Supplementary materials for Perovskite $ThTaN_3$: a Large Thermopower Topological Crystalline Insulator

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I. TOPOLOGICAL PROPERTIES

In this brief Supplemental Material file, first we provide more evidence of the topological crystalline insulator character of $ThTaN_3$. One type of evidence involves the number of hybrid Wannier center crossings (HWCC) across the zone. Figure 1 reveals two crossings, an even number representative of a topological crystalline insulator (TCI).

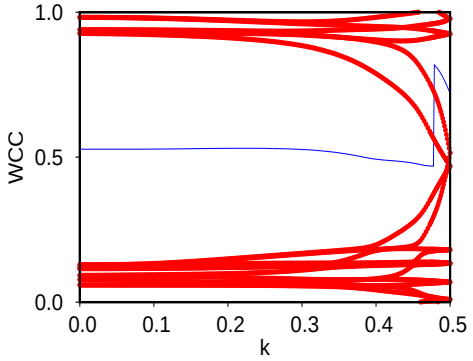

FIG. 1: (Color online) Hybrid Wannier charge center (red, thick lines) plot of $ThTaN_3$ across half of the Brillounin zone in the $k_z = 0$ plane, showing an even number of crossings between the charge center and largest gap function. The blue (thin) line denotes largest gap function. Here, the wave vector k along the (100) direction is given in unit of π/a.

It was noted in the main text that destruction of mirror or 4-fold rotation symmetries destroyed the TCI character. In Fig. 2 the band structures are displayed after destruction of these symmetries by displacement of the Ta ion.

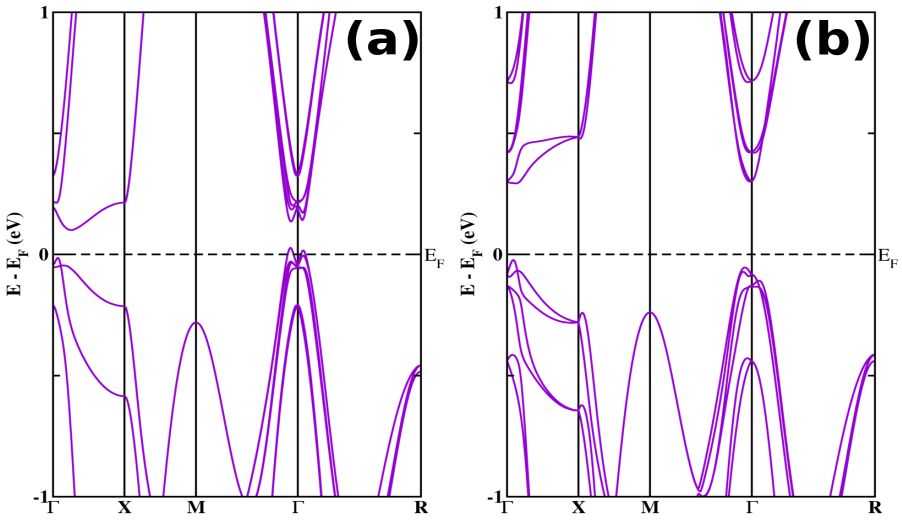

FIG. 2: (Color online) Enlarged GGA+SOC band structures, near the Fermi energy E_F, for breaking (a) only mirror and (b) both mirror and rotational symmetries.

II. THERMOELECTRIC PROPERTIES

Additionally, thermoelectric parameters of $ThTaN_3$ are calculated by a constant scattering time approximation τ. The results are shown in Fig. 3. Note that these include only electronic contributions. Thus, the figure of merit $zT = S^2\sigma(E,T)/\kappa_{el}(E,T)$, given here, is an upper bound.

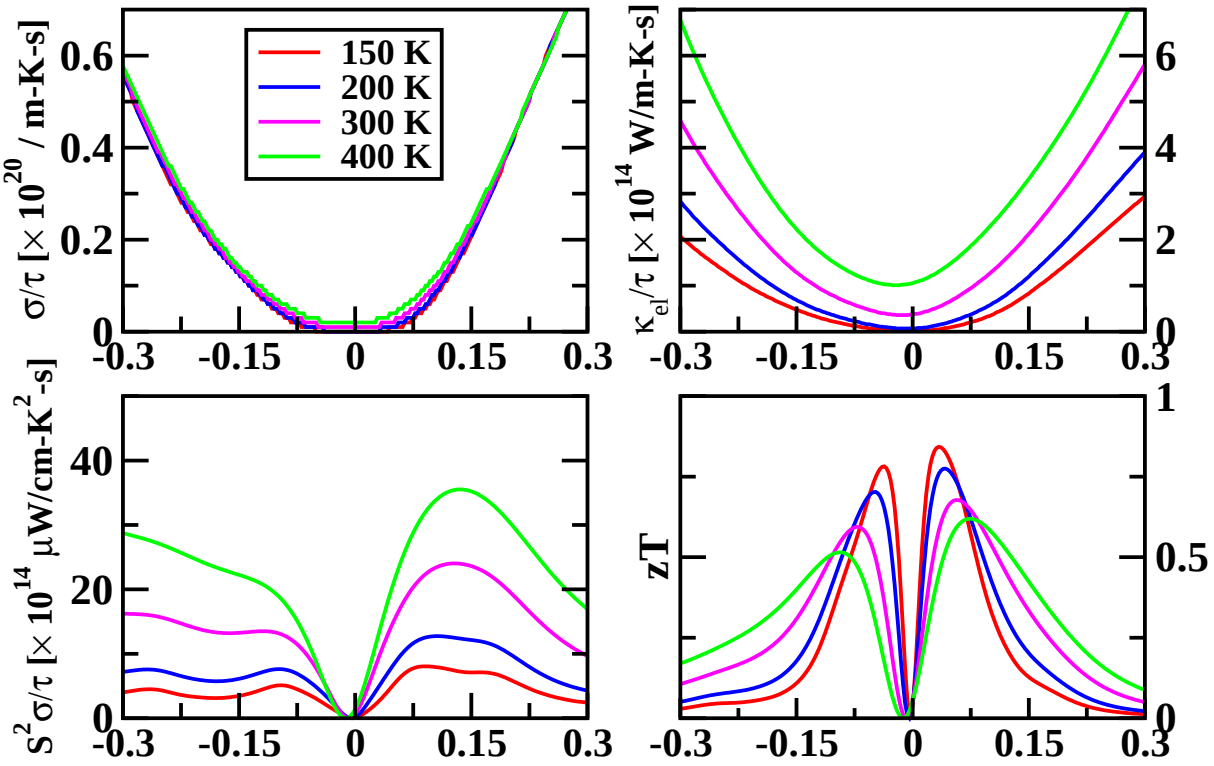

FIG. 3: (Color online) (a) Electric σ and (b) electronic thermal κ_{el} conductivities, divided by the scattering time $\tau = 0.8\times10^{-14}$ sec. (c) Power factor and (d) figure of merit, contributed by electrons.