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Spin-Charge-Orbital States and Electric Polarization in Multiferroic RFe_2O_4 SUMIO ISHIHARA, MAKOTO NAKA, JYOJI NASU, AYA NAGANO, Department of Physics, Tohoku University — Layered iron oxides RFe_2O_4 (R: rare-earth ion) is recognized to be an electronic ferroelectric and multiferroic compounds. Crystal structure of this compound consists of stacked FeO triangle layers. Charge and spin states have been studied by the electron and neutron diffraction experiments. Long range charge and spin orders characterized by the momentum (1/3, 1/3) appear around 320K and 250K, respectively, in $LuFe_2O_4$. Electric polarization is induced around the charge ordering temperature of Fe^{2+} and Fe^{3+}, and is enhanced around the magnetic ordering temperature. We examine theoretically spin-charge-orbital structures and electric polarization in RFe_2O_4. We suggest that Fe^{2+} ion has the doubly degenerate orbital degree of freedom. Effective Hamiltonian for spin, charge and orbital degrees of freedom is derived. Numerical analyses with the multi-canonical Monte-Carlo simulation and the mean-field approximation show that the electric polarization is attributed to the charge order with momentum (1/3, 1/3). A magnitude of the polarization is enhanced around the magnetic ordering temperature due to the coupling between spin and charge. Conventional orbital order is not expected from the numerical calculation, and possible orbital states at low temperatures are discussed.

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