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Vibrational properties of MnO and NiO from DFT + *U*-based density functional perturbation theory

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A. Floris[1,2], S. de Gironcoli[3], E. K. U. Gross[2,4], and M. Cococcioni[5]

[1]*Department of Physics, King's College London, London, Strand WC2R 2LS, United Kingdom*

[2]*European Theoretical Spectroscopy Facility (ETSF)*

[3]*SISSA Condensed Matter Theory sector and CNR-IOM DEMOCRITOS Simulation Centre, via Bonomea 265, I-34136 Trieste, Italy*

[4]*Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany*

[5]*Department of Chemical Engineering and Materials Science, University of Minnesota, 421 Washington Avenue SE, Minneapolis, Minnesota 55455, USA*

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We introduce an extension of the density functional perturbation theory (DFPT) that allows self-consistent linear-response calculations from a DFT + *U* ground state. Using this scheme, the full phonon dispersion of strongly correlated materials, whose ground state can be captured with Hubbard-corrected functionals, can be accessed with unprecedented accuracy and numerical efficiency. The tool is applied to the study of MnO and NiO in their antiferromagnetic (AFII) ground state. Our results confirm the highly noncubic behavior of these systems and show a strong interplay between features of the phonon spectrum and the occupation of specific *d* states, suggesting the possibility to investigate the electronic structure of these materials through the analysis of their phonon spectrum.

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