Lattice normal modes and electronic properties of the correlated metal \textsf{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 LaNiO$_3$. Using the landau theory of phase transitions and \textit{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 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 LaNiO$_3$. 

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