Citation of the 2017 (the 5th) Nishina Asia Award

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For his theoretical contributions to the discovery of Weyl semimetals

Weyl semimetal is a new topological state of matter that differs from topological insulators. Its remarkable property provides an opportunity to realize the so-called Weyl fermions as low-energy quasi-particles — a long sought massless chiral particle proposed as the building block of the Standard Model, but is yet to be observed in particle physics experiments. In recent years, we have witnessed the rapid development of this field, stimulated by the discovery of real Weyl semimetal materials, to which Weng has made crucial contributions. Weng's work in collaboration with his colleagues, using the first-principles calculations, predicted the unique topological electronic structure of TaAs family compounds [1], which had been known. Weng *et al.* has put the material in new perspective, leading to the discovery of Weyl semimetals [2] and Weyl fermions [3]. This work constitutes a good example that computational predictions can drive fundamental discovery and materials design.

In 1928, Paul Dirac proposed the 4-component Dirac equation to describe the motion of relativistic electrons. In the following year, in 1929, Hermann Weyl found that Dirac equation can be further simplified if electrons are massless. This led to the Weyl equation with 2-component chiral Weyl fermions as its low energy particles. Since then, the simplest Weyl representation has been widely accepted in quantum field theory and used as the building block of the Standard Model for particle physics. Unfortunately, all fundamental particles found up to now are massive (including neutrinos) due to symmetry breaking, therefore none of them are true Weyl fermions.

In contrast, in condensed matter physics, the progress in studying topological states has opened up the possibility of finding Weyl fermions as low-energy quasi-particles of a new topological state, called Weyl semimetals. In 2011, a couple of candidates were theoretically proposed as Weyl semimetals, although they are difficult to realize. In the following years, 2012-2014, further progress was made. Topological Dirac semimetals, where two Weyl nodes with opposite chirality coexist and overlap in the momentum space, were theoretically predicted and experimentally demonstrated. Weng has made important contributions in the studies of both kinds of materials.

The true challenge has been: how to find a realistic compound with separated Weyl nodes at the Fermi level? For that purpose one needs to break either time reversal or inversion symmetry, and the latter should be a better choice for experimental measurements. First-principles calculations should play an important role towards that end. After trying numerous compounds, the breakthrough was made by Weng *et al*. in 2014 [1]. They theoretically predicted that TaAs family compounds are non-centrosymmetric (with an inversion-symmetry broken crystal structure) Weyl semimetals. Soon after the theoretical prediction, Weng *et al*., collaborating closely with experimental groups, finally observed the Weyl nodes in the bulk and related Fermi arcs on the surface of TaAs in 2015 [2, 3]. This series of work leads to the discovery of Weyl semimetals and Weyl fermions. The other members of TaAs family compounds, such as NbAs, TaP and NbP, have also been all confirmed to be Weyl semimetals by recent experiments. It should be mentioned that this field is highly competitive, and a similar experimental discovery has been made almost simultaneously by a few groups worldwide. Nevertheless, the predictive role played by Weng *et al*. is crucial in this endeavor. For this reason, Weng well deserves the Nishina Asia Award.

References:

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