Supplementary Information: A Public Database of Thermoelectric Materials and System-Identified Material Representation for Data-Driven Discovery of High-Performance Thermoelectric Materials

Gyoung S. Na
Korea Research Institute of Chemical Technology
Republic of Korea
ngs0@krict.re.kr

1 Elemental Distribution of ESTM Dataset

The collected ESTM dataset contains 880 unique thermoelectric materials covering various elements, as shown in Fig. 1. The three most common elements in ESTM dataset were Se, Sb, and Te, which are popular in high-performance thermoelectric materials. The most common host materials in ESTM dataset were $Mg_{3.5}Sb_2$, SnSe, and SnTe. In addition to the host materials, ESTM dataset contains the thermoelectric materials with various dopants, such as Sb, Mn, Pb, and Ag.

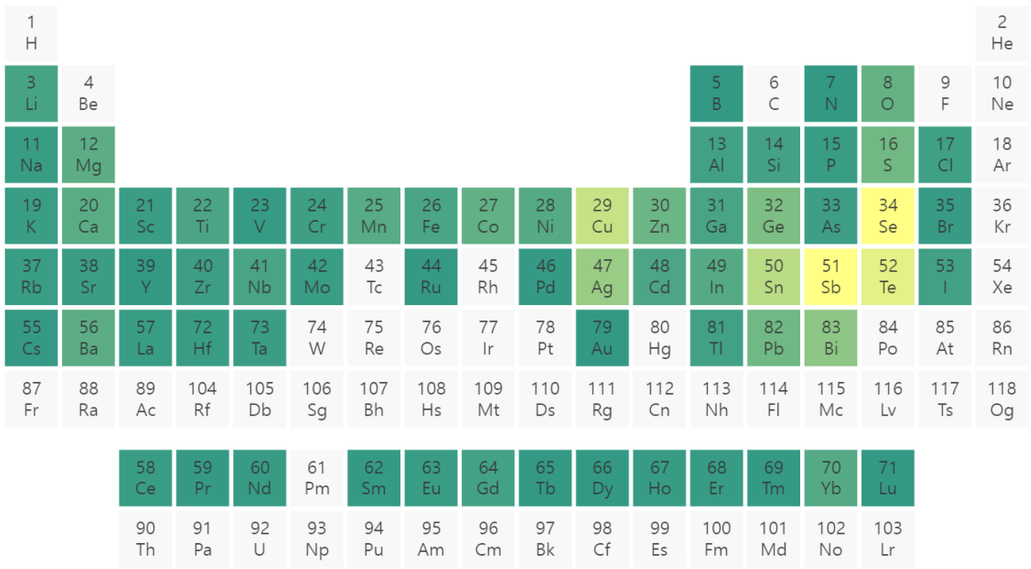

Figure 1: Distribution of the elements in the collected thermoelectric materials in ESTM dataset. The color of the periodic table indicates the frequency of the elements, and bright color means the high frequency of the element.

2 Target Distributions of ESTM Dataset

Fig. 2 shows the data distribution of ESTM dataset for the measuring temperatures. For the visualization, we categorized the observations in ESTM dataset based on four meausring temperatures: (1) low temperature ($T \leq 280$ K), (2) near room temperature (280 K $< T \leq 300$ K), (3) common thermoelectric temperature ($300 < T \leq 700$ K), and (4) high temperature (700 K $< T$). As shown in the pie chart, the thermoelectric properties measured at the common thermoelectric temperature are dominant in ESTM dataset. The proportions of the data for low, near room, common thermoelectric, and high temperatures were 2.11%, 5.94%, 71.82%, and 20.13%, respectively. We presented the distributions of the target thermoelectric properties at the common thermoelectric temperature where most data was collected in ESTM dataset. Although ESTM dataset contains various high-ZT materials (e.g., SnSe), the data distribution of ZT is biased to zero. This target distribution shows the difficulty of discovering high-ZT thermoelectric materials.

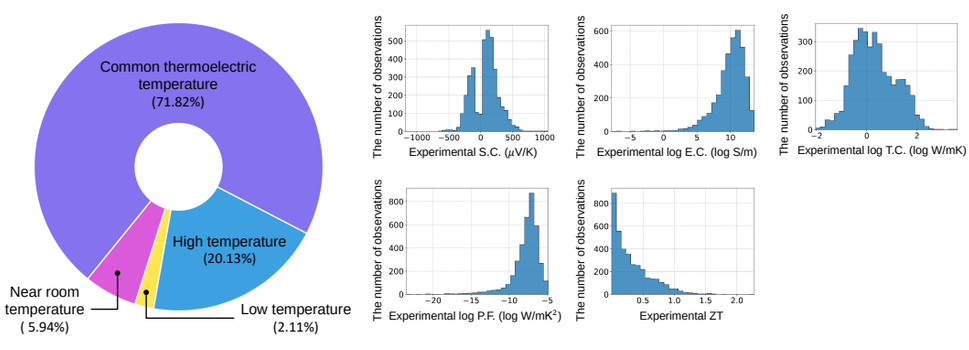

Figure 2: Data distribution of ESTM dataset and target distributions of the data at the common thermoelectric temperatures. We categorized the observations collected in ESTM dataset into four ranges of the measuring temperatures: (1) low temperature, (2) near room temperature, (3) common thermoelectric temperature, and (4) high temperature.

3 Search Results of SIMD-Based Material Space Exploration for Discovering High-ZT Thermoelectric Materials

In the experiments, we performed the SIMD-based global search for discovering high-ZT theremoelectric materials beyond the training datasets. In the search results, we selected top-100 materials based on their predicted ZTs. Table 1 shows the search results of the SIMD-based exploration of the material space.

Table 1: SIMD-based global search results to discover high-ZT thermoelectric materials. The predicted ZTs of the discovered materials are presented with the chemical compositions of the materials.

Index	Composition	Host Material	Dopant	Predicted ZT
1	Ge0.8Te1.2In0.003Sb0.035	Ge0.8Te1.2	In, Sb	1.77
2	Ge0.9Te1.1In0.003Sb0.036	Ge0.9Te1.1	In, Sb	1.768
3	Ge1.7Te2.2In0.014Sb0.1	Ge1.7Te2.2	In, Sb	1.611
4	Ge0.9Sb0.036Pb0.085	Ge0.9	Sb, Pb	1.475
5	Ge9Sb0.37Pb0.83	Ge9Sb0.37Pb0.83		1.457
6	Ge0.9Te1.1Mn0.023In0.007	Ge0.9Te1.1	Mn, In	1.442
7	Ge3Sn1.3Te2.7Sb0.006	Ge3Sn1.3Te2.7	Sb	1.42
8	Ge0.8Te1.2In0.003	Ge0.8Te1.2	In	1.41
9	Ge0.9Ag0.1Sb0.034	Ge0.9	Ag, Sb	1.403
10	Ge0.9Mn0.012Sb0.035Pb0.07	Ge0.9	Mn, Sb, Pb	1.388
11	Ge0.9Ag0.003Sb0.1Pb0.04	Ge0.9	Ag, Sb, Pb	1.385
12	Ge0.9Mn0.016Zn0.01Sb0.098	Ge0.9	Mn, Zn, Sb	1.369
13	Ge9Sb0.84Pb0.17	Ge9Sb0.84Pb0.17		1.343
14	Ge0.9Mn0.038Ag0.003Sb0.1	Ge0.9	Mn, Ag, Sb	1.336
15	Ge96SbMn0.1	Ge96Sb1	Mn	1.331
16	Ge0.9Te0.1Zn0.01Sb0.036	Ge0.9	Te, Zn, Sb	1.328
17	Ge0.9Sb0.1	Ge0.9	Sb	1.311
18	Ge0.9Sb0.1Mn0.031	Ge0.9	Sb, Mn	1.307
19	Ge0.9Ag0.001Sb0.1	Ge0.9	Ag, Sb	1.305
20	Ge0.9Mn0.008Sb0.1	Ge0.9	Mn, Sb	1.298
21	Ge0.6Te0.4Mn0.016Sb0.033	Ge0.6Te0.4	Mn, Sb	1.296
22	Ge0.9Se2.3Bi0.8	Ge0.9Se2.3Bi0.8		1.271
23	Bi3Zn0.015Ag0.024Sb0.006	Bi3	Zn, Ag, Sb	1.259
24	Bi3Zn0.015Ag0.026Sb0.006	Bi3	Zn, Ag, Sb	1.259
25	Bi3Zn0.015Ag0.029Sb0.006	Bi3	Zn, Ag, Sb	1.259
26	GeSe3Te3In0.011	Ge1Se3Te3	In	1.254
27	Bi3Zn0.013Ag0.025Sb0.006	Bi3	Zn, Ag, Sb	1.203
28	Ge0.9Mn0.005Zn0.069Sb0.062	Ge0.9	Mn, Zn, Sb	1.202
29	Bi3Zn0.034Ag0.003Sb0.006	Bi3	Zn, Ag, Sb	1.201
30	Bi3Zn0.04Ag0.004Sb0.006	Bi3	Zn, Ag, Sb	1.201
31	Bi3Zn0.032Ag0.003Sb0.006	Bi3	Zn, Ag, Sb	1.201
32	Bi3Ag0.003In0.003Sb0.006	Bi3	Ag, In, Sb	1.198
33	Bi3Ag0.004Sb0.006Pb0.014	Bi3	Ag, Sb, Pb	1.188
34	Bi3Ag0.027Sb0.006	Bi3	Ag, Sb	1.175
35	Bi3Ag0.024Sb0.006	Bi3	Ag, Sb	1.175
36	Bi3Ag0.025Sb0.006	Bi3	Ag, Sb	1.175
37	Bi3Ag0.003Sb0.006	Bi3	Ag, Sb	1.172
38	Bi3Zn0.014Sb0.006Pb0.013	Bi3	Zn, Sb, Pb	1.165
39	Bi3Zn0.021Sb0.006Pb0.014	Bi3	Zn, Sb, Pb	1.165
40	Bi3Zn0.031Sb0.006Pb0.013	Bi3	Zn, Sb, Pb	1.165
41	Bi3Zn0.016Sb0.006Pb0.014	Bi3	Zn, Sb, Pb	1.165
42	Bi3Zn0.02Sb0.006Pb0.014	Bi3	Zn, Sb, Pb	1.165
43	Bi2.9Zn0.1Sb0.006	Bi2.9	Zn, Sb	1.158
44	Ge0.9Bi0.1Zn0.034Sb0.006	Ge0.9	Bi, Zn, Sb	1.155
45	Te0.1Bi0.9Sb0.006	Bi0.9	Te, Sb	1.134
46	Te0.2Bi2.8Ag0.004	Te0.2Bi2.8	Ag	1.132
47	Te0.2Bi2.8Ag0.003	Te0.2Bi2.8	Ag	1.132
48	Bi3Zn0.032Sb0.006	Bi3	Zn, Sb	1.128
49	Bi3Zn0.038Sb0.006	Bi3	Zn, Sb	1.128
50	Bi3Zn0.04Sb0.006	Bi3	Zn, Sb	1.128
51	Bi3Zn0.034Sb0.006	Bi3	Zn, Sb	1.128
52	Bi3Zn0.01Sb0.006	Bi3	Zn, Sb	1.127
53	BiZn0.021Sb0.006	Bi1	Zn, Sb	1.125
54	Ge0.7Te0.3Sb0.045	Ge0.7Te0.3	Sb	1.124
55	Bi3In0.003Sb0.006	Bi3	In, Sb	1.123
56	Bi3Mn0.031Sb0.006	Bi3	Mn, Sb	1.114
57	Bi3Sb0.006Pb0.013	Bi3	Sb, Pb	1.113
58	Bi3Sb0.006Pb0.014	Bi3	Sb, Pb	1.113
59	BiSb0.006Pb0.028	Bi1	Sb, Pb	1.109
60	Bi3Sb0.006	Bi3	Sb	1.096
61	BiSb0.006	Bi1	Sb	1.095
62	BiAg0.002Sb0.033	Bi1	Ag, Sb	1.072
63	Bi3Zn0.033Ag0.003Pb0.014	Bi3	Zn, Ag, Pb	1.072

Index	Composition	Host Material	Dopant	Predicted ZT
64	Ge0.9Te0.9Bi0.2Pb0.001	Ge0.9Te0.9Bi0.2	Pb	1.063
65	Ge0.6Bi1.4Ag0.004	Ge0.6Bi1.4	Ag	1.062
66	Ge0.8Bi1.2Ag0.004	Ge0.8Bi1.2	Ag	1.059
67	Te0.2Bi2.8	Te0.2Bi2.8		1.056
68	Bi2.9Zn0.099Ag0.003	Bi2.9	Zn, Ag	1.055
69	Bi3Zn0.026Ag0.003In0.003	Bi3	Zn, Ag, In	1.053
70	Se0.1Te1.8Bi0.1Sb0.032	Te1.8	Se, Bi, Sb	1.052
71	Sn0.5Bi1.4Zn0.1	Sn0.5Bi1.4	Zn	1.05
72	SeMn0.017Ag0.024Sb0.006	Se1	Mn, Ag, Sb	1.05
73	SeMn0.016Ag0.026Sb0.006	Se1	Mn, Ag, Sb	1.05
74	Te0.1Bi2.9	Bi2.9	Te	1.047
75	BiSb0.008Pb0.019	Bi1	Sb, Pb	1.046
76	Ge0.9Te1.1	Ge0.9Te1.1		1.04
77	Te1.8Bi0.1In0.006Sb0.098	Te1.8	Bi, In, Sb	1.037
78	Te2Ag0.032In0.003Sb0.013	Te2	Ag, In, Sb	1.036
79	BiAg0.001Sb0.007	Bi1	Ag, Sb	1.034
80	Te0.1Bi0.9Ag0.004	Bi0.9	Te, Ag	1.032
81	Te3Ag0.026In0.004Sb0.006	Te3	Ag, In, Sb	1.031
82	Te3Ag0.028In0.004Sb0.006	Te3	Ag, In, Sb	1.031
83	Bi2.9Zn0.1Pb0.017	Bi2.9	Zn, Pb	1.026
84	Se0.8Te0.2Mn0.014Sb0.034	Se0.8Te0.2	Mn, Sb	1.024
85	Ge0.4Se1.6Sb0.035Pb0.001	Ge0.4Se1.6	Sb, Pb	1.024
86	Se0.8Bi0.2Sb0.032Pb0.015	Se0.8Bi0.2	Sb, Pb	1.024
87	Bi3Mn0.028Ag0.003	Bi3	Mn, Ag	1.013
88	SeAg0.03Sb0.006	Se1	Ag, Sb	1.01
89	SeAg0.026Sb0.006	Se1	Ag, Sb	1.01
90	SeAg0.023Sb0.006	Se1	Ag, Sb	1.01
91	SeAg0.027Sb0.006	Se1	Ag, Sb	1.01
92	SeAg0.028Sb0.006	Se1	Ag, Sb	1.01
93	Ge3Mn0.016Sb0.032	Ge3	Mn, Sb	1.005
94	BiSb0.001Pb0.012	Bi1	Sb, Pb	1.004
95	Se0.9Mn0.072Sb0.037	Se0.9	Mn, Sb	1.002
96	Bi3Ag0.003	Bi3	Ag	0.995
97	TeMn0.015In0.003Sb0.017	Te1	Mn, In, Sb	0.988
98	Se0.8Te1.2Sb0.034	Se0.8Te1.2	Sb	0.988
99	Se3Te3Mn0.014Sb0.034	Se3Te3	Mn, Sb	0.984
100	Ge0.1Se0.9Sb0.006	Se0.9	Ge, Sb	0.982