



UncorrelaTED

Solid-liquid thermoelectric systems with uncorrelated properties



Deliverable 5.1: Advanced simulator constructed

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Project partners

LOGO	Partner full name	Acronym
 UNIVERSITAT JAUME I	Universitat Jaume I	UJI
 IREC <small>Institut de Recerca en Energia de Catalunya Catalonia Institute for Energy Research</small>	Institut de Recerca en Energia de Catalunya	IREC
 KTH <small>VETENSKAP OCH KONST</small>	Kungliga Tekniska Högskolan	KTH
 WARWICK <small>THE UNIVERSITY OF WARWICK</small>	University of Warwick	UW
 SOLVIONIC	Solvionic	SOLV
 SPECIFIC POLYMERS	Specific Polymers	SP



Deliverable Name: Advanced simulator constructed.

Led by: UW

Partners: UJI, UW

Version	Date	Changes
1.0	30/11/2021	Original version

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1 Introduction

A code has been developed for the electron transport in a complex nanostructured material. Using Monte Carlo electron transport formalism, it solves for the electron conductivity in a two-dimensional porous structure domain.

2 Simulator

Taking few material parameters of interest, it gives the pristine material transport distribution function and the electrical conductivity. From the analytical Boltzmann Transport equation and from our Monte Carlo approach, we obtain a multiplication factor that optimises the further calculation when we introduce porosity in the domain. With this, electronic conductivity can be found for the porous material.

The simulator can be accessed [here](#).

3 References

- Dhritiman Chakraborty, Joshua Brooke, Nicholas C S Hulse, and Neophytos Neophytou, "Thermal rectification optimization in nanoporous Si using Monte Carlo simulations", Journal of Applied Physics 126, 184303 (2019) <https://doi.org/10.1063/1.5119806>
- Chakraborty, Dhritiman and Foster, Samuel and Neophytou, Neophytos, Monte Carlo phonon transport simulations in hierarchically disordered silicon nanostructures, Phys. Rev. B, 98, 11, (2018) 10.1103/PhysRevB.98.115435