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First-principles study of electronic and magnetic structures of the triangular-lattice magnet $PdCrO_2$ TATSUYA SHISHIDOU, TAMIO OGUCHI, ADSM, Hiroshima University — Quite recently *unconventional* anomalous Hall effect has been observed in some geometrically frustrated magnets, where the Hall resistivity does not follow the empirical relation and the noncollinear spin configuration seems to play the key role. $PdCrO_2$[1] is a perfect example of such magnets. It crystallizes in delafossite structure, which is made of alternating stack of triangular layers of Pd and Cr. Its metallic conductivity is attributed to Pd 4d electrons and shows strong two-dimensional anisotropy. Cr^{3+} localized moments show antiferromagnetic ordering at 37.5 K, forming 120 degree noncollinear spin structure. At temperatures lower than 20 K, unconventional Hall effect was measured. So far, its microscopic mechanism has not been clarified yet. In this study, we carry out noncollinear LSDA FLAPW calculations for $PdCrO_2$. We will investigate several magnetic structures with and without spin-orbit coupling. We will focus on the conducting states at the Fermi level and examine how they are affected by the Cr spin structure. [1] H. Takatsu H. Yoshizawa, S. Yonezawa, and Y. Maeno, PRB **79**, 104424 (2009).

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