Supporting Information

The n- and p-type thermoelectric response of semiconducting Co-based quaternary Heusler alloy: A Density Functional approach

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Here, we provide the details of band structure and transport related coefficients obtained using the PBE and the HSE06 functional respectively.

1 Electronic structure using PBE functional

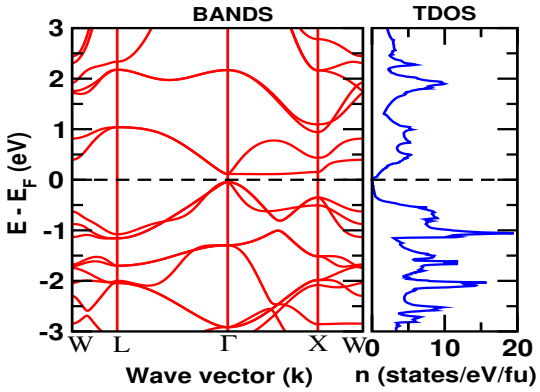

Figure 1: Electronic structure of CoFeTiAl using PBE exchange functional at relaxed lattice constant(a_{rlx} = 5.80Å). A small but finite band gap of 0.04 eV is obtained. Dashed line and TDOS represents the Fermi level(E_F) and total density of states respectively.

2 transport coefficients using hybrid functional (HSE06)

In this section, we present the optimal carrier concentration(n) at 900K, which corresponds to the maximum power factor[$(S^2\sigma/\tau)_{max}$] and upper limit of ZT [i.e. $(ZT_e)_{max}$] as depicted in table1.

*HSE*06	n	S	σ/τ	κ_e/τ	$(S^2\sigma/\tau)_{max}$	$(S^2\sigma/\tau)_{cal}$	$(ZT_e)_{max}$	$(ZT_e)_{cal}$
n-type	-0.0043	-6.68	0.0132	0.055	—	5.9×10^{10}	0.97	—
p-type	0.0022	6.04	0.0103	0.036	—	3.74×10^{10}	0.94	—
n-type	-1.65	-1.71	4.26	1.72	1.25×10^{12}	—	—	0.0007
p-type	9.14	0.913	11.9	3.17	9.96×10^{11}	—	—	0.0003

Table 1: The given values of transport coefficients (n, S, σ/τ, and κ_e/τ) are corresponding to the maximum power factor $[(S^2\sigma/\tau)_{max}]$ and upper limit of ZT [i.e $(ZT_e)_{max}$]. The other parameters, $[(S^2\sigma/\tau)_{cal}]$ and $(ZT_e)_{cal}$ are calculated from the given value of transport coefficients. The value of n, S, σ/τ, κ_e/τ, power factor are measured in 10^{21}cm^{-3}, 10^{-4}V/K, $10^{19}(\Omega ms)^{-1}$ and $10^{15}W/Kms$ and W/K^2ms. ALL the transport coefficients are calculated under the HSE06 exchange functional at $900K$.

From table1, it is clear that the carrier concentration obtained at maximum power factor $[(S^2\sigma/\tau)_{max}]$ does not corresponds to the maximum ZT [i.e. $(ZT_e)_{max}$] or, in other words, the values of n corresponding to $(S^2\sigma/\tau)_{max}$ and $(ZT_e)_{max}$ are different. For example, considering the n-type behavior, the optimal n corresponding to $(ZT_e)_{max}$ is -4.32 $\times 10^{18}$ cm^{-3} and the corresponding calculated power factor [i.e $(S^2\sigma/\tau)_{cal}$] is 5.9×10^{10} (W/K^2ms), which is different from the obtained value of maximum power factor (1.25×10^{12} W/K^2ms).