Prediction of Topological Quantum Materials

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We are dedicated to theoretical prediction of exotic topological quantum materials, such as topological insulators (TIs), quantum anomalous Hall (QAH) insulators, and topological semimetals. Guided by the materials design strategy, we search for topological materials by accurate *ab initio* calculations and close interactions with solid-state chemists in our institute. Among many of our achievements, we have predicted the first weak TI materials (e.g. KHgSb) [1,2], the stanene (Sn honeycomb lattice) as the first large-gap 2D TI [3] and the room-temperature QAH insulator [4], the strong TI with the largest energy-gap of 0.7 eV ($BaBiO_3$) [5], and recognized the famous Shockley states on the gold surface as the topological surface states [6]. Our research paves the way to realize novel topological phenomena in realistic materials and promises appealing applications as well.

We combine materials simulations to design state-of-art functional materials. A*b initio* calculations assisted by phenomenological models are employed to find the most promising candidates in the materials world with topological properties that we are interested. Benefit from the surrounding by solid-state chemists, we can gain feedback about the properties of predicted materials and optimize our theory in a realistic materials design routine.

Topological insulators are characterized by the robust gapless surface states inside the bulk energy gap. The metallic surface states are due to the bulk band topology induced by a band inversion. TIs have 2D (such as HgTe quantum wells) and 3D versions. The 3D TIs are further classified into strong TIs (such as Bi_2Se_3) and weak TIs. The weak TI can be regarded as stacking layers of 2D TIs and corresponding materials have been missing for a long time. Ferromagnetic (FM) doping in the 2D TI can lead to the QAH state. For example, the first QAH effect was realized in dilute magnetic doped $(Bi,Sb)_2Te_3$ thin films that works only in very low temperature (30 mK). For the known topological materials, one major obstacle to hinder experiments and further application is the relatively small size of the bulk band-gap, which is usually around 0.3 eV for a 3D TI (e.g. Bi_2Se_3) and in order of meV for a 2D TI or a QAH insulator.

The first weak TI materials. In the design of weak TIs, we obtained important insights from Heulser TIs (XYZ) [*S. Chadov, et al. Nature Mater. 9, 541 (2010)*], an expertise of our Dresden group. Heusler TIs crystalize in a filled diamond-lattice and are treated as a ternary version of the known TI HgTe, where the band-inversion between conduction and valence bands induces the topology. Alternatively, we propose to transfer the Heusler TI into the graphite-lattice, giving rise to a layered compound. Because each layer is a 2D TI where the band inversion still preserves, the stacked 3D compound becomes a 3D weak TI [1]. In this way, we found many ternary honeycomb compounds as the first-predicted weak TI candidates, some of which were indeed synthesized in previous experiments (such as KHgSb). Topological surface states were predicted to exist on the side surface, as illustrated in Fig. 1. We note that strong TIs were also predicted in this type of materials by band engineering [2].

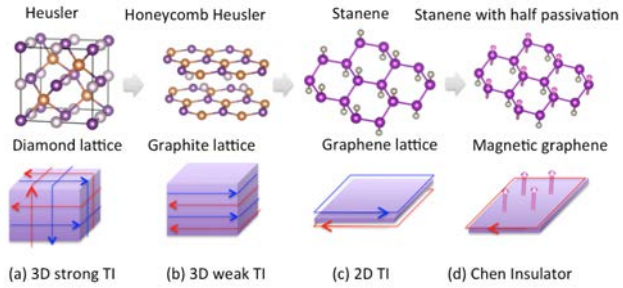

Fig. 1 Evolution of topological materials from (a) Heusler compounds to (b) the honeycomb version of Heuslers, (c) stanene and (d) half-passivated stanene where the unpaired electrons form a ferromagnetic order. The blue and red lines represent opposite spin directions and the arrows stand for current directions, which indicates the spin-momentum locking in topological surface and edge states.

Stanene as the first large-gap 2D TI and the room-temperature QAH insulator. (i) Above weak TI materials offer a fantastic possibility to design a 2D TI by extracting a single honeycomb layer from the weak TI. Collaborating with the Prof. Shou-Cheng Zhang's group in Stanford, we found that a Sn honeycomb layer with the dangling-bond passivation mimics the simplest 2D case of the monolayer of the KHgSb-type weak TIs. The 2D Sn lattice, called stanene in analogue to grpahene, exhibit 0.3 ~ 0.4 eV energy gap, which is in orders of magnitude large than that of HgTe quantum wells. Recently the stanene layer has been successfully grown by the MBE technique [*F. Zhu et al. arXiv:1506.01601 (2015)*] and awaits for the further identification of the topological edge states. (ii) The large-gap 2D TI provokes us to design a large-gap QAH insulator by introducing FM doping. We propose

a simple way to realize stable FM order by passivation of only half of the stanene lattice. Subsequently strong exchange coupling drives the 2D TI into the QAH phase. Large energy-gap (0.3 eV) and high T_c of the FM order promise a novel QAH system that can work at near room temperature [4].

The 3D TI $BaBiO_3$ with the largest energy gap. One important intuition from above weak TIs and 2D TIs is that the large energy-gap is purely due to the intrinsic SOC split. The Bi-6*p* states exhibits probably the largest intrinsic SOC split. Therefore, we may use Bi to design a TI with the record band gap. We choose the famous perovskite $BaBiO_3$, which has been known as a superconductor in the hole-doping case (T_c ~ 30 K). We found that a large band gap (more than 1 eV) opens due to SOC in the electron doped region with a band inversion at the same time, which has been omitted for decades in previous study. As a consequence, we found a 3D TI in this material with an indirect energy gap 0.7 eV, which is the largest gap among all known 3D TIs [5].

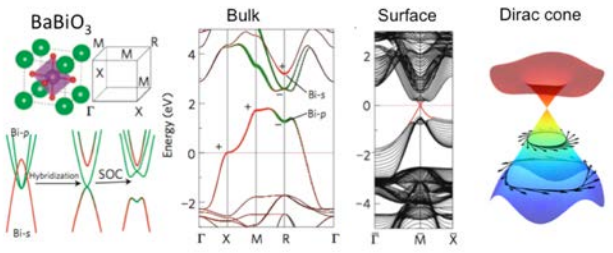

Fig. 2 The perovskite superconductor $BaBiO_3$ as a 3D TI with large energy gap. The bulk and surface band structures are in the middle panels. The Dirac-cone-like surface states is in the right panel.

A surprise from the topological gold. Gold surfaces host special electronic states that have been understood as a prototype of Shockley surface states. These surface states are commonly employed to benchmark the capability of ARPES and STS. We found that these Shockley states can be reinterpreted as topologically derived surface states of a TI [6]. Based on band structure calculations, the Z_2 topological invariant can be well defined to characterize the nontrivial features of gold that we detect by ARPES, in collaboration with Prof. Martin Aeschlimann's group in Kaiserslautern. The same topological states are also recognized on surfaces of other well-known noble metals (e.g., silver, copper, platinum, and palladium). Besides providing a new understanding of noble metal surface states, finding topological states on late transition metals provokes interesting questions on the role of topological effects in surface-related processes, such as adsorption and catalysis.

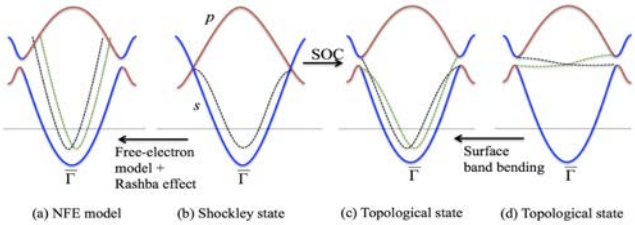

Fig. 3. Illustration of relations between Shockley surface states and topological surface states on the gold surface. Shockley states are commonly described by a nearly-free-electron (NFE) model with Rashba spin-split. We find that the origin of these surface states is indeed the topology of a TI, which is confirmed by our APRES measurement of empty states.

In addition, we also tackled new challenges in correlated topological states. In collaboration with Prof. Zhong Wang at the Tsinghua University, we proposed a topological Hamiltonian as an exact and simple tool to calculate topological invariants of strongly correlated materials [7]. This method was already employed with state-of-art DMFT and Monte-Carlo calculations to identify the topological Z_2 index. Due to the recognized contributions in predicting topological materials, we were pleased to be invited for review and perspective articles on Heusler TIs [8] and general topological materials [9-11].

References

[1] ***B. Yan***, *L. Müchler, and C. Felser, Phys. Re. Lett. 109, 116406 (2012).*
[2] *H.-J. Zhang, S. Chadov, L. M uchler,* ***B. Yan****, X.-L. Qi, J. K ubler, S.-C. Zhang, and C. Felser, Phys. Rev. Lett. 106, 156402 (2011).*
[3] *Y. Xu,* ***B. Yan****, H.-J. Zhang, J. Wang, G. Xu, P. Tang, W. Duan, and S.-C. Zhang, Phys. Re. Lett. 111, 136804 (2013).*
[4] *S.-C. Wu, G. Shan,* ***B. Yan****, Phys. Re. Lett. 113, 256401 (2014).*
[5] ***B. Yan****, M.Jansen, C.Felser, Nature Phys. 9, 709 (2013).*
[6] ***B. Yan****, B. Stadtmüller, N. Haag, S. Jakobs, J. Seidel, D. Jungkenn, S. Mathias, M. Cinchetti, M. Aeschlimann, and C. Felser, arXiv:1504.01971 (2015).*
[7] *Z. Wang and* ***B. Yan****, J. Phys. CM 25, 155601 (2013).*
[8] ***B. Yan*** *and A. de Visser, MRS Bull. 39, 859 (2014).*
[9] ***B. Yan****, S.-C. Zhang, Rep.Prog.Phys. 75, 096501 (2012).*
[10] *L. Müchler, H. Zhang, S. Chadov,* ***B. Yan****, F. Casper, J. Kübler, S.-C. Zhang, and C. Felser, Angew. Chem. 124, 7333 (2012).*
[11] *L. Müchler, F. Casper,* ***B. Yan****, S. Chadov, and C. Felser, Phys. Status Solidi RRL 7, 91 (2013).*

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