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A-site magnetic ordering in quadruple perovskite oxides MASAYUKI TOYODA, CREST, Japan Science and Technology Agency, KUNIHIKO YAMAUCHI, ISIR, Osaka University, TAMIO OGUCHI, CREST, Japan Science and Technology Agency — Magnetic exchange interaction in A-site ordered quadruple perovskites $AA'_3B_4O_{12}$ is comprehensively investigated by using first-principles calculations. The ideal crystal structure ($Im\bar{3}$) is characterized by the square-planer oxygen coordination around A' cations as well as the $a^+a^+a^+$ type tilting of BO_6 octahedra. Owing to these structural features, the compounds can include transition-metal ions both at the A' and B sites. Consequently, there are two magnetic sublattices with different oxygen coordination. Unlike the B-site magnetism that has been investigated for decades, detailed mechanisms for the A'-site magnetism and A'-B intersublattice magnetism are still unclear. In insulating compounds such as $CaCu_3Ge_4O_{12}$ and $YMn_3Al_4O_{12}$, it is found that the nearest-neighbor superexchange interaction between the A' sites determines the ground-state magnetic ordering. Furthermore, in our simulation, it is shown that magnetic phase transition from antiferromagnetism to ferromagnetism will occur along with insulator-to-metal transition in $YMn_3Al_4O_{12}$ by modulating the tilting of AlO_6 octahedra. Possible strategies are suggested to realize such a modulation, for example, by imposing chemical or physical pressure.

Masayuki Toyoda
CREST, Japan Science and Technology Agency

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