High-Temperature Performance of Ho–Sb–Te Thermoelectrics: Substrate Compatibility and Geometry-Driven Efficiency Optimization

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Abstract

This work integrates numerical simulation with experimental material ranking to assess thermoelectric power generation from 500–1200 K. We analyze how Seebeck coefficient (α), electrical conductivity (σ), and thermal conductivity (κ) govern voltage, power, and efficiency. High-temperature leaders—ScCoSb and SiGe—deliver sustained power at ≥900 K; skutterudites and Zn_2Sb_3 excel in the mid-temperature range; Bi_2Te_3/Bi_2SbTe_3 remain optimal for <500 K applications. The combined framework accelerates screening and de-risks device prototyping for waste-heat recovery, automotive, aerospace, and space systems.

Background

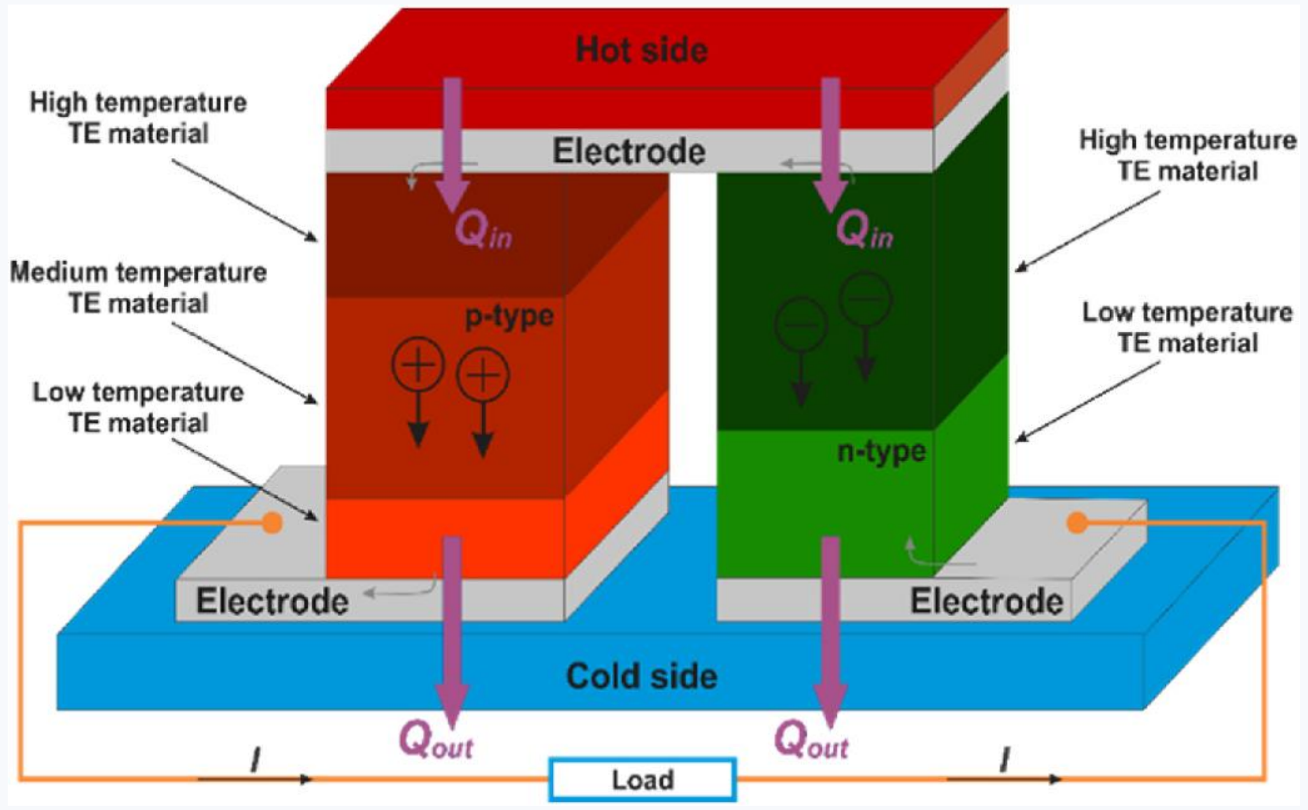
Thermoelectrics (TE) convert heat → electricity with no moving parts. High-T (≥900 K) applications demand materials that maintain high Seebeck (α), adequate electrical conductivity (σ), and low thermal conductivity (κ).We integrate synthesis/characterization with finite-element simulations to rank materials for industrial waste-heat recovery, automotive, and aerospace power systems

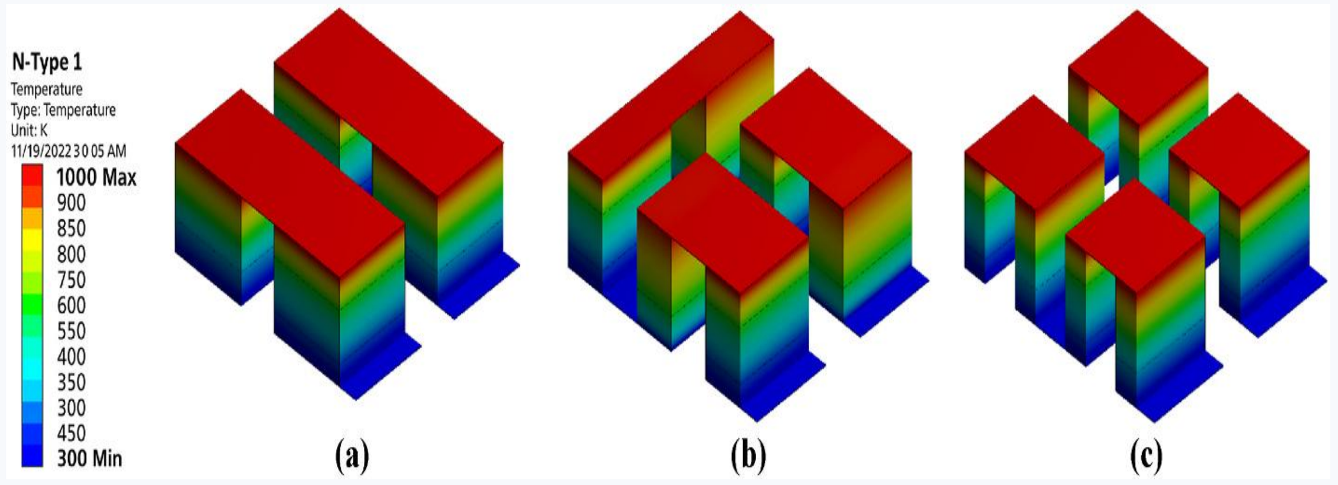
Objectives

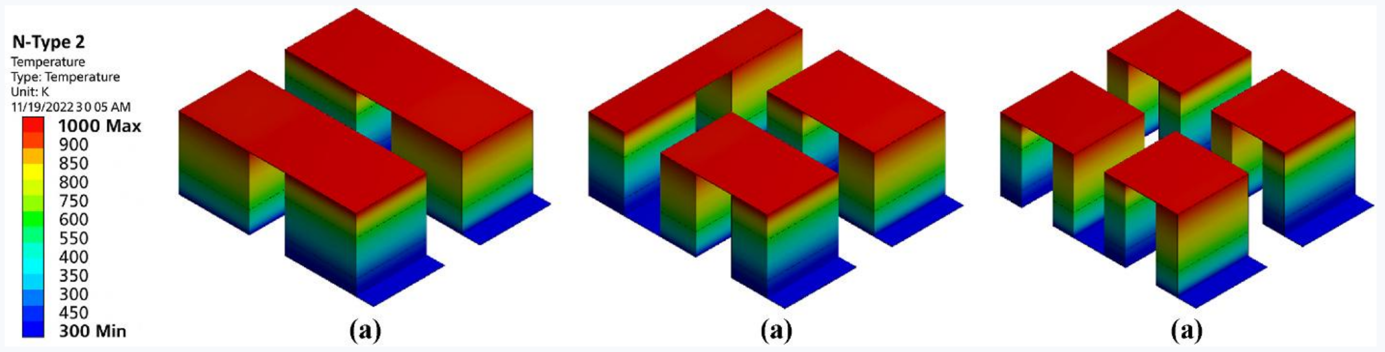
- Quantify voltage, power, and efficiency vs. T (500–1200 K)
  - Benchmark ScCoSb, SiGe, skutterudites, Zn_2Sb_3, Bi_2Te_3, Bi_2SbTe_3, $Mo_3Sb_4Te_{1.6}$
  - Map application windows: <500 K, 500–900 K, ≥1000 K
- Synthesize HoSbxTex and deposit onto TE substrates

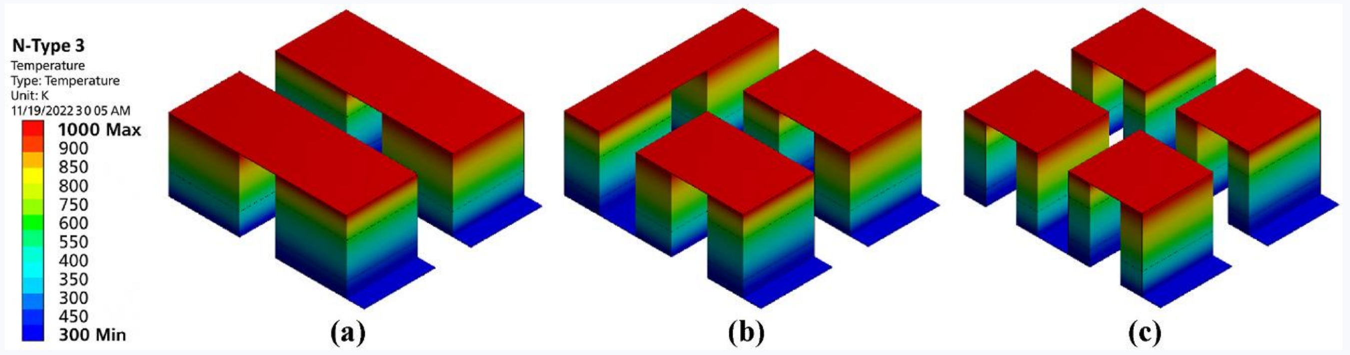
Method

- Experiments: transport (α, σ, κ) and ZT calculations; thin-film compatibility tests.
  - FEM (ANSYS): coupled thermal–electric model with realistic leg geometry and convective boundaries.
  - Metrics: V = ∫α(T)dT; P = V²/(R_int+R_load); η = P/Q̇_h.
  - Ranking: max power/efficiency, stability under ΔT>900 K, integration readiness.









Governing Equations

$$ZT = \frac{\alpha^2 \sigma T}{\kappa}$$

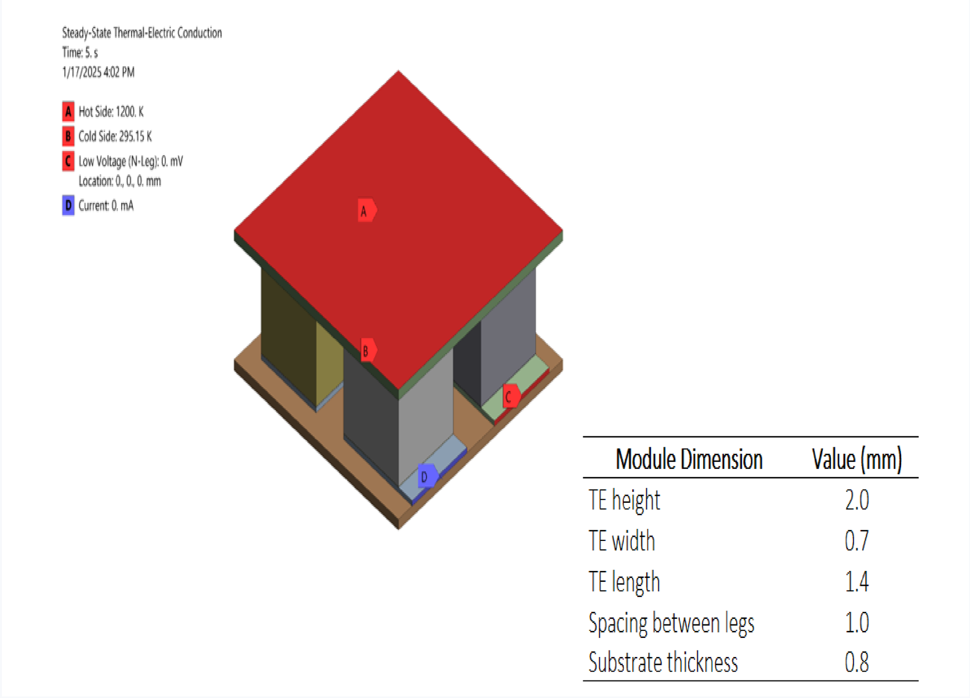
$$\mathbf{J} = \sigma(-\nabla V + \alpha \nabla T)$$

$$\mathbf{q} = -\kappa \nabla T + T\alpha \mathbf{J}$$

$$\nabla \cdot \mathbf{q} + \mathbf{J} \cdot \nabla V = 0$$

$$V = \int_{T_c}^{T_h} \alpha(T)\, dT \qquad P = \frac{V^2}{R_{\text{int}} + R_{\text{load}}} \qquad \eta = \frac{P}{\dot{Q}_h}$$

Key Results — Figures



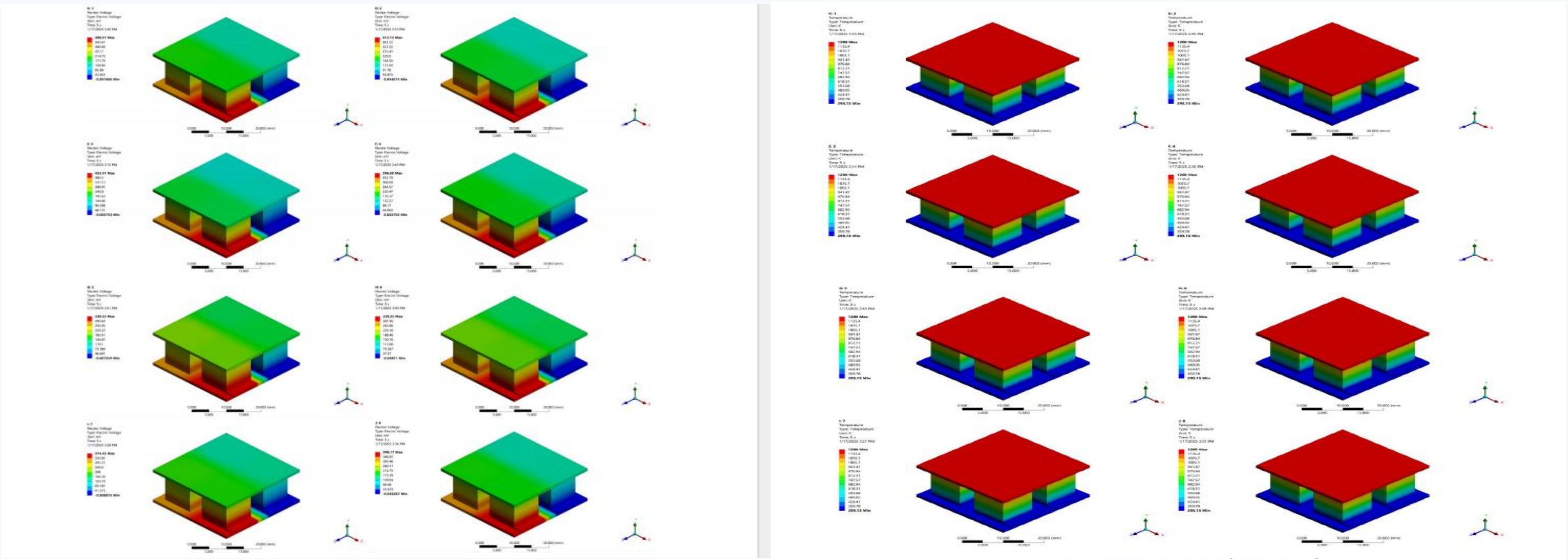
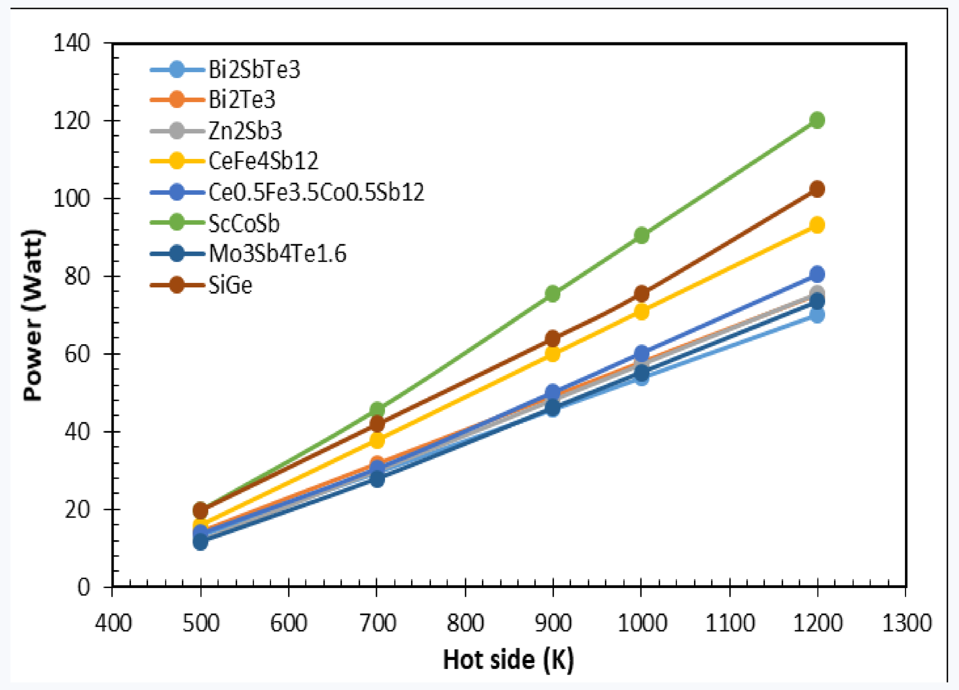
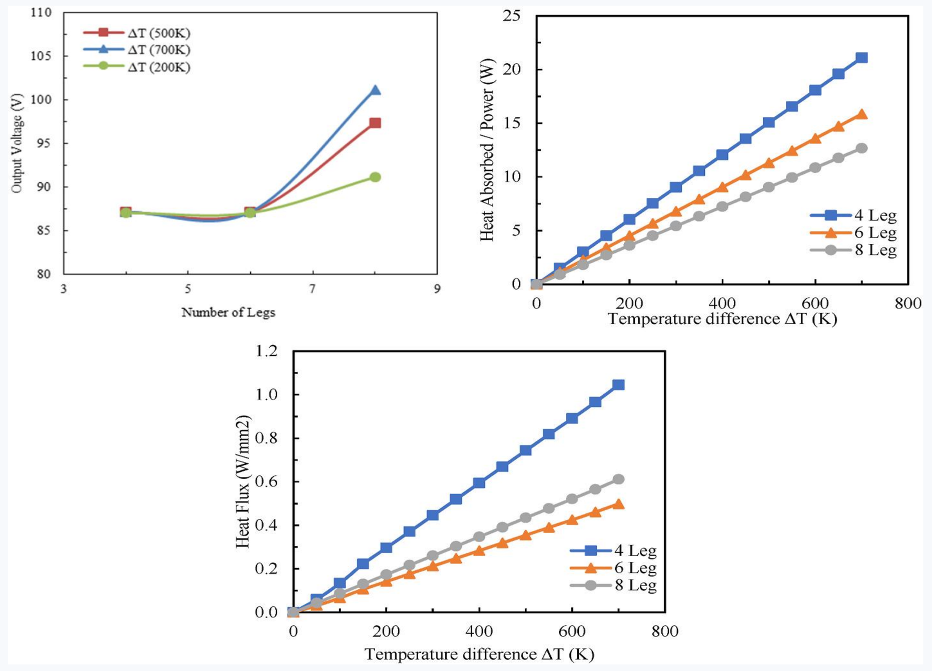


Figure 5. Temperature Distribution Graph





Transport & Ranking — Table 1

Material	σ (S/m)	κ (W/mK)	Temp Range	ρ (Ω·m)	S (μV/K)	ZT
Bi_2SbTe_3	1e4–1e5	1.0–1.5	300–400K	1e-4–1e-5	±150–±220	1.40
Bi_2Te_3	3e4–2e5	1.2–1.8	300K	3e-4–2e-5	±150–±250	1.43
Zn_2Sb_3	1e3–1e4	1.0–2.0	450–550K	1e-3–1e-4	+150–+300	1.44
$CeFe_4Sb_{12}$	1e4–1e5	2.0–3.0	450–550K	1e-4–1e-5	±150–±250	1.45
$Ce_{0.5}Fe_{3.5}Co_{0.5}Sb_{12}$	1e4–5e4	1.5–2.5	600–800K	1e-4–5e-4	+100–+200	1.56
ScCoSb	~1e4	3.0–5.0	500–700K	~1e-4	+100–+200	1.61
$Mo_3Sb_4Te_{1.6}$	1e4–1e5	1.0–2.0	500–700K	1e-4–1e-5	+100–+250	1.58
SiGe	1e3–1e4	3.0–6.0	900–1200K	1e-4–1e-5	+200–+400	1.60

Derived Parameters — Table 2

Material	σmid	κmid	Tlow	Thigh	Tmid	Smid	ρmid	PFmid	ZTmid	ΔT_ex	V_ex
Bi_2SbTe_3	5.5e4	1.25	300	400	350	185	1.82e-5	1.9e-3	0.53	100	0.0185
Bi_2Te_3	1.15e5	1.50	300	300	300	200	8.7e-6	4.6e-3	0.92	300	0.0600
Zn_2Sb_3	5.5e3	1.50	450	550	500	225	1.82e-4	2.8e-4	0.093	100	0.0225
$CeFe_4Sb_{12}$	5.5e4	2.50	450	550	500	200	1.82e-5	2.2e-3	0.44	100	0.0200
$Ce_{0.5}Fe_{3.5}Co_{0.5}Sb_{12}$	3.0e4	2.00	600	800	700	150	3.3e-5	6.8e-4	0.24	200	0.0300
ScCoSb	1.0e4	4.00	500	700	600	150	1.0e-4	2.3e-4	0.035	200	0.0300
$Mo_3Sb_4Te_{1.6}$	5.5e4	1.50	500	700	600	175	1.82e-5	1.7e-3	0.69	200	0.0350
SiGe	5.5e3	4.50	900	1200	1050	300	1.82e-4	5.0e-4	0.12	300	0.0900

Conclusions

High-T (1000–1200 K): SiGe, ScCoSb maximize power and operate stably.
Mid-T (500–800 K): Skutterudites & Zn_2Sb_3 balance α, σ, κ for strong output.
Near-room-T: Bi_2Te_3 family remains the benchmark for cooling/small ΔT harvesters.
Synthesis ↔ simulation loop accelerates material–device co-optimization.

Acknowledgements & Contact

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Contact: Christian.Idogho@uvm.edu | Full paper & code available on request.