Electronic Supplementary Material (ESI) for Dalton Transactions.

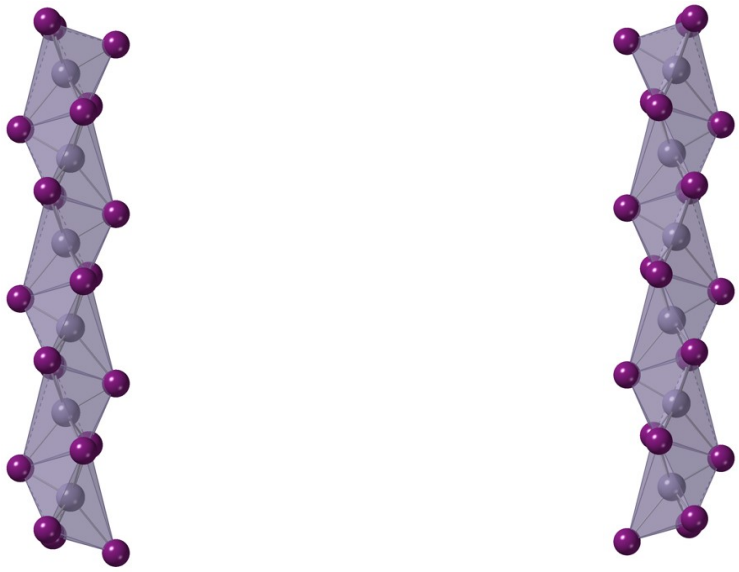
Tuning the dimensionality in chiral and racemic organic/inorganic hybrid Tin halide Compounds

Louis Caussin, Abdelaziz Jouaiti, Daniel Chartrand, W. G. Skene, Sylvie Ferlay

Supplementary Information

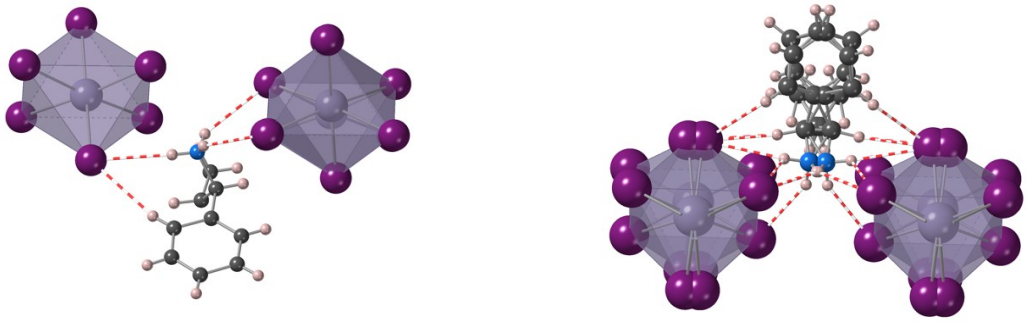
	((*R*)-**EBA**)$_2$-SnBr$_6$	((*S*)-**EBA**)$_2$-SnBr$_6$	(*rac*-**EBA**)$_2$-SnBr$_6$	(*S*)-**EBA**-SnI$_3$	(*R*)-**EBA**-SnI$_3$	*rac*-**EBA**-SnI$_3$
d_{SnX}	2.5794(6) 2.5795(6) 2.5815(6) 2.5924(7) 2.6119(6) 2.6244(6)	2.5808(12) 2.5802(11) 2.5836(12) 2.5926(12) 2.6099(11) 2.6222(11)	2.5908(6) 2.5999(6) 2.6006(7)	2.9434(10) 2.9576(10) 3.1024(10)	2.9439(6) 2.9607(7) 3.1042(7)	2.9804(10) 3.0414(6)
X-Sn-X	87.46(2) 88.21(2) 88.41(2) 89.24(2) 89.33(2) 90.30(2) 90.37(2) 90.43(2) 90.50(2) 90.97(2) 91.91(2) 92.96(2) 176.60(3) 177.42(2) 178.40(3)	87.45(4) 88.28(4) 88.58(4) 89.23(4) 89.42(4) 90.24(4) 90.27(4) 90.44(4) 90.56(4) 90.96(4) 91.78(4) 92.88(4) 176.84(5) 177.52(5) 178.41(5)	91.43(2) 88.57(2) 89.37(2) 89.75(2) 90.63(2) 90.25(2) 180.00(3)	88.67(3) 91.29(3) 94.28(3)	88.663(18) 91.321(18) 94.362(18)	86.58(2) 93.94(2) 94.11(3)
d_{N-X}	3.4128 (4) 3.4198 (4) 3.4413(4) 3.4718(4) 3.4986 (5) 3.5432 (5) 3.5591 (5) 3.6875(4) 3.7629(5)	3.4134(9) 3.4301(8) 3.4520(8) 3.4799(8) 3.5002(9) 3.5139(8) 3.5495(8) 3.5652(9) 3.6770(7) 3.7599 (9)	3.3985(6) 3.4243(6) 3.4324(6) 3.5646(5) 3.6519(6)	3.6340(11) 3.6893(11) 3.7721(10) 3.7827(10) 3.8000(10)	3.6259(7) 3.6923(7) 3.7712(7) 3.7825(8) 3.7894(7)	3.5180(11) 3.5775(9) 3.8142(9) 3.8420(11) 3.8965(9)
d_{C-X}	3.6231(6) 3.6663(5) 3.7233 (6)	3.6141(12) 3.6720(10) 3.7197 (10)	3.5845(6) 3.7151(6)	3.8783(13) 3.9476(11)	3.8599(9) 3.9526(8)	3.6158(14) 3.8647(14) 3.9282(17)

Table S1. Main distances (standard deviation in parentheses) measured for ((*S*)-**EBA**)$_2$-SnBr$_6$, ((*R*)-**EBA**)$_2$-Sn Br$_6$, (*rac*-**EBA**)$_2$-Sn Br$_6$, (*S*)-**EBA**-SnI$_3$, (*R*)-**EBA**-SnI$_3$ and *rac*-**EBA**-SnI$_3$.



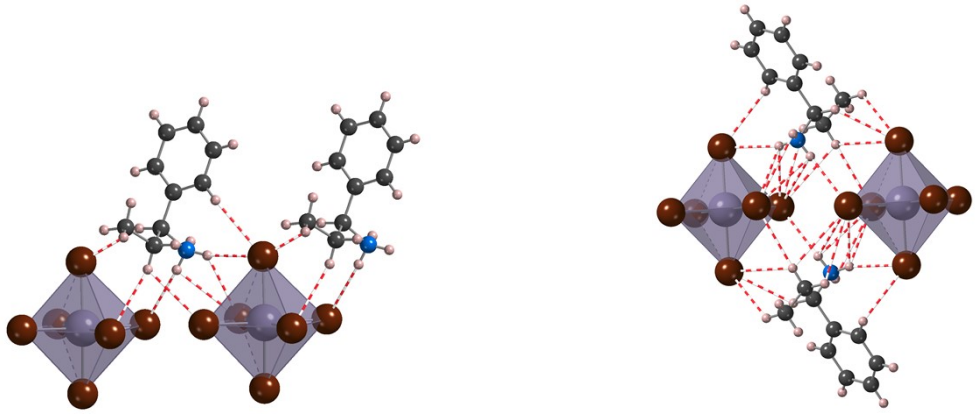
a **b**

Figure S1: Representation of the inorganic $(SnI_3)_n$ chains for (*S*) (a)- or (*R*)-**EBA**-SnI$_3$ (b) ; the chains are mirror images.



a **b**

Figure S2: Representation of the structures and short contacts in (a) (*S*)- or (*R*)-**EBA**-SnI_3 and (b) (rac)-**EBA**-SnI_3.



a **b**

Figure S3: Representation of the structures and short contacts in (a) ((*S*)- or (*R*)- **EBA**)$_2$-$SnBr_6$ and (b) ((rac)- **EBA**)$_2$-$SnBr_{63}$.

SHAPE program analysis[1]

Deviation considering 6-coordinated Sn
(CShM, Continuous Shape Measures)

	((*R*)-**EBA**)$_2$-SnBr$_6$	((*S*)-**EBA**)$_2$-SnBr$_6$	(*rac*-**EBA**)$_2$-SnBr$_6$	(*S*)-**EBA**-SnI$_3$	(*R*)-**EBA**-SnI$_3$	*rac*-**EBA**-SnI$_3$
Deviation from Oh CShM	19.056	19.046	19.324	17.124	17.127	Too much disorder

XRPD measurements

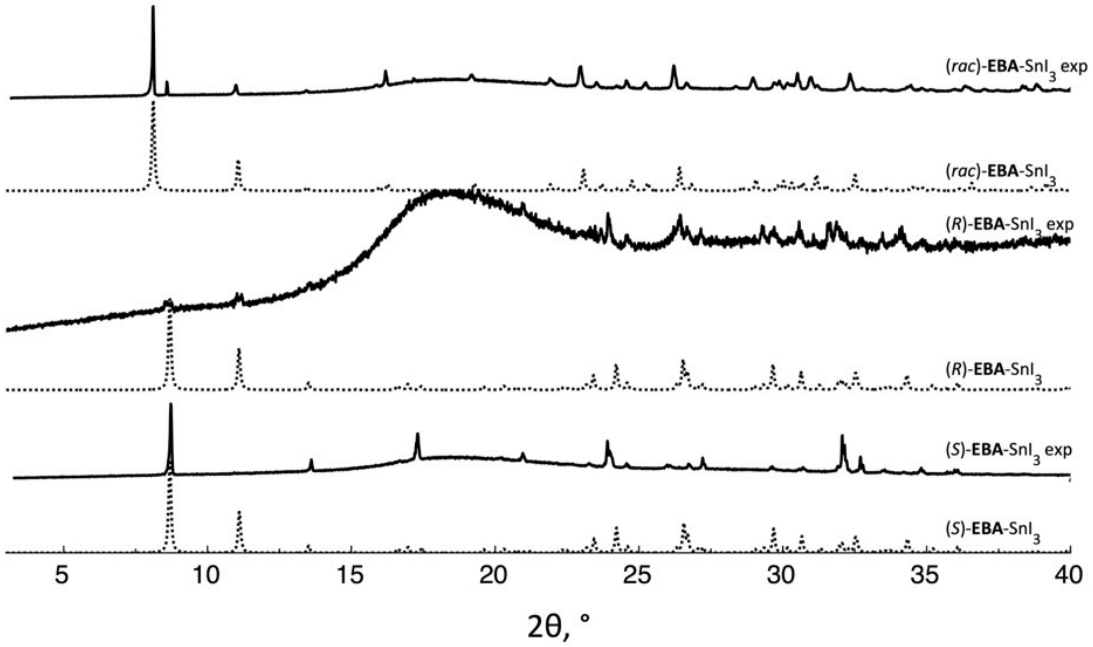


Figure S4: (*S*)- or (*R*)-**EBA**-SnI$_3$ and (rac)-**EBA**-SnI$_3$, comparison of the simulated and experimental powder X-Ray diffraction studies (PXRD) diagrams.

a

1 a) M. Llunell, D. Casanova, J. Girera, P. Alemany, S. Alvarez, SHAPE, version 2.1, Universitat de Barcelona, Barcelona, Spain ; b) S. Alvarez, P. Alemany, D. Casanova, J. Cirera, M. Llunell, D. Avnir, Shape maps and polyhedral interconversion paths in transition metal chemistry, *Coord. Chem. Rev.*, 2005, **249**, 1693-1708.

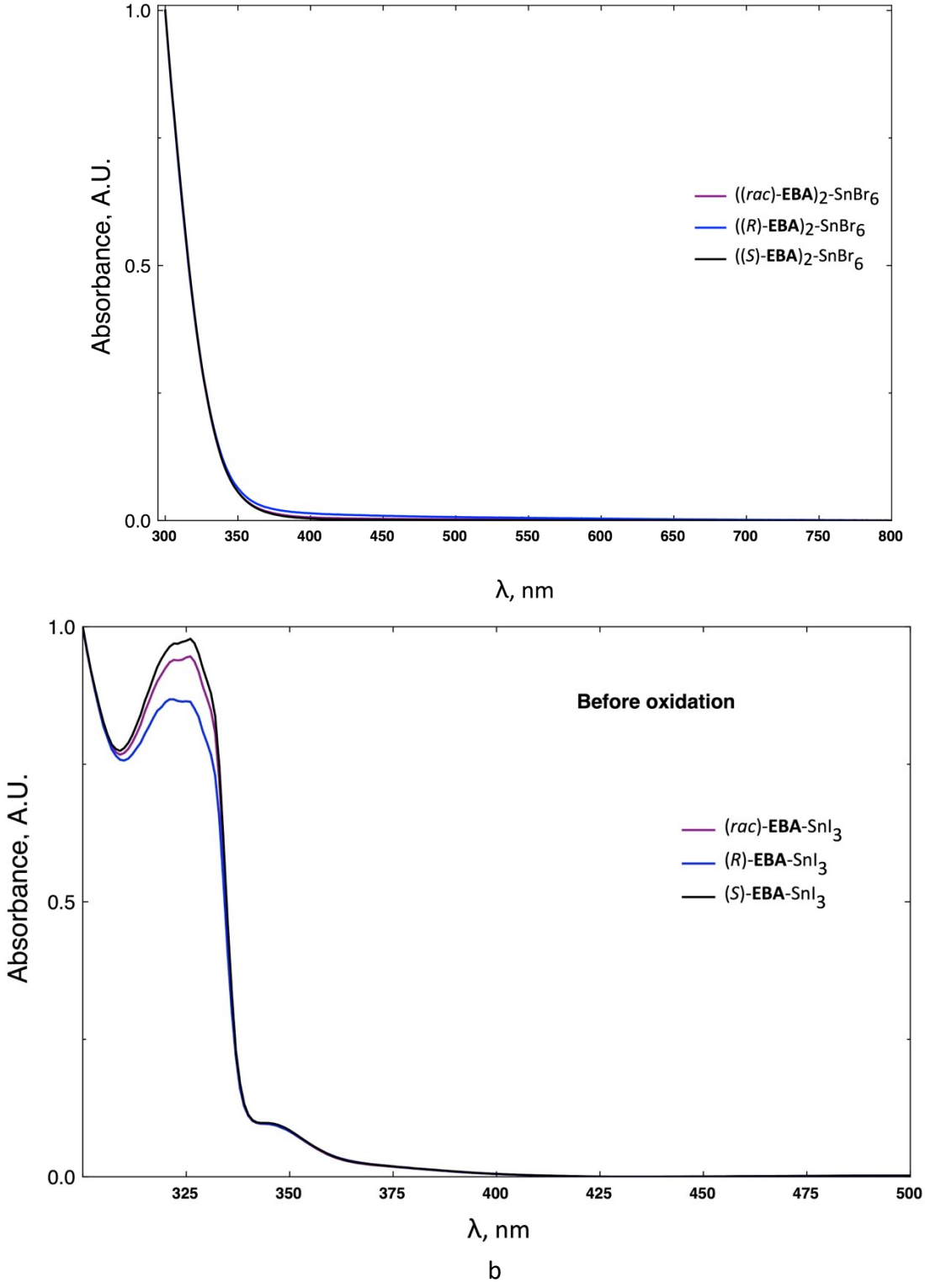


Figure S5: UV-vis spectra in a DMF solution of chiral antimony halide compounds (a) 0D ((S)- or (R)-**EBA**)$_2$-SnBr$_6$ and ((rac)-**EBA**)$_2$-SnBr$_6$ series and (b) 1D series. (b) (*S*)- or (*R*)-**EBA**-SnI$_3$ and (rac)-**EBA**-SnI$_3$.

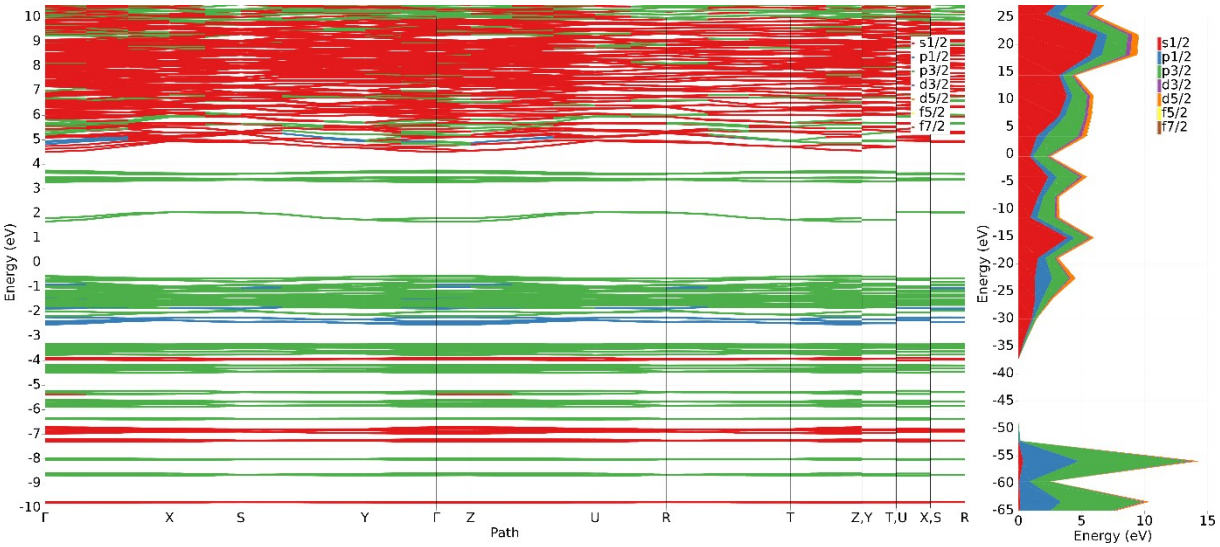


Figure S6: Computed electronic band structures (left) and density of states (right) for (rac-**EBA**)2-SnBr6.

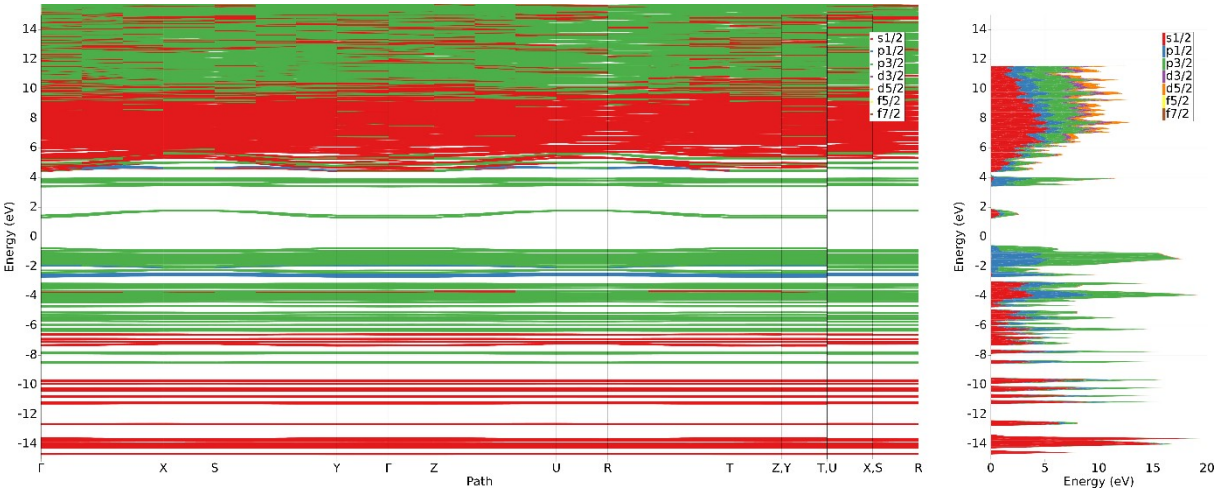


Figure S7: Computed electronic band structures (left) and density of states (right) for (*S*-**EBA**)2-SnBr6.

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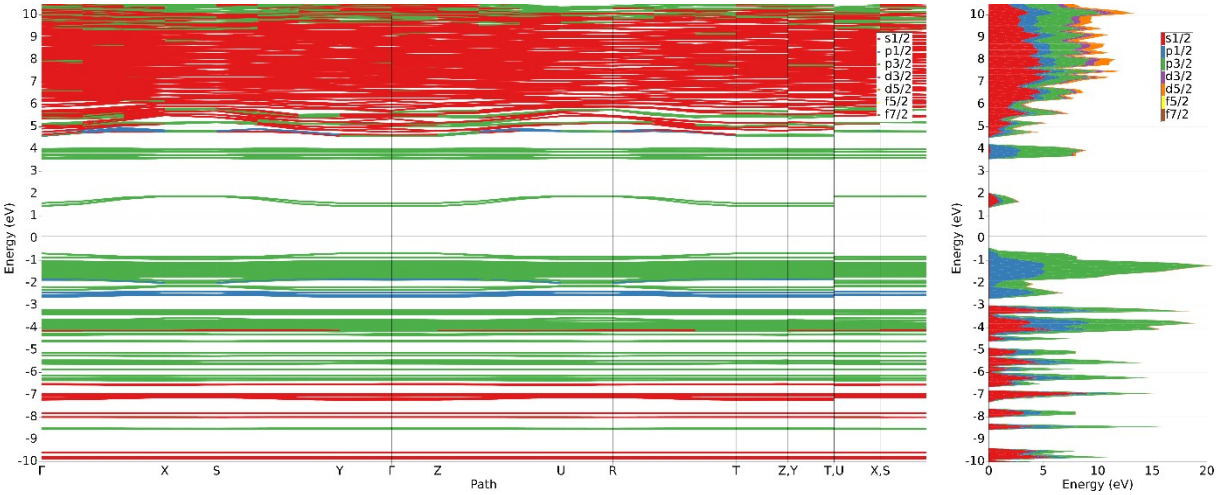

Figure S8: Computed electronic band structures (left) and density of states (right) for (*R*-**EBA**)2-SnBr6.

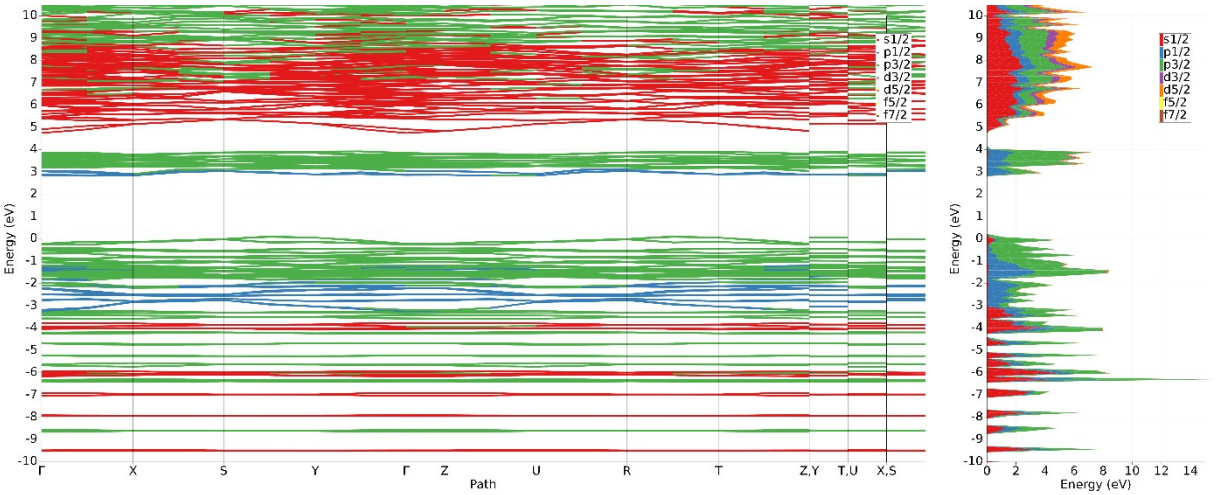

Figure S9: Computed electronic band structures (left) and density of states (right) for (*S*-**EBA**)-SnI_3.

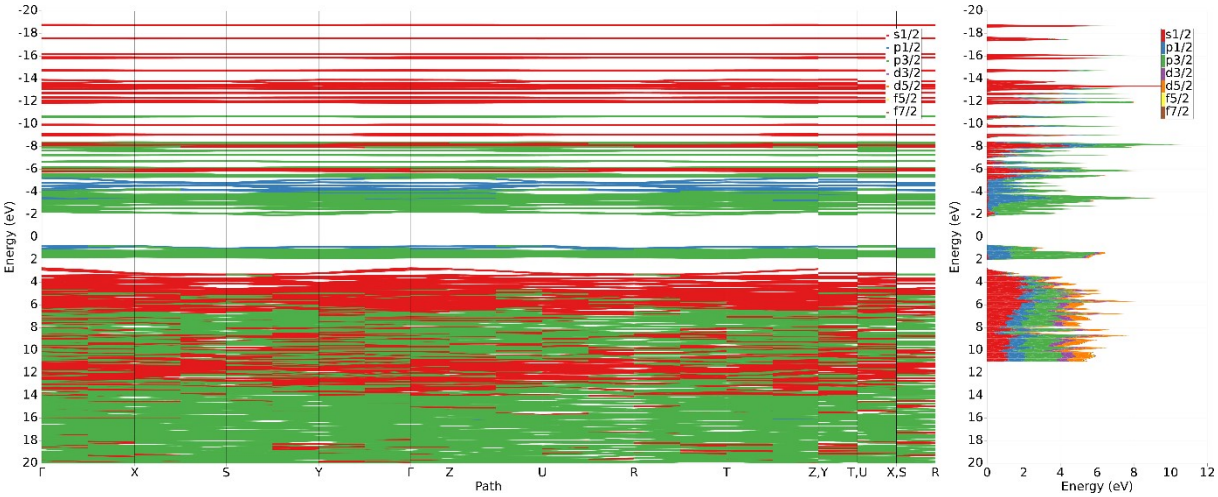

Figure S10: Computed electronic band structures (left) and density of states (right) for (*R*-**eba**)-SnI_3.