Supporting Information

Material Descriptors for the Discovery of Efficient Thermoelectrics

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Table S1. The scattering parameters as used in the simulations presented in this work, extracted from the literature.[9, 32, 33]

Material	ρ [kg/m^3 ×10^3]	u_s [m/s ×10^3]	ADP [a)] [eV]	ODP [a)] [eV/m ×10^{10}]	$\hbar\omega$ [eV]	ε_r [ε_0]
HfCoSb	9.54	5.64	0.2 / 0.4	1.4 / 1.85	0.028	17.51
HfNiSn	10.3	3.39	0.1 / 0.7	1.8 / 2	0.028	20.88
NbCoSn	8.43	5.36	0.2 / 0.5	2.6 / 2.16	0.034	22.6
NbFeSb	8.45	3.99	1 / 0.8	1.6 / 2.1	0.036	22.99
ScNiBi	8.48	3.1	0.8 / 0.2	2.2 / 1.4	0.028	29
ScNiSb	6.6	3.9	0.7 / 0.4	2.3 / 1.8	0.032	19.66
TiCoSb	7.4	4.04	1 / 0.5	1.75 / 2.2	0.036	19.09
TiNiSn	7.2	3.9	0.7 / 0.2	2.3 / 0.9	0.034	22.92
YNiBi	8.6	2.9	0.5 / 0.9	2.3 / 2.7	0.022	26.55
YNiSb	6.9	3.5	0.4 / 0.9	2.35 / 3.14	0.026	19.74
ZrCoBi	9.83	3.2	0.2 / 0.8	2.1 / 1.8	0.028	20.37
ZrCoSb	7.14	5.55	0.2 / 1	2.05 / 1.75	0.028	17.87
ZrNiSn	7.62	3.97	0.35 / 0.3	2.8/ 1.8	0.029	20.9
ZrNiPb	9.6	3.39	0.36/0.60	2.8/1.6	0.024	23.6

[a)] electrons / holes

Table S2. Extracted bandstructure parameters for *n*-type materials. The effective masses are in units of the electron rest mass and the total number of valleys considers the valleys within 0.1 eV from the band edge. n_b is the number of bands.

Material	m_{DOS}	m_{cond} T = 300 K	m_{cond} T = 600 K	m_{cond} T = 900 K	n_v	n_b
HfCoSb	2.87	0.95	0.88	0.84	3	1
HfNiSn	1.88	0.55	0.56	0.58	3	1
NbCoSn	2.42	0.89	0.86	0.88	6	2
NbFeSb	0.92	0.33	0.37	0.61	3	1
ScNiBi	3.12	0.75	0.73	0.72	3	1
ScNiSb	3.02	0.79	0.78	0.77	3	1
TiCoSb	3.32	1.41	2.03	2.03	3	1
TiNiSn	2.42	0.84	0.89	0.94	3	1
YNiBi	3.26	0.63	0.61	0.6	3	1
YNiSb	3.45	0.77	0.73	0.71	3	1
ZrCoBi	2.99	0.96	0.89	0.85	3	1
ZrCoSb	2.91	1.06	0.99	0.94	3	1
ZrNiSn	1.94	0.58	0.6	0.61	3	1
ZrNiPb	1.93	0.55	0.57	0.58	3	1

Table S3. Extracted bandstructure parameter for *p*-type materials. The effective masses are in units of the electron rest mass and the total number of valleys considers the valleys within 0.1 eV from the band edge. n_b is the number of bands.

Material	m_{DOS}	m_{cond} T = 300 K	m_{cond} T = 600 K	m_{cond} T = 900 K	n_v	n_b
HfCoSb	5.22	0.96	1.04	1.16	11	3
HfNiSn	4.1	0.93	0.96	1	3	3
NbCoSn	3.86	0.72	0.8	0.89	16	3
NbFeSb	5.08	1.05	1.08	1.13	8	2
ScNiBi	1.92	0.44	0.49	0.52	3	3
ScNiSb	2.2	0.49	0.55	0.58	3	3
TiCoSb	4.9	1.06	1.88	2.14	11	3
TiNiSn	6.11	1.64	1.64	1.69	3	3
YNiBi	1.43	0.3	0.37	0.41	3	3
YNiSb	1.79	0.39	0.46	0.51	3	3
ZrCoBi	4.39	0.94	0.97	1.05	11	3
ZrCoSb	4.42	0.97	1.02	1.13	8	3
ZrNiSn	4.49	1.15	1.2	1.36	3	3
ZrNiPb	3.34	0.93	0.95	1	3	3

Extraction of the density of states and conductivity effective masses from bandstructure

The data analysis and proposed descriptors make use of the DOS and conductivity effective masses m_{DOS} and m_{cond}, respectively. These are effective quantities that include information from the entire bandstructure, rather just specific valleys. To extract these, we consider non-degenerate conditions, where the Fermi level is placed in the bandgap, several k_BT from the bands. Then the m_{DOS} is the effective mass of an isotropic parabolic band that provides the same carrier density as the actual bandstructure. The m_{cond} is the effective mass of an isotropic parabolic band that has the same average velocity as all that of the entire bandstructure.[69]

To compute m_{DOS} we utilize the common expression for the carrier density in a non-degenerate semiconductor:

$$N = N_c e^{-\frac{E_C - E_F}{k_B T}} \quad \text{(S1)}$$

where E_c is the band edge, E_F is the Fermi level, k_B is the Boltzmann constant, T is the temperature and $N_c = 2\left(\frac{m_\mathrm{DOS} k_\mathrm{B} T}{2\pi\hbar^2}\right)^{3/2}$ is the effective density of states in the conduction band. This expression is derived by approximating the Fermi Dirac statistics with Boltzmann statistics. The carrier density in the numerical DFT bandstructure is given by:

$$N = \frac{2}{(2\pi)^3}\sum_{\boldsymbol{k},n} f_{E_{\boldsymbol{k},n}} dV_{\boldsymbol{k}} \quad \text{(S2)}$$

where the sum runs over all the $\boldsymbol{k}$ points in the reciprocal unit cell (mesh used for the DFT calculations) and all the bands, $f_{E_{\boldsymbol{k},n}}$ is the Fermi-Dirac distribution evaluated at the energy of each state (approximated by Boltzmann statistics in the non-degenerate limit), and $dV_{\boldsymbol{k}}$ is the volume element in the $\boldsymbol{k}$ space that depends only on the mesh. By equating the carrier density from equations (S1) and (S2) for the same Fermi level and band edge, we can extract the effective density of states in the conduction band, m_DOS. The process is the same for the valence band.

The conductivity effective mass of the bandstructure, m_cond, is extracted from the so-called injection velocity v_inj of the carriers in non-degenerate conditions.[69] As this method is derived for MOSFET devices, [70] it considers the ballistic current that the positive velocity states of the bandstructure will allow for a specific Fermi level in the non-degenerate conditions as:

$$I_{+,n} = e\frac{1}{2}\frac{2}{(2\pi)^3}\sum_{\boldsymbol{k}_n} f_{(E_{\boldsymbol{k}_n} - E_{F,\mathrm{S}})} |v_{\boldsymbol{k}_n}| dV_{\boldsymbol{k}_n} \quad \text{(S3)}$$

where e is the electron charge, the ½ factor is to take into account only half of the states, and, $|v_{\boldsymbol{k}_n}|$ is the band carrier velocity in absolute terms in order to only account for positive velocities. Then, the injection velocity is extracted by dividing the positive going ballistic current with the carrier density (to get the average velocity per carrier):

$$v_\mathrm{inj} = \frac{I_{+,n}}{e\frac{1}{2}\frac{2}{(2\pi)^3}\sum_{\boldsymbol{k}_n} f_{(E_{\boldsymbol{k}_n} - E_{F,\mathrm{S}})} dV_{\boldsymbol{k}_n}} \quad \text{(S4)}$$

where the denominator in equation (S4) is the charge occupying the positive velocity states alone. Once the injection velocity is extracted, the conductivity effective mass can be computed as:

$$m_\mathrm{cond} = \frac{2k_\mathrm{B}T}{v_\mathrm{inj}^2 \pi} \quad \text{(S5)}$$

which is the corresponding quantity for a simple parabolic band.[69, 70]

This calculation is performed along the three Cartesian directions *x*, *y*, and *z*. Thus, three conductivity affective masses are extracted, $m_{\mathrm{cond},x}$, $m_{\mathrm{cond},y}$, and $m_{\mathrm{cond},z}$ and a final average

conductivity affective mass is then formed by $m_{\mathrm{cond}} = \frac{3}{m_{\mathrm{cond},x}{}^{-1} + m_{\mathrm{cond},y}{}^{-1} + m_{\mathrm{cond},z}{}^{-1}}$. The process is performed twice, once for the conduction and once for the valence bands.

As an example, we show in **Figure S1a** the numerically extracted DOS for HfCoSb (blue lines) and the DOS provided by the extracted m_{DOS}, assuming that it forms an isotropic, parabolic band (dashed-dot green line), indicating adequate match at low energies. In **Figure S1b** we show the HfCoSb valence band injection velocity using the numerical bandstructure (blue line), and the injection velocity for an isotropic parabolic band with the extracted m_{cond} value (dash-dot green line), again indicating adequate match in the low-density region.

The relevance of m_{cond} becomes clear when comparing the TDF computed for the actual numerical bandstructure and for an isotropic parabolic band of an effective mass equal to the extracted m_{cond}, **Figure S1c**. The blue solid line (numerical bandstructure) and the green dashed-dot line (parabolic band with m_{cond}) are for the ADP-limited scattering mechanism. The lines overlap for a large energy region, indicating that m_{cond} captures the core transport information for ADP scattering in complex bandstructures. In the ODP case, the TDFs for the solid orange line (for the numerical bands) and the purple dash-dot line (for the parabolic band of m_{cond}) also clearly overlap. The TDFs deviate far from the band onset, when the parabolicity is lost.

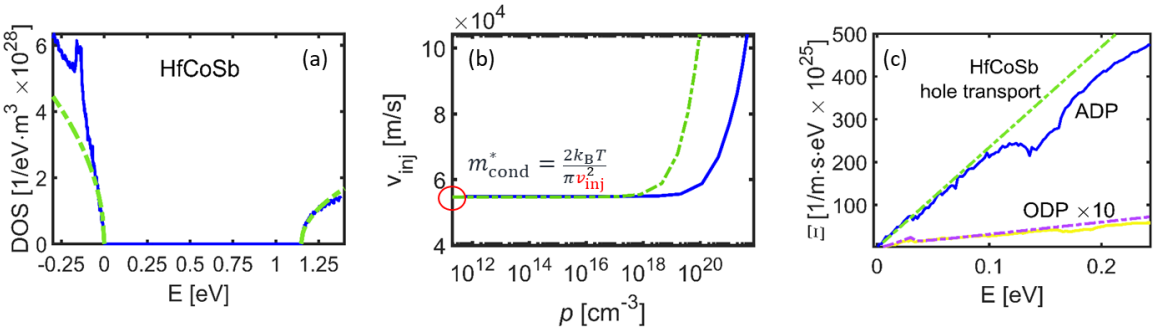

Figure S1: Comparisons between quantities extracted from the full numerical bandstructure and the corresponding quantities computed from the extracted m_{DOS} and m_{cond} for HfCoSb. (a) The DOS of HfCoSb, blue line, and the DOS of parabolic bands with the isotropic m_{DOS} values, green dashed lines. (b) Injection velocity versus carrier concentration for the positive going carriers of the HfCoSb valence band under ballistic conditions using the full bandstructure, blue solid line, and the parabolic isotropic band with the extracted effective mass value m_{cond}, green dashed line. (c) Transport distribution function versus energy for the HfCoSb valence band using the full bandstructure and the band formed with the extracted m_{cond}. The case of acoustic phonons (ADP – Acoustic Deformation Potential) transport and optical phonons (ODP – Optical Deformation Potential), transport are plotted. The blue and yellow lines indicate the full bandstructure extracted TDFs. The green and purple dashed lines indicate the TDFs for the parabolic isotropic band having an effective mass of m_{cond}.