Marie Skłodowska-Curie Innovative Training Network

HORATES

NEWSLETTER **#2** 2022

Hybrid and ORgAnic ThermoElectric Systems

The ongoing development of the **internet of things** (IoT) leads to completely new opportunities for **thermoelectric generators** based on **organic and hybrid materials**.

Our **mission** is to **train young professionals** that will be able to operate into this highly interdisciplinary field.

HORATES training will develop along three main guidelines:

Acquiring solid background in different **scientific and technological fields**, all related to hybrid and organic thermoelectrics;

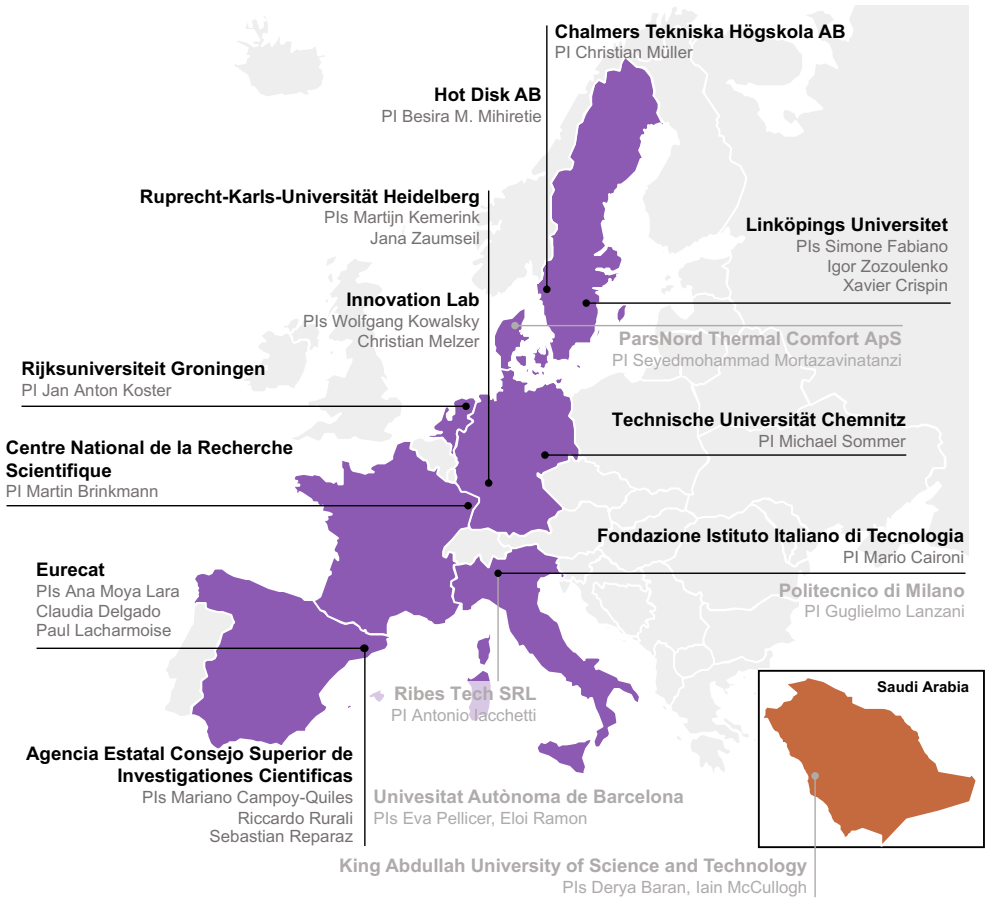
Exposing HORATES ESRs to **diverse sectors**, such as academia, technological research centers and industrial nodes;

Fostering the development of **transversal competencies**.

HORATES Mission

HORATES is a **Marie Skłodowska-Curie Innovative Training Network** (MSCA-ITN-ETN) aiming to train the **next generation of R&D innovators in hybrid and organic thermoelectrics** and develop prototype energy harvesters inspired by actual market demand.

The HORATES consortium:



11 Beneficiaries and **5 associate partners** from **7 European countries** and **1 non-European country**. This consortium brings together expertise from academic and non-academic nodes to ensure the **15 ESRs** are exposed to a real multisectoral exposure.

This project has received funding from the European Union's Horizon 2020 research and programme under the Marie Sklodowska-Curie grant agreement no. 955837

Marie Skłodowska-Curie Innovative Training Network

HORATES in numbers:

MEETINGS

- **1 kick-off meeting**
- **3 network meetings already implemented**
- **3 training workshops already implemented**

DISSEMINATION & COMMUNICATION

- **16 papers with ESRs and PIs as the co-authors already been published and many others are under review or in preparation**
- **42 oral/poster presentations at conferences and seminars**
- **6 conferences/workshops organized**

INTERACTIONS

- **1 graduate summer school attended**
- **2 trade fairs attended**
- **38 training activities implemented**

ESRs visiting KAUST (Saudi Arabia)

Related training and dissemination activities

Tutorial video on YouTube about a new method to measure thermal conductivity:

https://www.youtube.com/watch?v=vGWVGm4DDNI

Training workshops & schools

The HORATES Network offers a wide range of training opportunities to its ESRs, including 5 international schools on more specific scientific topics and 5 workshops on complementary and transferrable skills.

Workshops and international schools held thus far:

International School 1: *Basics of Thermoelectrics: Theory, Synthesis and Processing*; ***Workshop 1:*** *Team Building Workshop*

Göteborg (Sweden), 25-26 October 2021

International School 2: *Thermoelectric Characterization;* ***Workshop 2:*** *Academic Writing and Presentation, with focus on OTE*

Barcelona (Spain), 25-29 April 2022

International School 3: *Organic semiconductors and flexible electronics;* ***Workshop 3:*** *Thermal conductivity measurements – a company point-of-view*

KAUST (Saudi Arabia), 10-12 October 2022

More workshops and schools to come:

International School 4: *Advanced Topics in OTE;* ***Workshop 4:*** *From the initial idea to market entry*

International School 5: *Printed Electronics and Opportunities for OTE;* ***Workshop 5:*** *Career Development, incl. Postdoc Funding*

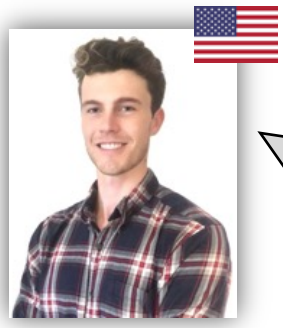
This project has received funding from the European Union's Horizon 2020 research and programme under the Marie Sklodowska-Curie grant agreement no. 955837

MARIE CURIE ACTIONS

The ESRs' scientific achievements thus far:

Aditya Dash (ESR1, Universität Heidelberg, Germany): *I am developing computational models to understand the electronic charge and heat transport in disordered or hybrid systems. My project aims to provide a quantitative description of the factors influencing thermoelectric efficiency considering the energetics and morphology. So far, I have developed a comprehensive model for the thermoelectric properties of SWCNT networks. In collaboration with Subhradip Guchait (ESR12), I am modelling the selective phase doping in organic polymers to understand the high power factor. And with Federico Ferrari (ESR 10), I am working towards simulating and linking the density of states to the conductivity and Seebeck coefficient in doped systems.*

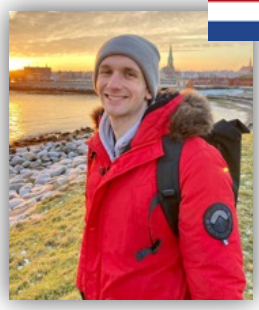
Angus Hawkey (ESR2, Heidelberg University, Germany): *I am working on developing composite thermoelectric materials consisting of semiconducting single-walled carbon nanotubes (SWNTs) and conjugated polymers. My project aims to fabricate, dope, and characterize these composites to understand role of the dopant counterion on the thermoelectric properties. This project is performed in collaboration with Aditya Dash (ESR1) in which he models the thermoelectric properties of the materials, and I perform the experimental work. Together, we aim to determine the design rules for improving the thermoelectric performance of SWNT based materials.*



Nathan James Pataki (ESR3, Istituto Italiano di Tecnologia, Italy): *I am working on the design, fabrication and characterization of organic thermoelectric generators (TEG) using organic semiconducting materials from within the HORATES ITN. My project aims to use existing and novel organic thermoelectric materials in combination with scalable fabrication techniques to produce proof-of-concept organic TEGs with output power densities exceeding 1 μW/cm^2. To this point, I have developed a thin and flexible TEG design to maximize thermocouple density and, thereby, output power density. The design was used to produce a fully organic TEG in collaboration with Qifan Li (ESR8) using the novel n-type ink developed in Prof. Simone Fabiano's lab, poly(benzimidazobenzophenanthroline):poly(ethyleneimine) (BBL:PEI). In addition, I have been working to characterize the thermoelectric properties of new n-type polymers based on benzodifuranone motifs synthesized by Diego Ropero Hinojosa (ESR11), while also working with Shubhradip Guchait (ESR12) to better understand the structure-property relationship in Diego's polymers.*

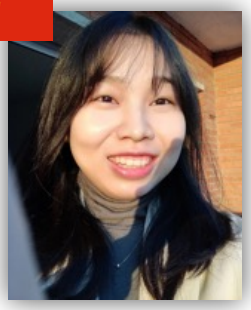
Mariavittoria Craighero (ESR4, Chalmers University of Technology, Sweden): *I work on the processing and doping of p-type conjugated polymers for thermoelectrics. My project aims to improve the thermoelectric performances of conjugated polymers by optimizing processing and doping efficiency. So far, I have studied the impact of side chain length on thermoelectric and mechanical properties of eligoethylene-substituted polythiophenes (in preparation). In collaboration with Joost Kimpel (ESR5), I am exploring the doping efficiency of novel thieno[3,2-b]thiophene polymers. With Shubhradip Guchait (ESR12), I am working on uniaxially aligned DPP-biEDOT copolymers for thermoelectric applications, and with Jiali Guo (ESR6), I am exploring the thermal conductivity of various polythiophenes.*

This project has received funding from the European Union's Horizon 2020 research and programme under the Marie Sklodowska-Curie grant agreement no. 955837



Joost Kimpel (ESR5, Chalmers University of Technology, Sweden): *I am working on the synthesis of novel p-type semiconducting polymers for thermoelectric applications, leveraging non-covalent interactions in conjugated polymers. My project aims to find facile synthesis routes to polymers with upscaling to multigram scale in hopes this accelerates research. Up to this day, I have shown the presence of non-covalent sulphur-oxygen interactions in compounds studied, which are postulated to aid in improving conductivity. Moreover, I have developed various novel thieno[3,2-b]thiophene semiconducting polymers through greener direct arylation methods (in preparation). In collaboration with Mariavittoria Craighero (ESR4), I am exploring doping effects on polymers, and with Diego Ropero Hinojosa (ESR11), I am working towards contextualizing difficulty of synthesis versus performance outcome using a synthetic complexity index analysis.*

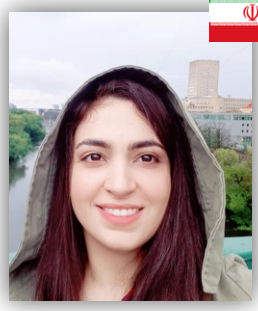
Jiali Guo (ESR6, Institute of Materials Science of Barcelona, Spain): *I am working on the advanced characterization of the thermoelectric properties of organic systems under the supervision of Prof. Mariano Campoy-Quiles (ICMAB-CSIC, Universitat Autònoma de Barcelona) and Dr. Sebastián Reparaz (ICMAB-CSIC, Universitat Autònoma de Barcelona). The main objective of my research project is to investigate experimentally the structural, electronic, and thermal properties of organic and hybrid thermoelectric materials based on their characterization using advanced tools and processing methods. So far, we are investigating the thermoelectric properties of conjugated polymers doped with different doping mechanisms in cooperation with Mariavittoria Craighero (ESR4). Fortunately, the preliminary results illustrate the correlation between electrical and thermal conductivities and the inevitable dependence of both on the microstructure and the dopant used.*



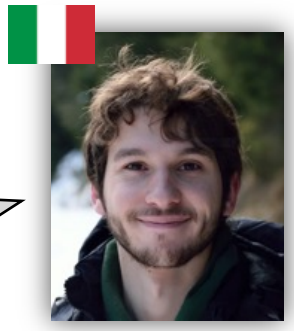
Paolo Sebastiano Floris (ESR7, ICMAB, Spain): *I'm working on developing a framework for the simulation of polythiophenes for the calculation of their lattice thermal conductivity based on previously existing classical force fields. My project aims to evaluate how doping affects thermal conductivity in organic thermoelectric materials. So far, I have studied the thermal conductivity of undoped P3HT as a function of its chain length and I have started to develop a force field for doped P3HT (work in preparation). In collaboration with Najmeh Zahabi (ESR9), I am exploring the thermal properties of crystalline PEDOT.*

Qifan Li (ESR8, Linköping University, Sweden): *I am developing dopant-free n-type organic conductors based on ground-state electron transfer in all-polymer blends. My project aims to synthesize new n-type organic semiconductor materials and investigate their ink formulation. So far, I have synthesized several ladder-type polymers with higher electron affinity (in preparation) and studied their charge transfer properties in combination with low-ionization energy donor polymers using Core-hole clock spectroscopy (in preparation). In collaboration with Nathan James Pataki (ESR 3), we fabricated ultra-flexible all-polymer thermoelectric generators based on poly(benzimidazobenzophenanthroline):poly(ethyleneimine) (BBL:PEI) and PEDOT:PSS.*

This project has received funding from the European Union's Horizon 2020 research and programme under the Marie Sklodowska-Curie grant agreement no. 955837

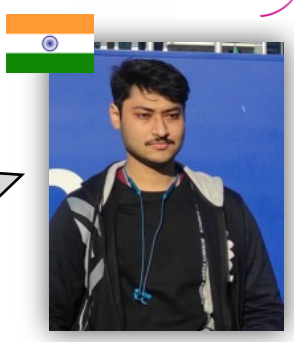


Najmeh Zahabi (ESR9, Linköping University, Sweden): *I am working on computational simulation and modeling of novel organic thermoelectric materials under Prof. Igor Zozoulenko's supervision. My research into charge carrier transport in the conducting polymer using the Car-Parrinello molecular dynamics method (in preparation). I have modeled thermoelectric devices made of PEDOT: PSS and Silver using the Seebeck effect by COMSOL Multiphysics software for a project in collaboration with Nathan James Pataki (ESR3). Also, I calculated crystallin PEDOT's thermal conductivity through classical molecular dynamics with Paolo Sebastiano Floris (ESR7) when I was in Barcelona (ICMAB-CSIC) during my secondment.*



Federico Ferrari (ESR10, University of Groningen, The Netherlands): *My PhD project combines numerical simulations and experimental work. In particular, I am focusing on understanding how the electronic structure affects the thermoelectric properties in n-type organic semiconductors. So far, I have been studying the effect of different regiochemistry of fullerene derivatives on their performance (work in preparation). In addition, I am exploring how the geometry of a thermoelectric generator influences its performance through multiphysics simulations. This last work is being carried out in collaboration with Irene Brunetti (ESR13).*

Diego Ropero Hinojosa (ESR11, TU Chemnitz, Germany): *I work on developing new n-type polymers based on benzodifuranone motifs for thermoelectric applications. My project aims to explore the tunability of these structures employing side chain modification, backbone modification, and exploration of different alternating co-monomers to achieve higher performances and lower LUMO levels to achieve higher stabilities and more ordered morphologies. So far, I have developed novel Single-Oxygen side chains that solubilize highly planar structures using simple synthetic procedures (in preparation). In collaboration with Nathan James Pataki (ESR3), I am exploring these new polymers' doping and thermoelectrical properties. With Joost Kimpel (ESR5), I am working towards developing a model to quantify the complexity, scalability, and performance of the different materials already published throughout the literature.*

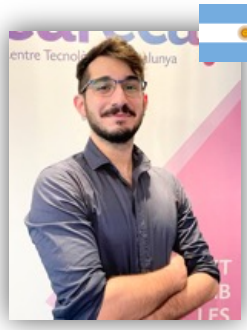


Shubhradip Guchait (ESR12, Institute Charles Sadron-CNRS, France): *I am working on developing organic semiconductor thin films for thermoelectric applications, based on inducing alignment, and structural control on p and n-type doped polymers. My project aims to enhance thermoelectric efficiency to establish correlations between structure and thermoelectric properties in anisotropic thin films by understanding the dopant intercalation mechanism. So far, I have developed the concept of selective phase doping in semi-crystalline polymers to provide a high power factor (Adv. Funct. Mater. 2022, 2202075). In collaboration with Mariavittoria Craighero (ESR4), I am exploring how the polar side chain influences the thermoelectric parameters. With Aditya Dash (ESR1), I am investigating the stability of doped organic polymers, and with Diego Ropero Hinojosa (ESR11) and Nathan James Pataki (ESR3), I am working towards oriented n-type polymers.*

This project has received funding from the European Union's Horizon 2020 research and programme under the Marie Sklodowska-Curie grant agreement no. 955837

Irene Brunetti (ESR13, InnovationLab GmbH, Germany): *I work on developing TEGs (Thermoelectric generators) based on organic materials. So far, I have developed reliable p-type screen-printed vertical TEGs made of silver and free-additive graphene legs (work in preparation). In collaboration with Federico Ferrari (ESR10), I am simulating the behavior of the TEGs. I am also collaborating with Nathan James Pataki (ESR3) to measure the devices' output power and with Zijn Zeng (ESR14) to measure the thermal conductivity of the materials that make up the TEGs. Furthermore, I am also working with the ink produced by Qifan Li (ESR8).*

Zijin Zeng (ESR14, HotDisk, Sweden): *My project aims to develop novel methods for determining thermal transport properties, such as thermal conductivity and heat capacity in organics. So far, I have proposed a measurement procedure based on the Transient Plane Source (TPS) method for quickly measuring the out-of-plane thermal conductivity of polymer films. I am working to verify the procedure and its corresponding simulation model in COMSOL Multiphysics. The work from my side is to provide another potential characterization method for the thermal-related properties of organic semiconductors.*



Matías Joglar (ESR15, Fundació Eurecat, Argentina): *I aim to develop devices that work powered by OTEGs, as well as circuits to adapt the OTEG energy to nominal voltage levels. So far, I have developed flexible circuits powered by commercial inorganic thermoelectric generators to sense atmospheric pressure, temperature, and humidity and report to a phone through NFC. I am currently working on transferring this circuit to printed electronics and a printed electronics circuit to be placed over wine bottles for quality control.*

To know more about HORATES, follow or contact us at:

https://horates.eu

https://twitter.com/horatesITN

https://horates.eu/blog/

This project has received funding from the European Union's Horizon 2020 research and programme under the Marie Sklodowska-Curie grant agreement no. 955837