Topological Insulators as Thermoelectrics

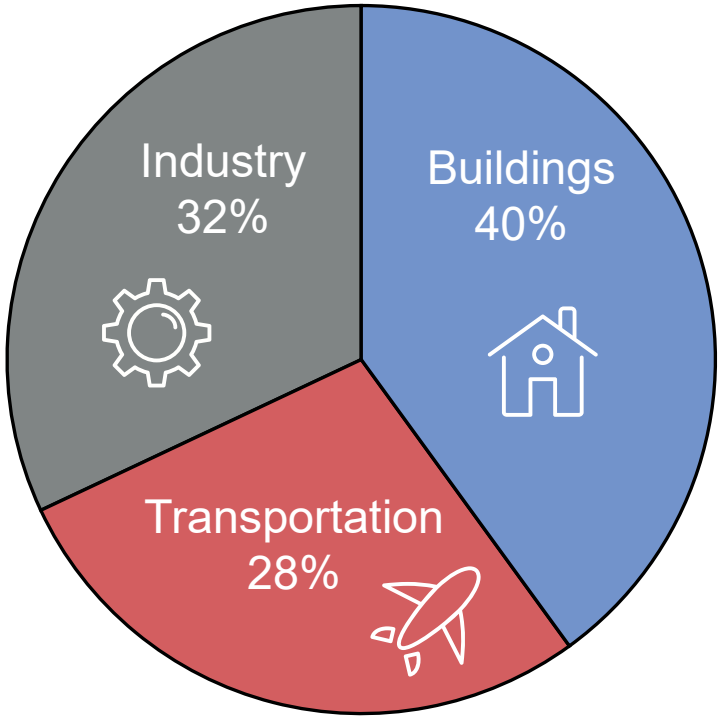
Michael Y. Toriyama, Prashun Gorai, G. Jeffrey Snyder

NORTHWESTERN
UNIVERSITY

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

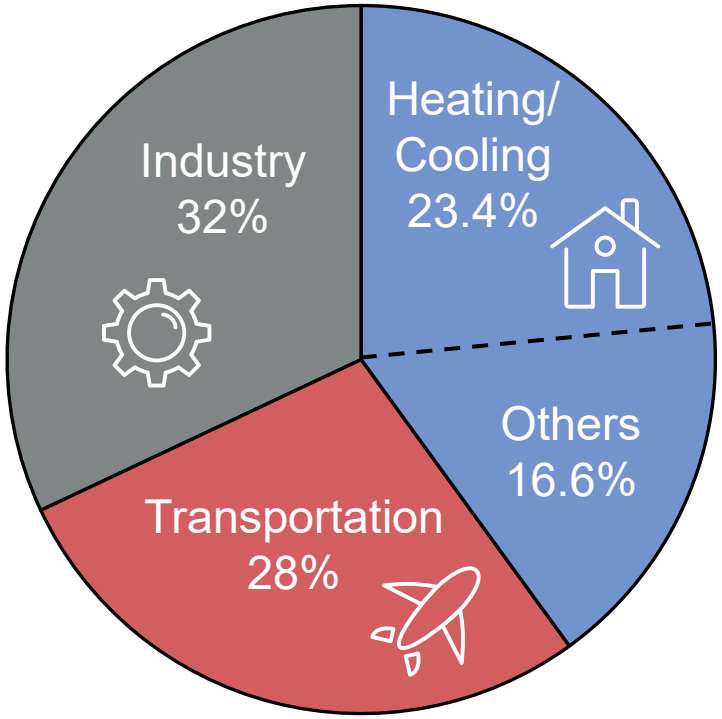
MichaelToriyama2024@u.northwestern.edu

Breakdown of energy consumption in the U.S.



https://needtoknow.nas.edu/energy/energy-use/

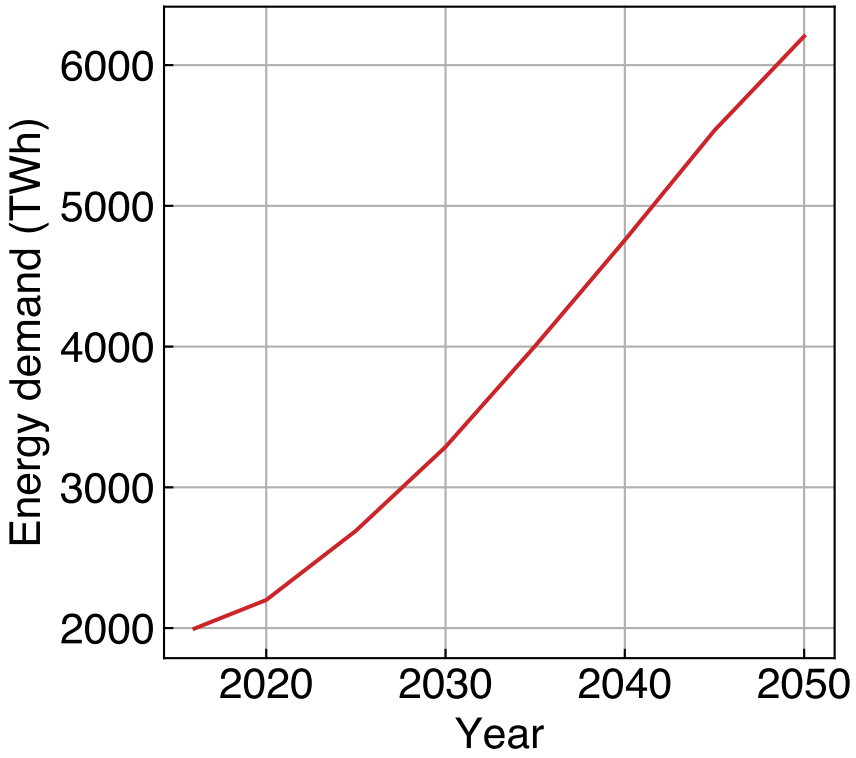
Breakdown of energy consumption in the U.S.

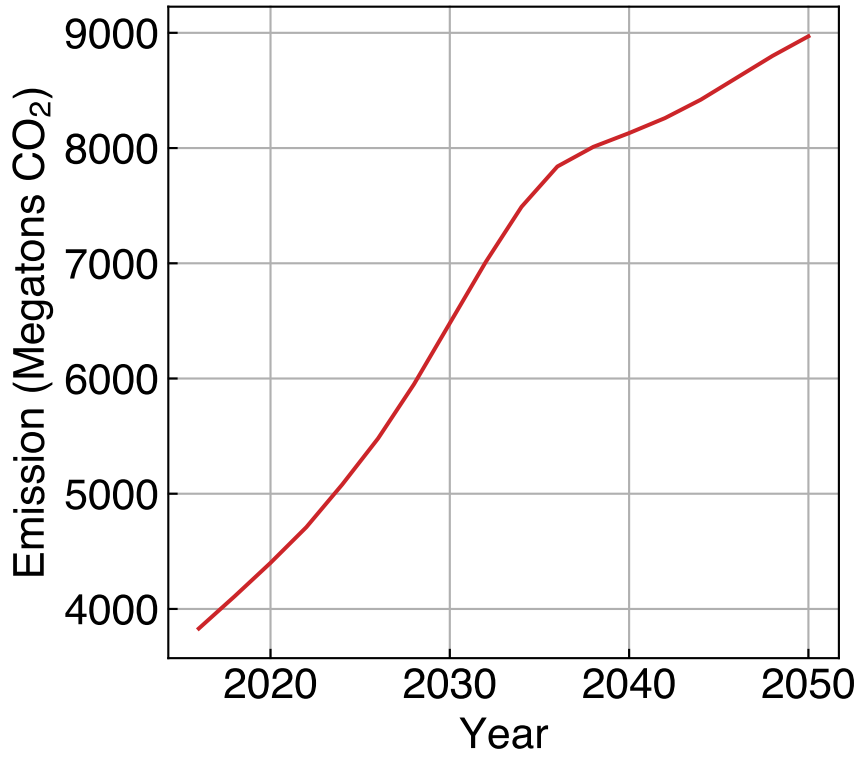


Key takeaway:
Substantial amount of energy is consumed by **heating and cooling**.

https://needtoknow.nas.edu/energy/energy-use/

Thermal management is a critical blind spot

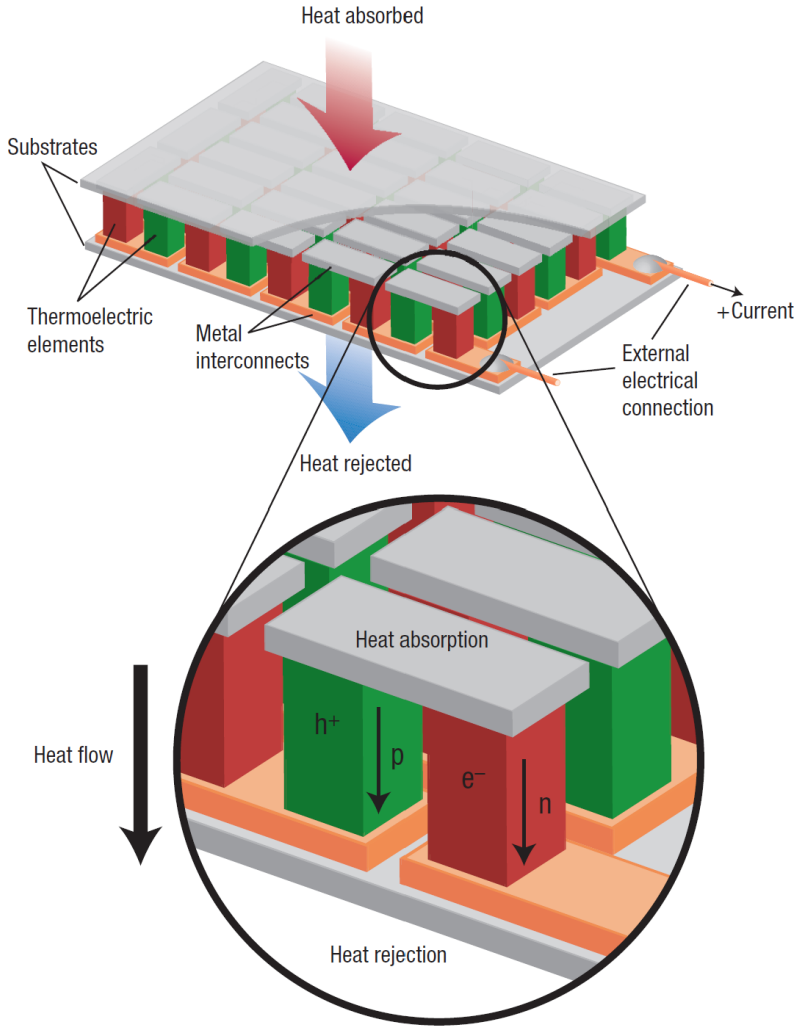


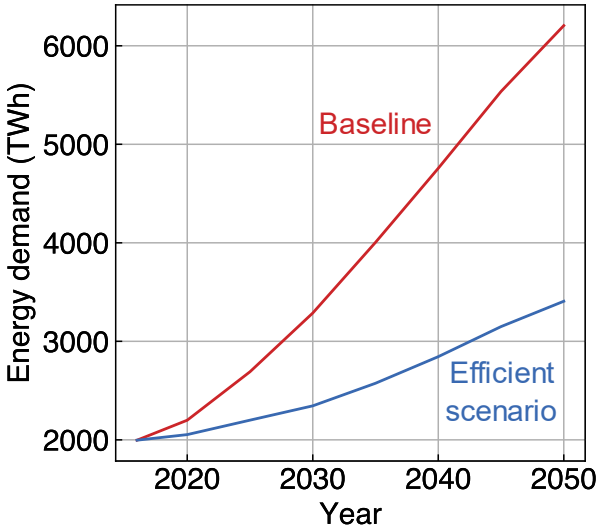


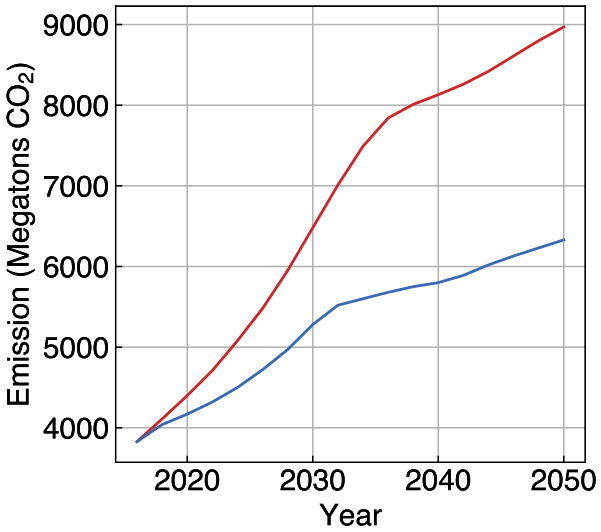
Problems with current cooling technologies:
1. High energy demand
2. Major source of greenhouse gas emissions

https://www.iea.org/reports/the-future-of-cooling
https://www.green-cooling-initiative.org/

Thermoelectrics for efficient thermal management







G. J. Snyder, et al., *Nat. Mater.* **7**, 101 (2008).

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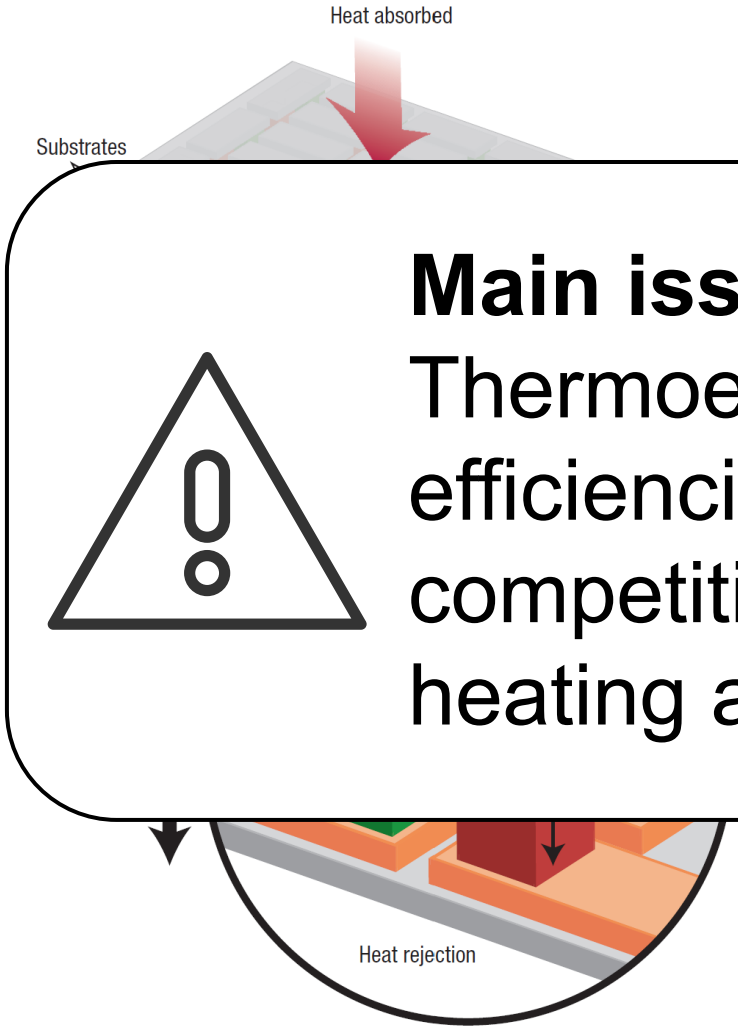
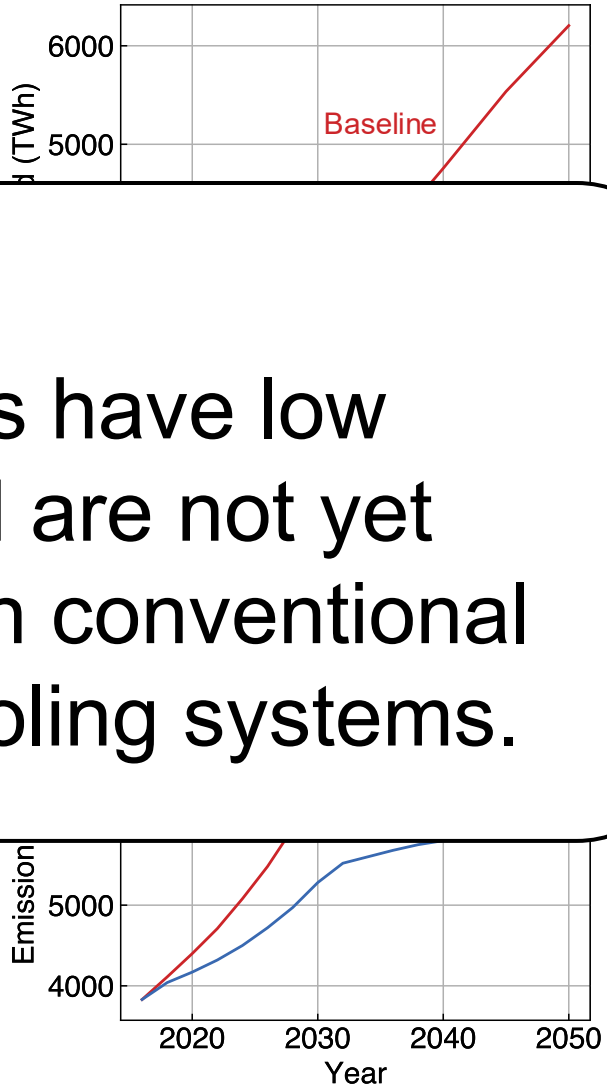
Thermoelectrics for efficient thermal management





Main issue:
Thermoelectrics have low efficiencies and are not yet competitive with conventional heating and cooling systems.

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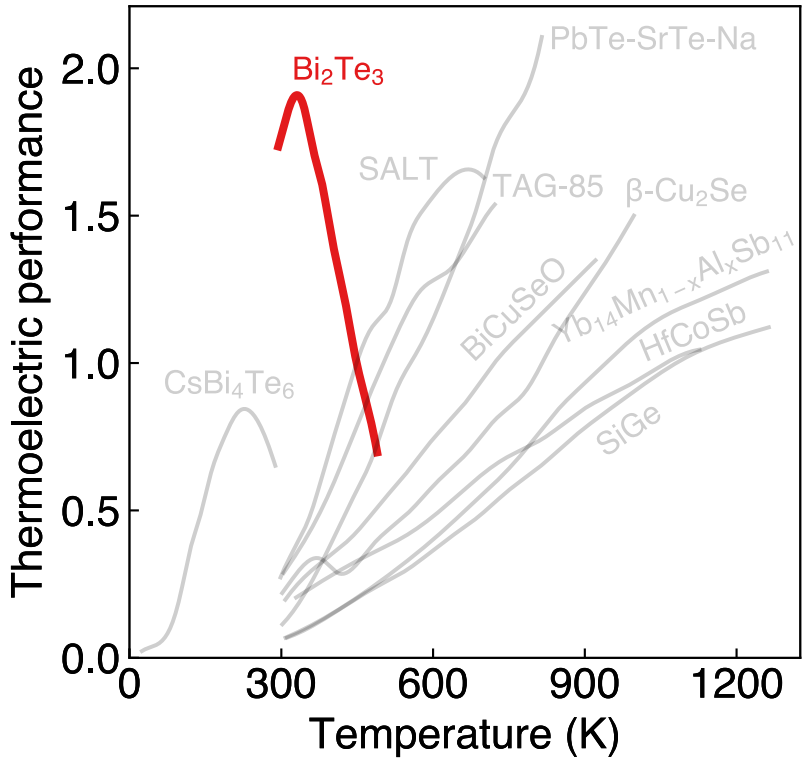
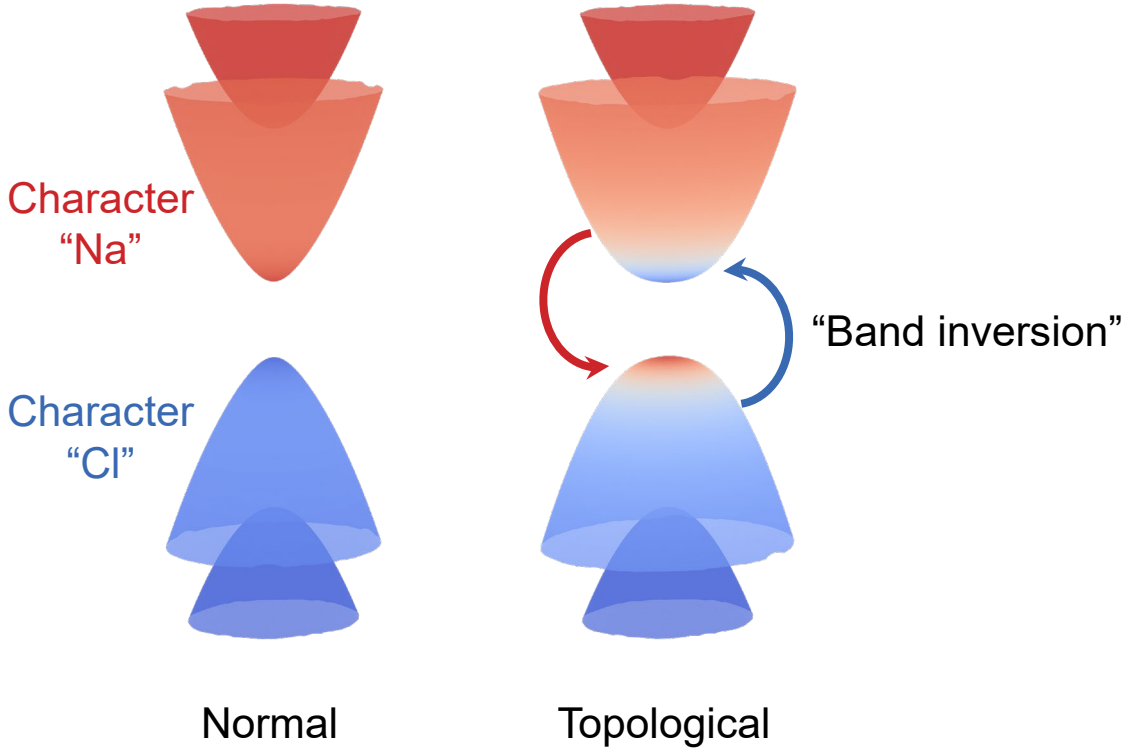
Bi_2Te_3: Good thermoelectric, also a topological insulator





M. Rull, et al., *RSC Adv.* **5**, 41653 (2015).

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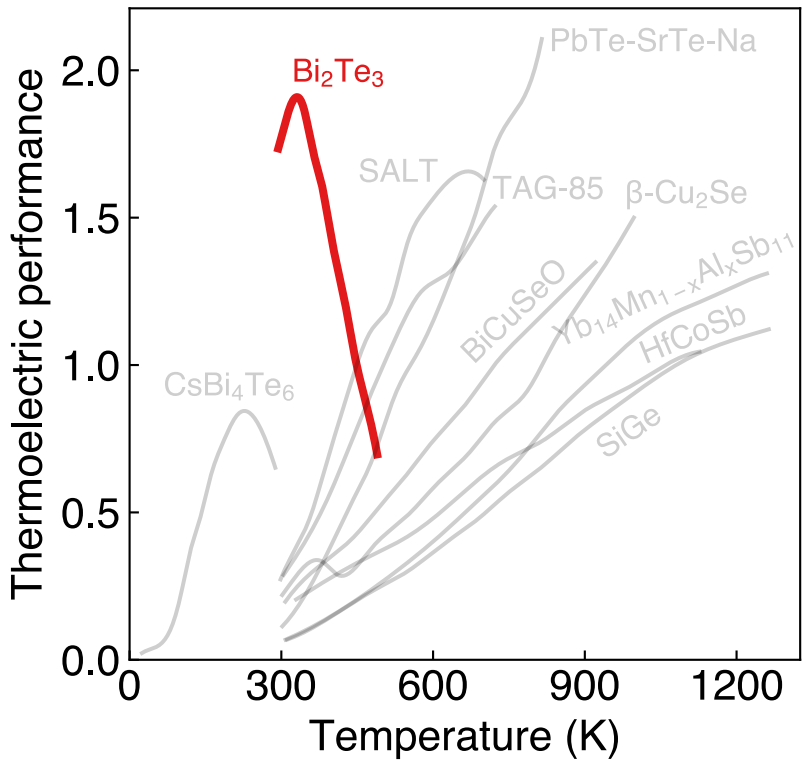
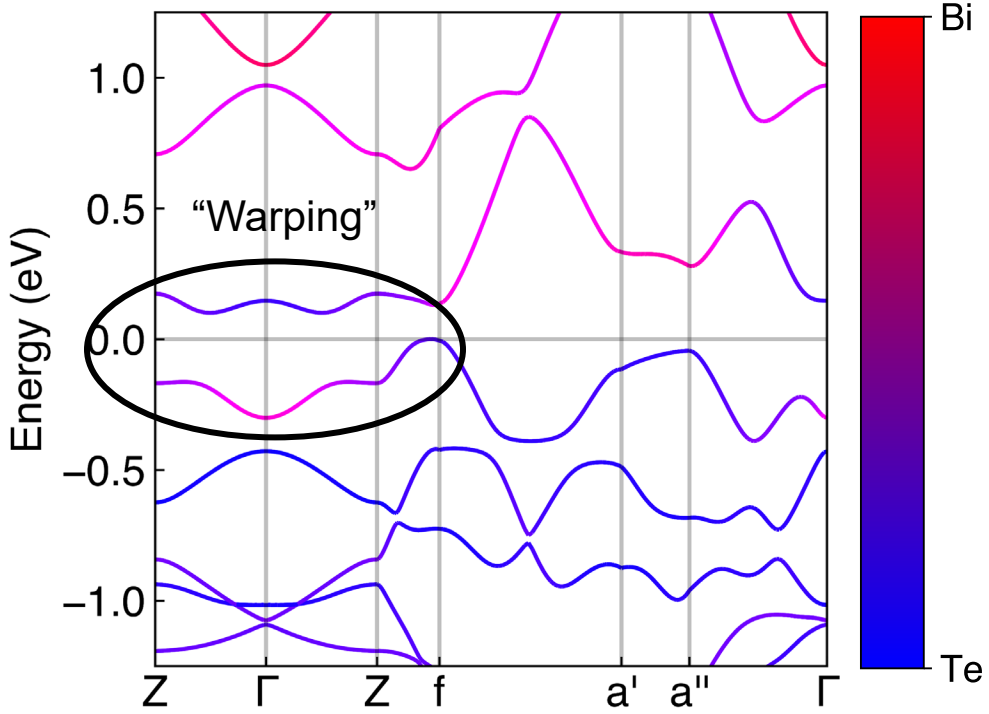
Bi_2Te_3: Good thermoelectric, also a topological insulator





Hypothesis:

Topological insulators, *in general*, are good thermoelectric materials due to band warping effects.

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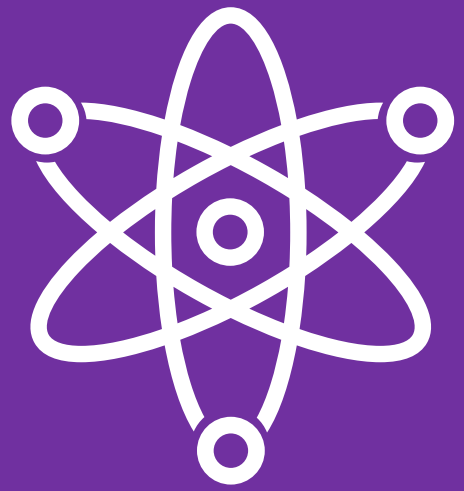
Key scientific questions

Does warping occur due to band inversion in topological insulators and, if so, when?



Are topological insulators linked to high thermoelectric performance?

How can we discover new efficient thermoelectric materials?

MichaelToriyama2024@u.northwestern.edu

Band inversion-driven warping: a theoretical understanding

Assumptions

Crystal Inversion Symmetry: $\mathcal{P} = \mathbb{1} \otimes \tau_z$

Time Reversal Symmetry: $\mathcal{T} = (-i\sigma_y \otimes \mathbb{1})\, K$

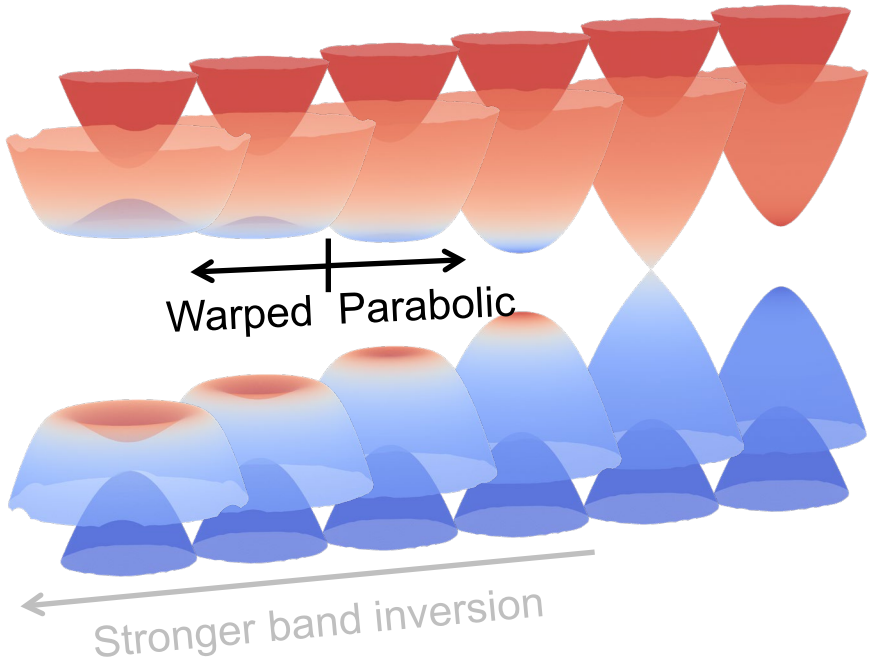
General Hamiltonian

$$H(\mathbf{k}) = \sigma_0 \otimes (A_0(\mathbf{k})\tau_0 + Y_0(\mathbf{k})\tau_y + Z_0(\mathbf{k})\tau_z) + \sum_{i=x,y,z} X_i(\mathbf{k})\sigma_i \otimes \tau_x$$

Warping Criterion

$$2\zeta_2 > \frac{f_2}{|M_0|} + 2\,|\alpha_2|$$

Band inversion strength



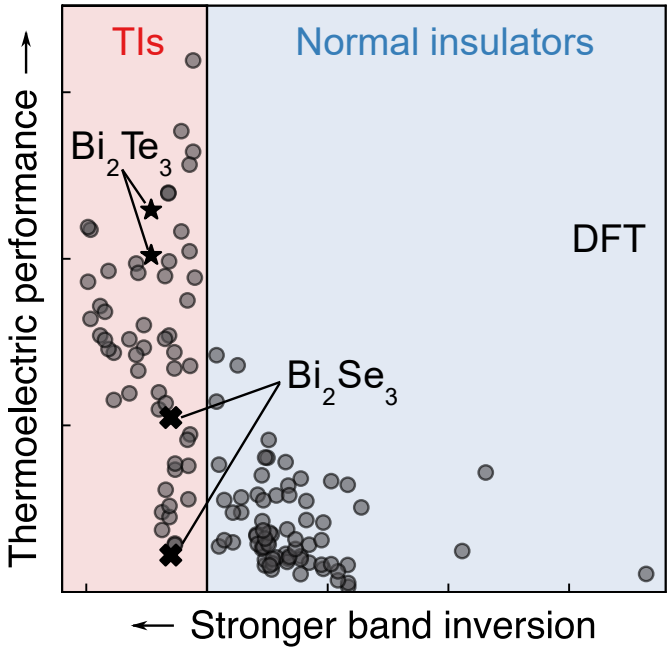
Rules for achieving warped bands:

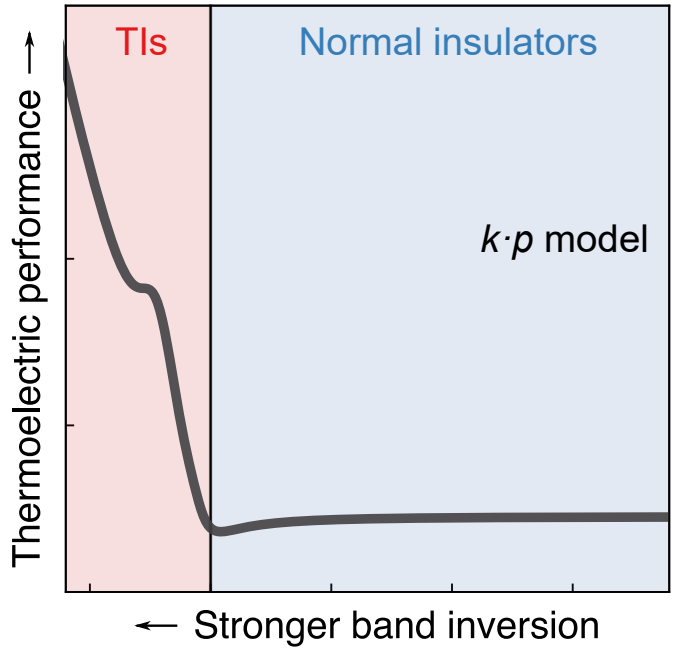
1. The material must be topological.
2. Bands must be sufficiently inverted.

M.Y. Toriyama, et al., *J. Mater. Chem. A,* **10**, 1588 (2022).
M.Y. Toriyama and G.J. Snyder, *Cell Rep. Phys. Sci.*, **4**, 101392 (2023).

MichaelToriyama2024@u.northwestern.edu

High thermoelectric performance driven by band inversion





Key conclusion:

Topological insulators outperform normal insulators as thermoelectrics due to band inversion and, as a result, warping.

M.Y. Toriyama and G.J. Snyder, *In Preparation*.

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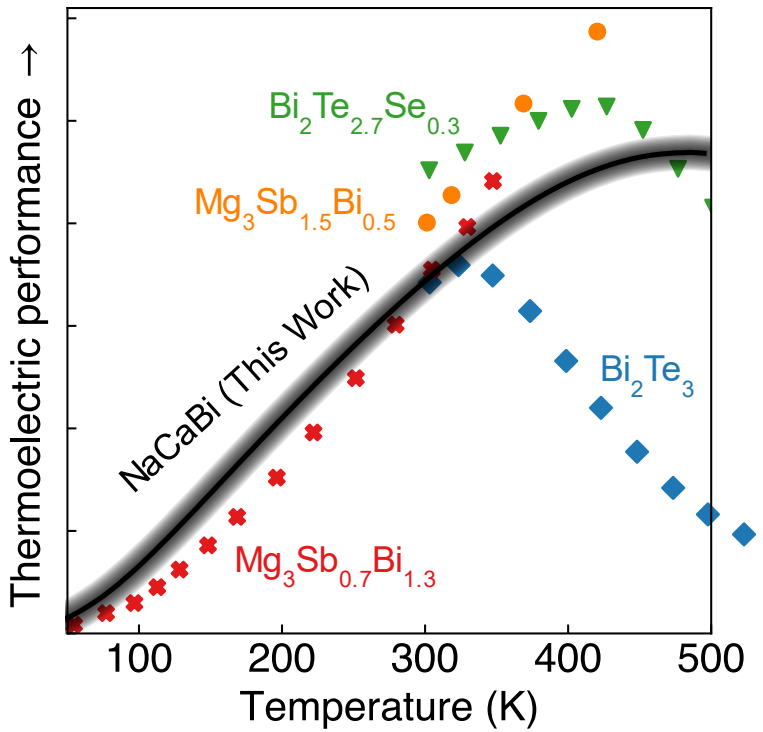
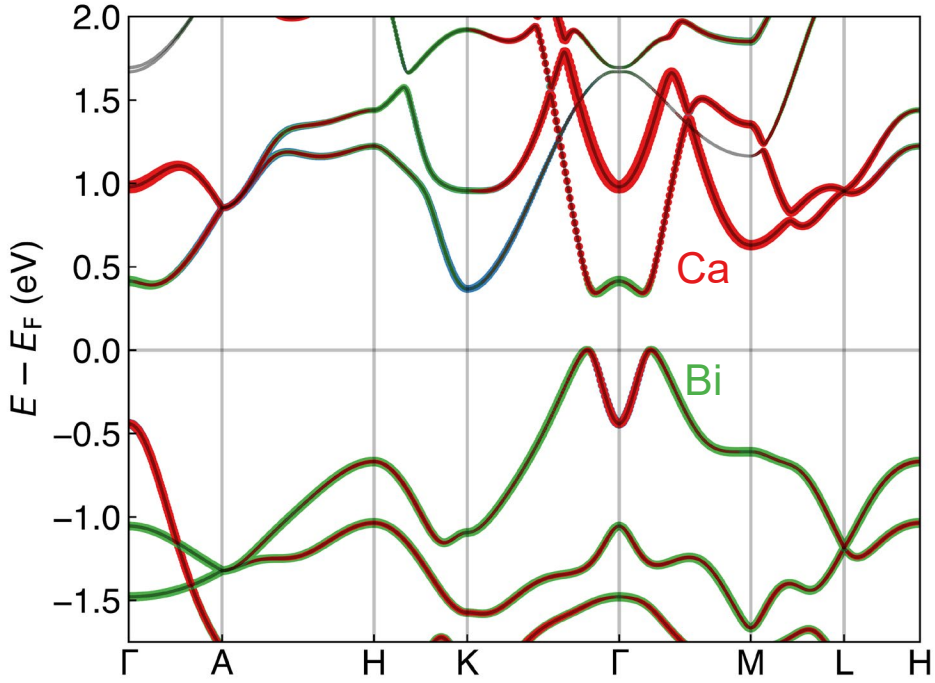
NaCaBi performs well, comparable to state-of-the-art





Conclusion:

NaCaBi is a good thermoelectric near room-temperature.

Key feature:

Band inversion-driven warping in the topological insulator

M.Y. Toriyama, P. Gorai, and G.J. Snyder, *In Preparation*.

Topological insulators: A new horizon for thermoelectrics

Does warping occur due to band inversion in topological insulators and, if so, when?

Are topological insulators linked to high thermoelectric performance?

How can we discover new efficient thermoelectric materials?

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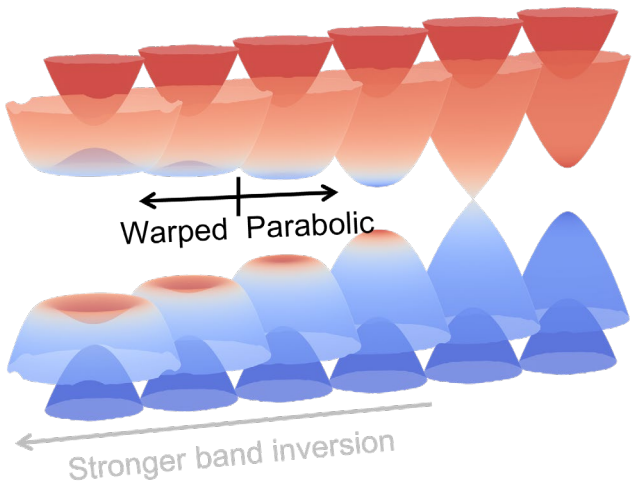
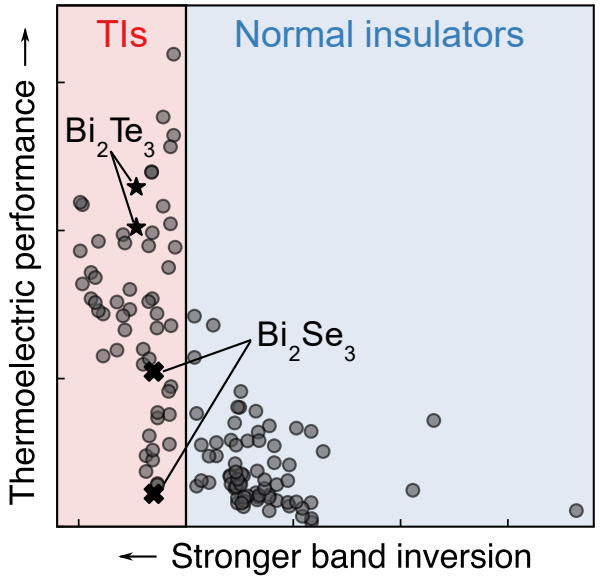
Topological insulators: A new horizon for thermoelectrics

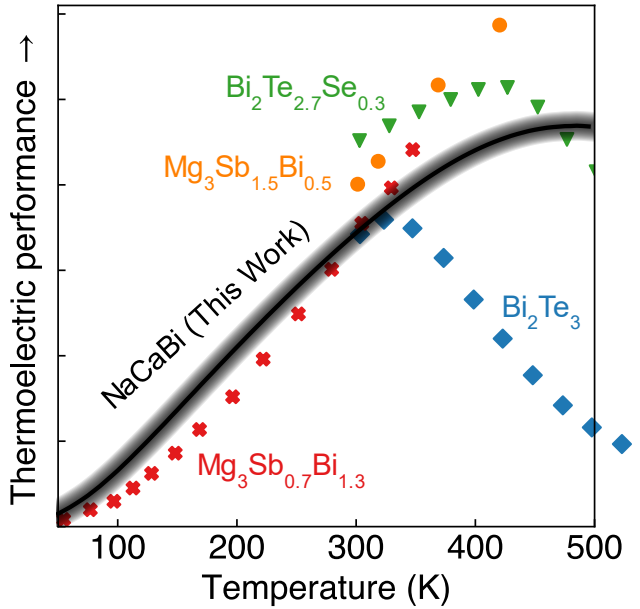
Band inversion strength is a key parameter in accessing warped bands.



Yes, materials with strongly inverted bands exhibit high thermoelectric performance.



Evaluate the band inversion strength to discover new thermoelectics.



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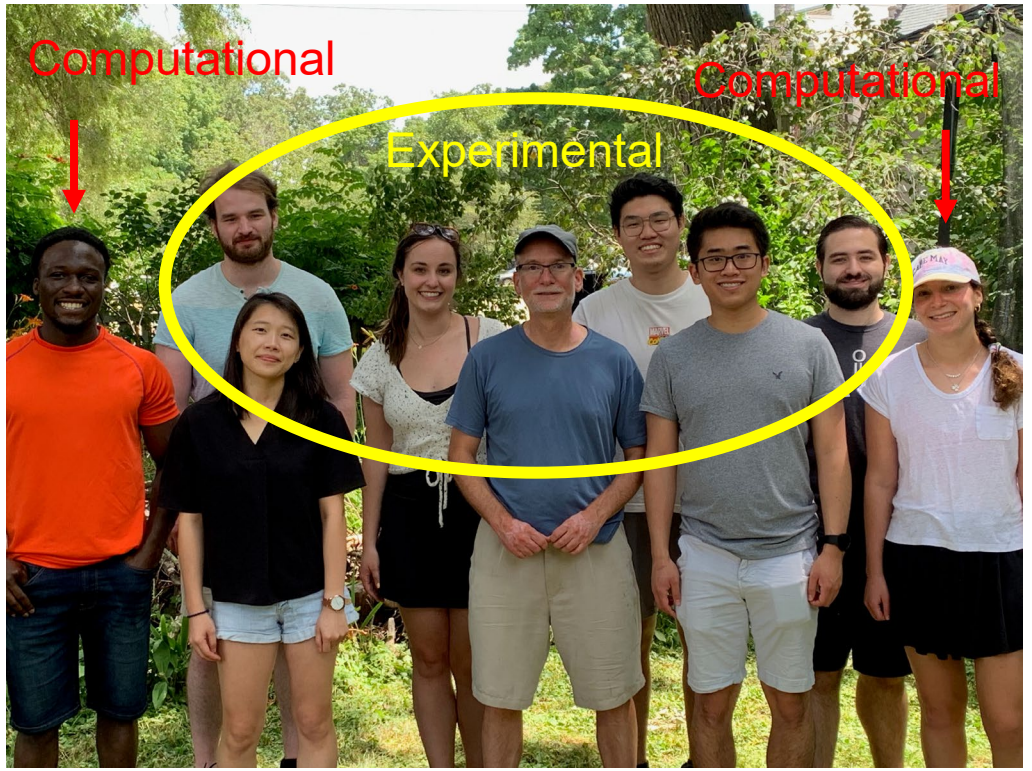
Thank You!

G. Jeffrey Snyder

Prashun Gorai



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