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DFT+U invstigation of doped-$PbPdO_2$ spin gapless semiconductors HAN HSU, SHENG-CHIEH HUANG, National Central University — Spin gapless semiconductors (SGSs), with a zero gap in one spin channel and a finite gap in the other, have attracted considerable attention due to its potential in spintronics. Ever since $PbPdO_2$ was predicted a gapless semiconductor by local density approximation (LDA) calculations and confirmed by experiments afterward, it is anticipated to be a backbone material for SGS. Using density functional theory + self-consistent Hubbard U (DFT+U_{sc}) calculations, we investigate doped $PbPdO_2$ with different kinds of transition-metal dopants, including V, Cr, Mn, Fe, Co, and Ni, at different dopant concentration. We show that doped $PbPdO_2$ can be a SGS with a proper choice of dopant and dopant concentration. Furthermore, different dopant and dopant concentration can lead to different types of SGS.

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