DIRAC ELECTRONS IN SINGLE-COMPONENT MOLECULAR CONDUCTOR [Pd(dddt)2] UNDER PRESSURE

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It has been shown that single-component molecular conductor [Pd(dddt)2] (dddt = 1,4-dithiin-2,3-dithiolate) exhibits Dirac electrons under pressure[1,2]. The crystal consists of four molecules per unit cell with the HOMO and LUMO orbitals which are symmetric and antisymmetric around the inversion center of the Pd atom, respectively. Compared with the well known case of organic conductor[3], this material provides the Dirac cone in three-dimensional momentum space $k=(k_x,k_y,k_z)$, which comes from transfer energies along the interlayer direction ($z$) in addition to those of the intralayer plane ($x,y$).

By using a tight-binding model corresponding to the pressure[4], which is described by 8 x 8 matrix Hamiltonian with the energy band with $E_j(k)$, ($j=1, ..., 8$), we examined the Dirac cone located between the conduction band $E_4(k)$ and valence band $E_5(k)$. A pair of the Dirac points given by the apex of the Dirac cone form a line with a closed loop. The contour of the gap function of $E_4-E_5$ gives a cylindrical shape along the line suggesting the energy dispersion of the Dirac cone on the plane perpendicular to the line which is almost parallel to the $k_z$ axis for small $k_z$, and is perpendicular to the $k_z$ axis for $k_z \sim \pi$. The typical Dirac points are given for $k_z=0$ (a), and $k_y=0$ (b) where the corresponding Dirac cones are shown in Figs. (a) and (b) as the function of $(k_x/\pi,k_y/\pi)$ with $|k_x/\pi|, |k_y/\pi| < 0.2$ (a) and $(k_x/\pi,k_y/\pi)$ with $|k_x/\pi| < 0.5$ and $|k_z/\pi-1| < 0.5$ (b), respectively.

Further, the Dirac electron is analyzed in terms of the parity at the time reversal invariant momentum (TRIM) where the level crossing of $E_4$ and $E_5$ occurs at a pressure of the emergence of the Dirac point.

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