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Understanding the Interplay of Polar, Magnetic, and Electronic Order in Ferroic $(LuFeO_3)_m/LuFe_2O_4$ Superlattices ALEJANDRO REBOLA, Cornell University, HENA DAS, Lawrence Berkeley National Laboratory, CRAIG FENNIE, Cornell University — Multiferroics are not only important from a technological point of view but also because of the rich and complex physics that results from the interplay between spin, charge and structural distortions. Hexagonal $LuFeO_3$ has recently been understood theoretical and experimentally, and shown to be an improper structural ferroelectric directly analogous to the hexagonal manganites. $LuFe_2O_4$ is structurally homologous to $LuFeO_3$ –both are characterized by a FeO_5 bipyramidal crystal field- but unlike the latter it exhibits a much larger magnetic moment and it is still a matter of debate whether it is ferroelectric. The double Fe-layer in $LuFe_2O_4$ is thought to be charge ordered and highly frustrated, resulting in possible polar, non-polar or anti-polar charge arrangements. Here we first investigate the relation between different charge and magnetic orders and structural distortions in bulk $LuFe_2O_4$ by DFT and Monte Carlo calculations. Then we concentrate on a system that combines both mechanisms -a structural improper ferroelectric and a charge frustrated polar structure- such as the $(LuFeO_3)_m/LuFe_2O_4$ superlattices.

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