Supporting Information
for
Effect of pressure on the electronic structure of antiferromagnetic and paramagnetic $YNiO_3$: role of disproportionation

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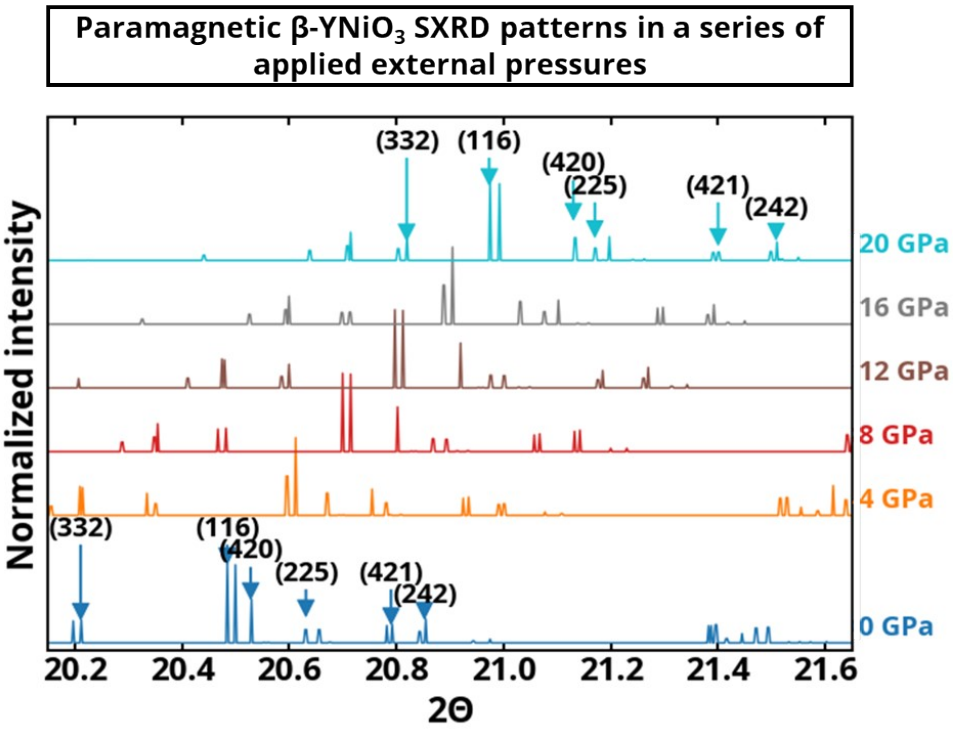

Figure S1. Synchrotron X-ray diffraction (SXRD) spectra of the simulated beta (paramagnetic) phase of $YNiO_3$ at ambient (0 GPa) and series of elevated pressures up to 20 GPa. The 2-Θ-scan diffractograms were computed assuming X-ray radiation source of λ=0.4166 Å corresponding to the beamline used in the referenced SXRD study of García-Muñoz et al.[1] For comparison with experiment the SXRD spectra are presented after reducing the polymorphous cell to the primitive cell neglecting small distribution of local structural motifs.

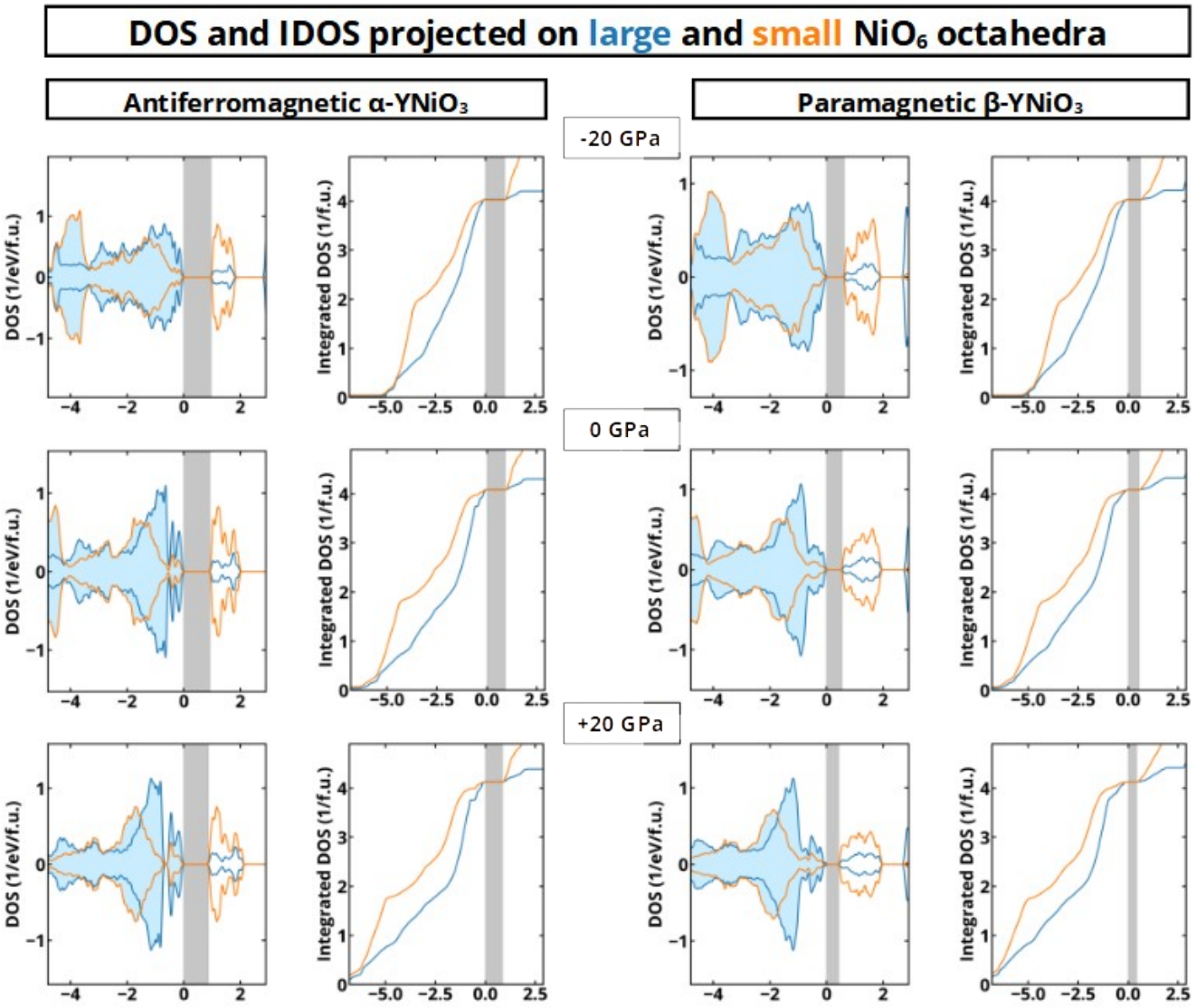

Figure S2. Ni-d density of states and integrated density of states with distinction between nickels in the center of large and small octahedra at ambient (0 GPa), elevated (+20 GPa), and decreased (-20 GPa) pressures.

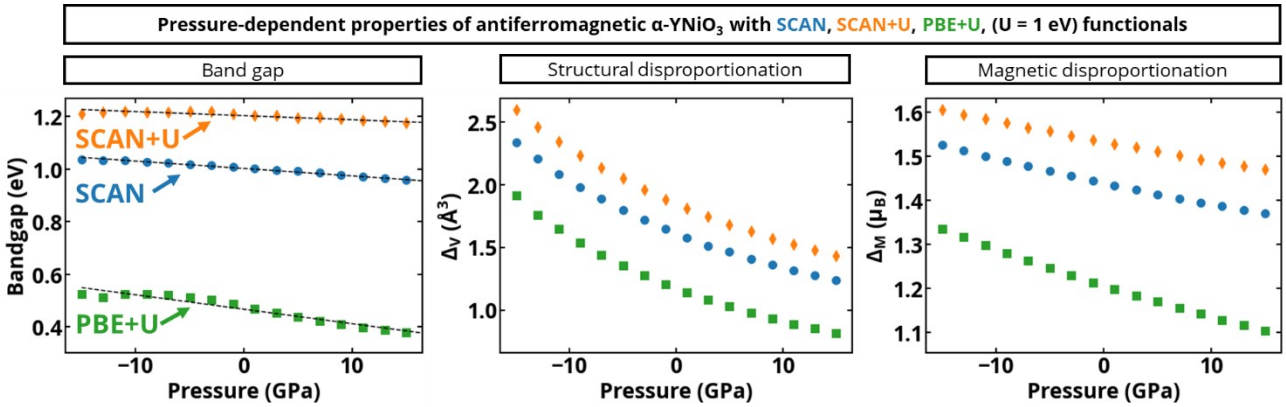

Figure S3. The pressure dependence of the electronic band gap and the two disproportionation factors present in the α-$YNiO_3$ system with different density functionals. Blue circles (labeled SCAN) correspond to the "SCAN, no U" results presented in Figure 2 and Figure 3 in the main text. Orange diamonds (labeled SCAN+U) have been obtained by applying the Hubbard U= 1 eV correction to Ni-d states using the Dudarev method[2]. Green squares (labeled PBE+U) have used the Perdew-Burke-Ernzerhof[3] functional with the same U correction.

References

1. J. L. García-Muñoz, M. Amboage, M. Hanfland, J. A. Alonso, M. J. Martínez-Lope and R. Mortimer, *Physical Review B*, 2004, **69**.
2. S. L. Dudarev, G. A. Botton, S. Y. Savrasov, C. J. Humphreys and A. P. Sutton, *Physical Review B*, 1998, **57**, 1505-1509.
3. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys Rev Lett*, 1996, **77**, 3865-3868.