Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Ab Initio study on structural, electronic, magnetic and dielectric properties of LSNO within Density Functional Perturbation Theory JOHN PETERSEN, Texas State University, FRIEDHELM BECHSTEDT, JÜRGEN FURTHMÜLLER, Friedrich-Schiller-Universität, LUISA SCOLFARO, Texas State University — LSNO ($La_{2-x}Sr_xNiO_4$) is of great interest due to its colossal dielectric constant (CDC) and rich underlying physics. While being an antiferromagnetic insulator, localized holes are present in the form of stripes in the Ni-O planes which are commensurate with the inverse of the Sr concentration. The stripes are a manifestation of charge density waves with period approximately 1/x and spin density waves with period approximately 2/x. Here, the spin ground state is calculated via LSDA + U with the PAW method implemented in VASP. Crystal structure and the effective Hubbard U parameter are optimized before calculating ε_∞ within the independent particle approximation. ε_∞ and the full static dielectric constant (including the lattice polarizability) ε_0 are calculated within Density Functional Perturbation Theory.

John Petersen
Texas State University

Date submitted: 18 Nov 2016 Electronic form version 1.4