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Noncollinear magnetic order in quadruple perovskite $LaMn_3V_4O_{12}$ MASAYUKI TOYODA, CREST, Japan Science and Technology Agency, KUNIHIKO YAMAUCHI, TAMIO OGUCHI, ISIR, Osaka University — The microscopic mechanism of noncollinear magnetic order in quadruple perovskite $LaMn_3V_4O_{12}$ has been investigated by first-principles density-functional theory calculations. Unlike other provskite-type manganites, Mn ions are located in the A'-sites that are surrounded by four oxygens with square-planar geometry, whereas the octahedrally coordinated B-sites are occupied by magnetically inactive V ions. In order to understand the magnetic interactions between the Mn spins, magnetic exchange coupling constants are estimated by mapping the numerically calculated energies with constraints on spin orientations onto an effective Heisenberg model. The antiferromagnetic coupling between the 2nd-nearest neighbors is found to satbilize the noncollinaer magnetic order which is relatively stronger in the present compound than in other G-type antiferromagnetic quadruple perovskites such as $YMn_3Al_4O_{12}$ and $LaMn_3Cr_4O_{12}$. We will also discuss on possibility of the ferroelectricity in the present compound in analogy with $CaMn_7O_{12}$, which is a multiferroic quadruple perovskite with noncollinear magnetic order.

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