

Abstract Submitted  
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**Lattice normal modes and electronic properties of the correlated metal  $\text{LaNiO}_3$**  GAOYANG GOU, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA, JAMES RONDINELLI, X-Ray Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, ILYA GRINBERG, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA — We present results from density functional calculations of lattice vibrations and electronic properties of the correlated metal  $\text{LaNiO}_3$ . Using the Landau theory of phase transitions and *ab initio* derived phenomenological coefficients obtained from local-spin density approximation (LSDA) calculation, we examine the evolution of the Raman-active phonon modes with temperature and find that the LSDA results give excellent agreement with experiments. To study the electronic structure of  $\text{LaNiO}_3$ , we extend to the post-LSDA functional methods, including the local spin density+Hubbard U (LSDA+U) method, and two hybrid exchange-correlation functionals, PBE0 and HSE. By comparing the results obtained from the various functionals with the experimental photoelectron spectroscopy (PES) and X-ray photoelectron spectroscopy (XPS) data, we argue that the screening effect coming from the delocalized O-2p and Ni- $t_{2g}$  electrons will be strong enough to reduce the electron correlation of  $\text{LaNiO}_3$ .

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