Accelerating the Clean Energy *Revolution with* Accelerated Nanomaterial Discovery

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Renewable Energy

https://www.youtube.com/watch?v=6UNB_nEDbGY&ab_channel=sarahkha

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Introduction

Thermoelectric (TE) materials *have attracted great attention in a wide range of applications and* **play a growing role in the clean energy revolution**

wearable devices

solar panels

cooling systems

TE materials

spacecrafts and automotive power generation

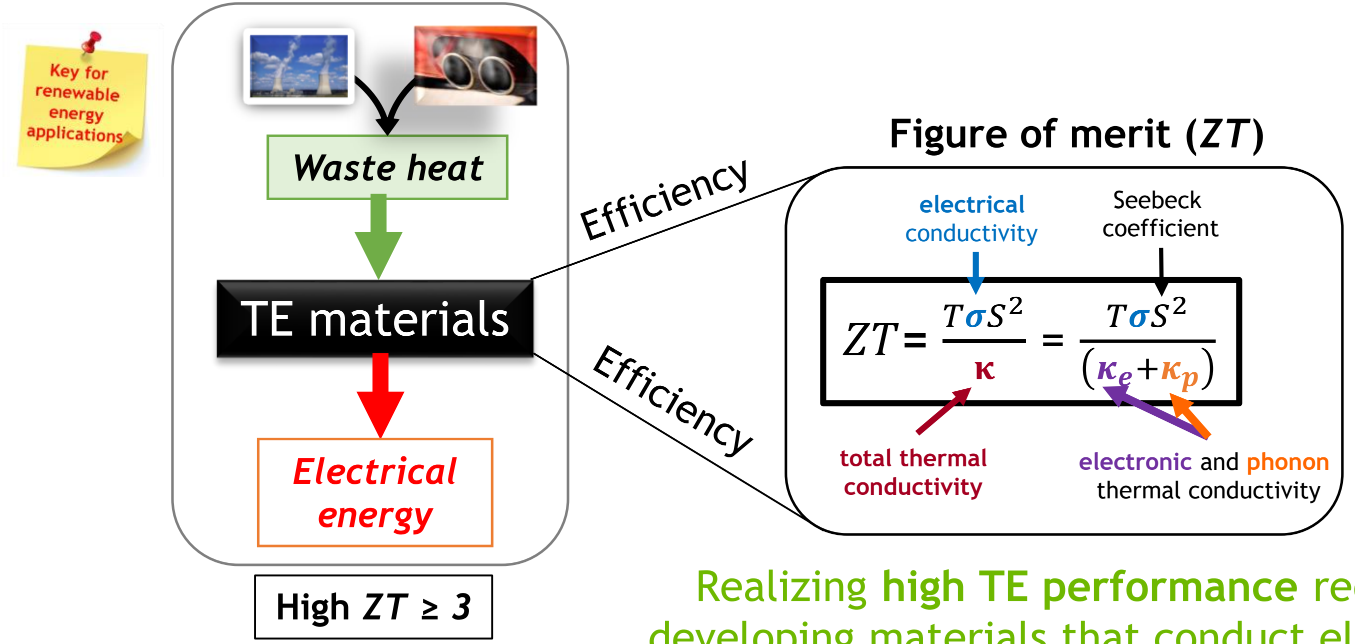
Key for renewable energy applications

Conversion of waste heat

However, the **efficiency** of thermoelectric devices is **yet to be sufficient** for a widespread use

Introduction (slide 2)

TE materials convert waste heat directly into electricity
without greenhouse gas emissions



Realizing **high TE performance** requires developing materials that conduct electricity but block heat from phonons (high *ZT*)

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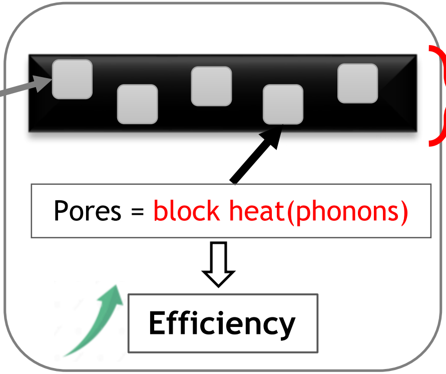
Objective

Nanoporous materials are of great interest for thermoelectric applications because they can conduct electricity easily, but block heat conduction

Nanoporous materials

Pore arrangement affects the efficiency of TE nanomaterials



?

Pores randomly oriented?
Aligned pores?
Optimum pore distribution?

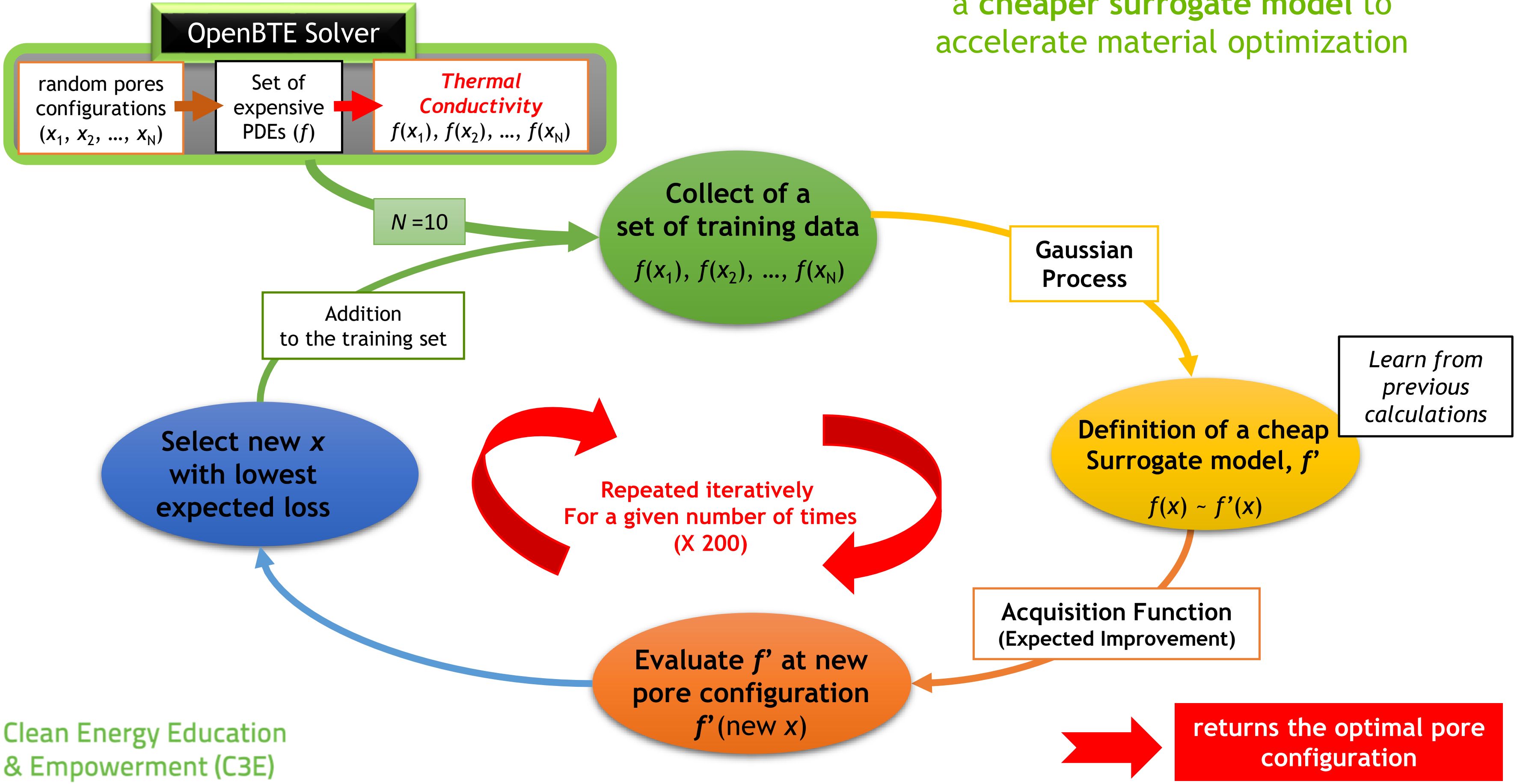
This work aims to optimize a 2D Si nanomaterial to achieve ***low thermal conductivity***.

To accelerate the discovery of novel pore patterns by combining machine learning with heat transport calculations

Nanomaterial optimization is a very challenging task. Identifying suitable pore patterns for every new material is extremely difficult to achieve

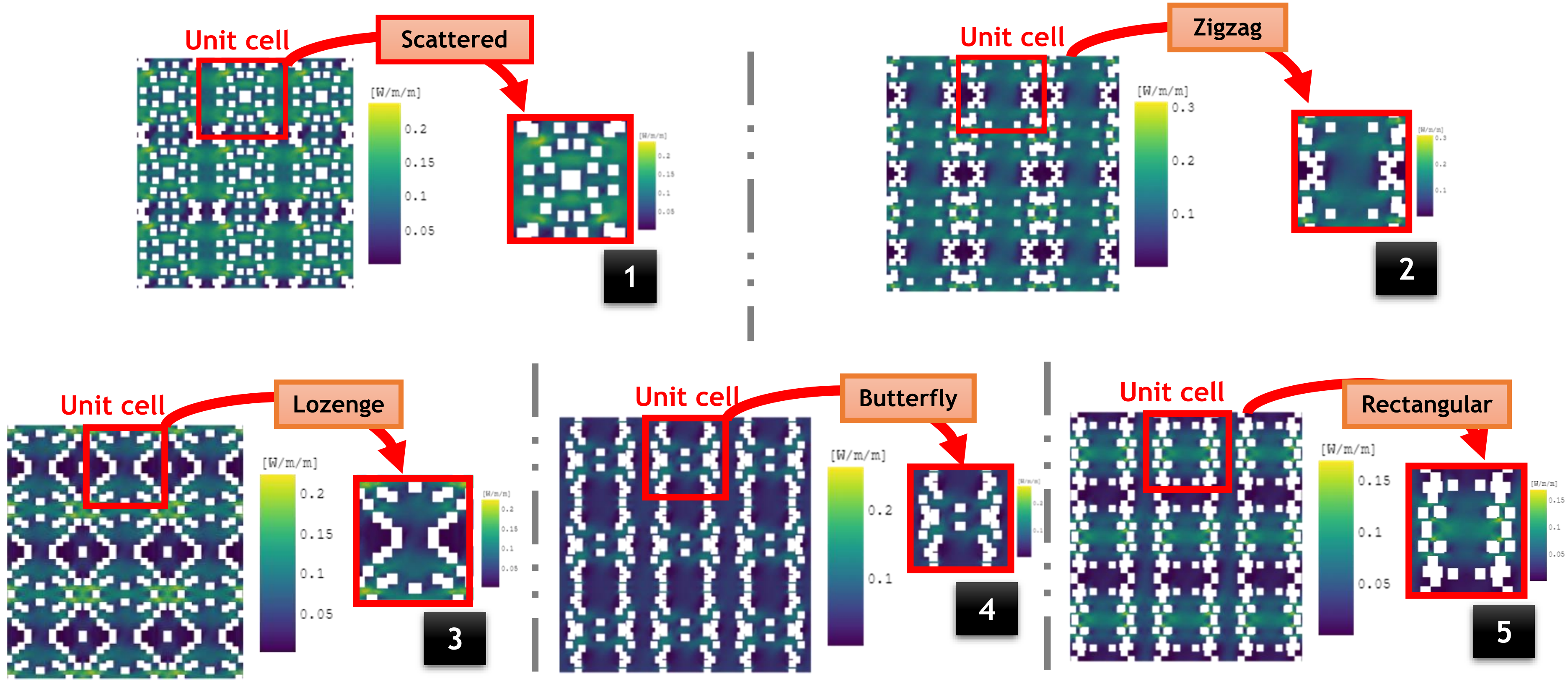
Methods

This methodology is powerful to build a **cheaper surrogate model** to accelerate material optimization



Results

5 novel pore patterns are presented in this work



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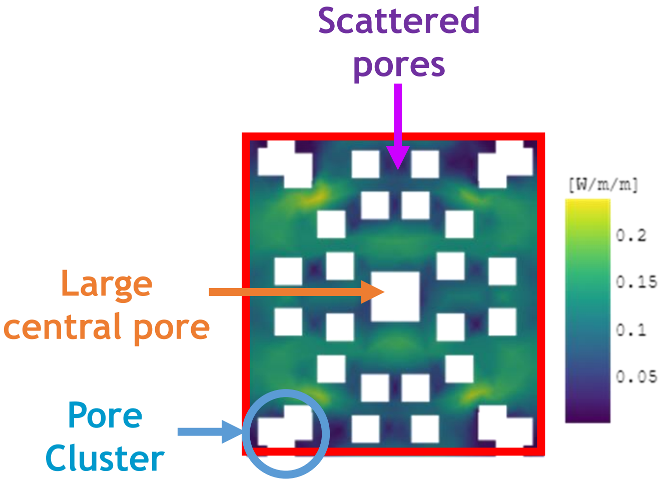
Results (slide 2)

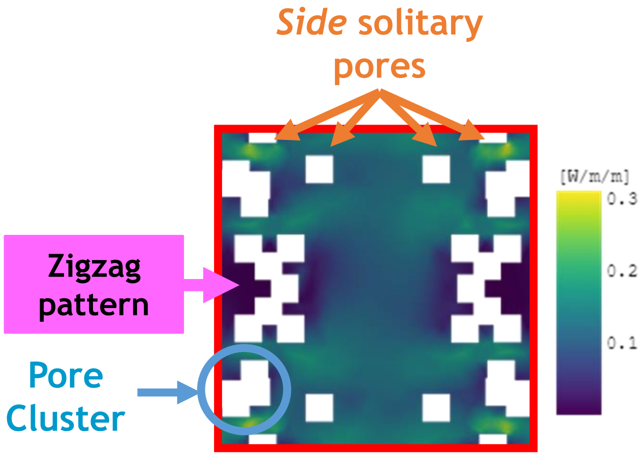
The "scattered" and "zigzag" patterns decrease the thermal conductivity (κeff) **below 10 W/m/K**

1 The Scattered pattern



κeff = 8.9 W/m/K

2 The Zigzag pattern



κeff = 6.1 W/m/K

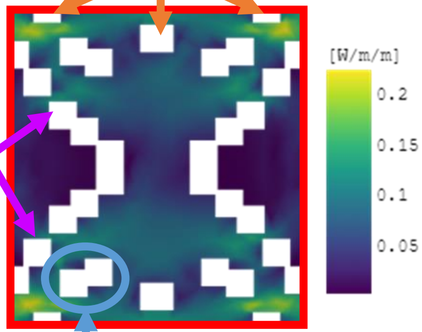
Results (slide 3)

The "lozenge", "butterfly" and "rectangular" patterns decrease the thermal conductivity (κeff) below 5 W/m/K

3 The Lozenge pattern

Isolated pores

Pores well packed



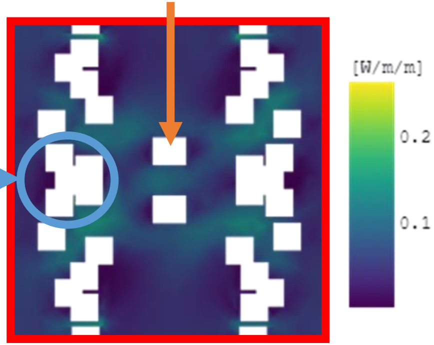
Set of 2 Interconnected pores

κeff = 4.9 W/m/K

4 The butterfly pattern

Central solitary pores

Pore Island

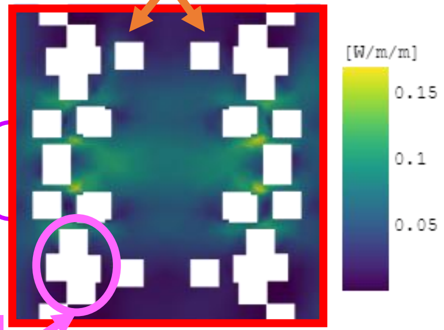


κeff = 4.0 W/m/K

5 The rectangular pattern

Aligned solitary pores

Contactless pores



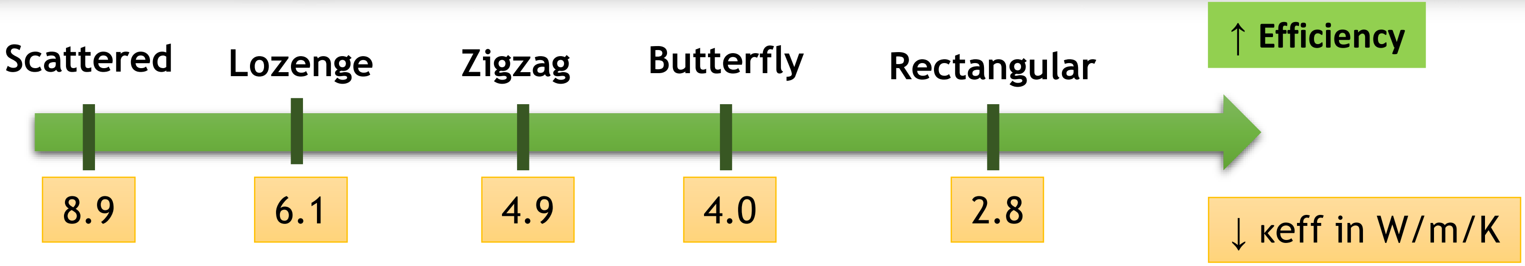
cross shape

κeff = 2.8 W/m/K

Conclusions

Nanomaterial optimization is a **very challenging task.** Combining thermal transport calculations with machine learning accelerate the discovery of new pore distribution.

Many **novel pore patterns** were identified in this work. We presented 5 of them. Pores can be found in clusters, very close to each others. Other pores are not connected to each others → *publication in preparation*



Nanomaterial discovery represents a key strategy in fighting climate change

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