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Hybrid-Improper Ferroelectricity in a Cation Ordered Ruddlesden-Popper Manganite[1] ANTONIO CAMMARATA, JAMES RONDINELLI, Drexel University — There is strong interest in uncovering new routes to design multiferroic compounds, which combine ordered magnetic states with electric polarizations, since they have great potential in novel multifunctional devices. Using first principles calculations based on density functional theory, we show the ground state of the the cation ordered (La,Sr)MnO_4 Ruddlesden-Popper oxide is polar. The electric polarization arises from an anharmonic coupling mechanism, which can be designed at the atomic scale. We find that in addition to cooperative polar cation displacements, two non-polar distortions of the oxygen lattice, *i.e.*, an octahedral rotation mode and Jahn-Teller bond distortions, are present in the polar phase. The latter originates from the *electronic* susceptibility of the Mn e_g orbitals to polarize, while the former is due to the La and Sr cation size mismatch. We find that the Jahn-Teller mode and the octahedral rotation mode are coupled through an anharmonic interaction and cooperatively stabilize the polar structure and induce a net electric polarization. Our survey of multiple transition paths reveal that this material is classified as a *hybrid-improper* ferroelectric, and the Mn d^4 configuration makes it a potential multiferroic oxide.

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