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Electronic Structure of novel Superconductor doped-ZrPSe

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Recently found superconductor $ZrP_{2-x}Se_x$ has the same structure with iron-based superconductor LiFeAs. $ZrP_{1.25}Se_{0.75}$ already has T_c ~ 5.8K, and the substitution of non-magnetic rare-earth elements for Zr even increases T_c [1-3]. Moreover, these doped-ZrPSe are also isostructural to ZrSiS, which has Dirac cone protected by non-symmorphic symmetry and three-dimensional Dirac line nodes [4-6].
Therefore, doped-ZrPSe can give a promising platform for investigating the interplay between the Dirac line nodes and the superconductivity. In order to study these points, it is necessary to clarify the electronic structure of doped-ZrPSe.

In this paper we report the results of the first-principles calculations for cation and anion co-doped system $(Zr_{1-y}Y_y)P(As_{0.25}Se_{0.75})$ using virtual crystal approximation. We found that the density of states at the Fermi level (=$D(E_F)$) shows a dome-shape with respect to the doping concentration y, as shown in the Figure. This result qualitatively explains the observed y dependence of T_c, especially for $(Zr_{1-y}Y_y)P_{1.25}Se_{0.75}$. We also found the similarity of the band structure between ZrSiS and doped-ZrPSe. Characteristic band crossing near E_F along M-G axis, which is found to be the Dirac line node in ZrSiS, is also found in doped-ZrPSe. This result strongly suggests that the superconductivity and the Dirac line node are co-existed in doped-ZrPSe.

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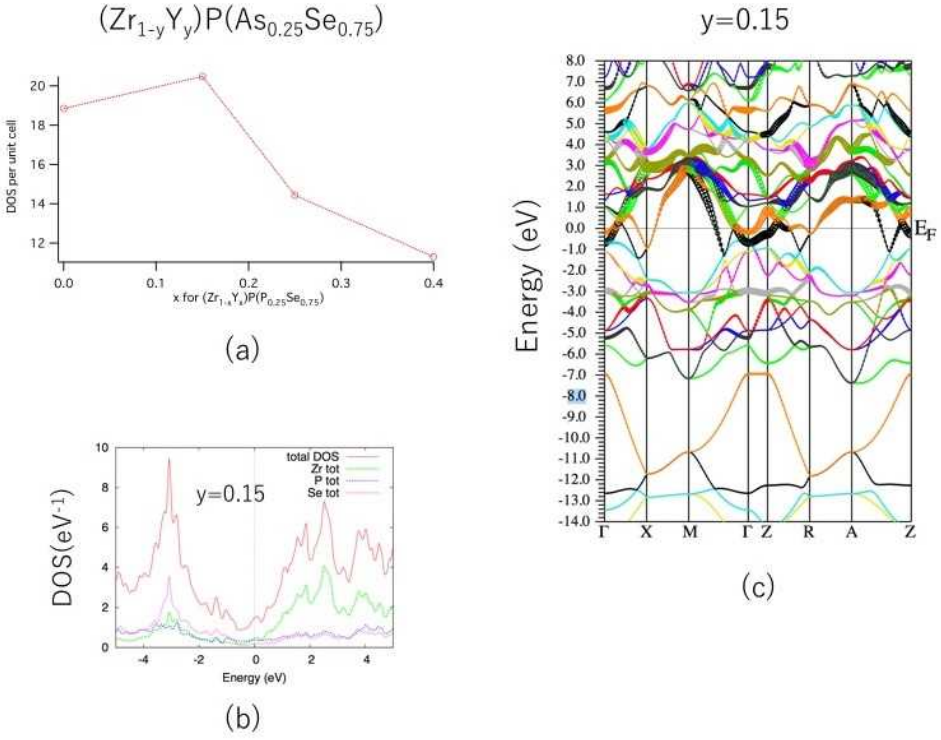

Fig. (a) Density of states at the Fermi level of $(Zr_{1-y}Y_y)P(As_{0.25}Se_{0.75})$ as a function of y. (b) Density of states curve of $(Zr_{0.85}Y_{0.15})P(As_{0.25}Se_{0.75})$. (c) Energy dispersion of $(Zr_{0.85}Y_{0.15})P(As_{0.25}Se_{0.75})$. The width of the band represents the contribution of Zr d-e_g orbitals.

Keywords: doped-ZrPSe, band structure calculation, doping dependence, Dirac line nodes