

## SUPPLEMENTARY DATA:

Realization of predicted exotic materials: The burden of proof

Supplementary S1: Methods

Convex hull calculations:

For the Bi-O system

the Ba-Bi system

For





Supplementary section S3: Spontaneous formation of Bi vacancy in  $\text{Ba}_4\text{Bi}_3$  resulting in the splitting of the Dirac cone in  $\text{Ba}_4\text{Bi}_3$

Figure S2.



Supplementary section S5: n-type doping destroying excited state band inversion in BaBiO<sub>3</sub>

Figure S3.

