

A powerful guiding principle for topological quantum synthesis

December 27 2017

Science Bulletin

Volume 62 · Number 24 · December 2017

Science Bulletin

Volume 62 · Number 24 · December 2017 · pp 1619–1680



 SCIENCE CHINA PRESS

Chinese Academy of Sciences
National Natural Science Foundation of China

The collaborative team of Prof. Huijun Liu at Wuhan University, Prof. Xingqiu

Chen at the Institute of Metal Research, Chinese Academy of Sciences, and Prof. Zhenyu Zhang at the University of Science and Technology of China proposes an efficient criterion that allows ready screening of potential topological insulators, a powerful guiding principle in synthesizing topological quantum materials. The work has been published as a cover paper in 2017, Issue 24 of Science Bulletin. Credit: Science China Press

Topological materials can be classified into topological insulators (TIs), topological crystalline insulators, topological Dirac semimetals, topological Weyl semimetals, topological nodal-line semimetals, and others. Such materials are attracting attention in condensed matter physics and materials science due to their intriguing physical properties and promising technological applications. For a given compound system, identification of its topological nature is generally complex, demanding specific determination of the appropriate topological invariant through detailed electronic structure and Berry curvature calculations.

The topologically nontrivial nature is tied to the appearance of inverted bands in the electronic structure. For most [topological materials](#), band inversions have been demonstrated to be induced by delicate synergistic effects of different physical factors, including chemical bonding, crystal field and, most notably, spin-orbit coupling (SOC). In particular, for the most widely studied topological systems of three-dimensional (3D) TIs, SOC has been identified to play the vital role in inducing band inversion. Recently, several so-called high-throughput methods were successfully developed for predicting TIs. For example, by using a certain descriptor, tens of new candidate TIs have been proposed by a research group in Duke University. Yet at the implementation level, all these approaches rely on detailed band structure calculations based on first principles.

In this cover paper, a simple and efficient criterion that allows ready

screening of potential topological insulators was proposed by the collaborative team of Prof. Huijun Liu at Wuhan University, Prof. Xingqiu Chen at the Institute of Metal Research, Chinese Academy of Sciences, and Prof. Zhenyu Zhang at the University of Science and Technology of China. The criterion is inherently tied to the band inversion induced by SOC, and is uniquely defined by a minimal number of two elemental physical properties of the constituent elements: the atomic number and Pauling electronegativity, rather than inputs from detailed computations of electronic band structures within density functional theory. The idea of the criterion is:

1. The energy gap (Δ) at certain high-symmetry k point is largely opened by the local chemical binding of the constituent elements and crystal field splitting, while the SOC tends to pull down the conduction band minimum and push up the valence band maximum in inducing the occurrence of the band inversion with an anti-crossing shape.
2. As an order of magnitude criterion, to induce the band inversion it would be desirable if a TI candidate material has a larger SOC strength λ and a smaller Δ . The critical or transitional case would require λ to be comparable to Δ .
3. In principle, the SOC strength λ is proportional to the atomic number, while the band gap of a compound is closely related to the electronegativity difference between the constituent atoms. In terms of the average atomic number (Z) of the formula unit and the Pauling electronegativity difference ($\Delta\{\chi\}$) of the constituent elements, one can define a simple Δ ratio ($\Delta a = 0.0184Z / \Delta a\{\chi\}$), and a candidate material is topologically nontrivial if Δ is larger than 1. The validity and predictive power of such criterion is demonstrated by rationalizing many known [topological insulators](#) and potential candidates in the tetradymite and half-Heusler families, and the underlying design principle is naturally also extendable to predictive discoveries of other classes of

topological [materials](#), which offers a powerful guiding principle in synthesizing topological quantum materials.

More information: Guohua Cao et al, A simple and efficient criterion for ready screening of potential topological insulators, *Science Bulletin* (2017). [DOI: 10.1016/j.scib.2017.11.016](https://doi.org/10.1016/j.scib.2017.11.016)

Provided by Science China Press

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