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).

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. 1: (Color online) Hybrid Wannier charge center (red, thick lines) plot of ThTaN$_3$ across half of the Brillouin 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 $\pi/a$.

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 $\tau$. 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.

![Graphs showing electric conductivity $\sigma/\tau$, electronic thermal conductivity $\kappa_{el}/\tau$, power factor $S^2\sigma/\tau$, and figure of merit $zT$.](image)

FIG. 3: (Color online) (a) Electric $\sigma$ and (b) electronic thermal $\kappa_{el}$ conductivities, divided by the scattering time $\tau = 0.8 \times 10^{-14}$ sec. (c) Power factor and (d) figure of merit, contributed by electrons.