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Supplemental material for Thermoelectric Properties of Materials with Nontrivial Electronic Topology

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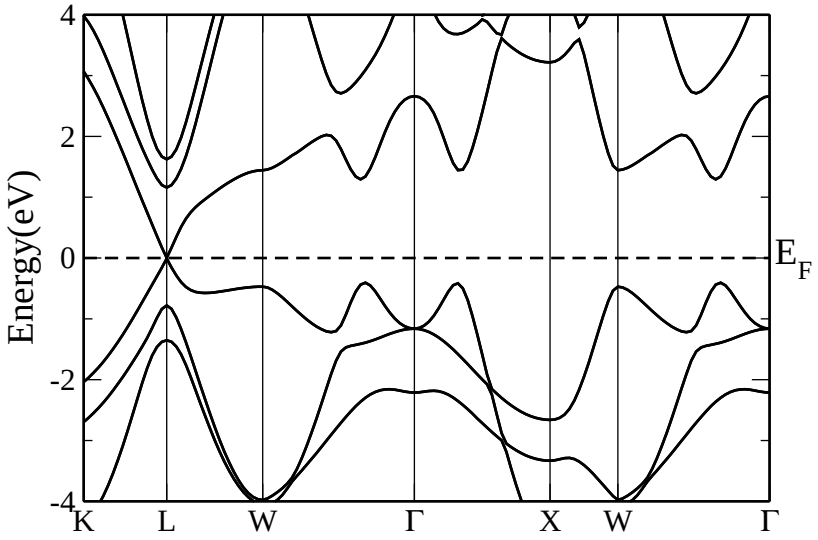

Figure S 1. Electronic structure of PbTe at the experimental lattce constant (a_{exp}=6.4384 $\mathring{A}^2$) which shows that it has zero band gap. This band gap is underestimated within density functional theory and it is far from the experimental band gap of 0.3-0.4 eV.

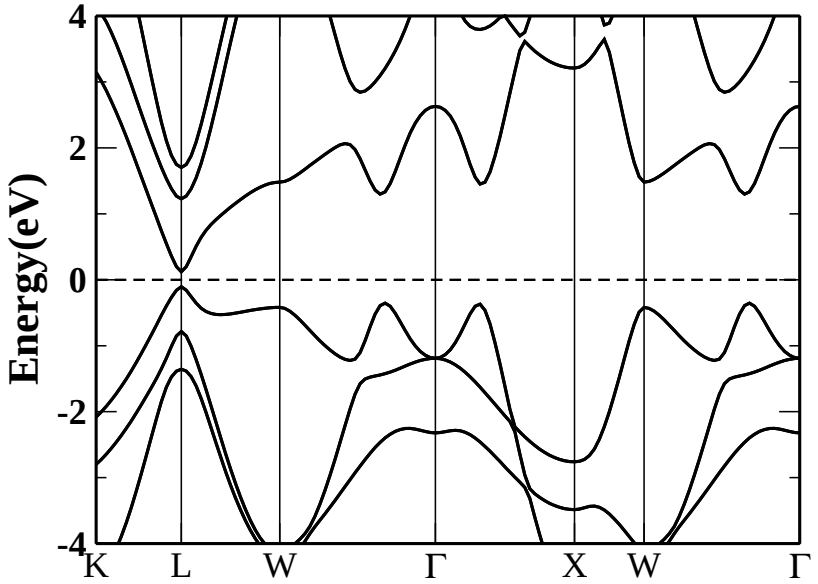

Figure S 2. Electronic structure of PbTe with isotropic strain ϵ_h= -0.014 (a= 6.348 $\mathring{A}$), applied with respect to the experimental lattce constant. At this value of the strain, PbTe is in the TCI state with band gap of 0.23 eV.

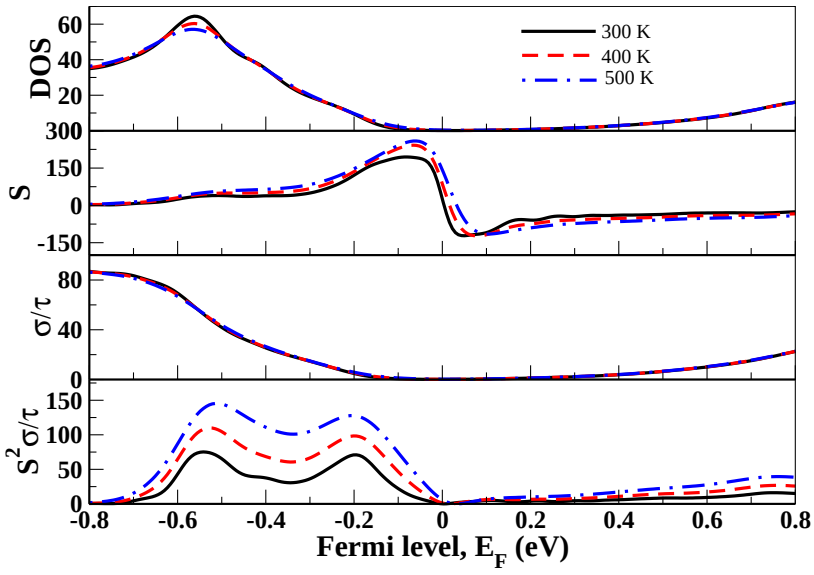

Figure S 3. Transport properties of PbTe at isotropic strain ϵ_h= -0.014 (a=6.348 $\mathring{A}$).

I. APPENDIX

Following the work by Ishida el el[1], we showed that Eq. (6) of the main article can be reduced to Eq. (3) of the main article for the metallic limit, which further can be reduced to Eq. (1) of the main article for the case of a free electron gas.

Within the Boltzmann transport theory, the expression for thermopower (S) is given by

$$\sigma_{\alpha\beta}(T, E_F) = \frac{1}{\Omega}\int \Sigma_{\alpha\beta}(\varepsilon)[-\frac{\partial f_0(T, \varepsilon, E_F)}{\partial \varepsilon}]d\varepsilon \tag{1}$$

and

$$S_{\alpha\beta}(T, E_F) = \frac{1}{eT\sigma_{\alpha\beta}(T, E_F)}\int (\varepsilon - E_F)\Sigma_{\alpha\beta}(\varepsilon)[-\frac{\partial f_0(T, \varepsilon, E_F)}{\partial \varepsilon}]d\varepsilon, \tag{2}$$

where α, β are Cartesian indices, Ω, f_0 are volume of unit cell, and Fermi-Dirac distribution function of the carriers respectively. Central to these relations is the transport distribution function ($\Sigma_{\alpha\beta}$),

$$\Sigma_{\alpha\beta}(\varepsilon) = \frac{e^2}{N}\sum_{i,\mathbf{k}} \tau v_\alpha(i, \mathbf{k}) v_\beta(i, \mathbf{k})\delta(\varepsilon - \varepsilon_{i,\mathbf{k}}), \tag{3}$$

Dropping all the indices and functional variables in the tensor quantities (for sake of simplicity) in the above three equations and substituting Eq. (1) and Eq. (3) in Eq. (2) we get,

$$S = \frac{1}{eT}\frac{\sum\int \tau v^2(\varepsilon)(\varepsilon - E_F)[-\frac{\partial f_0}{\partial \varepsilon}]D(\varepsilon)d\varepsilon}{\sum\int \tau v^2(\varepsilon)[-\frac{\partial f_0}{\partial \varepsilon}]D(\varepsilon)d\varepsilon}, \tag{4}$$

where we have used the identity, $\frac{1}{N}\sum_{i,\mathbf{k}}\delta(\varepsilon - \varepsilon_{i,\mathbf{k}}) = D(\varepsilon)$, where $D(\varepsilon)$ is the density of states.

For a simple metal the expression for S becomes[1],

$$S \approx -\frac{1}{eT}\frac{\sum\int \tau v^2(\varepsilon)(\varepsilon - E_F)^2[f_0(1-f_0)]D(\varepsilon)d\varepsilon}{\sum\int \tau v^2(\varepsilon)[f_0(1-f_0)]n(\varepsilon)d\varepsilon}, \tag{5}$$

where we assumed τ is constant and used $\frac{\partial f_0}{\partial \varepsilon} = f_0(1-f_0)$, $D(\varepsilon) = \frac{dn(\varepsilon)}{d\varepsilon} = \frac{3n(\varepsilon)}{2\varepsilon}$, $n(\varepsilon) \approx n(E_F) + (\frac{dn(\varepsilon)}{d\varepsilon})_{\varepsilon=E_F}$ and $\sigma(\varepsilon) = e^2\tau n(\varepsilon)/m$. $n(\varepsilon)$ is the number of state below ε, $f_0 = \frac{1}{1+(\varepsilon-E_F)/k_BT}$ and k_B is the Boltzmann constant.

Now substituting $x = \frac{(\varepsilon-E_F)}{k_BT}$ in Eq. (5), we get[1]

$$S = -\frac{k_B^2T}{e}\frac{D(E_F)\int_{-\infty}^{\infty}\frac{x^2e^x}{(1+e^x)^2}dx}{N(E_F)\int_{-\infty}^{\infty}\frac{e^x}{(1+e^x)^2}dx}, \tag{6}$$

$$S = -\frac{\pi^2k_B^2T}{3e}[\frac{d\ ln\ n(\varepsilon)}{d\varepsilon}]_{\varepsilon=E_F}, \tag{7}$$

For a free electron gas, we know that,

$n(\varepsilon) = \frac{N(\varepsilon)}{V} = \frac{1}{3\pi^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}\varepsilon^{\frac{3}{2}}$, where V is the volume and $\frac{d\ ln\ n(\varepsilon)}{d\varepsilon} = \frac{3}{2\varepsilon}$. Substituting these relations in Eq. (7), we get

$$S = \frac{8\pi^2k_B^2T}{3e}m(\frac{\pi}{3n})^{\frac{2}{3}}. \tag{8}$$

[1] A. Ishida, T. Yamada, T. Nakano, Y. Takano, and S. Takaoka, Japanese J. of App. Phys., 2011, **50**, 031302.

[2] Y. Noda, K. Masumoto, S. Ohba, Y. Saito, K. Toriumi, Y. Iwata, I. Shibuya, *Acta Cryst.*, Section C: *Crys. Struc. Comm.*, 1987, **43**, 1443.