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Lattice normal modes and electronic properties of the correlated metal $LaNiO_3$ 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 *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 $LaNiO_3$.

Gaoyang Gou
The Makineni Theoretical Laboratories, Department of Chemistry,
University of Pennsylvania, Philadelphia, PA 19104, USA

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