

## Supplementary Materials for: Double perovskites as p-type conducting transparent semiconductors: A high-throughput search

Hai-Chen Wang,<sup>1</sup> Paul Pistor,<sup>1</sup> Miguel A. L. Marques,<sup>1,\*</sup> and Silvana Botti<sup>2</sup>

<sup>1</sup>*Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany*

<sup>2</sup>*Institut für Festkörperteorie und -Optik, Friedrich-Schiller-Universität Jena and European Theoretical Spectroscopy Facility, Max-Wien-Platz 1, 07743 Jena, Germany*

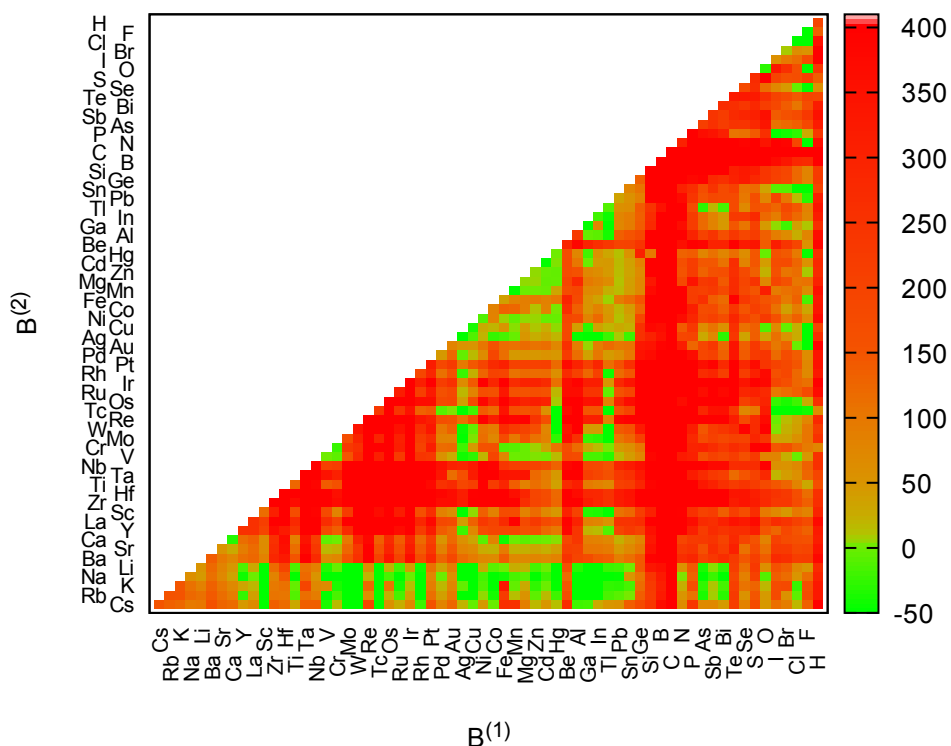


FIG. S1: Distance to the convex hull for the  $\text{Rb}_2\text{B}^{(1)}\text{B}^{(2)}\text{F}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

\* [miguel.marques@physik.uni-halle.de](mailto:miguel.marques@physik.uni-halle.de)

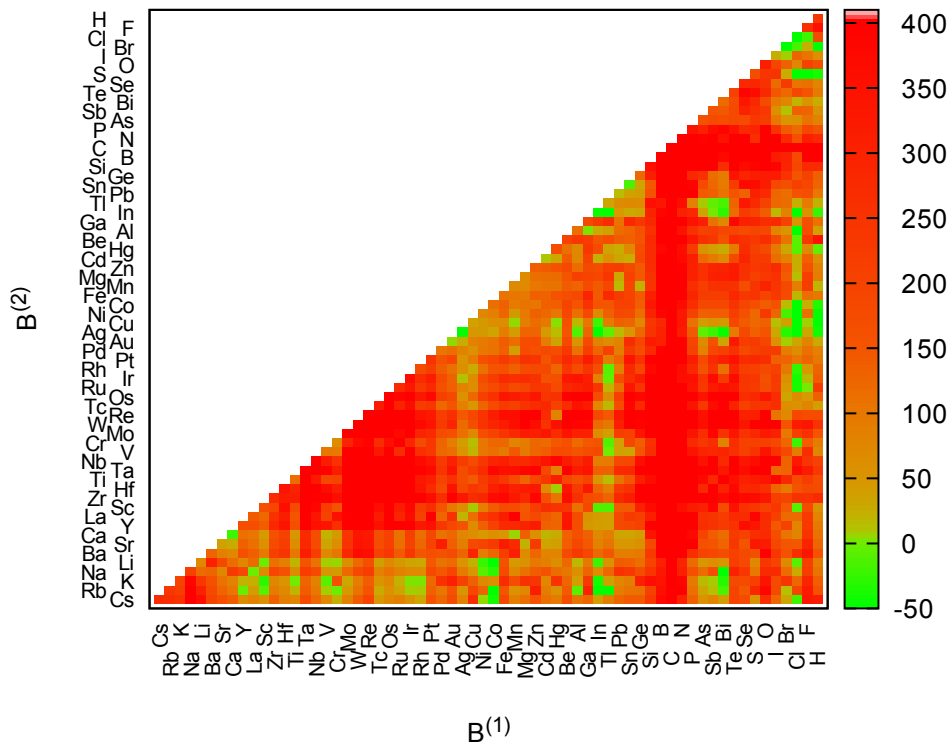


FIG. S2: Distance to the convex hull for the  $\text{Rb}_2\text{B}^{(1)}\text{B}^{(2)}\text{Cl}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

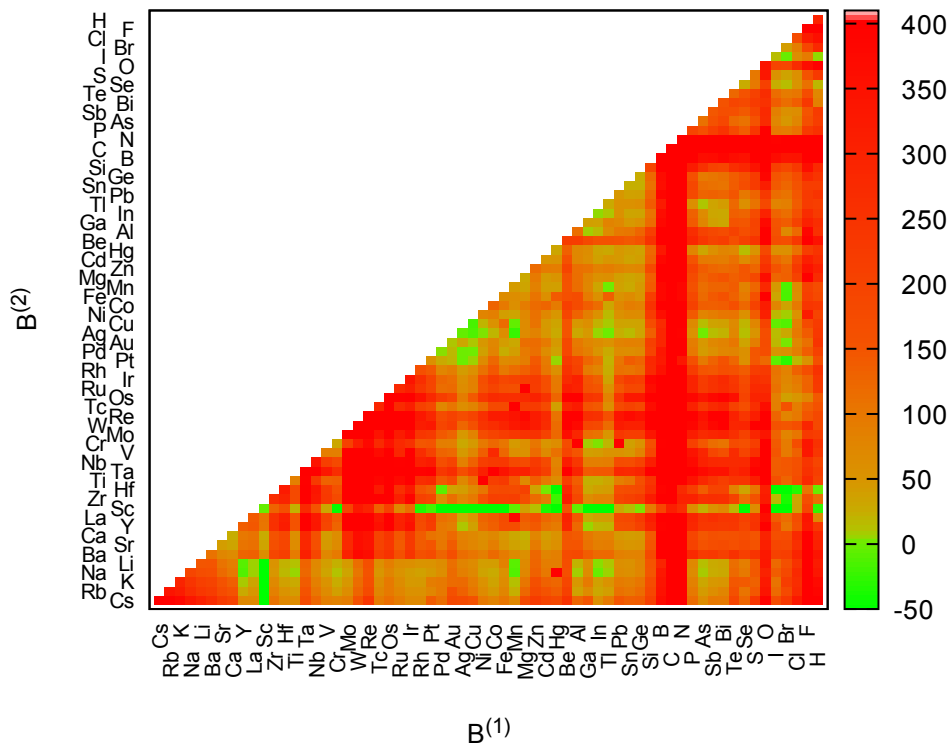


FIG. S3: Distance to the convex hull for the  $\text{Rb}_2\text{B}^{(1)}\text{B}^{(2)}\text{Br}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

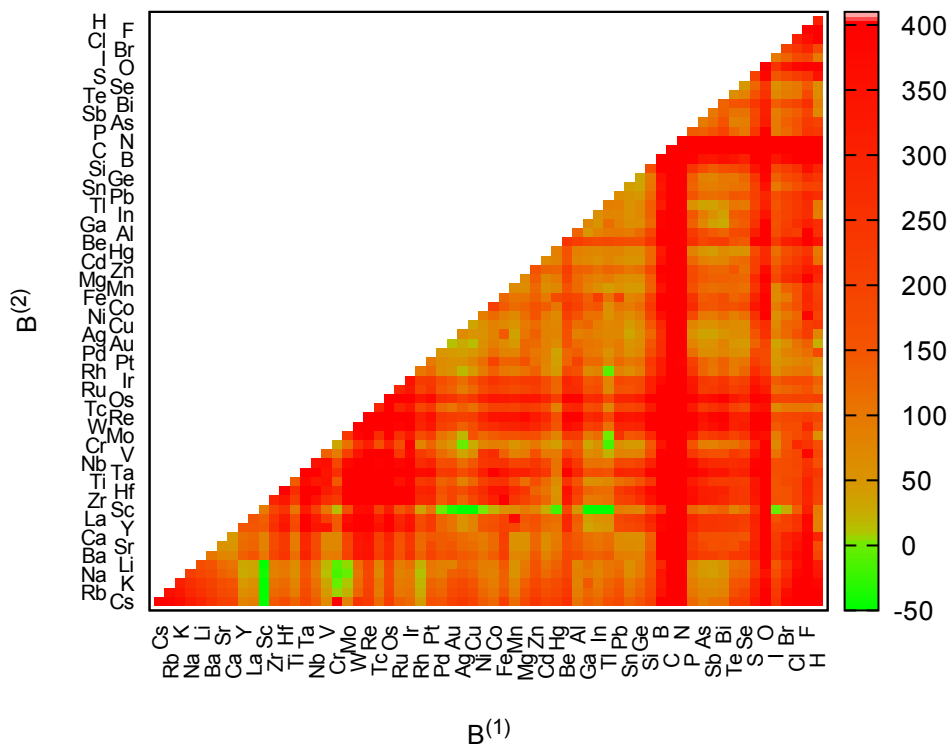


FIG. S4: Distance to the convex hull for the  $\text{Rb}_2\text{B}^{(1)}\text{B}^{(2)}\text{I}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

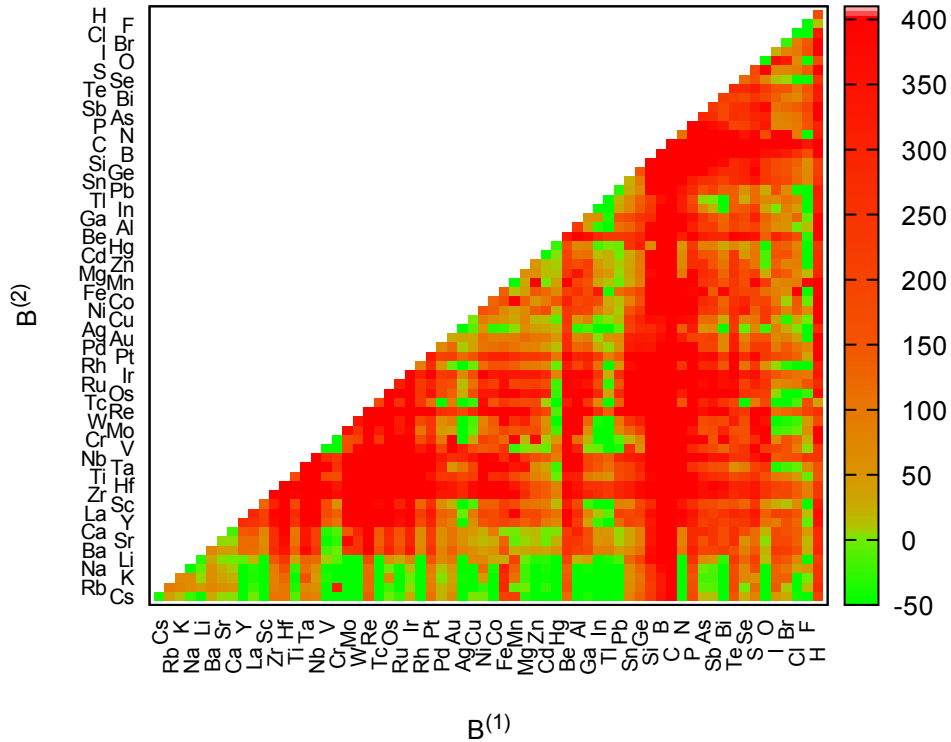


FIG. S5: Distance to the convex hull for the  $\text{Cs}_2\text{B}^{(1)}\text{B}^{(2)}\text{F}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

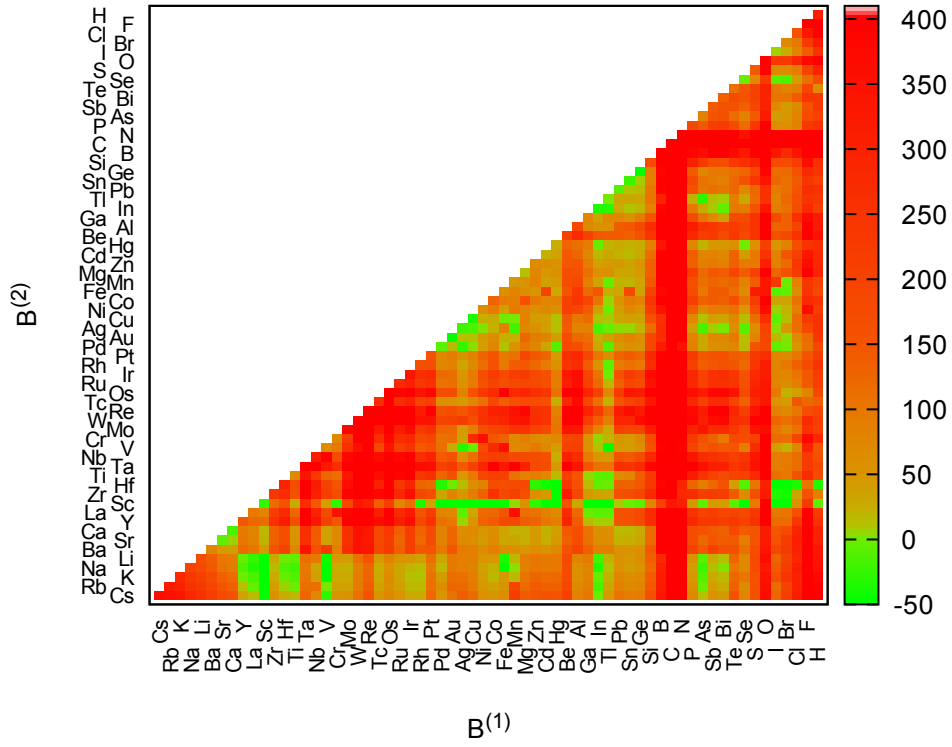


FIG. S6: Distance to the convex hull for the  $\text{Cs}_2\text{B}^{(1)}\text{B}^{(2)}\text{Br}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

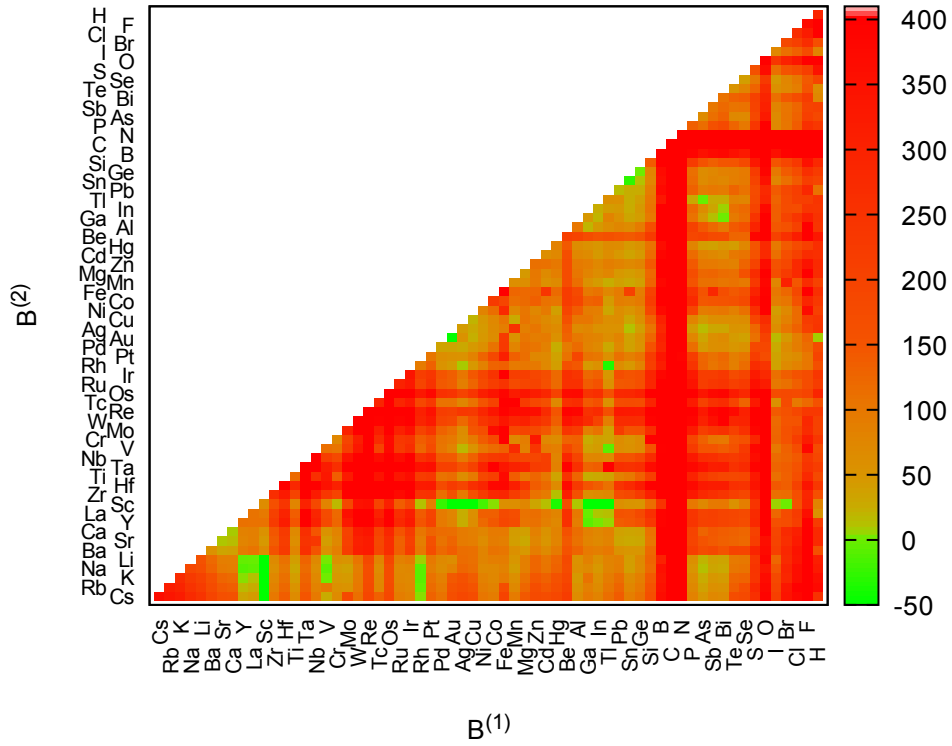


FIG. S7: Distance to the convex hull for the  $\text{Cs}_2\text{B}^{(1)}\text{B}^{(2)}\text{I}_6$  double perovskites in meV/atom. Green corresponds to theoretically stable compounds.

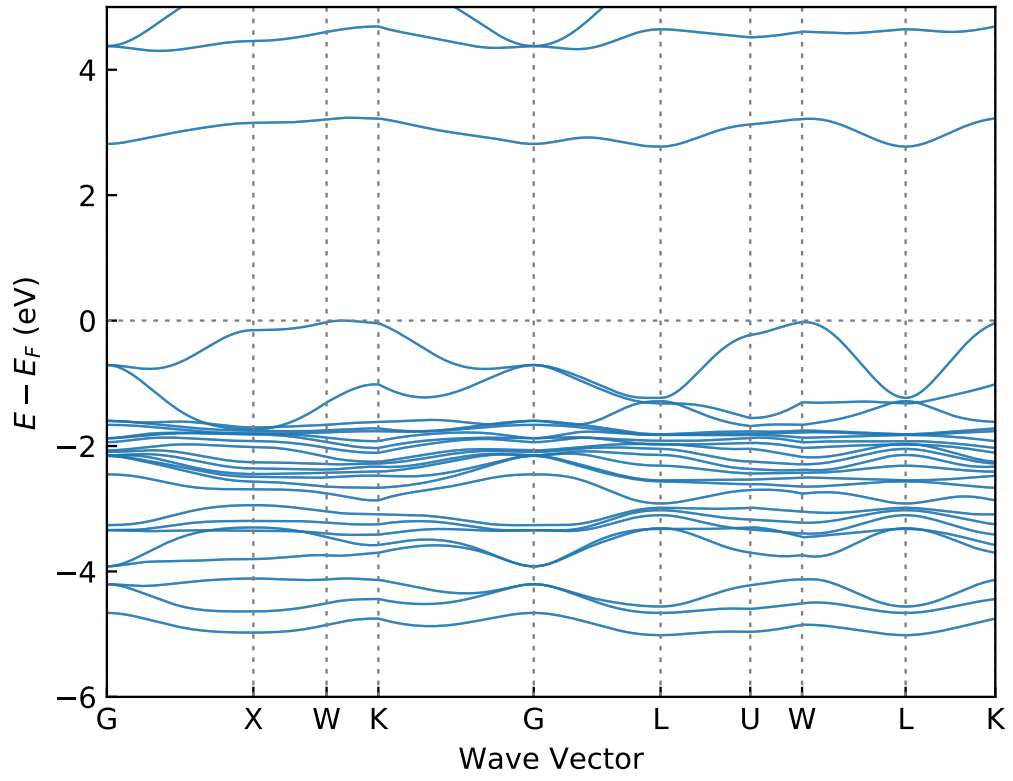


FIG. S8: The band structures of  $\text{Cs}_2\text{AgBiCl}_6$ .

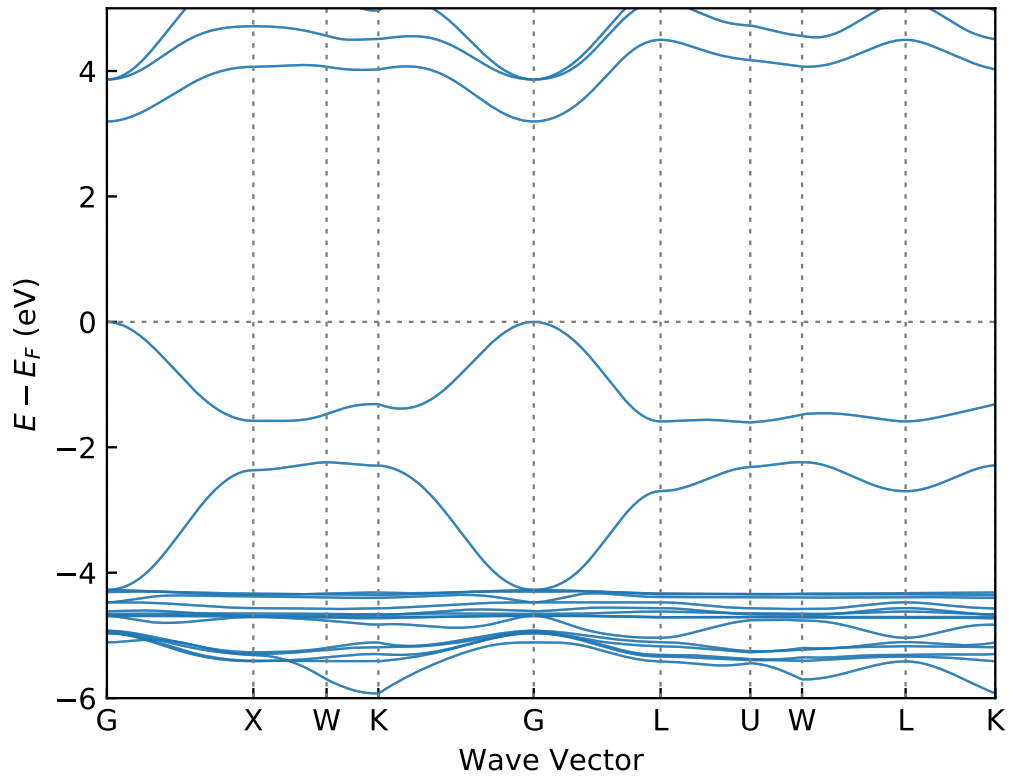


FIG. S9: The band structures of  $\text{Cs}_2\text{AsTiF}_6$ .

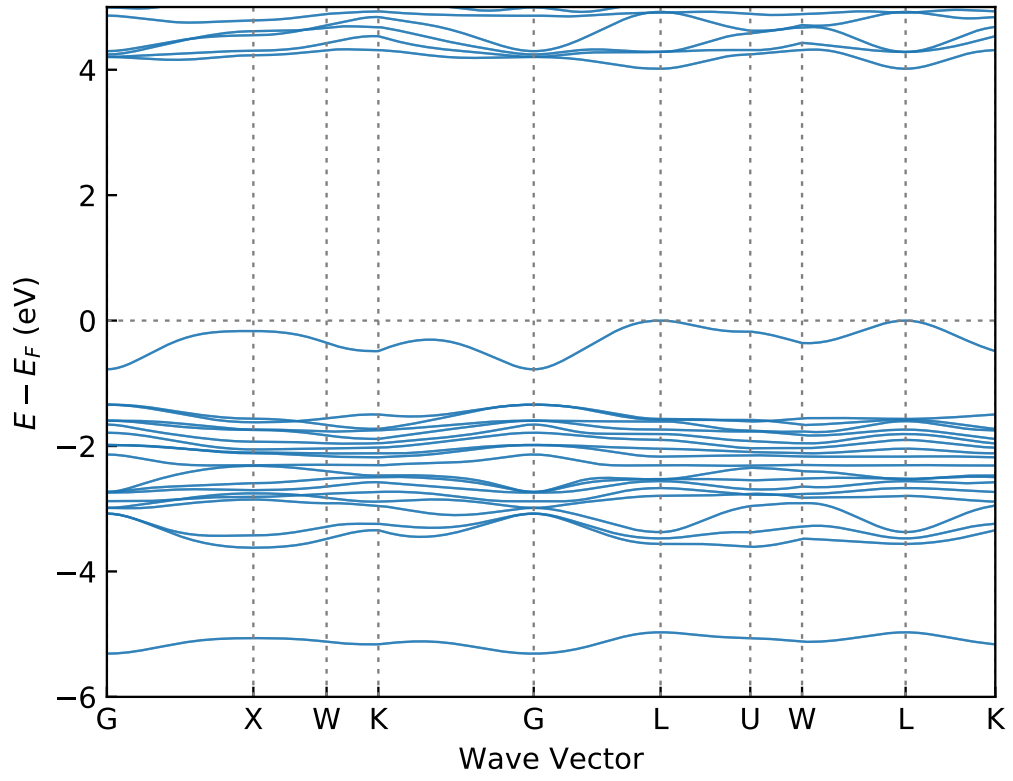


FIG. S10: The band structures of  $\text{Cs}_2\text{GaLaBr}_6$ .

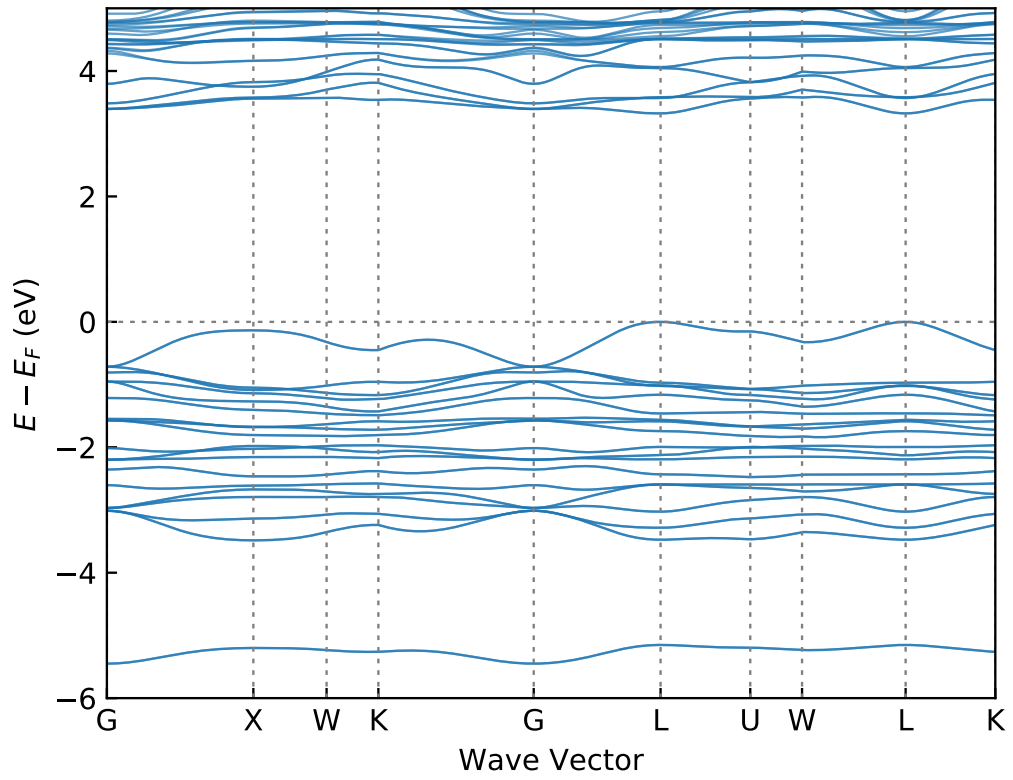


FIG. S11: The band structures of  $\text{Cs}_2\text{GaLaI}_6$ .

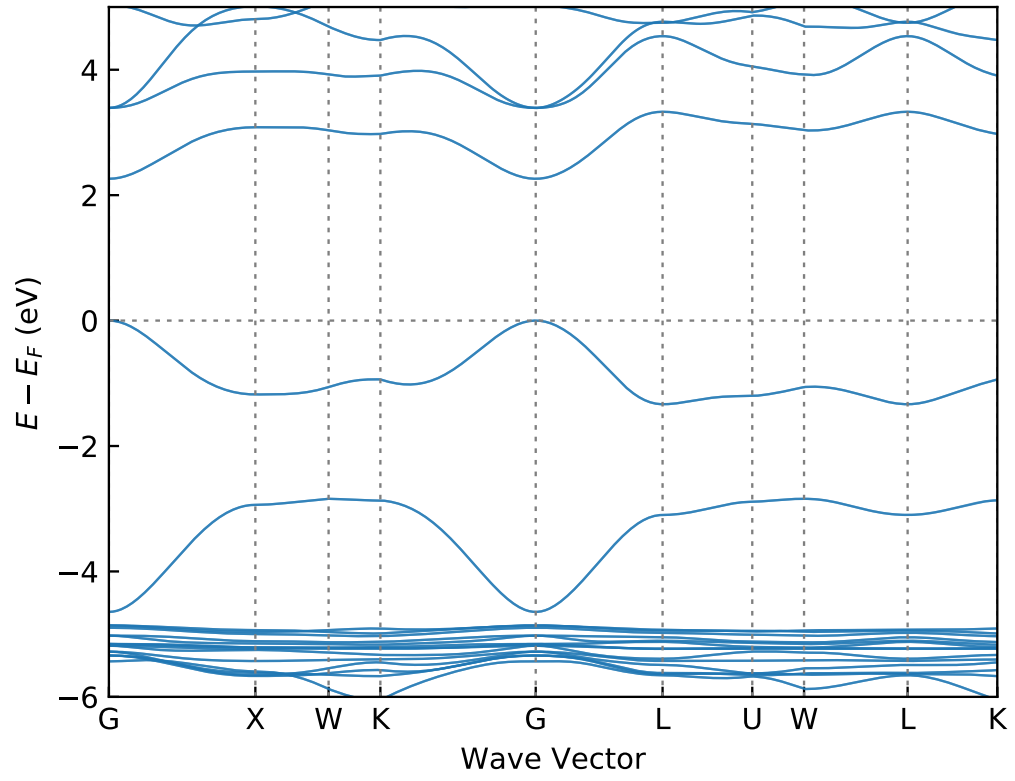


FIG. S12: The band structures of  $\text{Cs}_2\text{InBiF}_6$ .

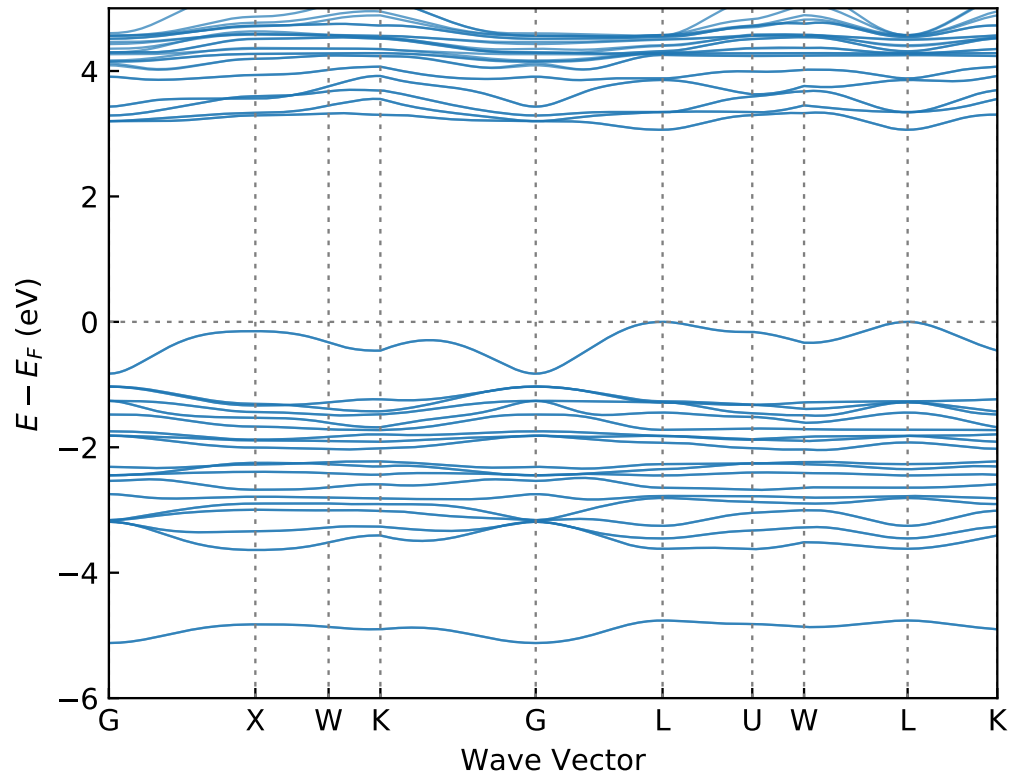


FIG. S13: The band structures of  $\text{Cs}_2\text{InLaI}_6$ .

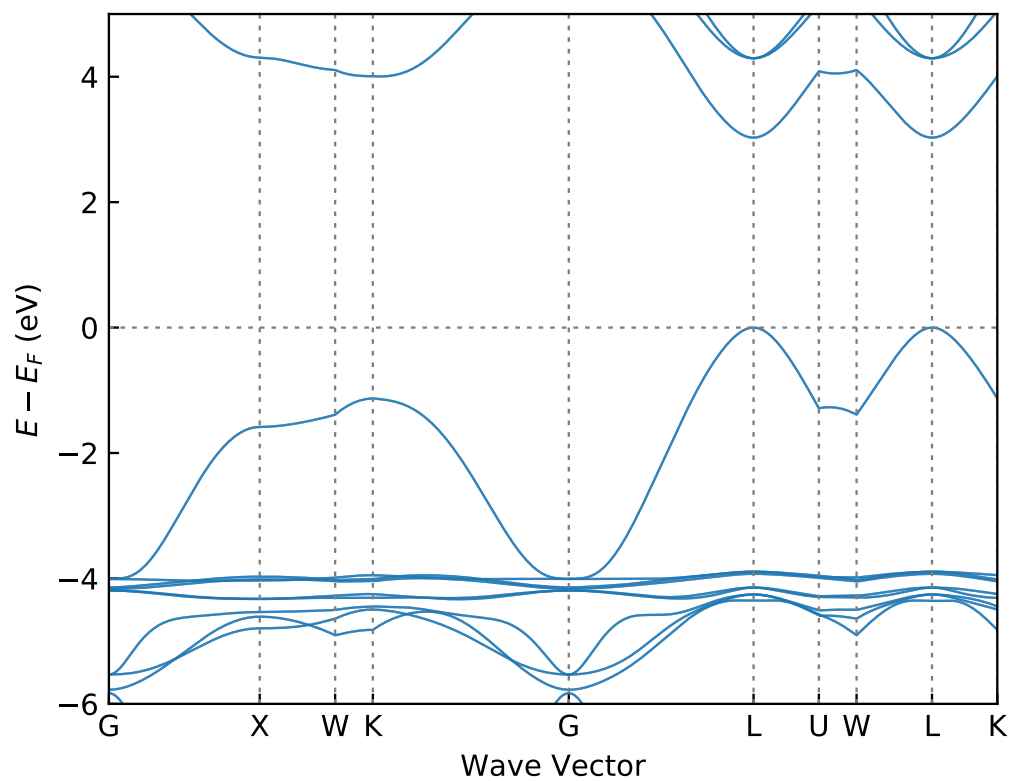


FIG. S14: The band structures of CsPbF<sub>3</sub>.

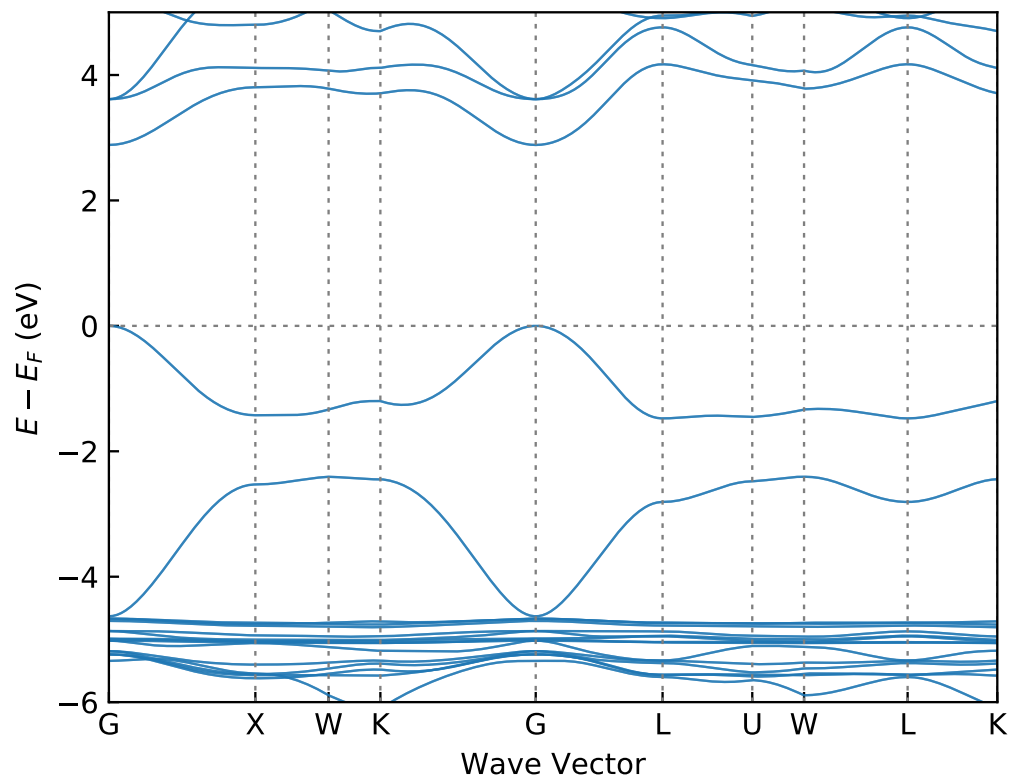


FIG. S15: The band structures of Cs<sub>2</sub>SbTlF<sub>6</sub>.



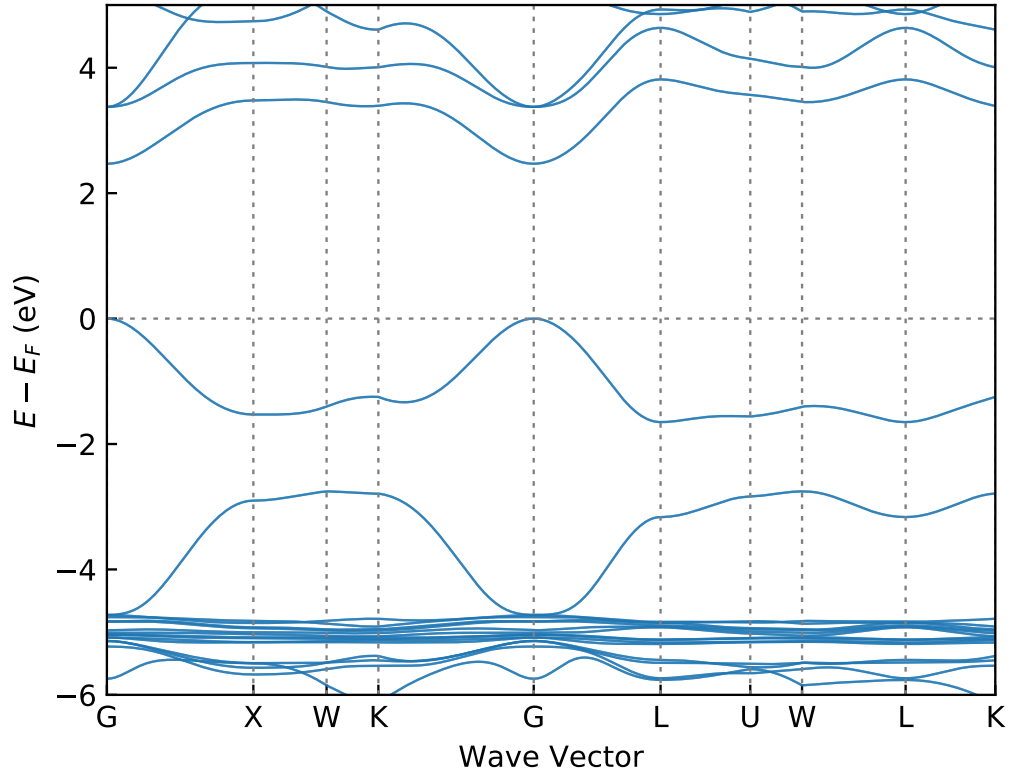


FIG. S16: The band structures of  $\text{Cs}_2\text{SnPbF}_6$ .

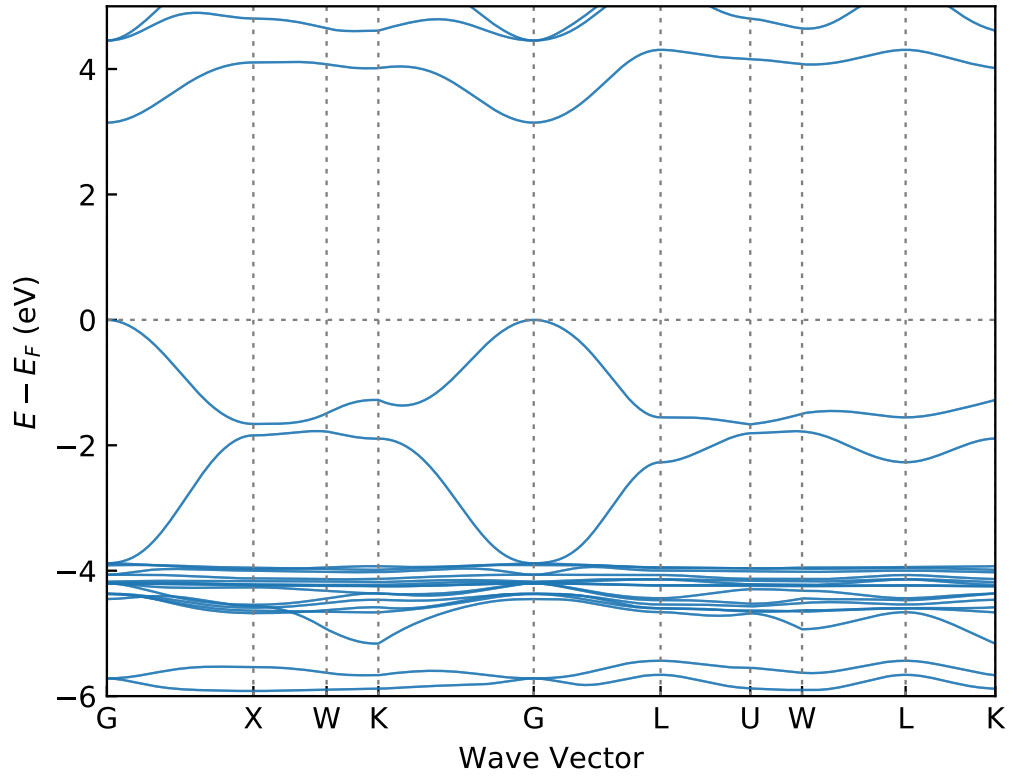


FIG. S17: The band structures of  $\text{Cs}_2\text{TlBiF}_6$ .

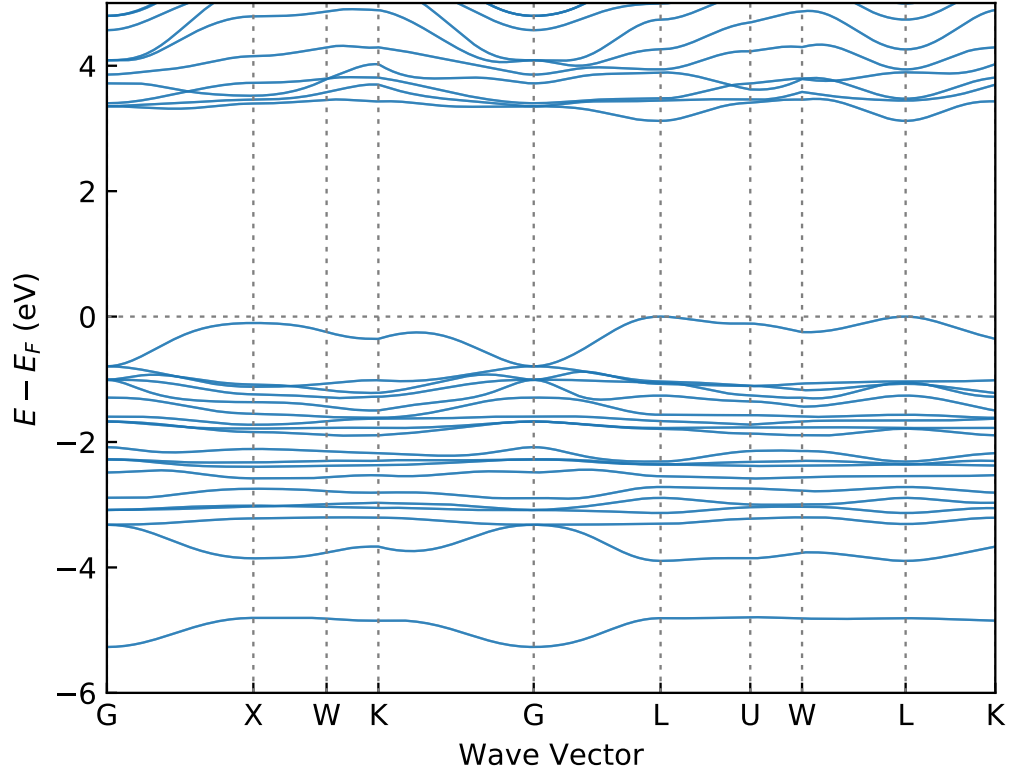


FIG. S18: The band structures of  $\text{Cs}_2\text{YInI}_6$ .

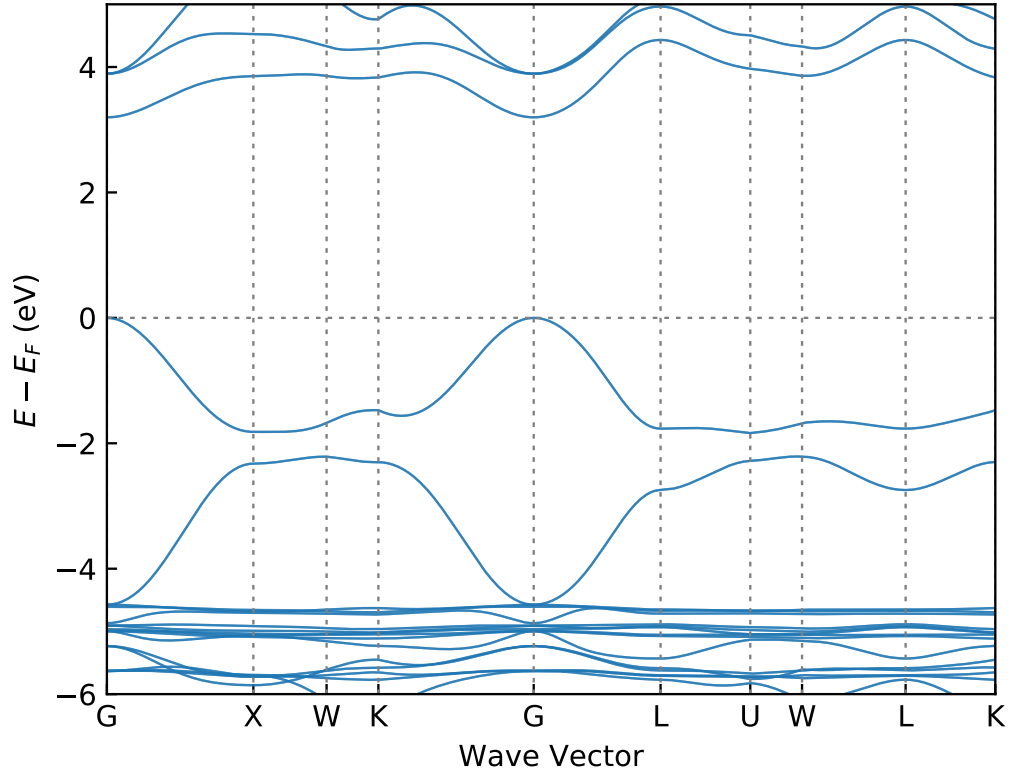


FIG. S19: The band structures of  $\text{Rb}_2\text{AsTlF}_6$ .

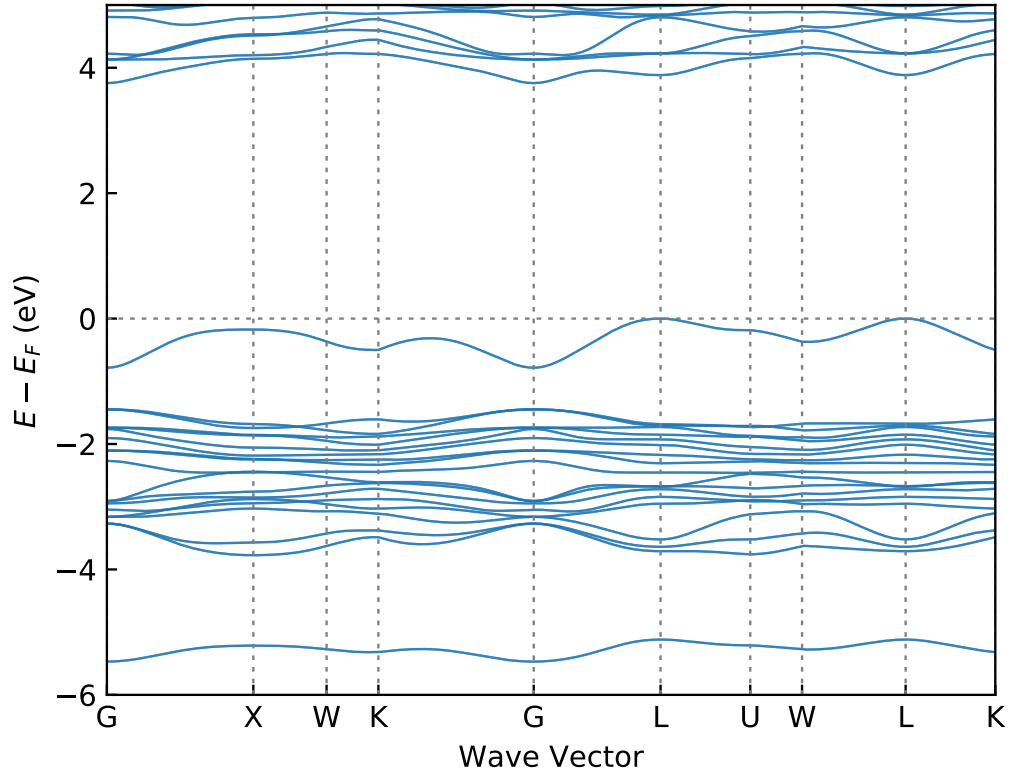


FIG. S20: The band structures of  $\text{Rb}_2\text{GaLaBr}_6$ .

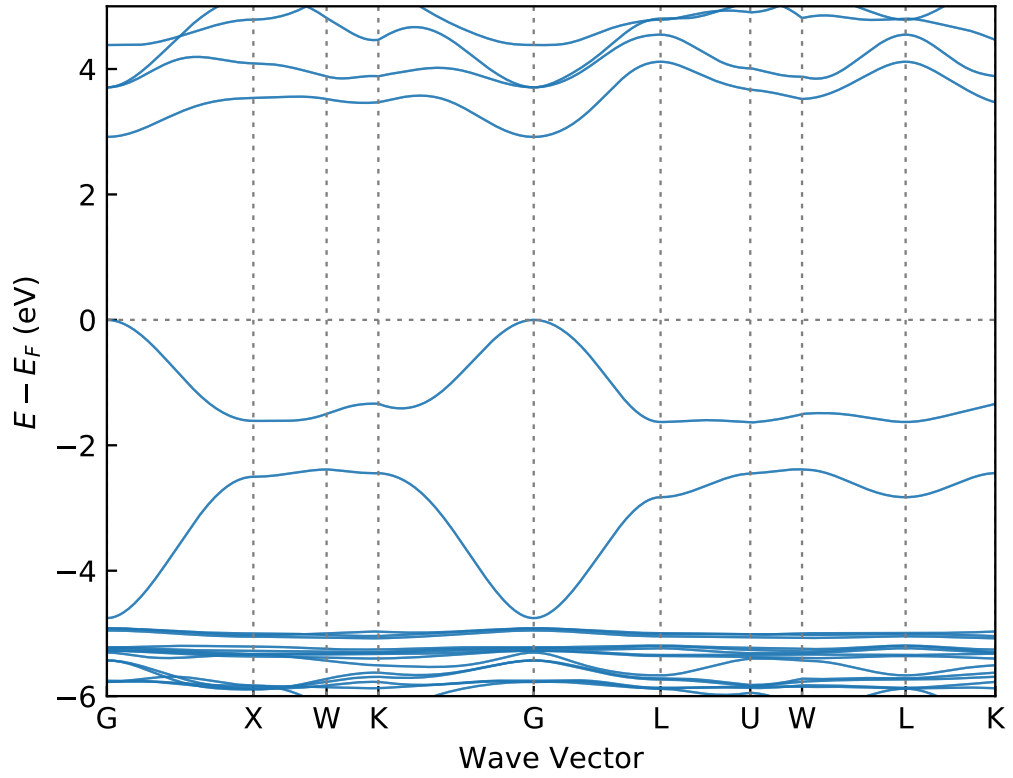


FIG. S21: The band structures of  $\text{Rb}_2\text{SbTlF}_6$ .

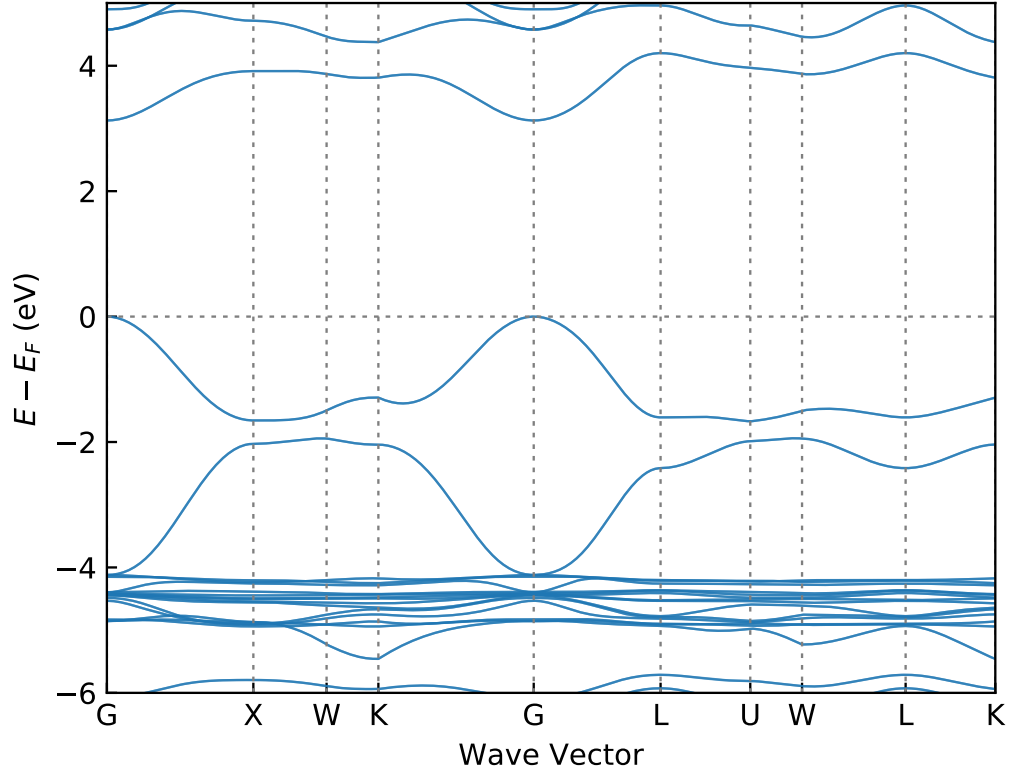


FIG. S22: The band structures of  $\text{Rb}_2\text{TlBiF}_6$ .

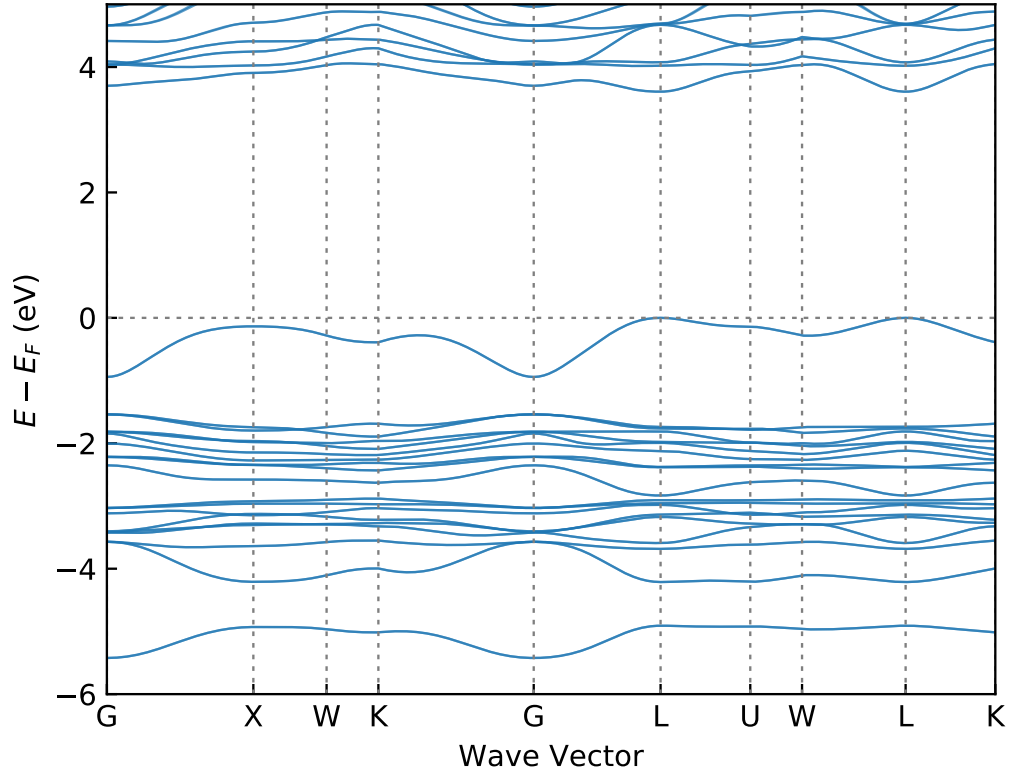


FIG. S23: The band structures of  $\text{Rb}_2\text{YInBr}_6$ .