

Electronic structure of the superconducting $\text{ZrP}_{2-x}\text{Se}_x$ with having Dirac nodal lines

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In recent years, attempts to find topological superconductor have become more and more active. Here we investigated the electronic structure of superconducting compound $\text{ZrP}_{2-x}\text{Se}_x$ with layered structure [1] by using first-principles calculation. Since compound has isostructural with ZrSiS which has Dirac nodal lines (DNLs) [2], topologically non-trivial electronic structure may be expected. In fact, a DNL-like band structure has been observed by angular-resolved photoemission spectroscopy [3].

Here we show the two (three) dimensionality of the P-3p (Zr-4d) partial DOS. As shown in Fig.1, the P-3p partial DOS of ZrPSe is almost unchanged when Se atoms are removed. Moreover, it almost retains its shape even in the ZrN monolayer. On the other hand, the Zr-4d partial DOS changes its shape drastically. More details are shown in the presentation.

[1] H. Kito *et al.* J. Phys. Soc. Jpn. 83, 074713 (2014).

[2] L. M. Schoop *et al.* Nat. Commun. 7, 11696 (2016).

[3] S. Ishizaka *et al.* Phys. Rev. B105, L121103 (2022).

Fig 1. Density of states curve of (a) ZrPSe , (b) ZrP with the same crystal structure as ZrPSe , and (c) quasi-monolayer ZrP .

