

334 A Material Prediction by ChatGPT

335 **Prompt:**

336 Rank the following 84 materials based on their thermoelectric performance, with 1 being the highest-
337 performing material and 84 being the lowest-performing material. Consider factors such as electrical
338 conductivity, thermal conductivity, and the Seebeck coefficient when determining their thermoelectric
339 performance.

340 ['WO_{2.9}', 'In₂O₃', 'Ni_{0.02}Zn_{0.98}O', ..., 'Mn_{1.3}Mo₆S₈']

341 **Answer from ChatGPT:**

342 Ranking materials based on their thermoelectric performance can be a complex task and depends on
343 various factors, including electrical conductivity, thermal conductivity, and the Seebeck coefficient.
344 Since I don't have access to the most up-to-date and specific thermoelectric performance data for
345 these materials, I can provide a general ranking based on the properties of common thermoelectric
346 materials. Keep in mind that this ranking may not be accurate for your specific application, as the
347 performance depends on various parameters and conditions.

348 Here's a general ranking of the provided materials from 1 (highest thermoelectric performance) to 84
349 (lowest thermoelectric performance):

350 Bismuth Antimony Telluride (Bi₂Te₃)
351 Lead Telluride (PbTe)
352 Silicon-Germanium Alloy (Si_{0.8}Ge_{0.2})
353 Zinc Antimonide (Zn₄Sb₃)
354 Strontium Titanium Niobium Oxide (SrTi_{0.8}Nb_{0.2}O₃)
355 Bismuth Selenide (Bi₂Se₃)
356 Calcium Cobaltate (Ca₃Co₄O₉)
357 Copper Selenide (Cu₂Se)
358 Magnesium Silicide (Mg₂Si)
359 Sodium Cobaltate (NaCo₂O₄)
360 Barium Strontium Titanate (Ba_{0.4}Sr_{0.6}TiO₃)
361 Nickel-based Thermoelectric Materials (Ni_{0.02}Zn_{0.98}O, Ni_{2.0}Mo₆S₈, Ni_{1.3}Mo₆S₈)
362 Copper-based Thermoelectric Materials (Cu_{1.98}Se, Cu_{4.0}Mo₆S₈, Cu₂Se)
363 Cerium-based Thermoelectric Materials (CeFe₄Sb₁₂, CeFe₃CoSb₁₂, CeFe_{3.5}Co_{0.5}Sb₁₂)
364 Cobalt-based Thermoelectric Materials (Ca_{0.9}Bi_{0.1}MnO₃, Ca_{0.9}Ho_{0.1}MnO₃, Ca_{0.9}Nd_{0.1}MnO₃,
365 LaCoO₃)
366 Tl-Bi-Te Compound (Tl₉BiTe₆, Tl₂SnTe₅, Tl₂GeTe₅)
367 Zinc Oxide (ZnO, Zn_{0.95}Al_{0.05}O, Zn_{0.98}Al_{0.02}O, Zn_{0.99}Al_{0.01}O)
368 Titanium-based Thermoelectric Materials (Zr_{0.25}Hf_{0.25}Ti_{0.5}NiSn, Zr_{0.98}Nb_{0.02}NiSn,
369 Zr_{0.5}Hf_{0.5}NiSn, ZrNiSn_{0.98}Sb_{0.02}, ZrNiSn, Zr_{0.35}Hf_{0.35}Ti_{0.3}NiSn)
370 Copper-Chromium Oxides (CuCr_{0.97}Mg_{0.03}O₂, CuCr_{0.98}Mg_{0.02}O₂, CuCr_{0.95}Mg_{0.05}O₂,
371 CuCrO₂)
372 Perovskite Oxides (La_{0.98}Sr_{0.02}CoO₃, La_{0.8}Sr_{0.2}CoO₃, Sr_{0.9}La_{0.1}TiO₃, Sr_{0.61}Ba_{0.39}Nb₂O₆,
373 Sr_{0.9}Y_{0.1}TiO₃)
374 Rare Earth-based Thermoelectric Materials (Yb₁₄MnSb₁₁, Sm_{0.5}Ca_{0.5}MnO₃, La_{1-x}Sr_xCoO₃,
375 La_{0.95}Sr_{0.05}CoO₃, LaFe₃CoSb₁₂, LaFe₃CoSb₁₂)
376 Other Oxides (BaPbO₃, Ba₈Ga₁₆Ge₃₀, Ca_{2.7}Bi_{0.3}Co₄O₉, Ca₃AlSb₃, Ca₂Co₂O₅,
377 Ca_{0.7}Y_{0.3}MnO₃, CaMn_{0.98}Nb_{0.02}O₃, CaMnO₃)
378 Iron-based Thermoelectric Materials (Fe_{1.94}Ti_{0.06}O₃, Fe_{1.3}Mo₆S₈, Cr_{1.3}Mo₆S₈, Mn_{1.3}Mo₆S₈)
379 Other Compounds (Nd₂CuO₄, K₂Bi₈Se₁₃, AgCrSe₂, Mo₃Te₄)

380 Please note that this ranking is based on general knowledge of thermoelectric materials and properties
381 as of my last update in September 2021. For specific applications or the most up-to-date information,
382 it's essential to refer to recent research and literature on thermoelectric materials. Additionally, the

383 actual performance may vary depending on factors like temperature, doping, and material preparation
 384 methods.

385 B Comparison of BERT tokenizer and MatBERT tokenizer

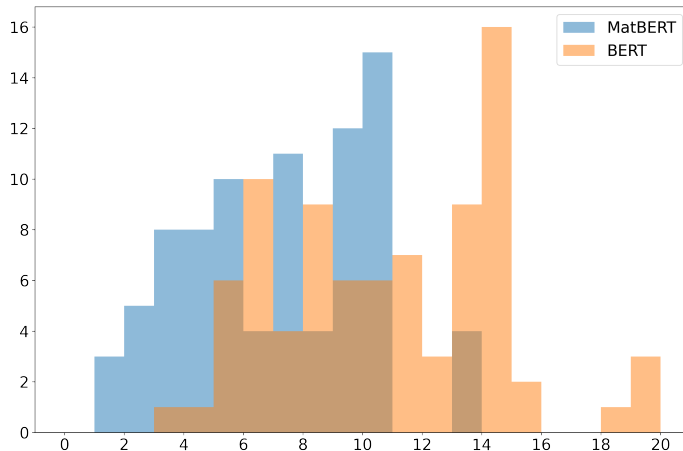


Figure 4: Comparison of length of tokenized 84 material names by different tokenizer

386 C Detailed Ranking Prediction

Table 2: Comparison of 79-material ranking by original experimental results and MatBERT (third-layer, context-average)

Rank	Experiment	MatBERT
1	Cu ₂ Se	Bi ₂ Te ₃
2	In _{0.25} Co ₄ Sb ₁₂	Sb ₂ Te ₃
3	Zr _{0.25} Hf _{0.25} Ti _{0.5} NiSn	Cu ₂ Se
4	Ba ₈ Ga ₁₆ Ge ₃₀	Cu _{1.98} Se
5	NaCo ₂ O ₄	CeFe ₄ Sb ₁₂
6	Tl _{0.02} Pb _{0.98} Te	Tl ₉ BiTe ₆
7	In _{0.2} Co ₄ Sb ₁₂	LaFe ₃ CoSb ₁₂
8	Na _{0.02} Pb _{0.98} Te	Tl ₂ GeTe ₅
9	Zn ₄ Sb ₃	Mo ₃ Te ₄
10	Ag ₉ TlTe ₅	Yb ₁₄ MnSb ₁₁
11	Zr _{0.35} Hf _{0.35} Ti _{0.3} NiSn	ZrNiSn
12	Cu _{1.98} Se	Bi ₂ Sr ₂ Co ₂ O ₈
13	Bi ₂ Sr ₂ Co ₂ O ₈	CeFe ₃ CoSb ₁₂
14	Ca ₂ Co ₂ O ₅	Na _{0.02} Pb _{0.98} Te
15	Tl ₉ BiTe ₆	TiNiSn
16	Bi ₂ Te ₃	ZrNiSn _{0.98} Sb _{0.02}
17	AgCrSe ₂	AgCrSe ₂
18	Ca ₃ Co ₄ O ₉	K ₂ Bi ₈ Se ₁₃
19	Sr _{0.61} Ba _{0.39} Nb ₂ O ₆	Tl _{0.02} Pb _{0.98} Te
20	In _{0.1} Co ₄ Sb ₁₂	Zr _{0.98} Nb _{0.02} NiSn
21	Mg ₂ Si _{0.98} Bi _{0.02}	In _{0.1} Co ₄ Sb ₁₂
22	Tl _{0.01} Pb _{0.99} Te	Ag ₉ TlTe ₅
23	LaFe ₃ CoSb ₁₂	In _{0.2} Co ₄ Sb ₁₂

24	Si0.8Ge0.2	Zr0.35Hf0.35Ti0.3NiSn
25	Yb14MnSb11	CeFe3.5Co0.5Sb12
26	CeFe3CoSb12	Tl0.01Pb0.99Te
27	CeFe4Sb12	NbCoSn
28	Zr0.98Nb0.02NiSn	SrTi0.8Nb0.2O3
29	Zr0.5Hf0.5NiSn	Zr0.5Hf0.5NiSn
30	Mg2Si	In0.25Co4Sb12
31	ZrNiSn	Zr0.25Hf0.25Ti0.5NiSn
32	Cu4.0Mo6S8	La0.95Sr0.05CoO3
33	TiNiSn	LaCoO3
34	Ba0.3Sr0.6La0.1TiO3	In1.8Ge0.2O3
35	SrTi0.8Nb0.2O3	Zn4Sb3
36	In1.8Ge0.2O3	KBi6.33S10
37	Ca2.7Bi0.3Co4O9	La0.8Sr0.2CoO3
38	In1.985Ge0.015O3	CaMn0.98Nb0.02O3
39	Zn0.95Al0.05O	CaMnO3
40	Zn0.98Al0.02O	Ca5Al2Sb6
41	Sr0.9La0.1TiO3	Si0.8Ge0.2
42	Cr1.3Mo6S8	Mg2Si0.98Bi0.02
43	Sb2Te3	Sr0.9La0.1TiO3
44	Sr0.9Y0.1TiO3	Fe1.3Mo6S8
45	CuRh0.9Mg0.1O2	In1.985Ge0.015O3
46	ZrNiSn0.98Sb0.02	Mn1.3Mo6S8
47	CaMn0.98Nb0.02O3	Ni2.0Mo6S8
48	Ca0.9Yb0.1MnO3	Sr0.9Y0.1TiO3
49	NbCoSn	In2O3
50	Mn1.3Mo6S8	Ba0.3Sr0.6La0.1TiO3
51	CeFe3.5Co0.5Sb12	NaCo2O4
52	WO2.9	CaMn0.96Ru0.04O3
53	Fe1.3Mo6S8	Nd2CuO4
54	Ca0.9Bi0.1MnO3	Sm0.5Ca0.5MnO3
55	CaMnO3	CuCr0.97Mg0.03O2
56	Ca0.9Ho0.1MnO3	Cr1.3Mo6S8
57	Zn0.99Al0.01O	Ca2.7Bi0.3Co4O9
58	In2O3	CuCr0.95Mg0.05O2
59	CaMn0.96Ru0.04O3	Ca0.9Yb0.1MnO3
60	WO2.722	Sr0.61Ba0.39Nb2O6
61	Ca5Al2Sb6	Cu4.0Mo6S8
62	La0.95Sr0.05CoO3	Mg2Si
63	CuCr0.97Mg0.03O2	Ca0.9Bi0.1MnO3
64	Ni2.0Mo6S8	CuCr0.98Mg0.02O2
65	CuCr0.95Mg0.05O2	Ca3Co4O9
66	Ca0.9Nd0.1MnO3	CuRh0.9Mg0.1O2
67	BaPbO3	Zn0.98Al0.02O
68	K2Bi8Se13	Ca0.9Nd0.1MnO3
69	Mo3Te4	Zn0.95Al0.05O
70	CuCr0.98Mg0.02O2	CuCrO2
71	Tl2GeTe5	Ni0.02Zn0.98O
72	Nd2CuO4	Ba8Ga16Ge30
73	La0.8Sr0.2CoO3	BaPbO3
74	CuCrO2	Ca0.9Ho0.1MnO3
75	Sm0.5Ca0.5MnO3	WO2.9
76	ZnO	WO2.722
77	LaCoO3	Zn0.99Al0.01O
78	KBi6.33S10	ZnO
79	Ni0.02Zn0.98O	Ca2Co2O5

Table 3: Comparison of 84-material ranking by original experimental results and GPT embedding

Rank	Experiment	GPT Embedding
1	Cu ₂ Se	Tl _{0.01} Pb _{0.99} Te
2	In _{0.25} Co ₄ Sb ₁₂	Tl _{0.02} Pb _{0.98} Te
3	Zr _{0.25} Hf _{0.25} Ti _{0.5} NiSn	Sb ₂ Te ₃
4	Ba ₈ Ga ₁₆ Ge ₃₀	Tl ₂ GeTe ₅
5	NaCo ₂ O ₄	Tl ₂ SnTe ₅
6	Tl _{0.02} Pb _{0.98} Te	Bi ₂ Te ₃
7	In _{0.2} Co ₄ Sb ₁₂	SrTi _{0.8} Nb _{0.2} O ₃
8	Na _{0.02} Pb _{0.98} Te	TiNiSn
9	Zn ₄ Sb ₃	Sr _{0.9} Y _{0.1} TiO ₃
10	Zr _{0.35} Hf _{0.35} Ti _{0.3} NiSn	Mo ₃ Te ₄
11	Cu _{1.98} Se	Na _{0.02} Pb _{0.98} Te
12	Bi ₂ Sr ₂ Co ₂ O ₈	Ni _{2.0} Mo ₆ S ₈
13	Ca ₂ Co ₂ O ₅	Zr _{0.5} Hf _{0.5} NiSn
14	Tl ₉ BiTe ₆	Zr _{0.98} Nb _{0.02} NiSn
15	Bi ₂ Te ₃	Cu _{1.98} Se
16	AgCrSe ₂	Sr _{0.9} La _{0.1} TiO ₃
17	Ca ₃ Co ₄ O ₉	ZrNiSn
18	Sr _{0.61} Ba _{0.39} Nb ₂ O ₆	Cu ₂ Se
19	In _{0.1} Co ₄ Sb ₁₂	Mg ₂ Si
20	Mg ₂ Si _{0.98} Bi _{0.02}	Zr _{0.35} Hf _{0.35} Ti _{0.3} NiSn
21	Tl _{0.01} Pb _{0.99} Te	In _{1.8} Ge _{0.2} O ₃
22	LaFe ₃ CoSb ₁₂	Fe _{1.3} Mo ₆ S ₈
23	Si _{0.8} Ge _{0.2}	In ₂ O ₃
24	Yb ₁₄ MnSb ₁₁	Fe _{1.94} Ti _{0.06} O ₃
25	CeFe ₃ CoSb ₁₂	ZrNiSn _{0.98} Sb _{0.02}
26	CeFe ₄ Sb ₁₂	In _{1.985} Ge _{0.015} O ₃
27	Zr _{0.98} Nb _{0.02} NiSn	Zr _{0.25} Hf _{0.25} Ti _{0.5} NiSn
28	Zr _{0.5} Hf _{0.5} NiSn	Si _{0.8} Ge _{0.2}
29	Mg ₂ Si	K ₂ Bi ₈ Se ₁₃
30	ZrNiSn	Cr _{1.3} Mo ₆ S ₈
31	Cu _{4.0} Mo ₆ S ₈	Ba ₈ Ga ₁₆ Ge ₃₀
32	TiNiSn	Cu _{4.0} Mo ₆ S ₈
33	Ba _{0.3} Sr _{0.6} La _{0.1} TiO ₃	Bi ₂ Sr ₂ Co ₂ O ₈
34	SrTi _{0.8} Nb _{0.2} O ₃	CuCrO ₂
35	In _{1.8} Ge _{0.2} O ₃	Tl ₉ BiTe ₆
36	Ca _{2.7} Bi _{0.3} Co ₄ O ₉	BaPbO ₃
37	In _{1.985} Ge _{0.015} O ₃	Zn ₄ Sb ₃
38	Zn _{0.95} Al _{0.05} O	Nd ₂ Cu _{0.98} Ni _{0.02} O ₄
39	Zn _{0.98} Al _{0.02} O	Mn _{1.3} Mo ₆ S ₈
40	Sr _{0.9} La _{0.1} TiO ₃	Ca _{0.9} Yb _{0.1} MnO ₃
41	Cr _{1.3} Mo ₆ S ₈	Ba _{0.4} Sr _{0.6} PbO ₃
42	Sb ₂ Te ₃	Ni _{0.02} Zn _{0.98} O
43	Sr _{0.9} Y _{0.1} TiO ₃	Zn _{0.99} Al _{0.01} O
44	CuRh _{0.9} Mg _{0.1} O ₂	Mg ₂ Si _{0.98} Bi _{0.02}
45	ZrNiSn _{0.98} Sb _{0.02}	Ba _{0.3} Sr _{0.6} La _{0.1} TiO ₃
46	CaMn _{0.98} Nb _{0.02} O ₃	In _{0.2} Co ₄ Sb ₁₂
47	Ba _{0.4} Sr _{0.6} PbO ₃	In _{0.25} Co ₄ Sb ₁₂
48	Ca _{0.9} Yb _{0.1} MnO ₃	In _{0.1} Co ₄ Sb ₁₂
49	NbCoSn	LaCoO ₃
50	Mn _{1.3} Mo ₆ S ₈	Nd ₂ CuO ₄
51	CeFe _{3.5} Co _{0.5} Sb ₁₂	AgCrSe ₂
52	WO _{2.9}	Ca _{0.7} Y _{0.3} MnO ₃
53	Fe _{1.3} Mo ₆ S ₈	Ca ₃ AlSb ₃
54	Ca _{0.9} Bi _{0.1} MnO ₃	Sr _{1.6} La _{0.4} Nb ₂ O ₇
55	Ca ₃ AlSb ₃	CeFe ₄ Sb ₁₂

56	CaMnO ₃	ZnO
57	Ca _{0.9} Ho _{0.1} MnO ₃	La _{0.98} Sr _{0.02} CoO ₃
58	Zn _{0.99} Al _{0.01} O	Yb ₁₄ MnSb ₁₁
59	In ₂ O ₃	Zn _{0.98} Al _{0.02} O
60	Tl ₂ SnTe ₅	CeFe ₃ CoSb ₁₂
61	WO _{2.722}	WO _{2.9}
62	Ca ₅ Al ₂ Sb ₆	Sr _{0.61} Ba _{0.39} Nb ₂ O ₆
63	La _{0.95} Sr _{0.05} CoO ₃	CeFe _{3.5} Co _{0.5} Sb ₁₂
64	CuCr _{0.97} Mg _{0.03} O ₂	Zn _{0.95} Al _{0.05} O
65	Fe _{1.94} Ti _{0.06} O ₃	La _{0.8} Sr _{0.2} CoO ₃
66	Ni _{2.0} Mo ₆ S ₈	Ca ₅ Al ₂ Sb ₆
67	Sr _{1.6} La _{0.4} Nb ₂ O ₇	LaFe ₃ CoSb ₁₂
68	CuCr _{0.95} Mg _{0.05} O ₂	Sm _{0.5} Ca _{0.5} MnO ₃
69	Ca _{0.7} Y _{0.3} MnO ₃	CaMnO ₃
70	Ca _{0.9} Nd _{0.1} MnO ₃	Ca ₂ Co ₂ O ₅
71	BaPbO ₃	La _{0.95} Sr _{0.05} CoO ₃
72	K ₂ Bi ₈ Se ₁₃	Ca _{0.9} Bi _{0.1} MnO ₃
73	La _{0.98} Sr _{0.02} CoO ₃	NaCo ₂ O ₄
74	Mo ₃ Te ₄	NbCoSn
75	CuCr _{0.98} Mg _{0.02} O ₂	WO _{2.722}
76	Tl ₂ GeTe ₅	CaMn _{0.98} Nb _{0.02} O ₃
77	Nd ₂ CuO ₄	Ca _{0.9} Nd _{0.1} MnO ₃
78	La _{0.8} Sr _{0.2} CoO ₃	Ca _{0.9} Ho _{0.1} MnO ₃
79	Nd ₂ Cu _{0.98} Ni _{0.02} O ₄	CuRh _{0.9} Mg _{0.1} O ₂
80	CuCrO ₂	Ca _{2.7} Bi _{0.3} Co ₄ O ₉
81	Sm _{0.5} Ca _{0.5} MnO ₃	CuCr _{0.97} Mg _{0.03} O ₂
82	ZnO	CuCr _{0.98} Mg _{0.02} O ₂
83	LaCoO ₃	CuCr _{0.95} Mg _{0.05} O ₂
84	Ni _{0.02} Zn _{0.98} O	Ca ₃ Co ₄ O ₉