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Supplementary Material for Computational Search for Strong Topological Insulators: An Exercise in Data Mining and Electronic Structure

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Abstract

We report a data-mining investigation for the search of topological insulators by examining individual electronic structures for over 60,000 materials. Using a data-mining algorithm, we survey changes in band inversion with and without spin-orbit coupling by screening the calculated electronic band structure for a small gap and a change concavity at high-symmetry points. Overall, we were able to identify a number of topological candidates with varying structures and composition. Our overall goal is expand the realm of predictive theory into the determination of new and exotic complex materials through the data mining of electronic structure.

Keywords: electronic structure, data mining, topological insulators, predictive theory

This supplementary material provides the electronic band structure (with and without spin-orbit coupling), as well as the partial and total density of states for each material predicted in this search. The material transforms from direct gap (no spin-orbit interaction included, green line) at specific k-points to an in-direct gap (around the same point in inverse space) when the spin-orbit is included (black line) in the electronic structure calculation, *i.e.* the upper most valence band is pushed way and the anti-crossing feature appears.

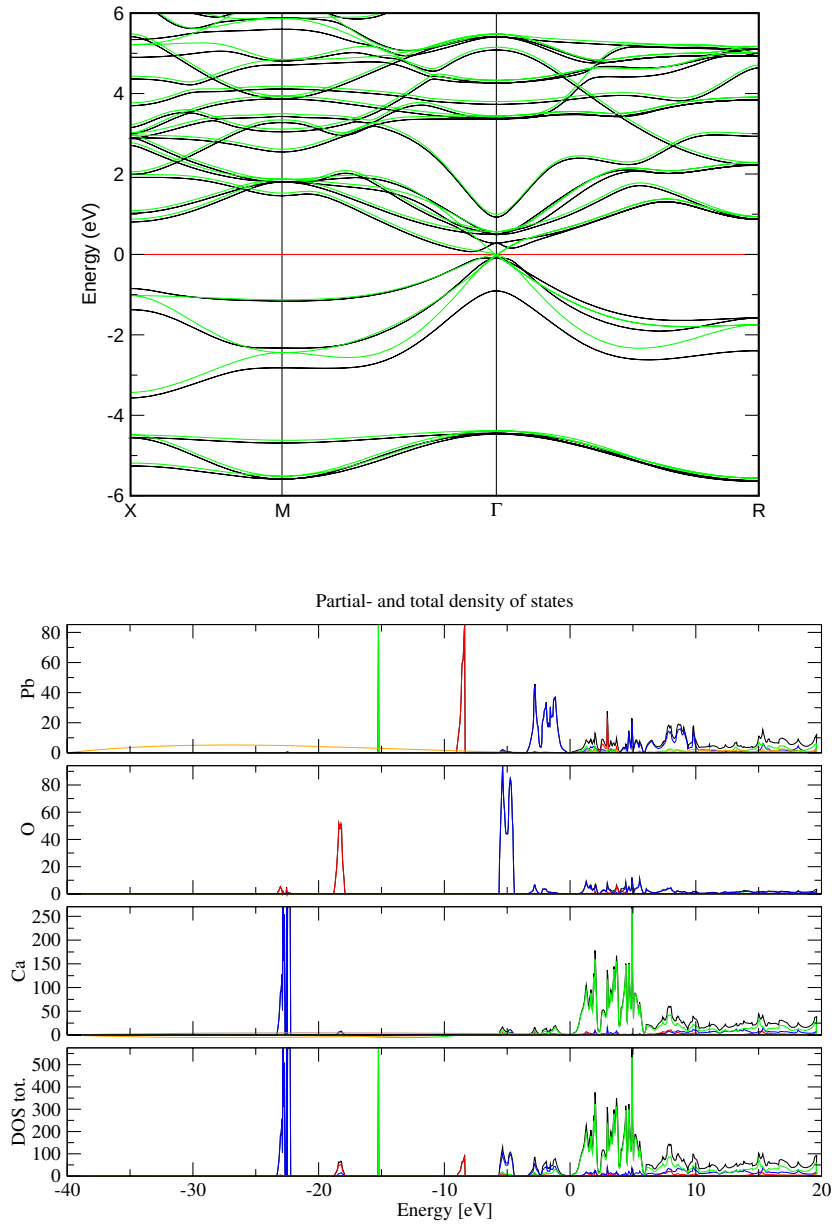
The starting point is the inorganic crystal structure database (ICSD) which is a collection of some 130,000 experimental crystal structures obtained by X-ray and neutron diffraction. Using only the crystal structure as input, we have calculated the electronic structure for about 60,000 entries in the ICSD using a full-potential linear muffin-tin orbital implementation (FP-LMTO) (Skriver, 1984) of density functional theory (DFT) within the local density approximation (LDA). The obtained library is maintained within the electronic structure project (ESP) and has been made available on the web (Ortiz, Eriksson, & Klintenberg, 2009; Klintenberg, Derenso, & Weber, 2002a, 2002b). The data-mining process in the search for new strong topological insulators is rather straight forward. Non-layered small gap materials ($\leq$0.5eV) with an anti-crossing feature at the Γ-point are identified. Furthermore it is verified that the anti-crossing feature disappears when the spin-orbit interaction is switched off. The data-mining identifies 17 compounds as potential strong topological insulators and these are presented in Table 1. These results were then submitted to the condensed matter ArXiv for experimental verification. Since that time, a number of these materials have been investigated further and some verified by experiment. These references are given in the last column of Table 1. Note that because the ESP takes crystal structures from the ICSD, all compounds identified in this study exist and have been structurally determined.

Table 1. Results of the mining algorithm for second generation non-trivial topological insulators. 17 compounds are identified as new potential topological insulators. ARPES measurements should confirm our findings. The materials that have been either confirmed or investigated further are cited in the last column. The electronic band structures, partial and total density of states are given for all materials in the supplementary information

Material	Space Group	Structure Type	Structure Reference	LDA gap [eV]	Other Reports
Ca_3PbO	P m -3 m	$CaTiO_3$	Widera & Schaefer (1980)	0.2	Examined further and verified by Kariyado & Ogata (2011) and Sun, Chen, Yunoki, Li, & Li (2010)
Sr_3PbO	P m -3 m	$CaTiO_3$	Widera & Schaefer (1980)	0.1	Examined further and verified by Kariyado & Ogata (2011) and and Sun et al. (2010)
Ba_3PbO	P m -3 m	$CaTiO_3$	Widera & Schaefer (1980)	0.1	Examined further and verified by Kariyado & Ogata and (2011) Sun et al. (2010)
Yb_3PbO	P m -3 m	$CaTiO_3$	Velden & Jansen (2004)	0.2	No further reports
Ca_3SnO	P m -3 m	$CaTiO_3$	Widera & Schaefer (1980)	0.2	Examined further and verified by Kariyado & Ogata (2011) and Sun et al. (2010)
Sr_3SnO	P m -3 m	$CaTiO_3$	Widera & Schaefer (1980)	0.1	Examined further and verified by Kariyado & Ogata (2011) and Sun et al. (2010)
Yb_3SnO	P m -3 m	$CaTiO_3$	Velden & Jansen (2004)	0.1	No further reports
GdPtSb	F -4 3 m	AlLiSi	de Vries, Thiel, & Buschow (1985)	0.2	No further reports
Bi_2SeTe_2	R -3 m H	Bi_2Te_3	Bland & Basinski (1985)	0.3	Verified by Dai et al. (2012)
Bi_2STe_2	R -3 m H	Bi_2Te_3	Harker (1934)	0.3	No further reports
$PbTl_4Te_3$	I 4/m c m	In_5Bi_3	Bradtmoeller & Boettcher (1993)	0.1	Verified by Arpino (2014)
$BiTl_9Te_6$	I 4/m c m	In_5Bi_3	Doert & Boettcher (1994)	0.1	No further reports
$BiTlTe_2$	R -3 m H	$NaCrS_2$	Hockings & White (1961)	0.0*	Verified by Chen et al. (2010)
$SbTlTe_2$	R -3 m H	$NaCrS_2$	Hockings & White (1961)	0.2	No further reports
Bi_2TeI	C 1 2/m 1	Bi_2TeI	Savilov et al. (2005)	0.1	No further reports
$GeSb_4Te_7$	P -3 m 1	$AgBiSe_2$	Petrov, Imamov, & Pinsker (1968)	0.2	No further reports
HgKSb	P 63/m m c	KZnAs	Vogel & Schuster (1980)	0.2	No further reports

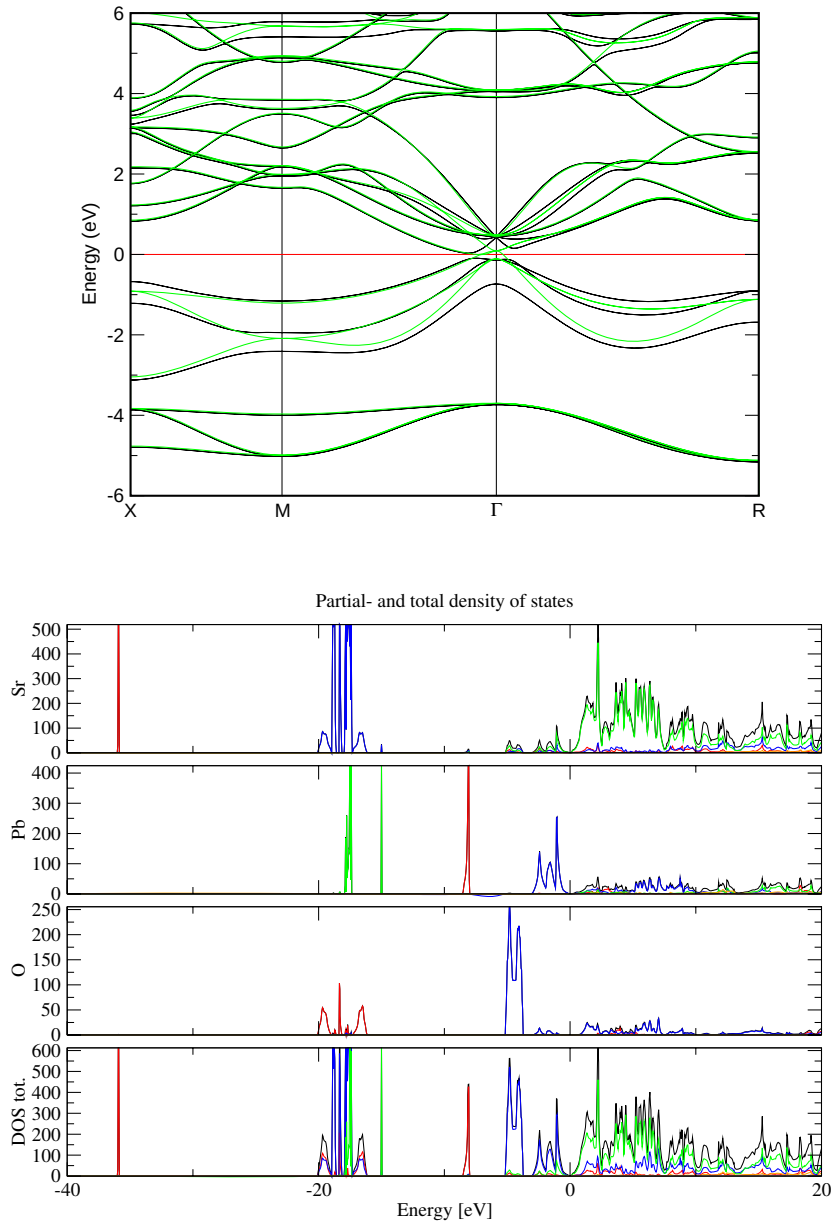
*The material has small hole pockets.

The electronic band structure and partial as well as total density of states for **Ca_3PbO**, P m -3 m.



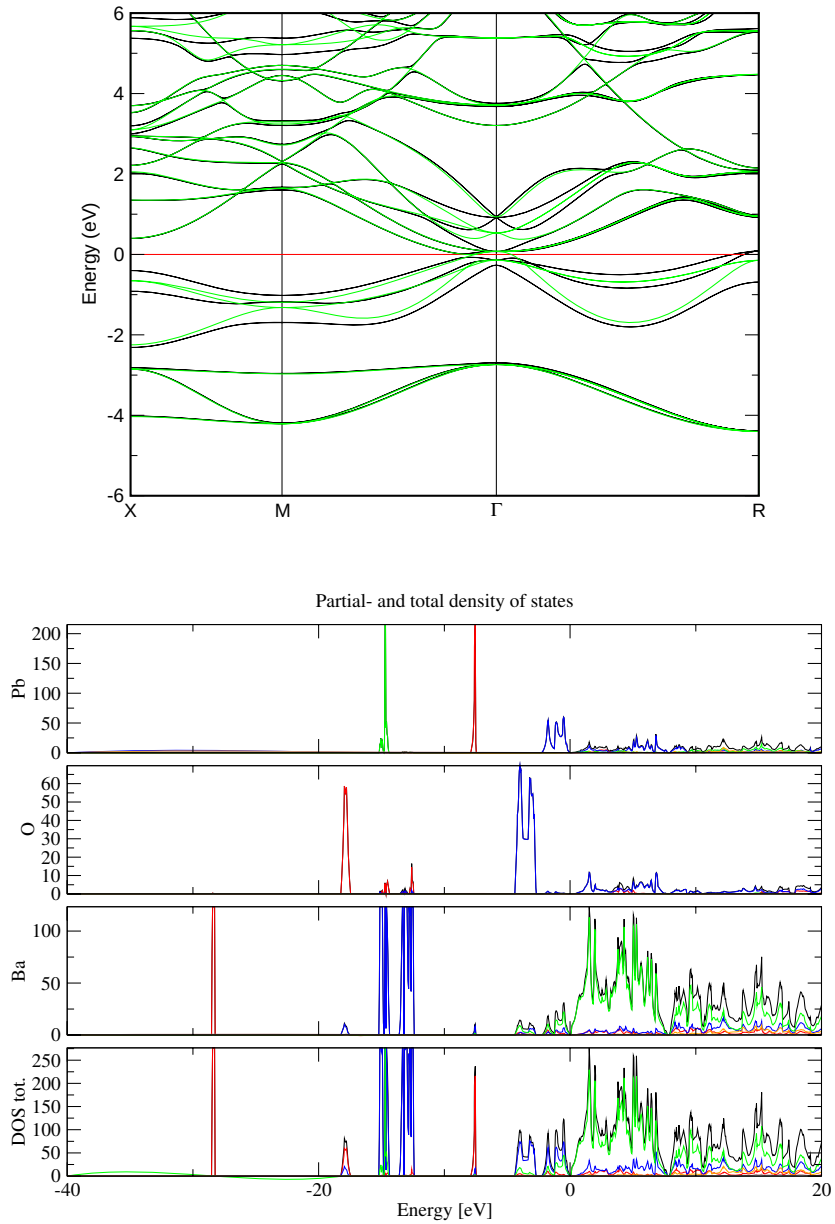
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Sr_3PbO**, P m -3 m.



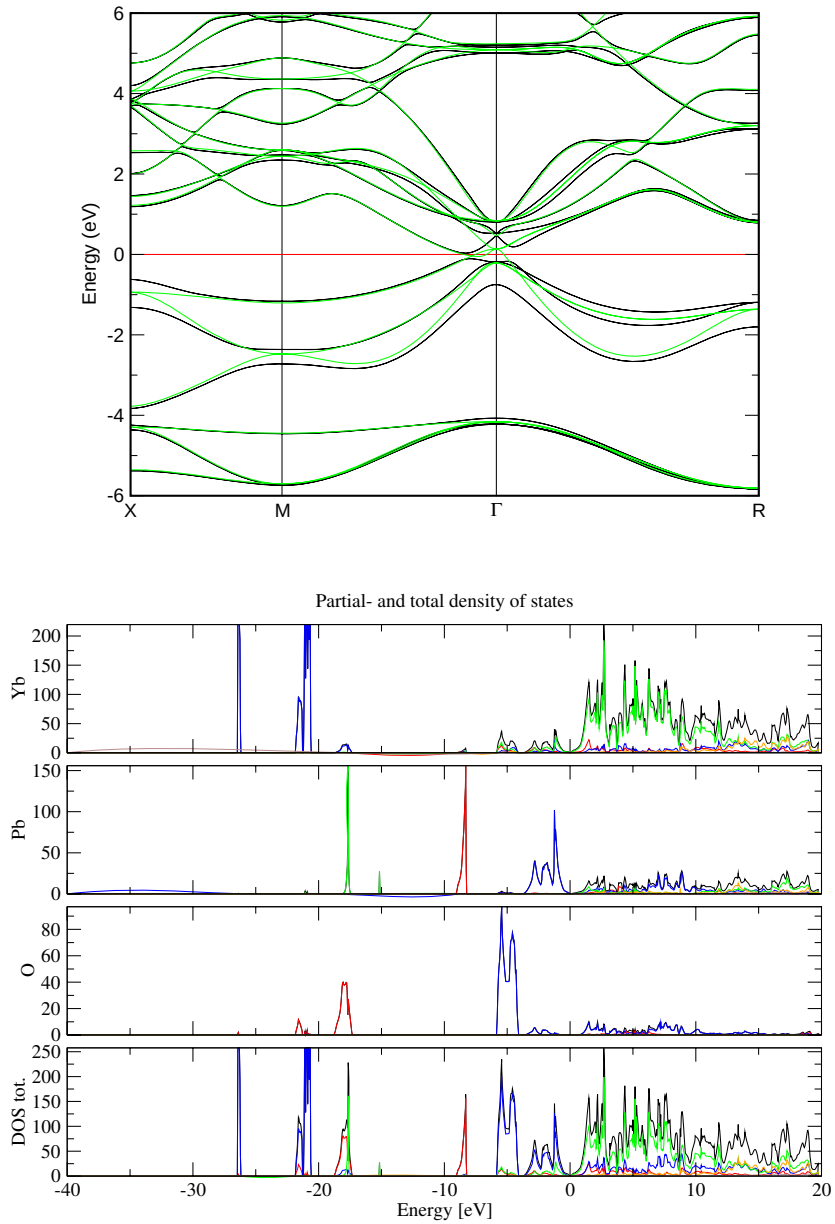
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Ba_3PbO**, P m -3 m.



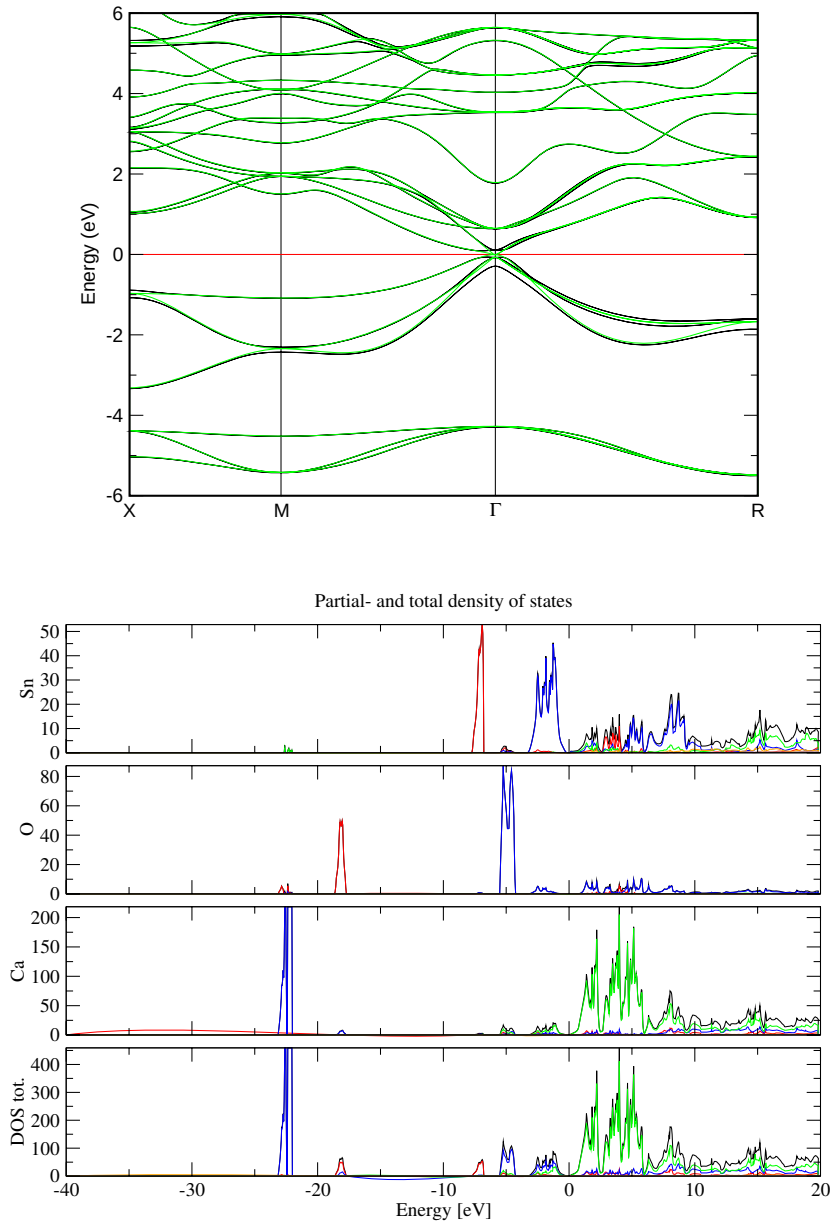
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Yb_3PbO**, P m -3 m.



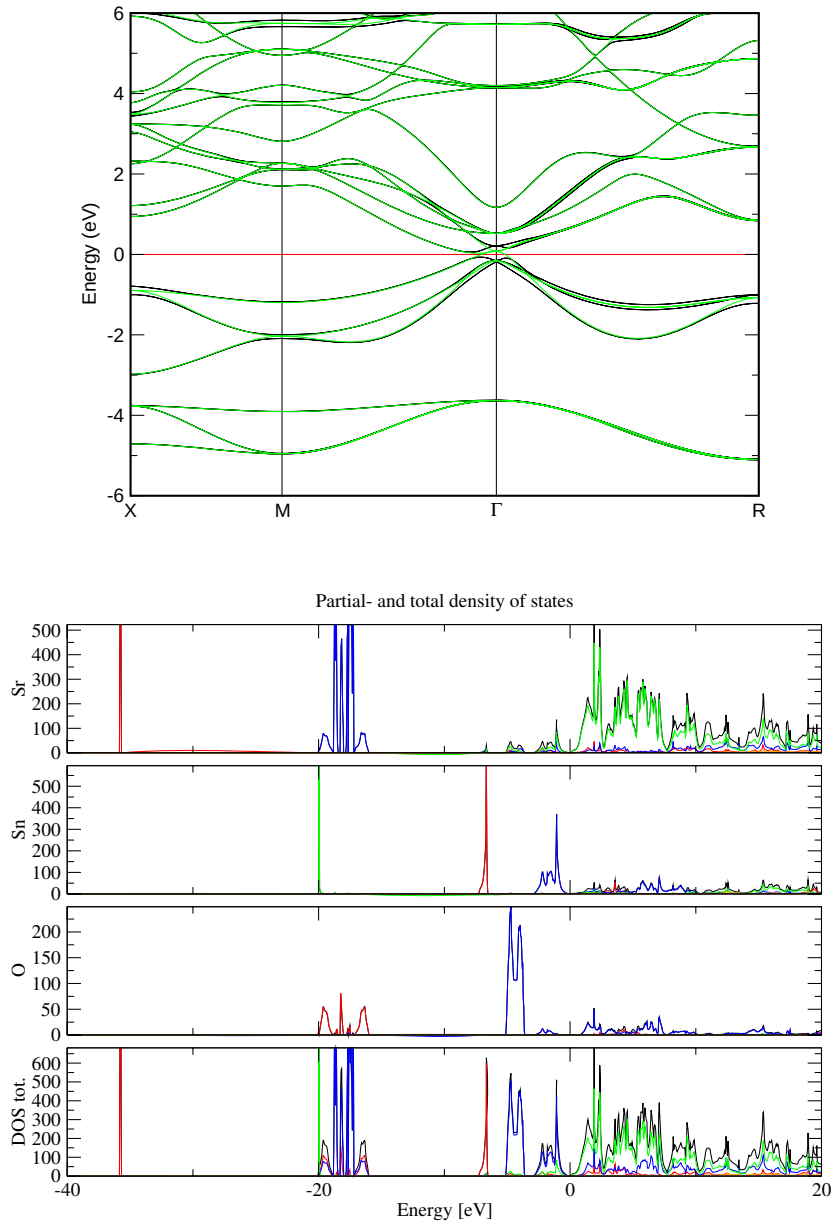
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Ca_3SnO**, P m -3 m.



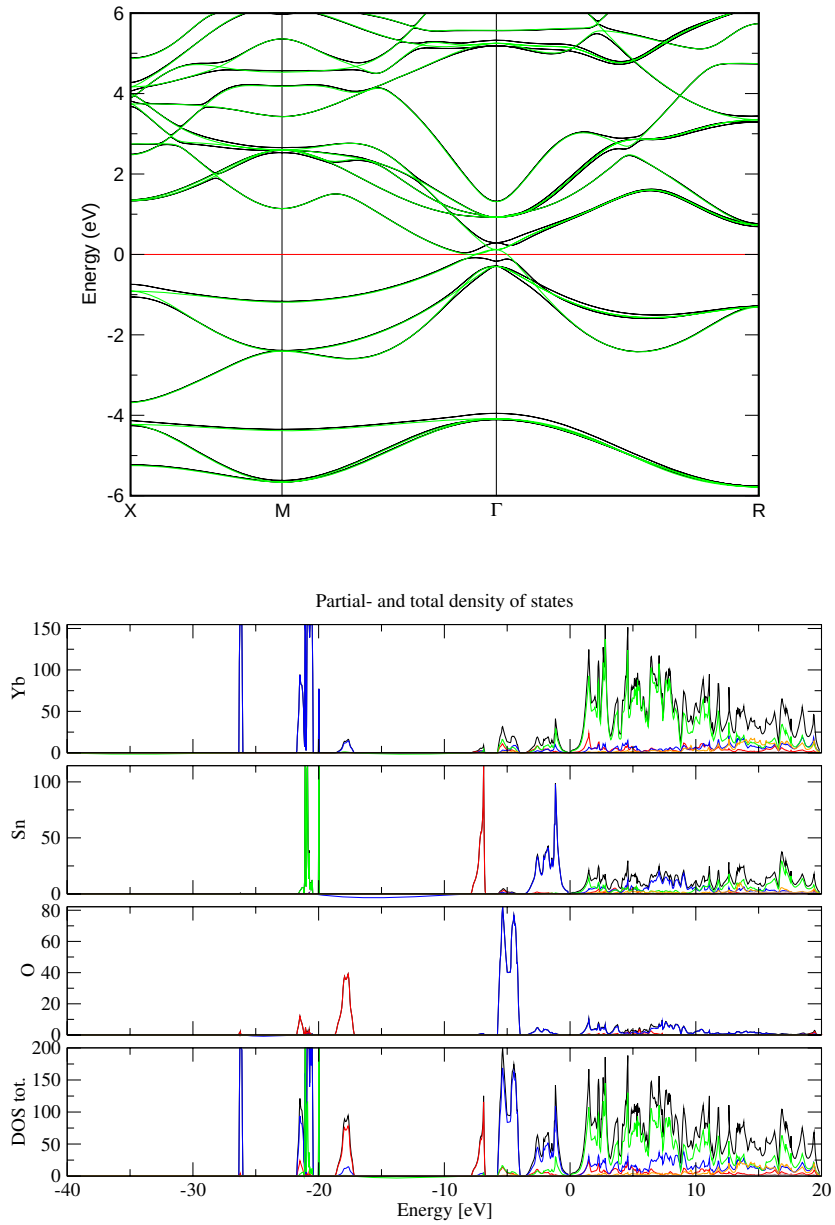
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Sr_3SnO**, P m -3 m.



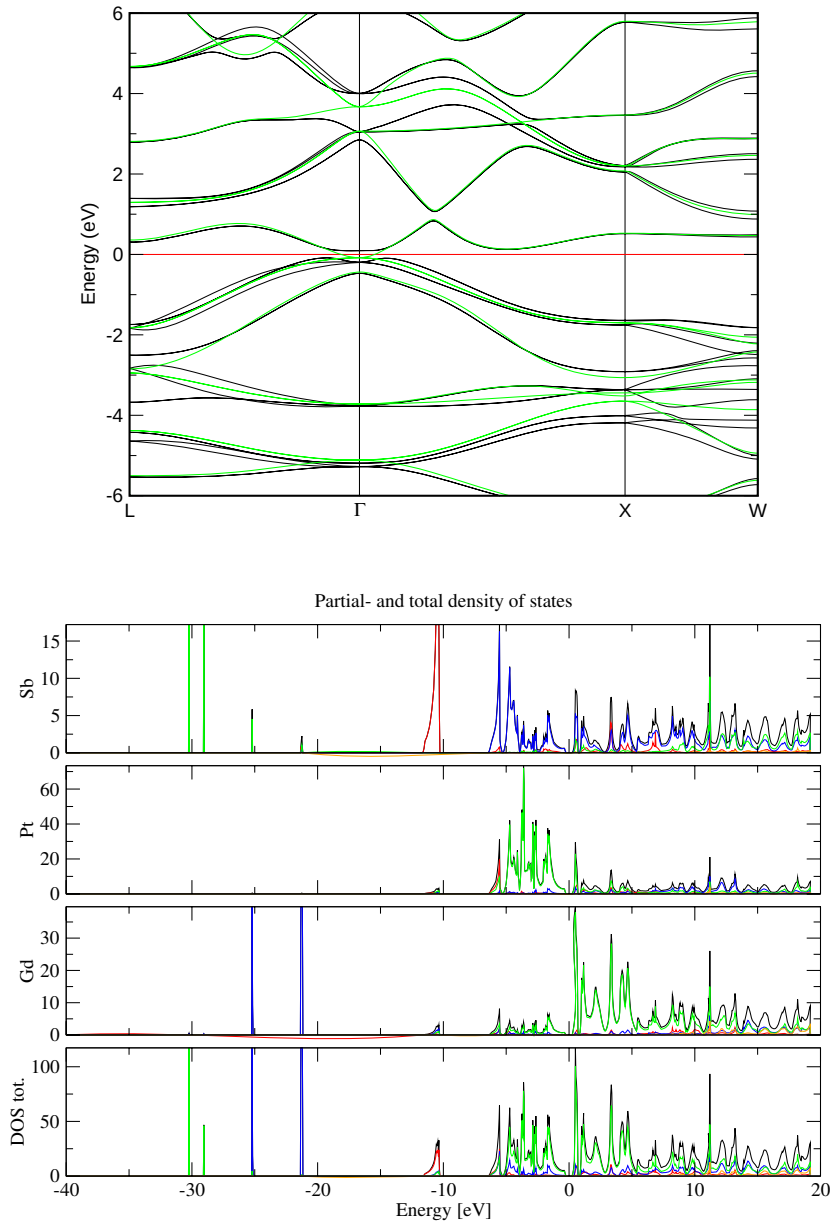
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Yb_3SnO**, P m -3 m.



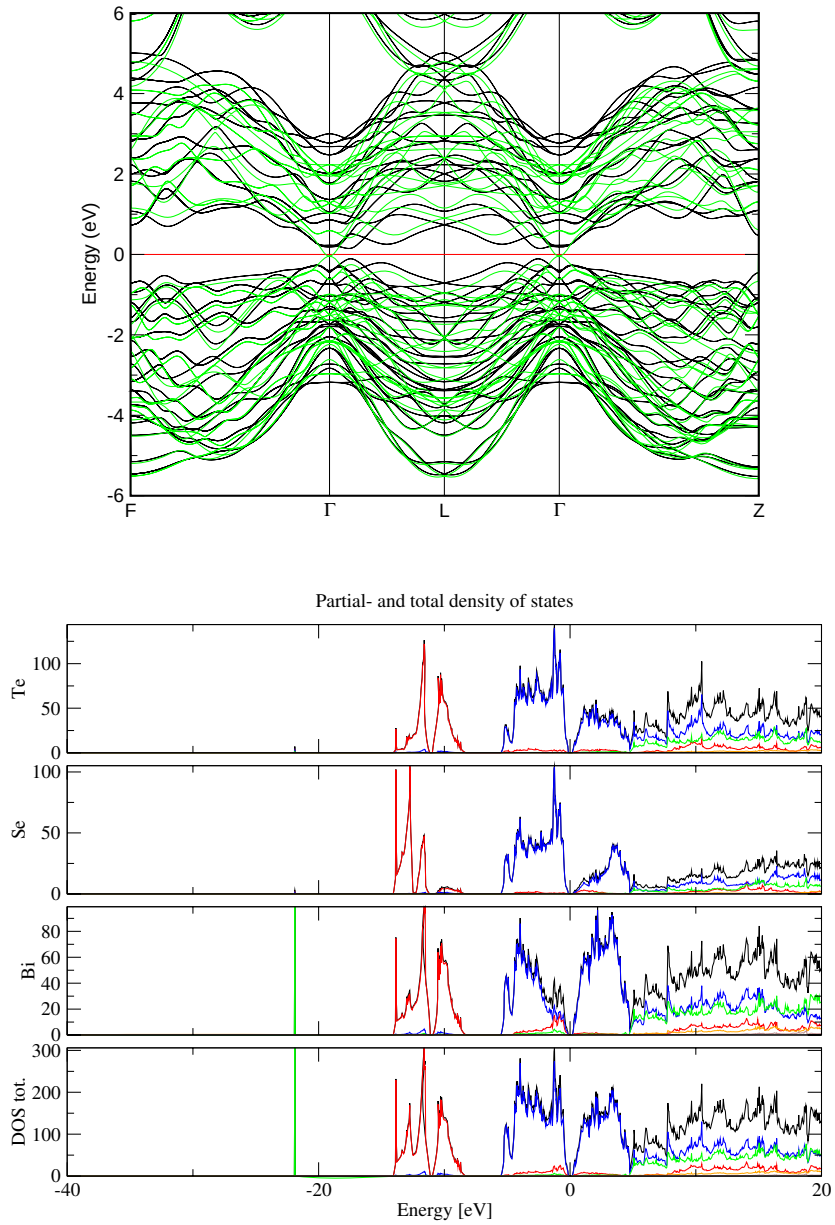
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **GdPtSb**, F -4 3 m.



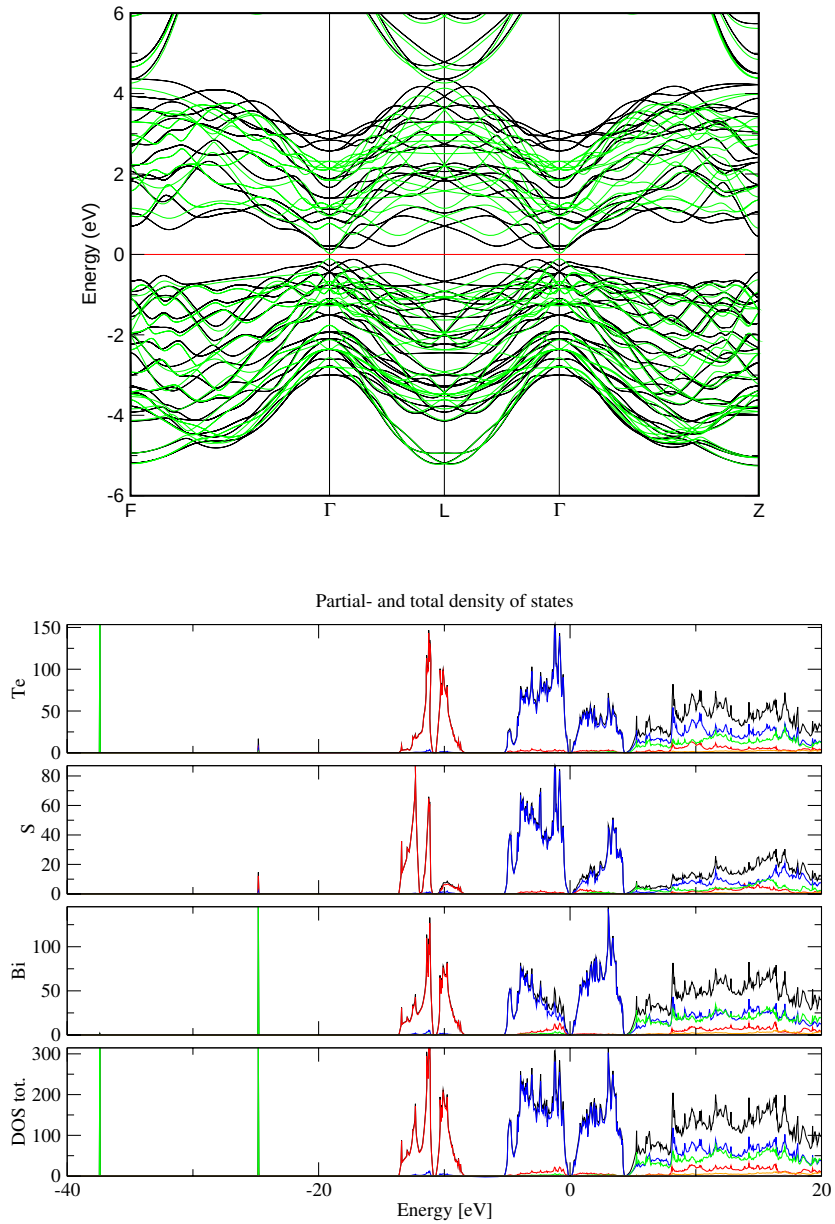
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Bi_2SeTe_2**, R -3 m H.



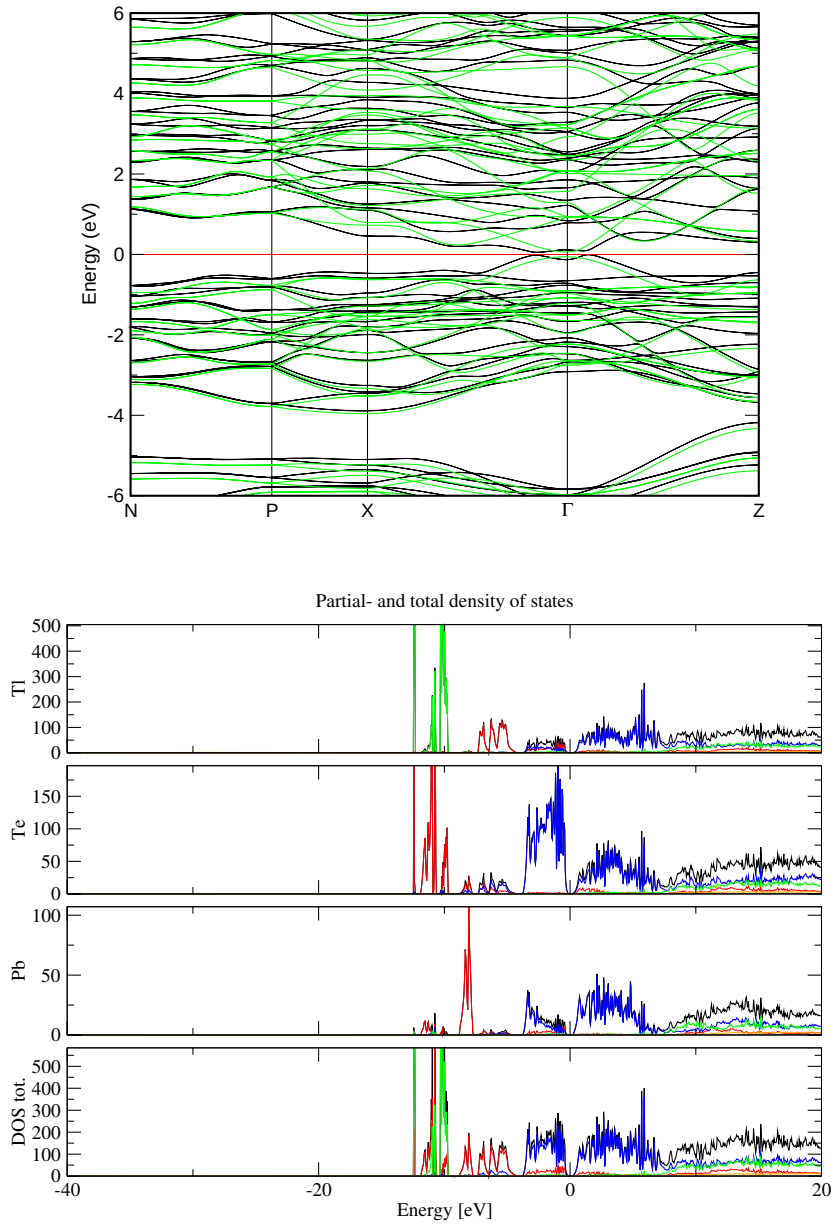
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Bi_2STe_2**, R -3 m H.



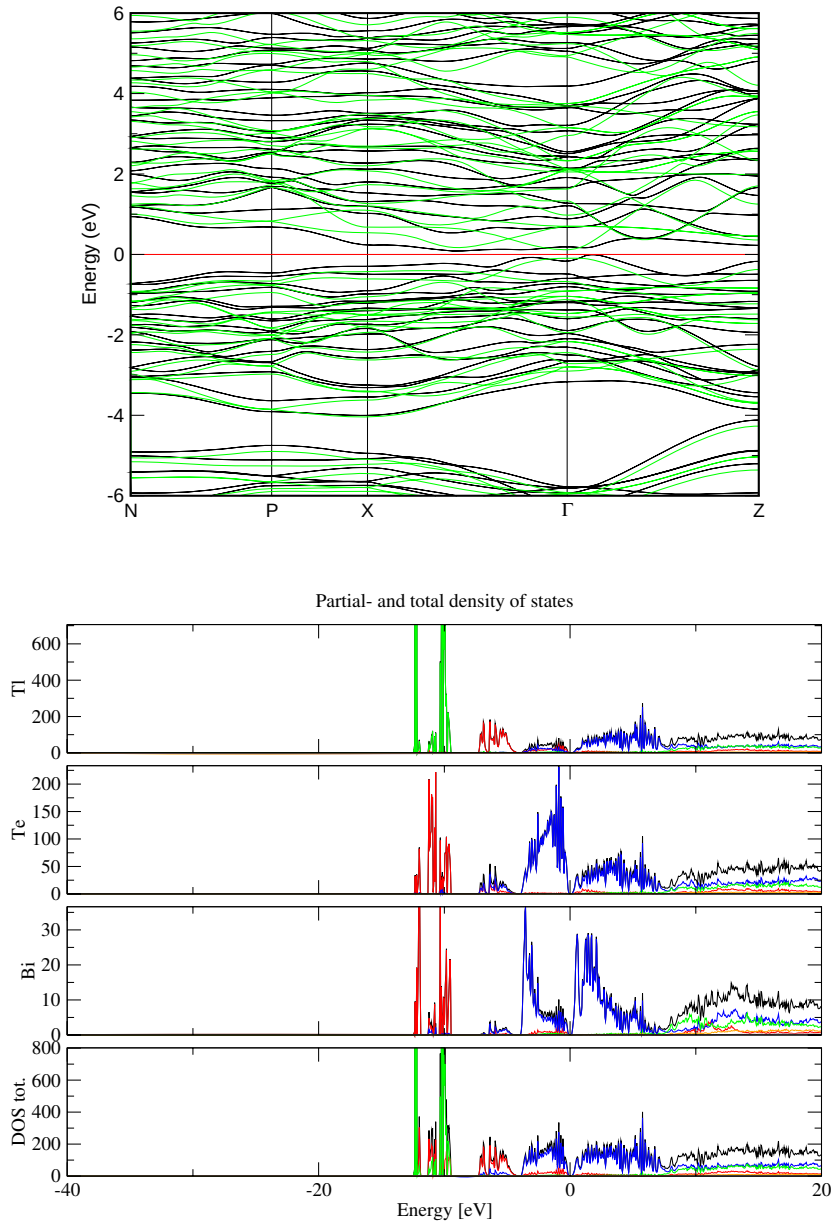
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **PbTl$_4$Te$_3$**, I 4/m c m.



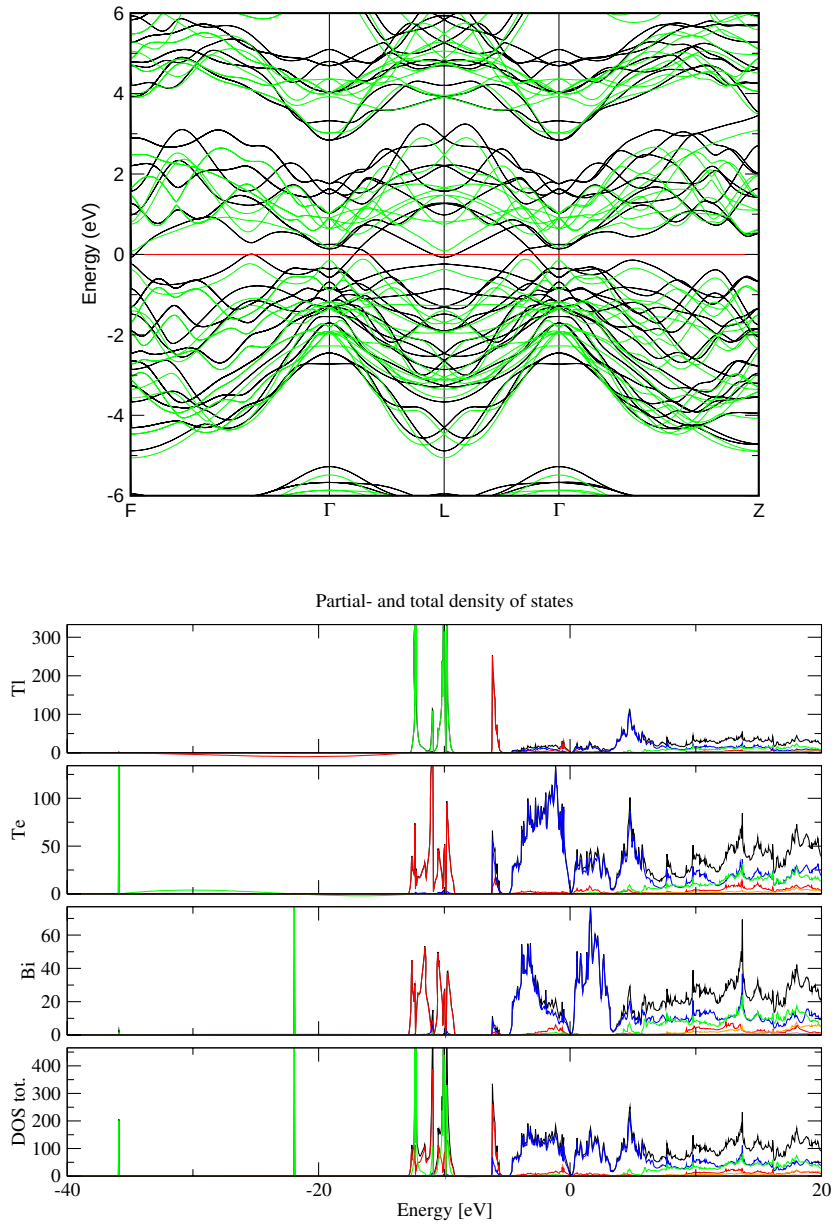
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **BiTl**$_9$**Te**$_6$, I 4/m c m.



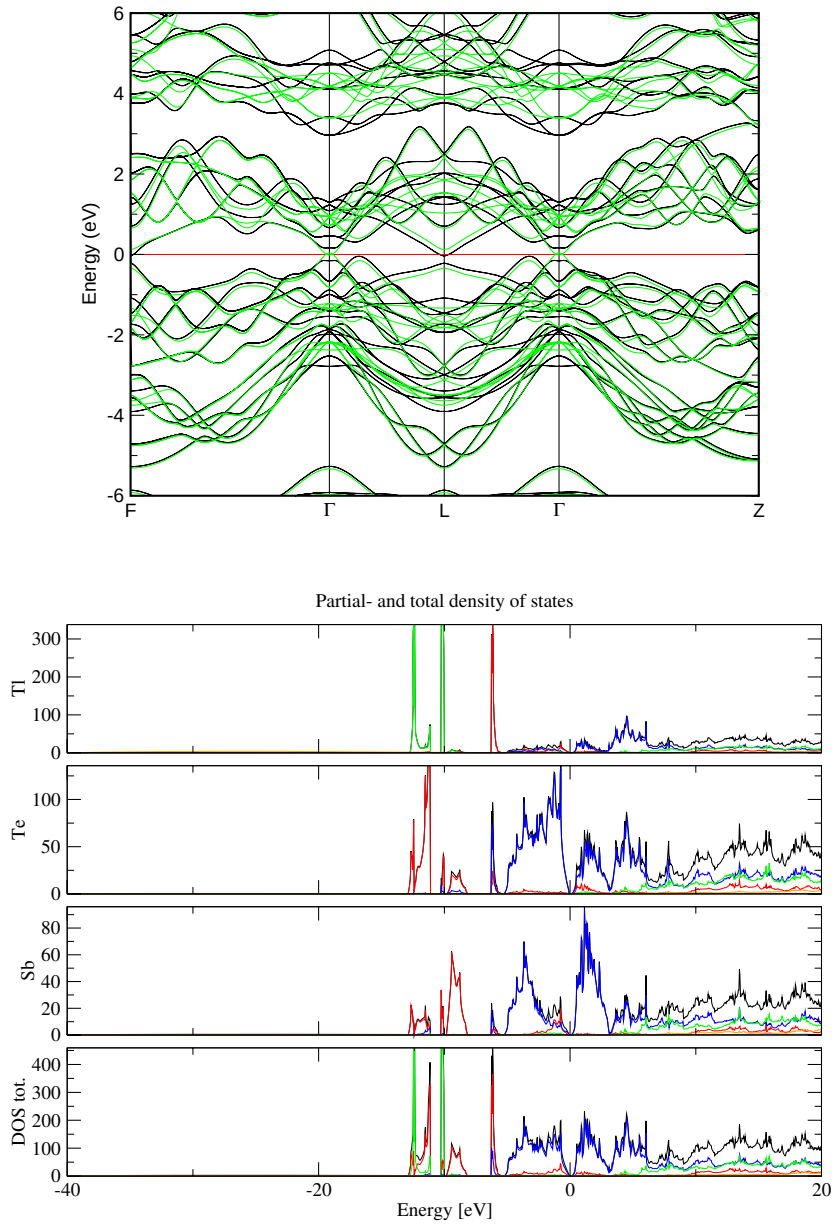
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **$BiTlTe_2$**, R -3 m H.



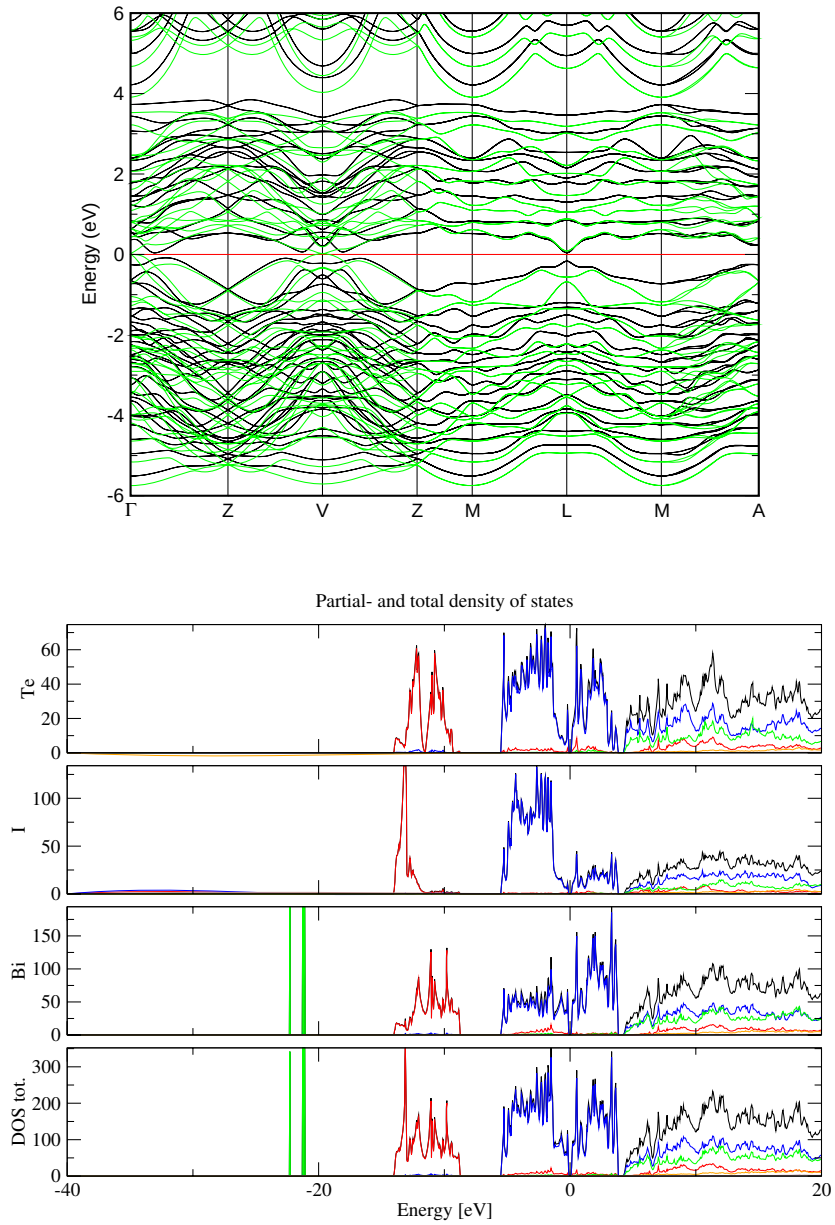
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **SbTlTe**$_2$, R -3 m H.



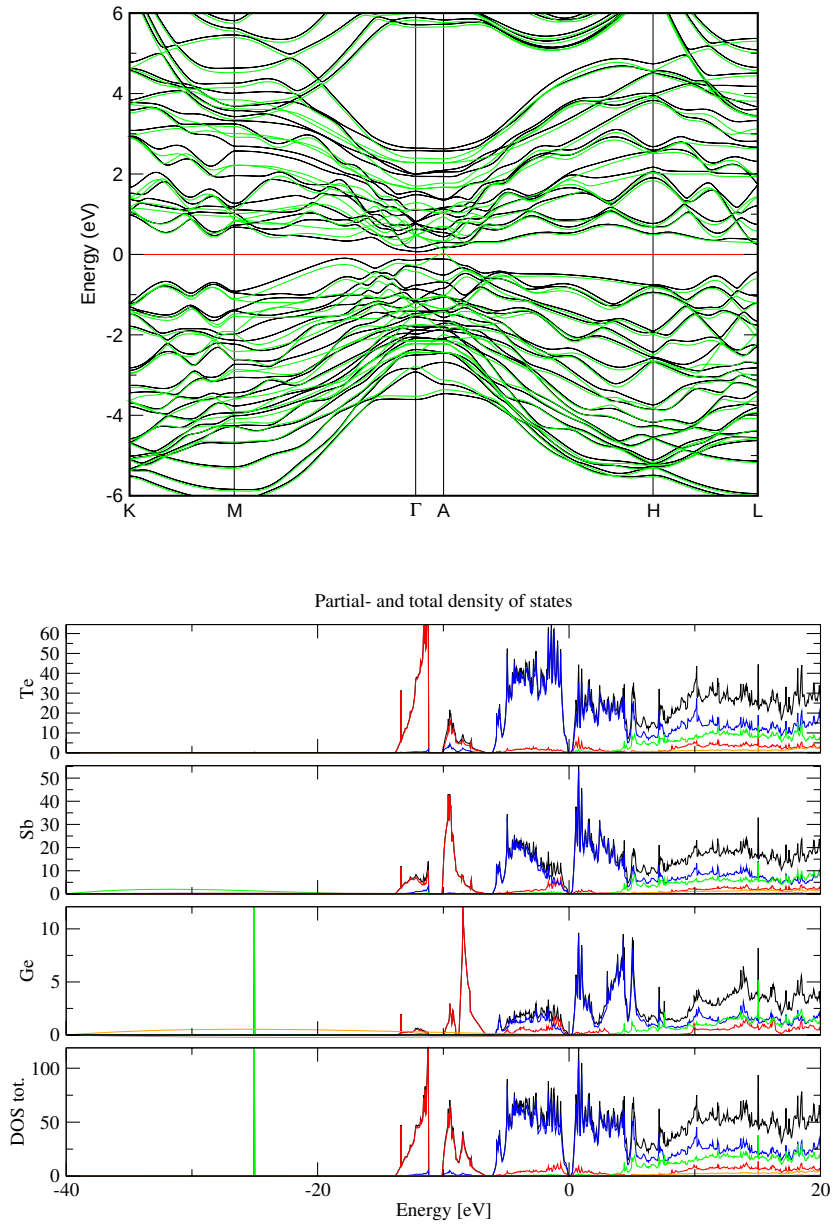
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **Bi_2TeI**, C 1 2/m 1.



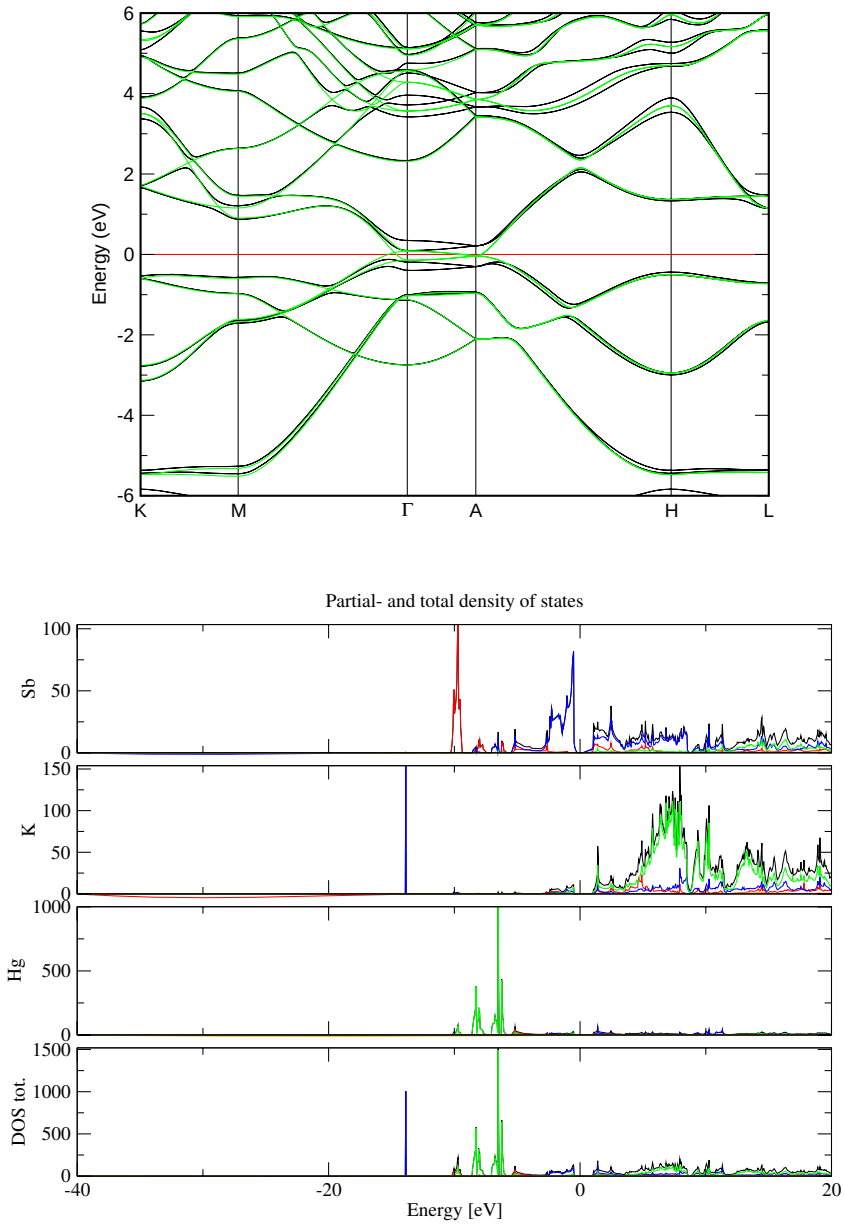
(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **GeSb$_4$Te$_7$**, P -3 m 1.



(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

The electronic band structure and partial as well as total density of states for **HgKSb**, P 63/m m c.



(Upper Panel) Black line with spin-orbit coupling and green line without. (Lower Panel) Black line shows the total density of states in each panel. Red, blue and green show s-, p- and d-type character, respectively.

Because the starting point in this search for new topological insulators is materials that have already been structurally characterized with X-ray diffraction or neutron diffraction, we speculate that there are more candidate compounds that belong to the same families of materials, *e.g.* the inverse perovskites or the Bi_2Te_3 structure type.

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