



# PROGRAM

## International Workshop

### Thermoelectric Materials: from materials chemistry and physics to devices (IWT2023)

<b>TUESDAY 11<sup>TH</sup> APRIL 2023</b>	
16:00-17:30	REGISTRATION
<b>WEDNESDAY 12<sup>TH</sup> APRIL 2023</b>	
8:15-9:00	REGISTRATION
9:00-9:10	OPENING CEREMONY, PR. ANNIE-CLAUDE GAUMONT, VICE-PRESIDENT UNIVERSITY OF CAEN NORMANDY, RESEARCH COMMITTEE
SESSION A : DEVICES / CHAIR : YOSHIAKI KIMEMUCHI	
9:10-9:35	<b>Woochul Kim</b> : Our journey toward operating wearable sensors and actuators based on body heat harvesting
9:35-10:00	<b>Guillaume Savelli</b> : Overview of research activities on thermoelectrics at CEA-LITEN
10:00-10:25	<b>Masashi Mikami</b> : Development of thermoelectric modules consisting of Heusler alloys
10:25-10:50	<b>Philippe Sauerschnig</b> : Improving the reliability and efficiency of nanostructured PbTe-based thermoelectric materials and modules
<b>COFFEE BREAK</b>	
Session B : PHYSICS / CHAIR : ERIC ALLENO	
11:25-11:50	<b>Yuzuru Miyazaki</b> : Incommensurate Nowotny Chimney-Ladder phases - Potential thermoelectric materials
11:50-12:15	<b>Subhajit Roychowdhury</b> : Large room temperature anomalous transverse thermoelectric effect in kagome antiferromagnet YMn <sub>6</sub> Sn <sub>6</sub>
12:15-12:40	<b>Christophe Candolfi</b> : Engineering the electronic band structure of SnTe with resonant levels and band convergence
<b>LUNCH</b>	
Session C : CHEMISTRY / CHAIR : JAN-WILLEM BOS	
14:10-14:35	<b>Maria Ibáñez</b> : Sintering solution processed nanoparticles: a way to tune microstructure through surface chemistry
14:35-15:00	<b>Pierric Lemoine</b> : Crystal structure and TE properties of new sphalerite derivative phases in the ternary system Cu-Sn-S: Cu <sub>5</sub> Sn <sub>2</sub> S <sub>7</sub> and Cu <sub>22</sub> Sn <sub>10</sub> S <sub>32</sub>
15:00-15:25	<b>Kazuki Imasato</b> : Synthesizing triple half-Heusler to explore larger compositional space
15:25-15:50	<b>Arnaud Le Febvrier</b> : Multifunctional nitride and oxide thin film for thermoelectrics and energy harvesting
<b>COFFEE BREAK</b>	
SESSION D : PHYSICS / CHAIR : XINGCHEN SHEN	
16:20-16:45	<b>Hidetoshi Miyazaki</b> : Improvement of thermoelectric conversion properties by controlling electronic structure in Heusler-type Fe <sub>2</sub> VAl compounds
16:45-17:10	<b>Ran He</b> : Enhancement of phonon scattering in thermoelectric half-Heusler compounds by non-equilibrium synthesis
17:10-17:35	<b>Eric Alleno</b> : Optimization of the thermoelectric properties in self-substituted Fe <sub>2</sub> VAl
17:35-18:15	POSTER PRESENTATIONS (See the list of posters in page 3 and the <a href="#">book of abstracts</a> )
18:15-20:00	POSTER SESSION – APERITIF DINNER

**THURSDAY 13TH APRIL 2023****SESSION E : PHYSICS / CHAIR : SUBHAJIT ROYCHOWDHURY**9:10-9:35 **Stéphane Pailhès** : Phonons in complex crystals9:35-10:00 **Francesco Rossella** : Semiconductor nanowire thermoelectrics: gate-controlled ZT, giant reduction of thermal conductivity, thermoelectric-gating10:00-10:25 **Mickaël Baudhuin** : Lattice dynamics and thermoelectric properties of type IX clathrates Ba<sub>24</sub>Ge<sub>100</sub>**COFFEE BREAK****Session F : CHEMISTRY / CHAIR : MARIA IBÁÑEZ**11:00-11:25 **Michitaka Ohtaki**: Carrier concentration tuning of highly conductive tungsten-based Magnéli phase oxide W<sub>18</sub>O<sub>49</sub> with inherently low lattice thermal conductivity11:25-11:50 **Mathieu Pasturel** : Magnesiothermy: an efficient route to mesostructured thermoelectric intermetallics11:50-12:15 **Jan-Willem Bos** : Exploration of half-Heusler and metal phosphide thermoelectric materials12:15-12:40 **David Bérardan** : BiCuSeO-based oxychalcogenides: recent developments and defect chemistry**LUNCH****Session G : THEORY / CHAIR : RÉGIS GAUTIER**14:10-14:35 **Marie-Christine Record** : First-principle investigations on n(PbTe)-m(Bi<sub>2</sub>Te<sub>3</sub>) system compounds14:35-15:00 **Masato Yoshiya** : Computational attempts to go beyond conventional theories for exploration of thermoelectric properties of practical materials15:00-15:25 **Céline Barreteau** : New intermetallic thermoelectric materials among using high-throughput calculations and machine learning15:25-15:50 **Pascal Boulet** : Chalcogenide-based high entropy alloys as thermoelectric materials for power generation15:50-16:15 **Nathalie Vast** : *ab initio* description of electron-phonon and phonon-phonon scattering processes in DFT for the calculation of charge and heat transports**COFFEE BREAK**

17:00-18:00 VISIT OF THE ABBAYE

19:30 GALA DINNER

**FRIDAY 14TH APRIL 2023****SESSION H : CHEMISTRY/DEVICES / CHAIR : DAVID BERARDAN**8:45-9:10 **Michihiro Ohta** : Materials development, module fabrication, and module evaluation in thermoelectric power generation9:10-9:35 **Dimitri Tainoff** : Thermal energy harvesting for the powering of industrial IoT sensors: from basic applications to complex measurements9:35-10:00 **Yohann Thimont** : Elaboration and the study of transparent p-type thermoelectric properties of CuCrO<sub>2</sub>:Mg and CuI thin films10:00-10:25 **Nicolas Stein** : Pulse electrodeposition of SnSe films for thermoelectric conversion**COFFEE BREAK****Session I : DEVICES / CHAIR : GUILLAUME SAVELLI**11:00-11:25 **Tsutomu Kanno** : High efficiency and output power in GeTe/Mg<sub>3</sub>Sb<sub>2</sub>-based thermoelectric generator11:25-11:50 **Yoshiaki Kinemuchi** : Thermographic detection of failure in thermoelectric module11:50-12:15 **Soufiane El Oualid** : Influence of thermoelectric properties on the output power density of a new design of planar  $\mu$ -TEG

12:15-12:30 CLOSING CEREMONY

# POSTERS

- 1) *ab initio* calculations of the thermoelectric phonon drag effect in semiconductor nanostructures, *R. Sen, N. Vast, J. Sjakste*
- 2) Bi<sub>2</sub>Te<sub>3</sub>: Towards a Se free n-Type, *A. Galodé, F. Gascoin*
- 3) Chemical synthesis of single crystalline Ag<sub>2</sub>Te and Cu<sub>2</sub>Te nanorods, *K. Al Hokayem, J. Ghanbaja, S. Michel, S. Legeai, N. Stein*
- 4) Efficient optimization of the synthesis parameters of thermoelectric legs using a machine learning approach, *S. Le Tonquesse, H. Bouteiller, K. Imasato, M. Ohta, T. Mori, D. Berthebaud*
- 5) Glassy thermal conductivity in Cs<sub>3</sub>Bi<sub>2</sub>l<sub>6</sub>Cl<sub>3</sub> single crystal, *P. Acharyya*
- 6) Graphical User Interface for using active learning assisted by Bayesian Optimization applied to thermoelectric materials, *C. Bajan, G. Lambard*
- 7) Implantation effect on the thermoelectric properties of scandium and chromium nitrides thin films, *R. Burcea, H. Bouteiller, P. Eklund, A. Le Febvrier, S. Dubois, J-F. Barbot*
- 8) In situ diffraction study of the phase transformations occurring in the thermoelectric colusite Cu<sub>26</sub>V<sub>2</sub>Sn<sub>6</sub>S<sub>32</sub>, *F. Guiot, A. Bourhim, G. Guélou, C. Dejoie, A. Fitch, E. Guilmeau, P. Lemoine, C. Prestipino*
- 9) Scalability of the magnesiothermic process for mass production of skutterudites: preliminary results, *A. Hodroj, M. Pasturel, V. Bouquet, V. Demange, C. Prestipino, R. Lebullenger*
- 10) Screening quaternary Heusler by machine learning for application in thermoelectricity, *R. Xie, J-C. Crivello, C. Barreteau*
- 11) Precursor phase with full phonon softening above the charge-density-wave phase transition in 2H-TaSe<sub>2</sub>, *X. Shen*
- 12) Structural analyses and thermoelectric properties of Cr<sub>2</sub>Sn<sub>3</sub>S<sub>7</sub>, *C. Prestipino*
- 13) Synthesis of β-FeSi<sub>2</sub> by reactive sintering, *L. Abbassi, D. Mesguich, D. Berthebaud, B. Srinivasan, S. Le Tonquesse, T. Mori, G. Chevallier, C. Estournès, E. Flahaut, R. Viennois, M. Beaudhuin*
- 14) Thermoelectric Materials for utilizing Automobile Waste Heat, *K. K. Johari, Y. Tsuchiya, M. Naruke, K. Imasato, T. Ishida, A. Yamamoto, M. Ohta*
- 15) Thermoelectric properties of the Mn(Sb,Bi)<sub>2</sub>(S,Se)<sub>4</sub> series, *M. Leproult, T. Barbier, E. Guilmeau*
- 16) Unconventional synthesis and characterization of substituted rare-earth antimonides for very high temperature thermoelectric applications, *H. Bouteiller, S. Le Tonquesse, T. Mori, J-F. Halet, D. Berthebaud, F. Gascoin*
- 17) A Tunable Structural Family with Ultralow Thermal Conductivity: Copper-Deficient Cu<sub>1-x</sub>Pb<sub>1-x</sub>Bi<sub>1+x</sub>S<sub>3</sub>, *K. Maji, P. Lemoine, A. Renaud, B. Zhang, X. Zhou, V. Carnevali, C. Candolfi, B. Raveau, R. Al Rahal Al Orabi, M. Fornari, P. Vaqueiro, M. Pasturel, C. Prestipino, E. Guilmeau*
- 18) Doping strategies in sphalerite derivative thermoelectric sulfides, *L. Le Gars, P. Lemoine, B. Malaman, K. Suekuni, B. Raveau, E. Guilmeau*
- 19) 3D scanning precession electron diffraction analysis of nanodomains in thermoelectrics, *S. Passuti, V. P. Kumar, B. Raveau, B. Zhang, X. Zhou, S. Fujii, M. Yoshiya, K. Yoshizawa, S. Le Tonquesse, Carmelo Prestipino, P. Lemoine, K. Suekuni, E. Guilmeau, and P. Boullay*
- 20) Investigation of the magnetism impact on the thermoelectric properties in the spinel family, *S. El Haber, D. Pelloquin, O. Lebedev, R. Daou, A. Maignan, S. Hébert*