

Nanocomposite Thermoelectric Design

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Quantum Systems & Nanomaterials

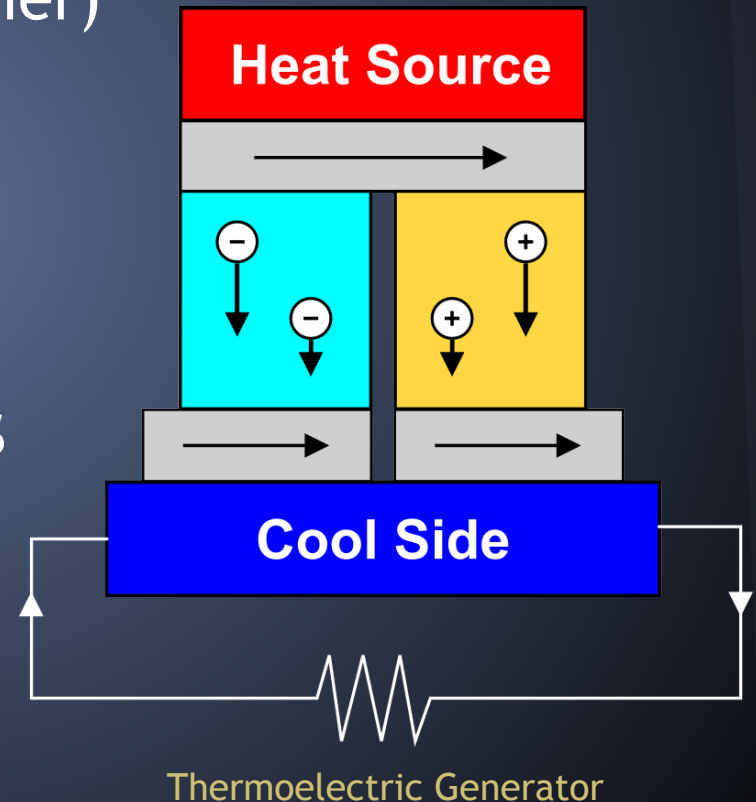


Presentation Overview

- What is a Thermoelectric?
- What is a Nanocomposite?
- History of Thermoelectrics
- Applications & The Future
- Thermoelectric Theory
- Assumptions & Core Theory
- Project Aims

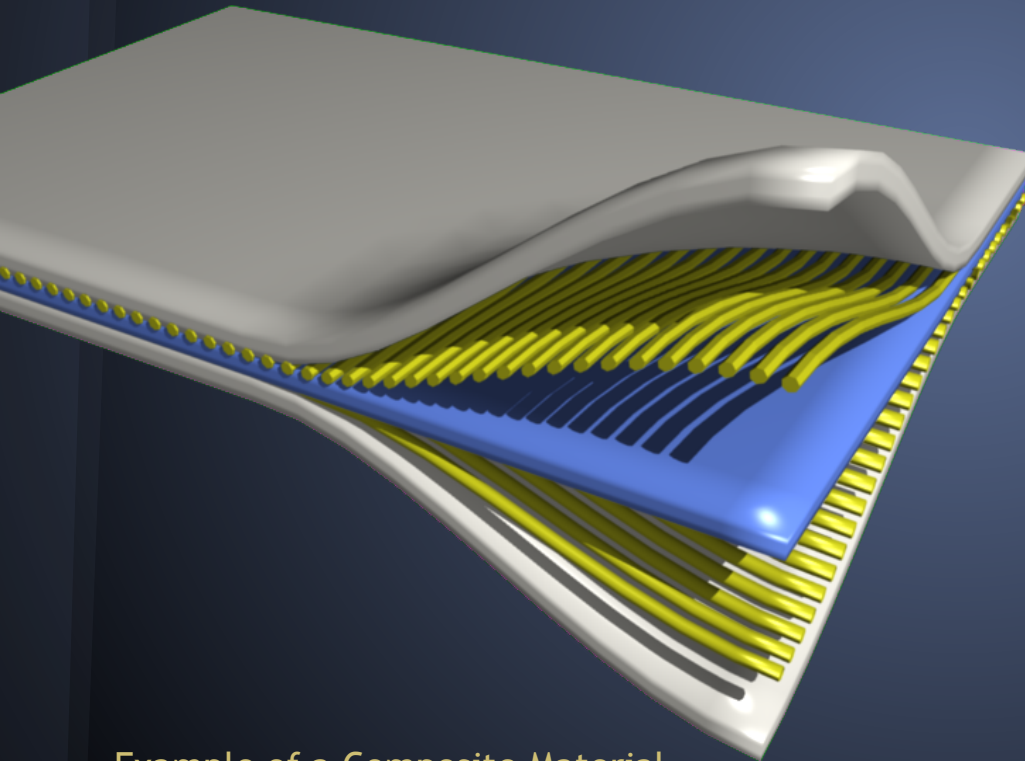
What is a Thermoelectric?

- Heat → Electricity (Seebeck effect)
 - Electricity → Cooling (Peltier)
- Carnot engine limits
 - Charge carriers like steam
- 2 Heat carriers
 - Electrons, phonons
- 5 Transport mechanisms

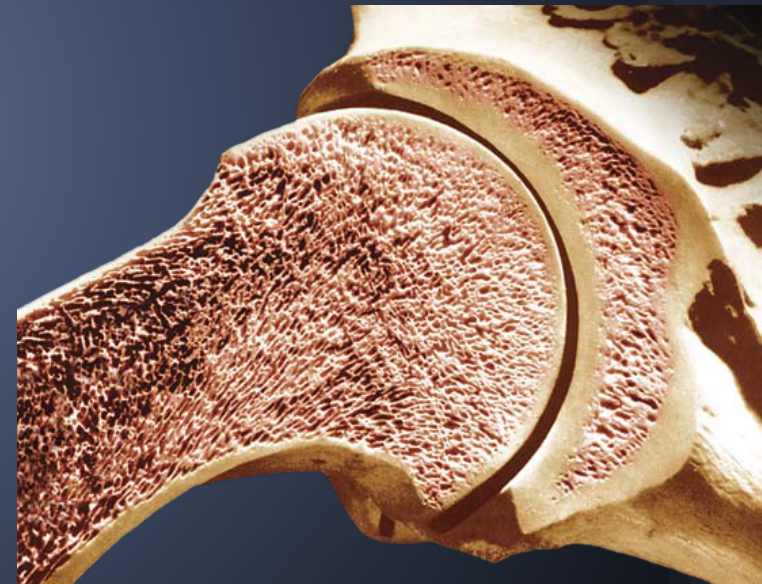


What is a Nanocomposite?

- Identical concept to traditional composites
 - Aeroplanes, cars, bones



Example of a Composite Material



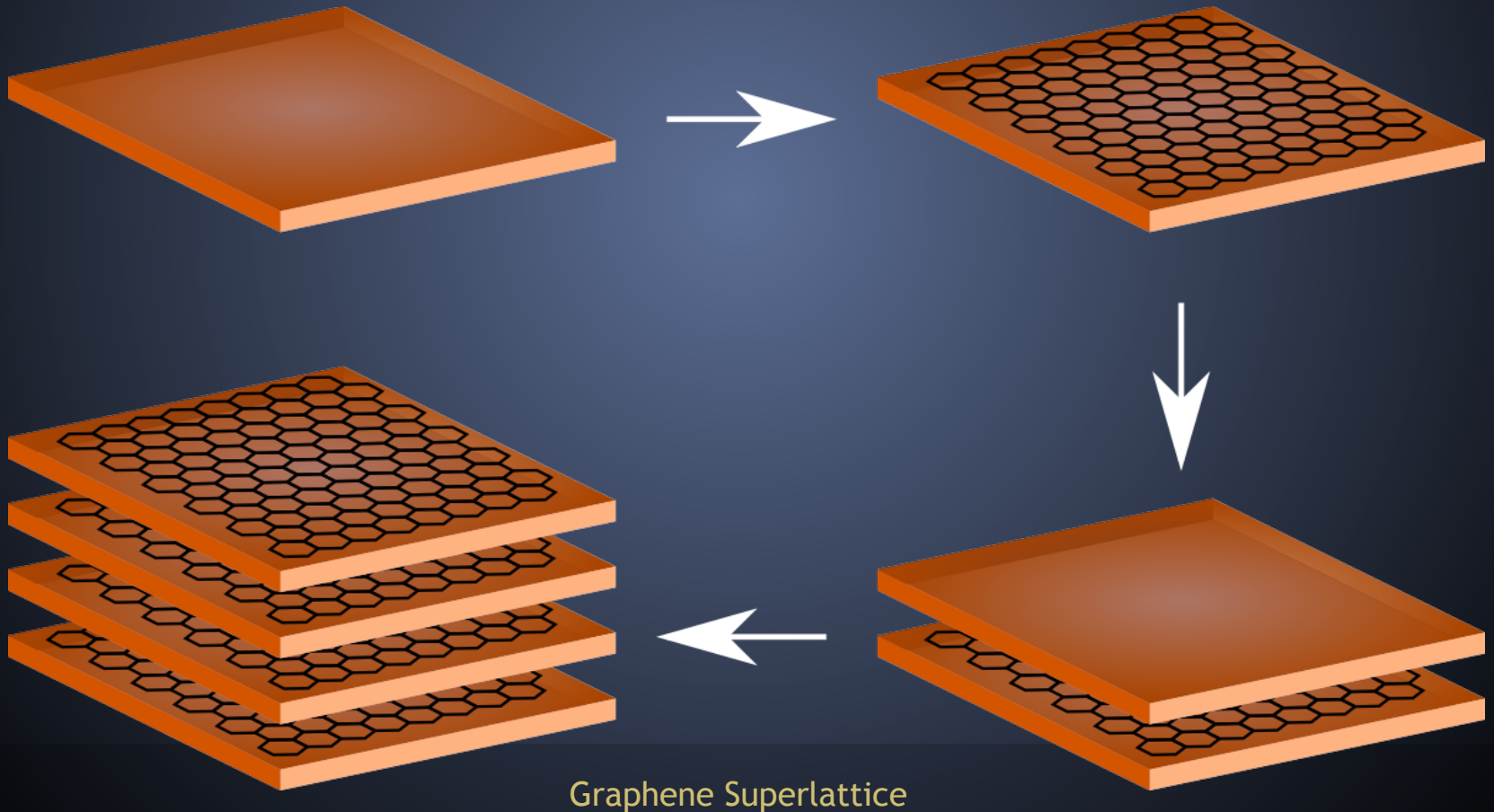
Inside Bone - Biological Composite

Left image credit: wikipedia.org/wiki/File:Composite_3d.png

Right image adapted from: media.web.britannica.com/eb-media/57/94557-004-CF63D396.jpg

Superlattice - 2D Nanocomposite

- Artificial 3D crystal (nano-sandwich)

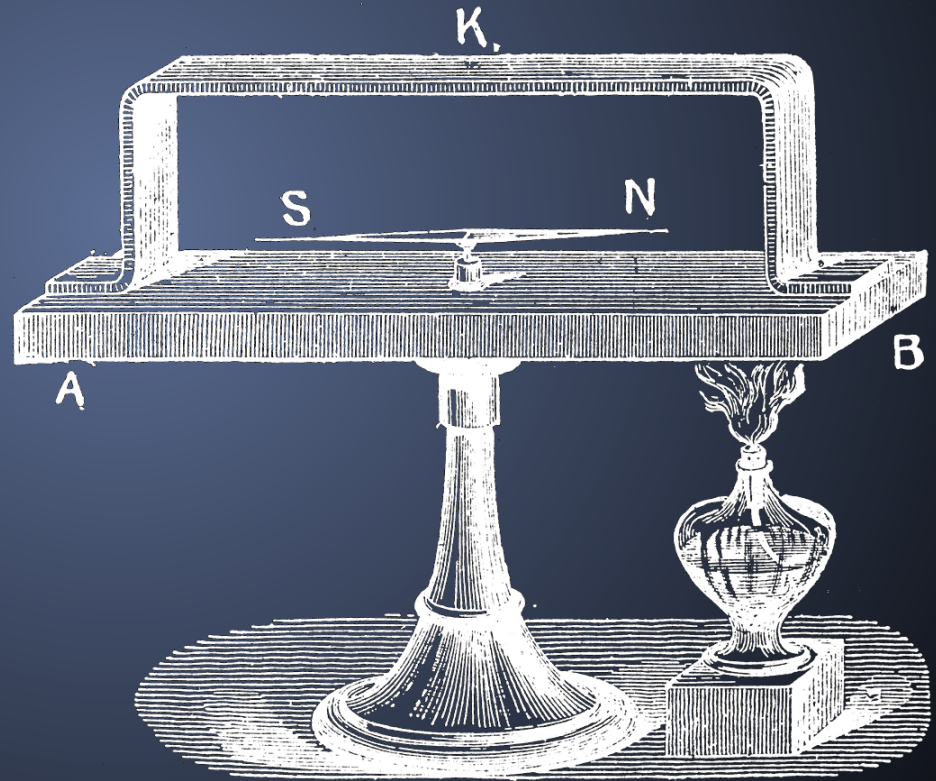


History of Thermoelectrics

- 1821 Seebeck discovers thermoelectricity



Thomas Seebeck



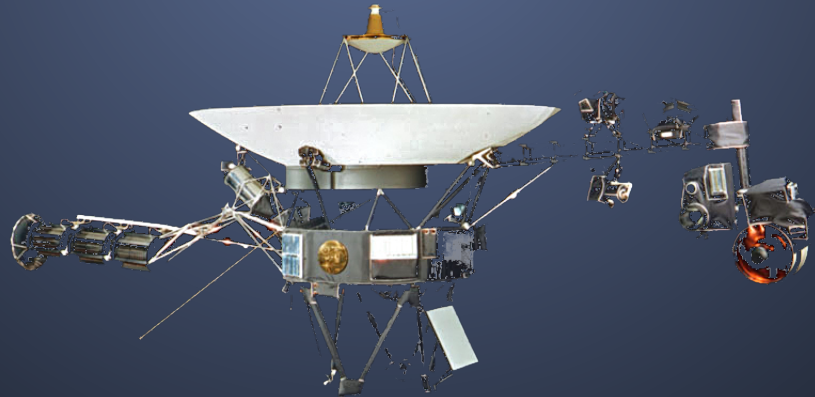
Seebecks Original Experiment

Left image credit: Hans Wahl, Anton Kippenberg: Goethe und seine Welt, Insel-Verlag, Leipzig 1932 S.204

Right image adapted from: etc.usf.edu/clipart/35600/35659/seebeck_35659_lg.gif

History of Thermoelectrics

- 1960's bulk materials - Bi_2Te_3 , PbTe , SiGe
 - Maximum practical efficiency of 4% [1]
 - Use in aerospace - deep space probes
 - Reliable, low weight
- 1990's nanocomposites research
 - Efficiencies of 20-30% possible [2]

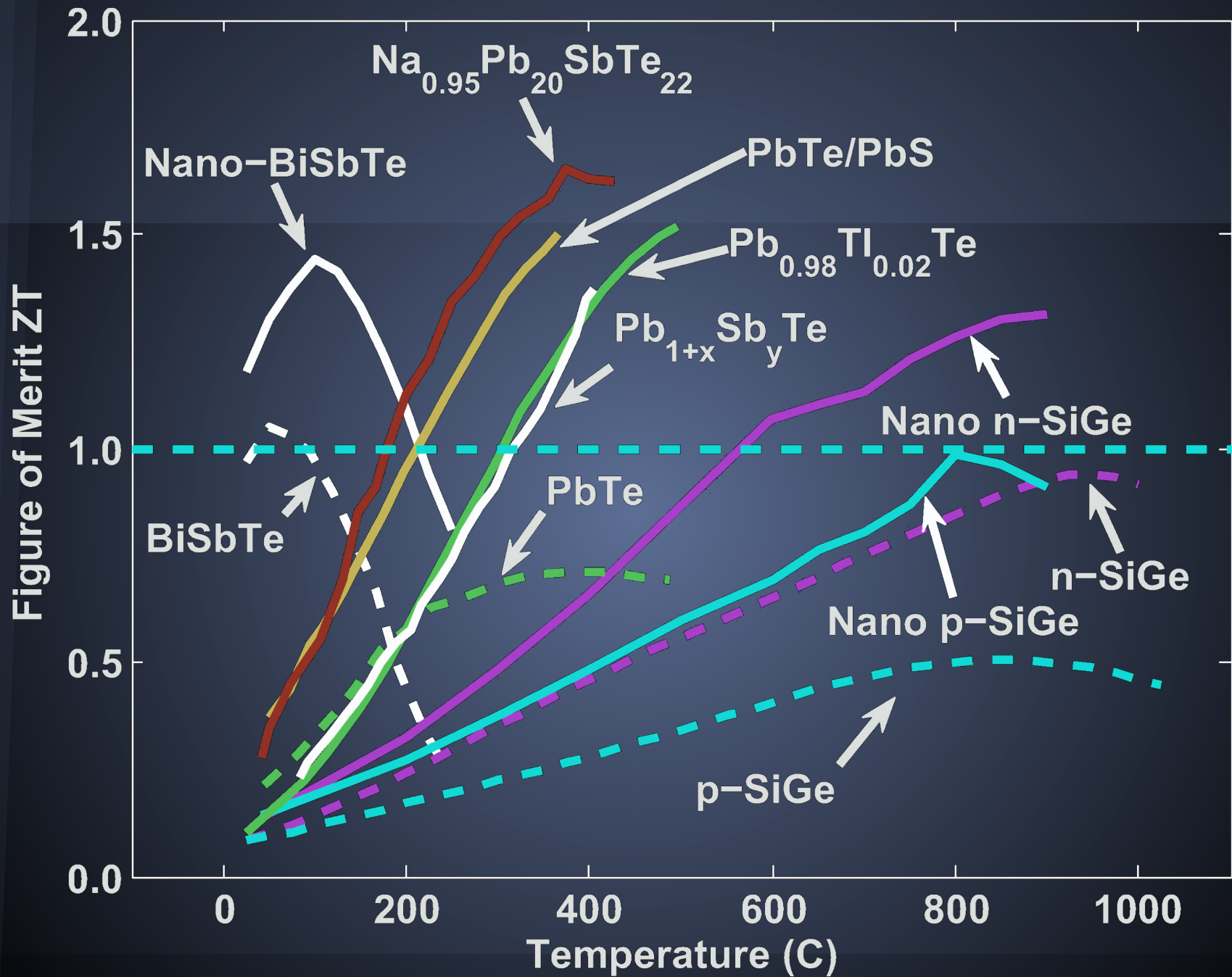


Voyager Space Probe

[1]: Vorobiev et al. Solar Energy 80 (2006) 170–176

[2]: Chen et al. International Materials Reviews 48 (2003) 45-66

Image adapted from: voyager.jpl.nasa.gov/image/images/spacecraft/Voyager.jpg



Graph adapted from: Minnich et al. Energy Environ. Sci. (2009) 466-479

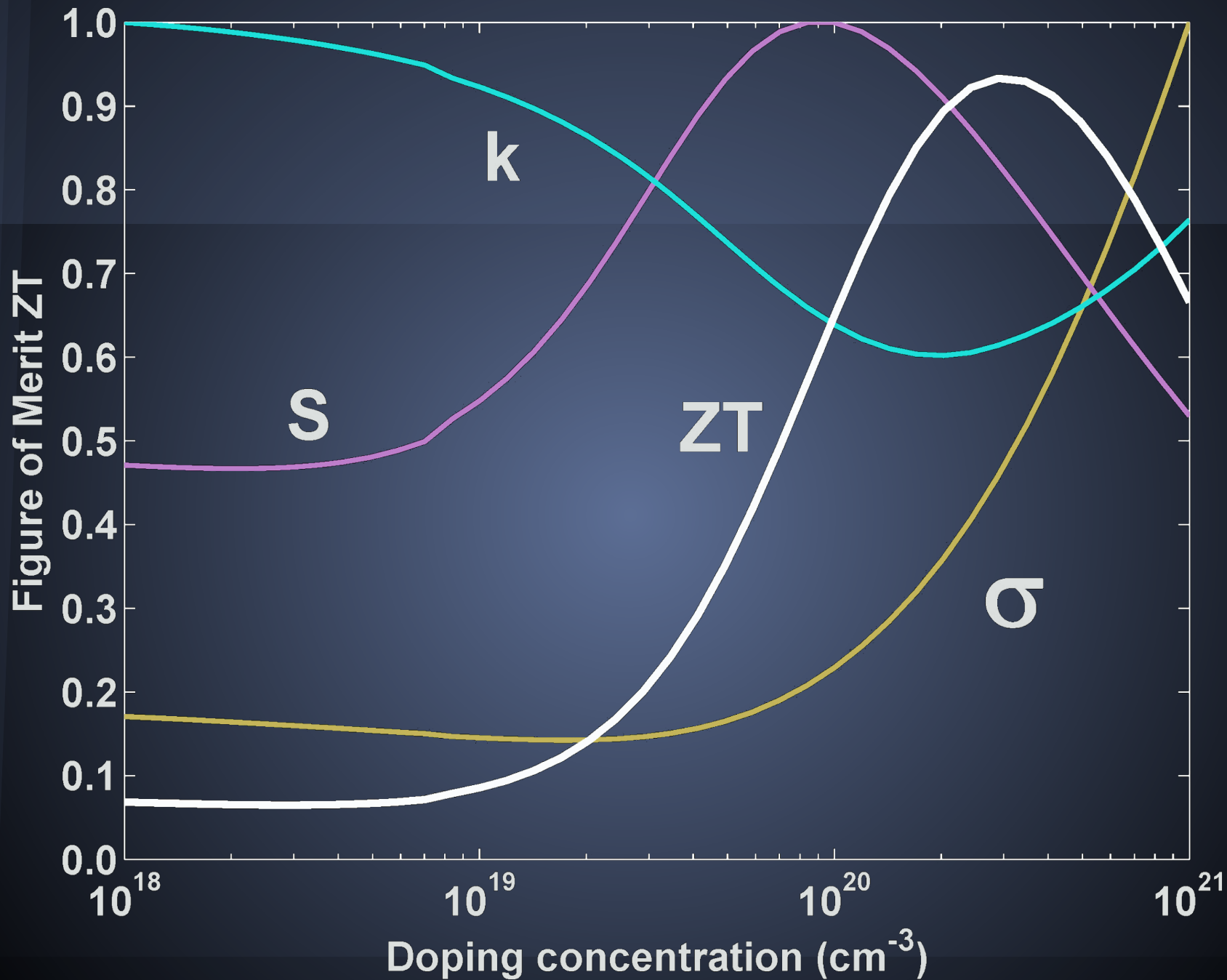
Applications & The Future

- $ZT > 3$ = “we’re in business”
 - Opens up novel applications
 - Heat recovery systems, solar thermal generators
 - Laptops recycling waste heat
- $ZT > 10$ = “we’re getting rich”
 - Thermoelectrics replace steam turbines
 - Greater reliability,
- $ZT \rightarrow \infty$ = “woah lots of power!”
 - Reach carnot limit
 - Thermal gradients exploitable for maximum electric output

Thermoelectric Theory - ZT

$$ZT = \frac{S^2 \sigma \bar{T}}{\kappa_{electron} + \kappa_{phonon}}$$

- $ZT \propto$ Total conversion efficiency
- Relationships between S , σ , $\kappa_{electron}$
 - Necessary compromise between variables
- κ_{phonon} independent
 - Key variable in our project
 - Can be minimised, 3-fold reduction [1]



Graph adapted from: Minnich et al. Energy Environ. Sci. (2009) 466-479

Assumptions & Core Theory

- Kinetic theory of gases
 - Assuming non-interacting, free gas of particles
- Nearly free electron model
 - Electrons perturbed by atomic lattice
 - Electrons and holes are free and non-interacting
- Phonon model
 - Collective excitations of the atomic lattice
 - Phonons are free and non-interacting
- Boltzmann transport equation
 - Describes kinetic change of macroscopic quantity
 - Thermal & electrical gradients

PGEC - Phonon Glass Electron Crystal

- Core concept for our research
 - Proposed thermoelectric method [1]
 - Properties of phonon scattering glasses and electron transmissive crystals
- Small perturbations to lattice?
 - Strong scattering effect on phonons
 - Electrons unaffected
 - Limited effectiveness?
- Multiple boundary defects?
 - Low dimensional systems
 - Many defects, may affect electrons
 - Phonons large range of mean free path

Project Aims

1. Understand phonon thermal conductivity
2. Develop theoretical methods to attain PGEC
3. Propose nanocomposite structures for PGEC
4. Computationally model proposed nanocomposite structures

Core references:

- [1]: D. M. Rowe (1995) CRC Handbook of Thermoelectrics
- [2]: Minnich et al. Energy Environ. Sci. (2009) 466-479