

Programme

Day 1: Monday July 3rd, 2017

15:45-16:15 Registration

16:15-16:30 Welcome

Plenary Session: New Material Design Concepts

Chair: Anke Weidenkaff, University of Stuttgart, Germany

16:30-17:15 **G. Jeffrey Snyder**, Northwestern University, USA
Fermi Surface Complexity Factor for Thermoelectric Materials

17:15-18:00 **David Singh**, University of Missouri, USA
Methods for Identifying New High Performance Thermoelectric Materials

Social Evening

19:30 Dinner at Bodega

Day 2: Tuesday July 4th, 2017

8:50-9:10 Registration

Session 1: Industrial Applications

Chair: Devendraprakash Gautam, Tyndall National Institute, Ireland

9:10-9:50 **Albert O'Grady**, Analog Devices, Ireland
Industrial Applications for Thermoelectric Energy Harvesting

9:50-10:30 **Ryan Enright**, Nokia Bell Labs, Ireland
Thermally Integrated Photonics Systems

Coffee Break

10:30-11:00

Session 2: Thermoelectric Devices

Chair: Ryan Enright, Nokia Bell Labs, Ireland

11:00-11:20 **Devendraprakash Gautam**, Tyndall National Institute, Ireland
Enhanced Seebeck Coefficient of Electroplated p-type $(\text{Sb}_{1-x}\text{Bi}_x)_2\text{Te}_3$ thin films by Te Encapsulation

11:20-11:40 **Maria Ibáñez**, ETH Zurich, Switzerland
Bottom-up Engineering of Thermoelectric Nanomaterials and Devices from Solution-Processed Nanoparticles

11:40-12:00 **Bruno Lorenzi**, University of Milano Bicocca, Italy
From Theoretical Modeling to Lab Testing, a Way towards the Development of
Optimized and Cost Effective Hybrid Thermoelectric-Photovoltaic Devices

Lunch Break

12:00-13:30

Session 3: IV-VI and Related Materials

Chair: G. Jeffrey Snyder, Northwestern University, USA

13:30-14:10 **Bo Brummerstedt Iversen**, Aarhus University, Denmark
Structural Thermoelectrics

14:10-14:50 **Matthieu J. Verstraete**, University of Liege, Belgium
Ab Initio Phonon Limited Transport

14:50-15:30 **Yaniv Gelbstein**, Ben Gurion University, Israel
Thermoelectric Efficiency of IV-VI and V₂-VI₃ Materials Driven near Phase Transitions

Coffee Break

15:30-16:00

Session 4: Thermal Conductivity Modelling

Chair: Matthieu J. Verstraete, University of Liege, Belgium

16:00-16:40 **Christian Carbogno**, Fritz-Haber Institute Berlin, Germany
Thermal Conductivities in Solids from First Principles: Accurate Computations and
Qualitative Insights

16:40-17:20 **Olle Hellman**, California Institute of Technology, USA
Temperature Dependent Vibrational Properties of Thermoelectric Materials

17:20-17:40 **Ivana Savić**, Tyndall National Institute, Ireland
Lattice Thermal Conductivity of PbTe Materials Driven near Ferroelectric Phase
Transition

Poster Session

17:40-18:40 **Perla Wahnón**, Universidad Politecnica de Madrid, Spain
Theoretical Calculation of Electronic and Thermoelectric Properties of Bi and Sn doped-
Cu₃SbSe₄ from First Principles

17:40-18:40 **Simon Corbett**, Trinity College Dublin, Ireland
Characterisation of Thermoelectric Devices with CCD – Thermoreflectance techniques

17:40-18:40 **Daniela Galliani**, University of Milano Bicocca, Italy
Thermoelectric Properties of Vapour Phase Polymerized
Poly(3,4 Ethylenedioxythiophene) -Trifluoromethanesulfonate (VPP PEDOT:Tf):
a Study on a Highly Performing Conductive Polymer

17:40-18:40 **Alessio Campo**, University of Basel, Switzerland
Semiconductor Nanowires as Efficient Thermoelectric Nanomaterials

- 17:40-18:40 **Neil M. Wight**, Heriot-Watt University, Edinburgh, UK
A Universal Method for Thermal Conductivity Measurements on Micro-/Nano-Films With and Without Substrates using Micro-Raman Spectroscopy
- 17:40-18:40 **Swatchith Lal**, Tyndall National Institute, Ireland
Optimization of Electrodeposited Bi₂Te₃-Based Thin Films for Realization of Thermoelectric Energy Harvester
- 17:40-18:40 **Javier Fernández Troncoso**, Queen's University Belfast, UK
Thermal Conductivity of PbTe from Classical Molecular Dynamics Simulations
- 17:40-18:40 **Maria Troppenz**, Humboldt University Berlin, Germany
Finite-Temperature Properties of the Thermoelectric Clathrate Ba₈Al_xSi_{46-x}
- 17:40-18:40 **Djordje Dangić**, Tyndall National Institute, Ireland
Thermal Expansion of Pb_{1-x}Ge_xTe Alloys from First Principles
- 17:40-18:40 **Jiang Cao**, Tyndall National Institute, Ireland
Effect of Electron-Phonon Scattering on Thermoelectric Figure-of-Merit
- 17:40-18:40 **Ronan Murphy**, Tyndall National Institute, Ireland
Reducing the Thermal Conductivity by Driving PbTe to a Phase Transition via Strain and/or Alloying

Conference Dinner

- 19:45 Dinner at South's Bar, Imperial Hotel

Day 3, Wednesday July 5th, 2017

Session 1: Tellurides

Chair: Yaniv Gelbstein, Ben Gurion University, Israel

- 8:30-9:10 **Juri Grin**, Max Plank Institute Dresden, Germany
Substitutional Behavior of Lead Telluride
- 9:10-9:50 **Oliver Oeckler**, University of Leipzig, Germany
Crystallography of Thermoelectric Tellurides
- 9:50-10:10 **Pavel Korotaev**, Dukhov Research Institute for Automatics, Moscow, Russia
Supercell Modeling of Na and Tl Doping of Lead Telluride

Coffee Break

- 10:10-10:40

Session 2: 2D and Layered Materials

Chair: Nicola Bonini, Kings College London, UK

- 10:40-11:20 **Troels Markussen**, QuantumWise, Denmark
First Principles Modelling of Thermo-electrics Using ATK, Comparison of Bulk and Full Device Approaches

11:20-11:40 **Graeme Cunningham**, Nokia Bell Labs, Ireland
Full Thermoelectric Characterisation of Hot Pressed Solution Processed Group VI TMD
Films around Room Temperature

11:40-12:00 **Jakub D. Baran**, University of Bath, UK
Insight into Thermoelectric Properties of High-Performance Layered Oxides: A
Cooperative Computational and Experimental Study

Lunch Break

12:00-13:30

Session 3: Half-Heuslers

Chair: Christian Carbogno, Fritz-Haber Institute Berlin, Germany

13:30-14:10 **Anke Weidenkaff**, University of Stuttgart, Germany
Thermoelectric Materials for the Medium- and High-Temperature Range ($600\text{ K} < T < 1200\text{ K}$)

14:10-14:50 **Georgy Samsonidze**, Bosch, USA
Thermoelectricity by Rational Design: New Materials and Insights from First-Principles
Computations of Carrier Scattering

14:50-15:30 **Ankita Katre**, CEA-Grenoble, France
Unveiling the Role of Defects in Thermal Transport: an Ab Initio Study Using AlmaBTE
Code

Coffee break

15:30-16:00

Session 4: Thermoelectric Transport Modelling

Chair: David Singh, University of Missouri, USA

16:00-16:40 **Giovanni Vignale**, University of Missouri, USA
Nonequilibrium Thermal Density Functional Theory - a Microscopic Approach to
Thermoelectric Transport

16:40-17:20 **Nicola Bonini**, Kings College London, UK
Thermoelectric Properties from First-Principles via the Exact Solution of the Boltzmann
Transport Equation

17:20-17:40 **Phillip Murphy-Armando**, Tyndall National Institute, Ireland
Study of the Effect of the Scattering rate on the Thermopower

17:40-18:00 **Fabio Ricci**, University of Liege, Belgium
About the Electronic Properties of Fe_2VAl and Related Thermoelectric Compounds

Social Evening

19:30 Dinner at Franciscan Well

Day 4: July 6th, 2017

Session 1: Discussion

9:00-11:00 Open Discussion and Future Directions