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Electric polarization and magneto-dielectric effect in charge ordered system with frustrated geometry TSUTOMU WATANABE, IMRAM, Tohoku University, SUMIO ISHIHARA COLLABORATION — Recently discovered multiferroics materials, where electric polarization and non-collinear spin structure coexist, are recognized as ferroelectric materials driven by spin ordering. There is another class of ferroelectricity where the electric polarization is attributed to the electronic charge ordering. Layered iron oxide $LuFe_2O_4$ belongs to this class of material. Ferroelectric transition occurs at almost the same temperature with the charge ordering one where Fe^{2+} and Fe^{3+} are aligned in the paired triangular lattices. Therefore, it is expected that the frustration plays important roles on breaking of the space inversion symmetry. We study theoretically a possibility of the charge-driven ferroelectric transition, and, in particularly, focus on the electron quantum transfer effects. We analyzed the V-t model, where t and V are the transfer integral and the Coulomb repulsion between nearest-neighbor sites, respectively, by using the variational Monte Carlo method. We found that the quantum fluctuation and frustration tend to enhance the stabilization of a three-fold charge ordered state and electric polarization, although the polarization is small. In addition, we studied the effect of the spin ordering. It is found that, in some spin ordered structures, the electric polarization is stabilized accompanying the three-fold charge ordered state.

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