05-2013 | 09:45 | Cu-As-Te glassy systems: challenges and prospects for thermoelectric applications. | VANEY | Jean-Baptiste |
| oral | C.IV-6 | 28-05-2013 | 10:00 | Disorder Induced Suppression of Lattice Heat Conduction in Crystalline Chalcogenides with thermoelectric properties | WUTTIG | Matthias |

BREAK **28-05-2013****Coffee Break****SESSION** **Thermoelectric Theory - I : Janusz Tobola**

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|---------|-------|------------|-------|---|----------------|---------|
| invited | C.V-1 | 28-05-2013 | 10:45 | Resonant levels in bulk thermoelectric semiconductors | P. HEREMANS | Joseph |
| oral | C.V-2 | 28-05-2013 | 11:15 | Thermoelectric efficiency in Si and Ge nanoribbons | DAGOSTA | Roberto |
| oral | C.V-3 | 28-05-2013 | 11:30 | Molecular dynamics calculations of the thermal conductivity of isotopically modulated silicon multilayer nanowires | Frieling | Rafael |
| oral | C.V-4 | 28-05-2013 | 11:45 | First principle calculations of alloy phase stability of ScN-based materials for thermoelectric application | KERDSONGPANY A | SIT |
| oral | C.V-5 | 28-05-2013 | 12:00 | Boltzmann transport and electronic structure calculations in disordered thermoelectrics: application to Ti(Fe-Ni)Sb half-Heusler alloys | KUTORASINSKI | Kamil |

BREAK **28-05-2013****Lunch****SESSION** **Nanostructured Bulk Materials : George Nolas**

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|---------|--------|------------|-------|--|-------|---------|
| invited | C.VI-1 | 28-05-2013 | 14:00 | Nanostructured Bulk Thermoelectric Materials | REN | Zhifeng |
| oral | C.VI-2 | 28-05-2013 | 14:30 | Evolution of phase segregation and spinodal structures in the AgPb ₁₈ SbTe ₂₀ system during melt | DADDA | Jayaram |

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|----------------|---------|-------------------|-------|---|----------------|--------------|
| | | | | synthesis and thermoelectric properties of Ag _{1-y} Pb ₁₈ Sb _{1+z} Te ₂₀ compounds | | |
| oral | C.VI-3 | 28-05-2013 | 14:45 | Novel Synthetic Process and Enhanced Thermoelectric Properties of CNT/Bi ₂ Te ₃ Nanocomposites- REMOVED | KIM | Kyung Tae |
| oral | C.VI-4 | 28-05-2013 | 15:00 | ZnSb Nanoparticles and Nanostructured Materials: Chemical Synthesis, Characterization and Thermoelectric Properties | NGUYEN THANH | Mai |
| oral | C.VI-5 | 28-05-2013 | 15:15 | Antimony as an additional n-type dopant in nanosilicon NOT PRESENTED | PETERMANN | Nils |
| oral | C.VI-6 | 28-05-2013 | 15:30 | Chemical synthesis and thermoelectric evaluation of nanostructured iron antimonide (FeSbx) - Changed to poster, session C.PI | SALEEMI | Mohsin |
| oral | C.VI-7 | 28-05-2013 | 15:45 | Interface crystallization and thermoelectric performance of n-type Bi ₂ (Te/Se) ₃ nanoplatelet composites NOT PRESENTED | XIONG | Qihua |
| BREAK | | 28-05-2013 | | Coffee Break | | |
| SESSION | | | | Films, Particles & Quantum Dots : Jan König | | |
| oral | C.VII-1 | 28-05-2013 | 16:30 | Te concentration and thickness dependence on the thermoelectric properties of p-type Bi _{0.5} Sb _{1.5} Te _{3+X} thin films deposited by Pulsed Laser Deposition - REMOVED | ATHANASOPOULOS | Georgios |
| invited | C.VII-8 | 28-05-2013 | 16:15 | How to Make That Breakthrough in Energy Conversion: Thermoelectricity | LEE | Wooyoung |
| oral | C.VII-2 | 28-05-2013 | 16:45 | Thickness dependence and giant high temperature thermoelectric response of Ca ₃ Co ₄ O ₉ thin films | Habermeier | Hanns-Ulrich |
| oral | C.VII-3 | 28-05-2013 | 17:00 | Enhancement of the Power Factor in Two-Phase Silicon-Boron Nanocrystalline Alloys | NARDUCCI | Dario |
| oral | C.VII-4 | 28-05-2013 | 17:15 | Fabrication of large scale single crystal Bi ₂ Te ₃ nanosheet arrays via one-step electrolysis process | Tsai | Hung-Wei |
| oral | C.VII-5 | 28-05-2013 | 17:30 | Seebeck effects of silicon and nickel silicide nanocrystals composite films | UCHIDA | Noriyuki |
| oral | C.VII-6 | 28-05-2013 | 17:45 | Sintering of Inkjet-printed Silicon Nanoparticles for Thermoelectric Devices | DRAHI | etienne |
| oral | C.VII-7 | 28-05-2013 | 18:00 | Synthesis of graphene based Cu-Ni quantum dots: An ideal thermoelectric material | KUAMR | Anil |

SESSION**Nanowires & Nanopillars : Claudia Felser**

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|---------|----------|------------|-------|---|------------|-----------|
| invited | C.VIII-1 | 29-05-2013 | 08:30 | Nanostructured bulk silicon for thermoelectricity: A model system to explore novel device concepts | SCHIERNING | Gabi |
| oral | C.VIII-2 | 29-05-2013 | 09:00 | Thermoelectric properties of nano-scale Si _{1-x} Gex pillars array and microcooling devices | CHING-CHI | Wang |
| oral | C.VIII-3 | 29-05-2013 | 09:15 | Thermoelectric Property of Nanostructure-Engineered Bi-Te Core/shell Nanowire Grown by On-Film Formation of Nanowires | KIM | Jeongmin |
| oral | C.VIII-4 | 29-05-2013 | 09:30 | Thermoelectric measurement of single nanowire using a microfabricated platform | SONG | Jae Yong |
| oral | C.VIII-5 | 29-05-2013 | 09:45 | Optimization prospects for geometry-modulated nanowires against their thermoelectric efficiency | ZIANNI | XANTHIPPI |
| oral | C.VIII-6 | 29-05-2013 | 10:00 | Coherent x-ray diffraction study of GaAs nanopillars embedded in air-gap heterostructures | ZOZULYA | Alexey |

BREAK**29-05-2013****Coffee Break****SESSION****Chalcogenides & Intermetallics : Dariusz Kaczorowski**

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|---------|--------|------------|-------|---|--------------|-----------|
| invited | C.IX-1 | 29-05-2013 | 10:45 | Topological insulators and thermoelectric materials | FELSER | Claudia |
| oral | C.IX-2 | 29-05-2013 | 11:15 | Layered oxychalcogenides: new high-ZT thermoelectric materials | BARRETEAU | Céline |
| oral | C.IX-3 | 29-05-2013 | 11:30 | Thermoelectric Properties of TS ₂ (T: Ti, Cr) Based Layer Sulfides Prepared by CS ₂ Sulfurization | OHTA | Michihiro |
| oral | C.IX-4 | 29-05-2013 | 11:45 | Thermoelectric Properties of Layered Antiferromagnetic CuCrSe ₂ NOT PRESENTED | TEWARI | GIRISH C |
| oral | C.IX-5 | 29-05-2013 | 12:00 | Tuning of the thermoelectric properties of intermetallic phases Ru _{1-x} TxIn ₃ (T = Re, Rh, Ir) by electron and phonon engineering | WAGNER-REETZ | Maik |

BREAK**29-05-2013****Lunch****SESSION****Posters-II : António Pereira Gonçalves**

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|----------------------------|---------|------------|-------|--|-------------------|------|
| Flash poster presentations | | | 14:00 | | all | |
| poster | C.PII-1 | 29-05-2013 | 14:00 | LixNayCoO ₂ as promising thermoelectric material: synthesis, structure, properties. | SEMENOVA | Anna |
| poster | C.PII-2 | 29-05-2013 | 14:00 | Anomalous enhancement of the thermoelectric figure of merit by V co-doping in SrTiO ₃ | SCHWINGENSCHL OGL | Udo |

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|--------|----------|------------|-------|---|-----------------|----------|
| poster | C.PII-3 | 29-05-2013 | 14:00 | CHEMICAL THERMOCOUPLE AS EFFECTIVE DEVICE FOR CONVERTING HEAT INTO ELECTRICITY IN LOW TEMPERATURE GRADIENTS | VASSEL | Sergei |
| poster | C.PII-4 | 29-05-2013 | 14:00 | First principles calculation of Seebeck coefficients of γ -Fe(OH) | MORI | MASAMI |
| poster | C.PII-5 | 29-05-2013 | 14:00 | Two-layer photo-thermal deflection model to study the non-radiative recombination process: Application to $\text{Ga}_{0.7}\text{In}_{0.3}\text{Al}_{0.23}\text{As}_{0.77}/\text{GaSb}$ and $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}_{0.08}\text{Sb}_{0.92}/\text{GaSb}$ laser structures NOT PRESENTED | ILAH | Soufiene |
| poster | C.PII-6 | 29-05-2013 | 14:00 | Reliable Characterisation of Thermoelectric Generators NOT PRESENTED | WINKLESS | Laurie |
| poster | C.PII-7 | 29-05-2013 | 14:00 | Computational studies of vacancies, antisite, and exchange pairs defects in bismuth telluride NOT PRESENTED | POKROPIVNY | Alex |
| poster | C.PII-8 | 29-05-2013 | 14:00 | Effect of transition metals doping on the thermoelectric properties of $\text{Zn}_{1-x}\text{Al}_x\text{O}$ | Zhang | Shaolin |
| poster | C.PII-9 | 29-05-2013 | 14:00 | Spark plasma preparation of $\text{Ti}_{1-x}\text{V}_x\text{O}_{1.9}$ ($x = 0 \div 0.1$) and their thermoelectric properties | VEREMCHUK | Igor |
| poster | C.PII-10 | 29-05-2013 | 14:00 | Using Crystallographic Shear to Reduce Lattice Thermal Conductivity: Magnesium Oxides for Thermoelectric Application | KIESLICH | Gregor |
| poster | C.PII-11 | 29-05-2013 | 14:00 | Misfit-layered cobalt oxides by hydrothermal synthesis | CHOU | Ta-Lei |
| poster | C.PII-12 | 29-05-2013 | 14:00 | Correlated transition metal oxides for thermoelectric power generation | POPULOH | Sascha |
| poster | C.PII-13 | 29-05-2013 | 14:00 | Oxide thermoelectric converters for waste heat recovery designed by applying the compatibility approach | Saucke | Gesine |
| poster | C.PII-14 | 29-05-2013 | 14:00 | Partial nitrogen substitution in thermoelectric EuTiO_3 | SAGARNA | Leyre |
| poster | C.PII-15 | 29-05-2013 | 14:00 | Thermal conductivity in compositionally-graded $\text{Si}_{1-x}\text{Ge}_x$ superlattices | RODRÍGUEZ-VIEJO | Javier |
| poster | C.PII-16 | 29-05-2013 | 14:00 | First-principle simulation of atomically-thin films and nanotubes of bismuth telluride NOT PRESENTED | POKROPIVNY | Alex |
| poster | C.PII-17 | 29-05-2013 | 14:00 | Tailoring properties of graphene with vacancies NOT PRESENTED | POKROPIVNY | Alex |

SESSION **Devices & Applications : John Stockholm**

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|--------------|-------|-------------------|-------|---|-----------------|----------|
| invited | C.X-1 | 30-05-2013 | 08:30 | Thermoelectric Generators for Direct Conversion of Automotive Waste Heat into Useful Electrical Power | MEISNER | Gregory |
| oral | C.X-2 | 30-05-2013 | 09:00 | Laser-assisted direct writing of thermoelectric generators | FEINAEUGLE | Matthias |
| oral | C.X-3 | 30-05-2013 | 09:15 | Development of Skutterudite Thermoelectric Modules | HEUER | Jana |
| oral | C.X-4 | 30-05-2013 | 09:30 | Performance evaluation of solar thermoelectric generator | HAN | Seungwoo |
| oral | C.X-5 | 30-05-2013 | 09:45 | CMOS compatible planar thermoelectric microgenerator based on top-down Si nanowires | RODRÍGUEZ-VIEJO | Javier |
| oral | C.X-6 | 30-05-2013 | 10:00 | Electrochemical Fabrication and Characterization of Thermoelectric Micro Generators | ROSTEK | Raimar |
| BREAK | | 30-05-2013 | | Coffee Break | | |

SESSION **Novel Thermoelectric Materials : Gregory Meisner**

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|--------------|--------|-------------------|-------|--|-----------|--------------|
| invited | C.XI-1 | 30-05-2013 | 10:45 | Complex Zintl Compounds for Discovering new High Efficiency Thermoelectric Materials | SNYDER | Jeff |
| oral | C.XI-2 | 30-05-2013 | 11:15 | Poly(3-hexylthiophene)-carbon nanotube composites for high-performance organic thermoelectrics | GOÑI | Alejandro R. |
| oral | C.XI-3 | 30-05-2013 | 11:30 | Synthesis and Thermoelectric Properties of p-type Hexaborides | TAKEDA | Masatoshi |
| oral | C.XI-4 | 30-05-2013 | 11:45 | Thermoelectric properties of CrN | RIVADULLA | Francisco |
| oral | C.XI-5 | 30-05-2013 | 12:00 | Novel thermoelectric sheets based on the spin Seebeck effect | KIRIHARA | Akihiro |
| BREAK | | 30-05-2013 | | Lunch | | |

SESSION **Half-Heusler & Silicides : Jeff Snyder**

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|---------|---------|------------|-------|---|-------------------|-----------|
| invited | C.XII-1 | 30-05-2013 | 14:00 | Rare-earth-based half-Heusler phases for thermoelectric applications | KACZOROWSKI | Dariusz |
| oral | C.XII-2 | 30-05-2013 | 14:30 | Phase stability and oxidation studies of (Ti _{0.33} Zr _{0.33} Hf _{0.33})NiSn half-Heusler compounds | Gał,ą,zka | Krzysztof |
| oral | C.XII-3 | 30-05-2013 | 14:45 | Significant ZT Enhancement in half-Heusler Nanocomposites via a Synergistic 'High Mobility Electron Injection, Energy filtering and Boundary Scattering' Approach | XIE | WENJIE |

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|------|---------|------------|-------|--|-------------------------------|-----------|
| oral | C.XII-4 | 30-05-2013 | 15:00 | Influence of power factor enhancement on the thermoelectric figure of merit in Mg ₂ Si _{0.4} Sn _{0.6} based materials | DASGUPTA | Titas |
| oral | C.XII-5 | 30-05-2013 | 15:15 | Nanostructure stability and thermoelectric properties of Mg ₂ (Si,Sn) thermoelectric material | BELLANGER | Philippe |
| oral | C.XII-6 | 30-05-2013 | 15:30 | Microstructure ? thermoelectrical properties relationships for a n-type polycrystalline Si _{1-x} Gex alloy sintered by SPS | BELLANGER for BERNARD-GRANGER | Guillaume |
| oral | C.XII-7 | 30-05-2013 | 15:45 | Thermoelectric properties of doped Mg ₂ Si _{1-x-y} Sn _x Gey Solid Solutions- REMOVED | KYRATSI | Theodora |

BREAK

30-05-2013

Coffee Break

SESSION

Thermoelectric Theory - II : Joseph Heremans

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|---------|----------|------------|-------|---|-----------------------|--------------|
| invited | C.XIII-1 | 30-05-2013 | 16:30 | Impact of electronic correlations on the transport in transition-metal oxides | LECHERMANN | Frank |
| oral | C.XIII-2 | 30-05-2013 | 17:00 | Micro-Meter-Scale Molecular Dynamics Simulation of the Lattice Thermal Conductivity of Graphene | KIM | Yong-Sung |
| oral | C.XIII-3 | 30-05-2013 | 17:15 | Modelling Thermoelectric Materials from First Principles | MURPHY ARMANDO | Felipe |
| oral | C.XIII-4 | 30-05-2013 | 17:30 | First-principle simulation of Ce and Yb filled superstructures of skutterudites | XIONG for POKROPIVNY | Alex |
| oral | C.XIII-5 | 30-05-2013 | 17:45 | Thermoelectric properties of Ni and Sn doped ZnO: A first principle study NOT PRESENTED | XIONG | Shiyun |
| oral | C.XIII-6 | 30-05-2013 | 18:00 | Strongly enhanced thermal transport in a lightly doped Mott insulator- REMOVED | ZLATIC | Veljko |
| | | 30-05-2013 | | Closing | Bühler-Paschen | Silke |