Topological property of exotic Dirac electrons in organic conductor [Pd(dddt)$_2$]

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The single-component molecular conductor [Pd(dddt)$_2$] (dddt = 1,4-dithiin-2,3-dithiolate) which displays exotic Dirac electrons under pressure has been found and studied using a tight-binding model consisting of four molecules per unit cell with HOMO and LUMO energy levels [1]. The model describes the following feature. The transition from the insulator to the zero-gap state (ZGS) with increasing pressure, is associated with an overlap between the convex HOMO band and the downward-convex LUMO band. The HOMO-LUMO interactions play an important role in the Dirac cone formation. In the present paper, we demonstrate a topological property to verify the exotic Dirac electron which exists as a pair of Dirac cones between the neighboring energy bands. The variation of the transfer energy with respect to the pressure, is estimated from an interpolation formula between the ambient pressure and the high pressure. The insulating state is a novel state which occurs as a merging of a pair of the Dirac electrons at the Gamma point. Further the ZGS is obtained by a pair of Dirac electrons which is located between the HOMO and LUMO bands. We calculate the parity of the wave function at the time reversal invariant momentum (TRIM), which is associated with the topological property originated from the inversion symmetry of the crystal [2]. It is shown that the product of all the parity of the wave functions below the Fermi level becomes negative in the presence of the Dirac electrons while it becomes positive in the absence of the Dirac electrons. Such a property is compared with that of organic conductor alpha-(BEDT-TTF)$_2$I$_3$, which has been well known as the two-dimensional Dirac electron system with the ZGS [3].