第55回トポロジカル物質科学セミナー
Topological Materials Science Seminar (55)

Spontaneous Ferroelectric Distortion Driven Weyl Semimetal State in $HgPbO_3$

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Time: 10:30 -12:00

Place: Room 525, Science Bldg. #5 (Physics), Kyoto University

Abstract:

The recent discoveries of ferroelectric metal [1] and Weyl semimetal (WSM) [2] have stimulated a natural question: whether these two exotic states of matter can coexist in a single material or not. These two discoveries ensure us that physically it is possible since both of them share the same necessary condition, i.e., the broken inversion symmetry.

Here, by using first-principles calculations, we demonstrate that the experimentally available nonmagnetic $HgPbO_3$ represents a unique example of hybrid "Ferroelectric Weyl semimetal" driven by spontaneous ferroelectric distortion [3]. The centrosymmetric R3-c phase of $HgPbO_3$ will undergo a ferroelectric phase transition to the ferroelectric R3c structure with both phases being metallic. The later phase can harbor six pairs of chiral Weyl nodes around the Fermi level as an oxide WSM. The ferroelectric distortion can be controlled to manipulate the creation and evolution of Weyl nodes in momentum space of $HgPbO_3$, which is promising for potential applications of integrated topotronic and ferroelectric devices. Recently, our experimental collaborators have observed a ferroelectric phase transition around 250 K on their polycrystalline samples as predicted by our calculations.

References:

[1] Y. Shi *et al.,* Nat. Mat. **12**, 1024 (2013).

[2] H. Weng *et al*., Phys. Rev. X **5**, 011029 (2015); B. Lv *et al*., Phys. Rev. X **5**, 031013 (2015);
B. Lv *et al.*, Nat. Phys. **11**, 724 (2015).

[3] R. Li *et al*., arXiv:1610.07142 (2016).

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