SURFACE PHYSICS BY NODAL LINES IN ALKALINE EARTH METALS

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In the presentation, we study surface physics characteristic in a nodal-line semimetal, which is one of the topological semimetals. We show by ab initio calculations that fcc Ca, Sr, and Yb have topological nodal lines near the Fermi level when the spin-orbit interaction is neglected (Fig.1(a)) [1]. These nodal lines (Fig.1(b)) are purely topological, characterized by the π Berry phase. Because of the topological nature of the nodal lines, the Zak phase, defined as an integral of Berry connection along a reciprocal vector, becomes π within the region (Fig.1 (c)) encircled by the nodal lines. This π Zak phase is related with charge polarization, and it means that there is an excess charge of e/2 or –e/2 within this wavevector region. This charge is screened by bulk carriers, leaving behind a large dipole at the surface and a potential dip at the surface. Eventually, this tends to cause a large Rashba spin-orbit coupling, when atoms with large spin-orbit coupling are added at the surface. It is demonstrated in Bi/Sr(111) surface, as well as in Bi/Ag(111) surface [1].

If time allows, we also show our results on Weyl semimetals (WS) [2], which are topological semimetals with nondegenerate 3D Dirac cones in the bulk. In the presentation we show that if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens [3]. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation [4].

Keywords: Nodal-line semimetal, Rashba splitting

References

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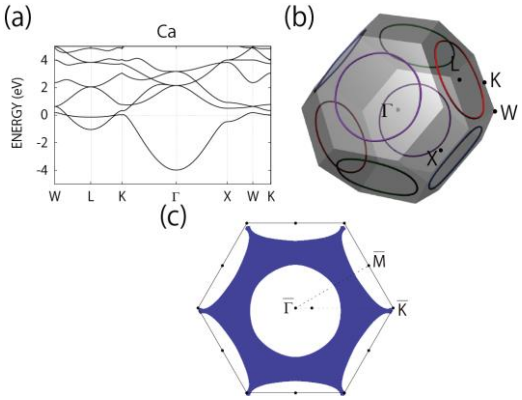

Fig. 1 (a) Band structure of Ca, (b) nodal lines of Ca, and (c) region with π Zak phase on the (111) surface