## SUPPLEMENTARY DATA:

Realization of predicted exotic materials: The burden of proof

Supplementary S1: Methods

Supplementary section S3: Spontaneous formation of Bi vacancy in  $Ba_4Bi_3$  resulting in the splitting of the Dirac cone in  $Ba_4Bi_3$ 

Figure S2.

Supplementary section S4: Energy stabilization by various magnetic arrangements in  $\mbox{CuBi}_2\mbox{O}_4$ 

Table SI

|             | Magnetic      | Relative total    |
|-------------|---------------|-------------------|
| Space Group | configuration | energy (meV/f.u.) |
|             |               |                   |
|             |               |                   |
|             |               |                   |
|             |               |                   |
|             |               |                   |
|             |               |                   |
|             |               |                   |
|             |               |                   |

Supplementary section S5: n-type doping destroying excited state band inversion in  $\mbox{BaBiO}_3$ 

Figure S3.

## References

- [1] G. Kresse, J. Hafner, Phys. Rev. B 47 (1993), 558
- [2] G. Kresse, J. Furthmüller, Comp. Mater. Sci. 6 (1996), 15
- [3] G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996), 11169
- [4] J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996), 3865
- [5] A. V. Krukau, O. A. Vydrov, A. F. Izmaylov, G. E. Scuseria, J. Chem. Phys. 125 (2006), 224106
- [6] S. L. Dudarev, G. A. Botton, S. Y. Savrasov, C. J. Humphreys, A. P. Sutton, Phys. Rev. B 57 (1998), 1505

[7] S. P. Ong, W. D. Richards, A. Jain, G. Hautier, M. Kocher, S. Cholia, D. Gunter, V. L. Chevrier, K. A. Persson, G. Ceder, Comp. Mater. Sci. 68 (2013), 314

[8] K. Momma, F. Izumi, J. Appl. Crystallogr. 44 (2011), 1272

[9] A. Belsky, M. Hellenbrandt, V. L. Karen, P. Luksch, Acta Crystallogr., Sect. B: Struct. Sci. 58 (2002), 364

[10] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K. A. Persson, APL Mat. 1 (2013), 011002

[11] S. Curtarolo, W. Setyawan, G. L. W. Hart, M. Jahnatek, R. V. Chepulskii, R. H. Taylor, S. Wang, J.

Xue, K. Yang, O. Levy, M. J. Mehl, H. T. Stokes, D. O. Demchenko, D. Morgan, Comp. Mater. Sci. 58 (2012), 218

[12] S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, A. M. Rappe, Phys. Rev. Lett. 108 (2012), 140405

[13] H. J. Monkhorst, J. D. Pack, Phys. Rev. B 13 (1976), 5188

[14] V. Stevanovi , S. Lany, X. Zhang, A. Zunger, Phys. Rev. B 85 (2012), 115104

[15] S. Lany, A. Zunger, Phys. Rev. B 78 (2008), 235104

[16] S. Lany, A. Zunger, Modell. Simul. Mater. Sci. Eng. 17 (2009), 084002

[17] A. Goyal, P. Gorai, H. Peng, S. Lany, V. Stevanovi, Comp. Mater. Sci. 130 (201) at (201) Comp. Mater. Sci. 130 (201) (201