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**Magnetic-induced polarization in charge-ordered $CaMn_7O_{12}$ system** DIOMEDES SALDANA-GRECO, JIN SOO LIM, ANDREW M. RAPPE, University of Pennsylvania — The electronic properties of $CaMn_7O_{12}$ yield interesting physical phenomena including charge-ordering, non-collinear magnetism, and improper ferroelectricity. The charge-ordered $CaMn_7O_{12}$ is a complex quadruple perovskite whose chemical formula is $(CaMn_3^{3+})(Mn_3^{3+}Mn^{4+})O_{12}$ where three $Mn^{3+}$ are on the $A$-site (Mn1), three $Mn^{3+}$ on the $B$-site (Mn2), and one $Mn^{4+}$ on the $B$-site (Mn3). Three parallel $c$-chains with alternating Mn1 and Mn2 form a Kagome lattice with either Mn3 or Ca at the center of the hexagonal rings. The non-collinear magnetic state consists of spin moments lying on the $ab$-plane, forming a helical pattern along the $c$-axis. Our DFT+$U$+$J$ study shows that the Mn3 spins adopt a (90°,30°) spin configuration with respect to the surrounding (Mn1,Mn2) spins, breaking the inversion symmetry and generating a Berry-phase computed ferroelectric polarization of 2975 $\mu C/m^2$ along the $c$-axis. We demonstrated that when the magnetic helicity of the system is reversed, the ferroelectric polarization flips. This study aims to explore how the electronic and magnetic properties are intertwined to give rise to a multiferroic, charge-ordered state.

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