Usage Report for Fiscal Year 2017

Project Title:

Numerical study of fractional topological phases on two-dimensional lattices

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Description of the project

1. Background and purpose of the project, relationship of the project with other projects

Topological phases of matter is an exciting field in condensed matter physics in the last decade. Recently, following the prediction of Weyl semimetal (WSM) in TaAs family, WSMs have attracted a lot of attention. WSMs host Weyl points (WPs) around the Fermi level. Each WP carry a nonzero topological charge, either +1 or -1. According to Nielsen-Ninomiya theorem, positive and negative charge WPs always appear in pair. On the surface of WSMs, open topological surface arcs connects two WPs with opposite topological charge.

Very recently, spin-1 WPs were proposed in FeSi. Due to point group symmetry, the three- and four- fold degenerate points at the Brillouin zone (BZ) center and corner are spin-1 WP and charge-2 Dirac point.

In this study, we have found that the band crossing points (BCPs) of phonon spectra between K(1/3,1/3,0) and H(1/3,1/3,1/2) in the 3D BZ of noncentrosymmetric WC-type materials are all WPs. These WPs are decribed by first- or second- order k.p theory. Furthermore, for those WPs described by second-order k.p theory, when some conditions are satisfied, there are three nearby surrounding WPs with the opposite charge. Then a charge-radius dependence effect is predicted and observed.

2. Specific usage status of the system and calculation method

My IPA program was terminated and my account on HOKUSAI has also be terminated. So I didn't know the usage status of HOKUSAI. My calculation method is first-principles calculations. We use the VASP package. The surface states are calculated by using the iteration Green's function method.

3. Result

We have studied the phonon spectra of a serious of WC-type materials and found that the BCPs between K(1/3,1/3,0) and H(1/3,1/3,1/2) in the 3D BZ are all WPs. These materials include HfS, HfSe, IrB, MoC, MoN, MoP, NbN, NbS, TaN, TaS, TiO, TiS, WN, ZrS, ZrSe, and ZrTe, but not WC. These materials belong to the space group P-6m2 (No. 187) with two sites in a hexagonal cell [see Fig. 1(a) for an example]. The two sites occupy Wyckoff positions 1a(0,0,0) and 1d(1/3,2/3,1/2), respectively. We find that the band crossing points (BCPs) of phonon dispersions between K(1/3,1/3,0) and H(1/3,1/3,1/2) are WPs. That is, two phonon bands contact at a single momentum in the

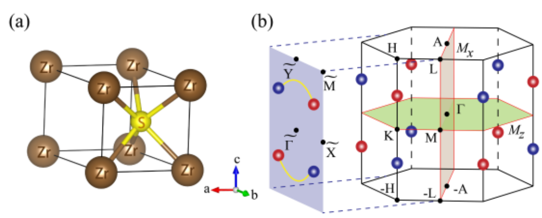

Fig 1. (a) Crystal structure of ZrS, an example of WC-type materials with space group P6m2. (b) Brillouin zone (BZ) and the Surfurterminated (10$\bar{1}$0) surface. Two shaded Mx

(brown) and Mz (green) planes are mirror planes. The WP at kz = 0:2058 and its symmetric counterparts in the bulk BZ and their projections on the $(10\bar{1}0)$ surface are indicated by spheres. Red (blue) sphere represents a WP with positive (negative) charge. The surface arcs are schematically depicted.

3D BZ. The topological charges are found to be ±1. Based on symmetry analysis, we derive two-band k.p models to describe these WPs. For majority of WPs, we find that a first-order theory is sufficient to well reproduce the phonon dispersions within the range of 0.002 $Å^{-1}$ and the topological charges. However, in many cases, a second-order theory is needed. Particularly, when the second-order term plays a dominant role, a charge c(±1) WP is surrounded by three nearby charge –c WPs. These nearby WPs appear at general k points and thus are difficult to locate in 3D BZ. Fortunately, when they are close to the fitting range 0.002 $Å^{-1}$, the second-order k.p model gives good estimations. In general, their existences can be confirmed by the total charge of all four WPs, which should be -2c. When WPs are projected onto crystal surfaces, two WPs with opposite charges are connected by topologically protected surface states. These surface states form open arc structures which terminate at the surface projections of the bulk WPs. To be concrete, we will take ZrS as an example to illustrate our results in the following.

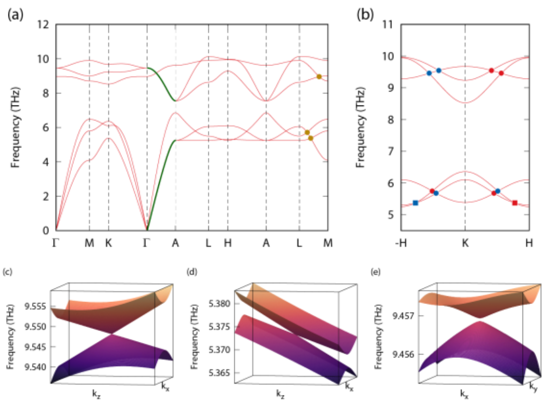

Fig 2. (a)-(b) The phonon spectra of ZrS along high symmetry momentum paths. The high-symmetry k points are indicated in Fig. 1(b). In (b), red (blue) circles and squares denote type-I and type-II WPs, respectively, with positive (negative) charges. (c) Phonon dispersion around a type-I WP at kz = 0.2058 on the zxplane. (d) Phonon dispersion around the type-II WP at kz = 0.3875 on the zx-plane. (e) Phonon dispersion around the #4 WP at kz = 0:2820 on the xy-plane. The spectrum show a C3 rotation symmetry. All dispersions in (c), (d) and (e) are calculated within the range of 0.002 Å-1.

The DFT optimized lattice constants of ZrS are a = b = 3.461 Å and c = 3.475 Å. We use these values throughout the calculations. The crystal structure is shown in Fig. 1 (a).

Figures 2 show the phonon spectra of ZrS. The band crossing points along KH are all WPs. Their positions are listed in Table I.

TABLE I. Weyl points at ($\frac{1}{3}, \frac{1}{3}, k_z$) in ZrS. Charge + (−) denotes positive (negative) topological charge and type I (II) indicates a type-I (type-II) WP.

No.	k_z	Frequency (THz)	Charge	Type
1	0.2058	9.547	+	I
2	0.2262	5.679	+	I
3	0.2562	5.746	−	I
4	0.2820	9.457	−	I
5	0.3875	5.373	+	II

Figure 3 show the Wannier center evolutions around a positive and a negative charge WPs and also the Berry curvature distributions. Positive and negative charge WPs are the source and sink and Berry curvature distributions, respectively.

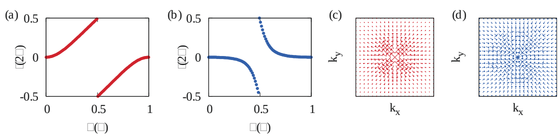

Fig 3. The Wannier center evolution around WPs with (a) positive and (b) negative charges at kz = 0.2058 and 0.2562, respectively. We use a sphere with radius 0.001 Å-1. Here theta is the polar angle of orbitals and phi the phase factor of the position operator on the orbitals. The Berry

curvature distributions xy around these two WPs at (c) kz = 0.2058 and (d) kz = 0.2562 on the xy-plane within 0.001Å-1.

Figure 4 show the results of a WP described by second-order k.p theory. There are three nearby WPs with the opposite charge. A charge-radius dependence effect was observed.

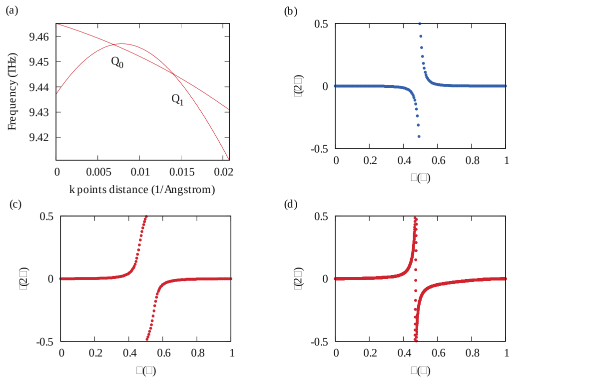

Fig 4. (a) Phonon dispersion along Q0 and Q1 from DFT calculation. Here Q0 is the #4 WP at kz = 0.2820. Q1 is a nearby WP of Q0 [The other two nearby WPs Qi (i = 2; 3) are not shown]. The Cartesian coordinates of Q1 is (6.9, 0.0, -0.5)×103 Å-1 relative to Q0. (b) and (c) Wannier center evolutions around Q0 and Q1. A radius r = 0.001 Å-1 < d is used in theWilson-loop method. It is clear that Q0 has charge -1 and Q1 has charge +1. (d) Wannier center evolutions around Q0. A radius r = 0.010 > d is used. Four WPs Qi (i = 0; 1; 2; 3) are included within this radius. The total charge of four WPs is +2. The positions of nearby WPs are obtained from analytically solving model H2(q). The fitting parameters and d are listed in Table II.

Figure 5 show then surface arc on the two (10-10) surface. Positve and negative charge WPs are connected by open surface arcs. On the (01-10) surface, we also observe similar results.

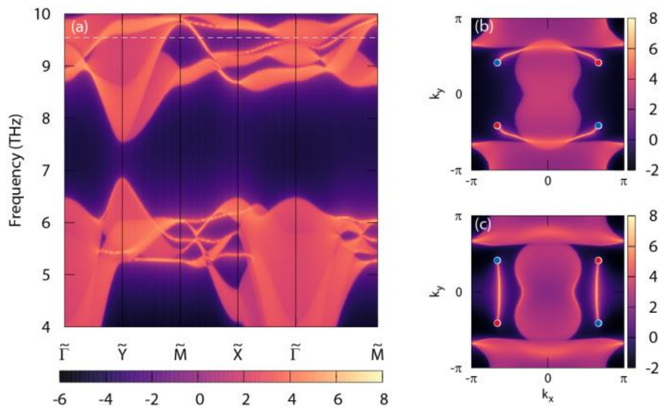

Fig. 5. (a) The surface DOS along high symmetry k path on the Surfur-terminated (10-10) surface of ZrS. The dashed white line is at 9.547 THz. The corresponding WPs is at kz = 0.2058. The surface DOS around the #1 WP on (b) Surfur- and (c) Zirconium-terminated (10-10) surfaces, respectively. Clear surface states are observed. The red (blue) surface WPs have positive (negative) charge.

4 . Conclusion

In summary, we have shown that in a series of WC-type materials the BCPs between K and H are all WPs. These WPs are described by first- or second-order k.p models. For those WPs described by second-order k.p model , when some special conditions are satisfied, there are three nearby surrounding WPs and these nearby WPs have the opposite charge with the WP on KH. Accoridingly, a charge-radius dependence effect is predicted and obseved around these WPs. The topological charges of all WPs are determined and the surface arcs on both (10-10) and (01-10) surfaces are observed.

5 . Schedule and prospect for the future

My IPA program was finished. So there is no schedule for future study.