Supporting Information

Formation, electronic structure and defects of Ni substituted spinel cobalt oxide: a DFT+U study

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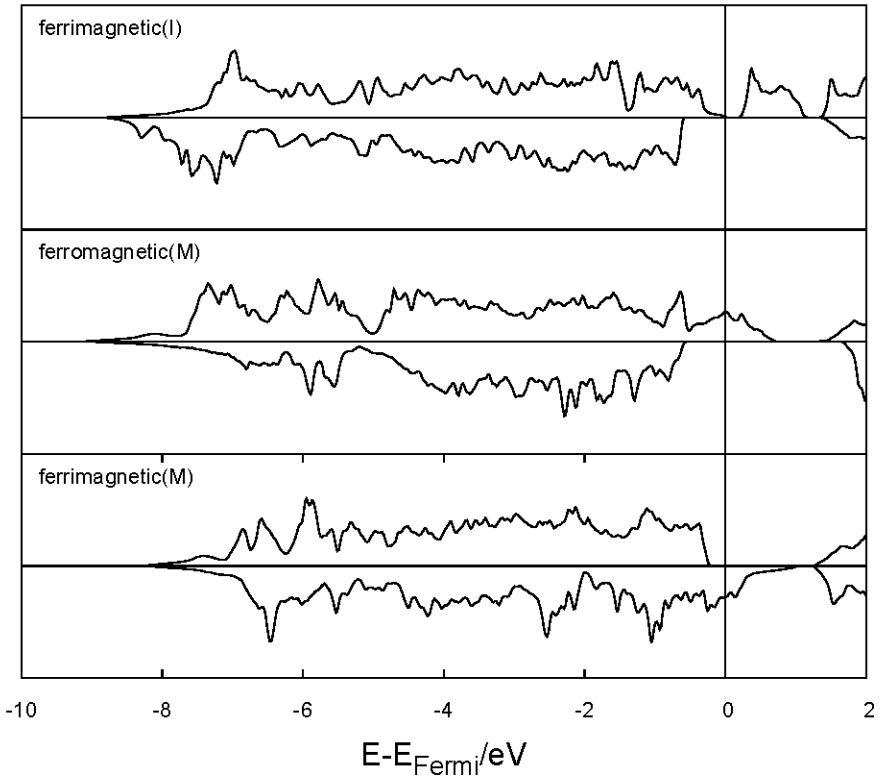

Figure S1,DOS calculated for the insulating ferrimagnetic (I) (top panel), metallic ferromagnetic (M) (middle panel), and metallic ferrimagnetic (M) (bottom panel) configurations of NiCo2O4.

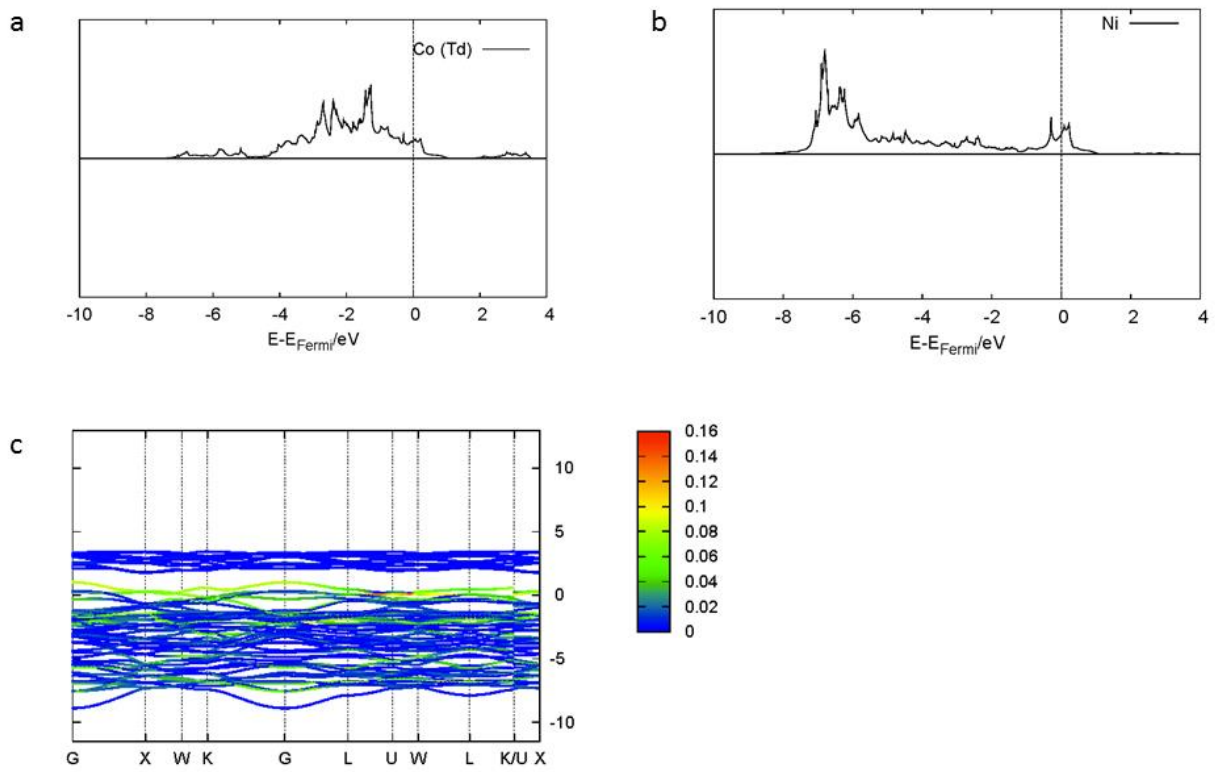

Figure S2 Projected DOS calculated for the e/e_g states of (a), Co (Td) and (b), Ni. The fractional valence calculated from this PDOS is ~2.1+ for both Co(Td) and Ni. (c) Band structure around the Fermi level; different colors indicate the contribution of the oxygen orbitals.

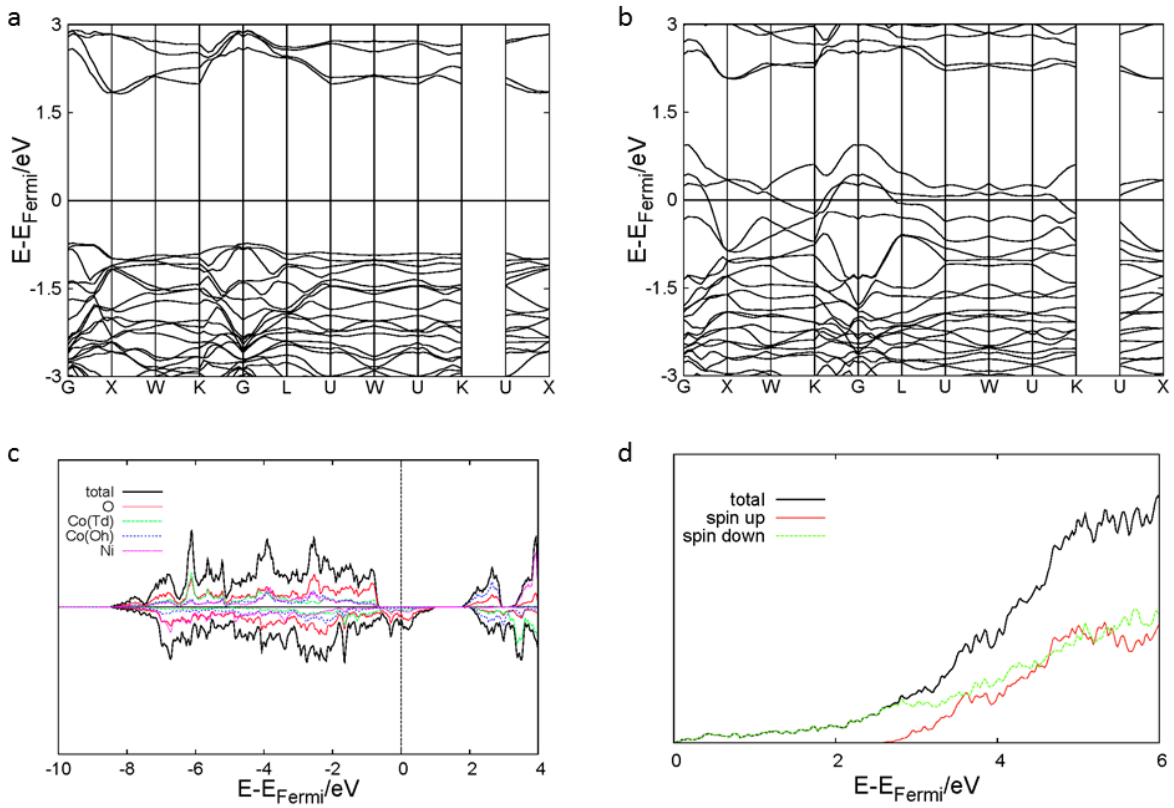

Figure S3 Electronic structure of NCO calculated using norm conserving pseudopotentials with U terms from linear response: band structure for (a) majority and (b) minority spins; (c) Projected DOS, and (d) Joint DOS. The JDOS suggests an optical band gap of ~ 2.5 eV for the majority spins and absorption at long wavelengths for the minority spins.

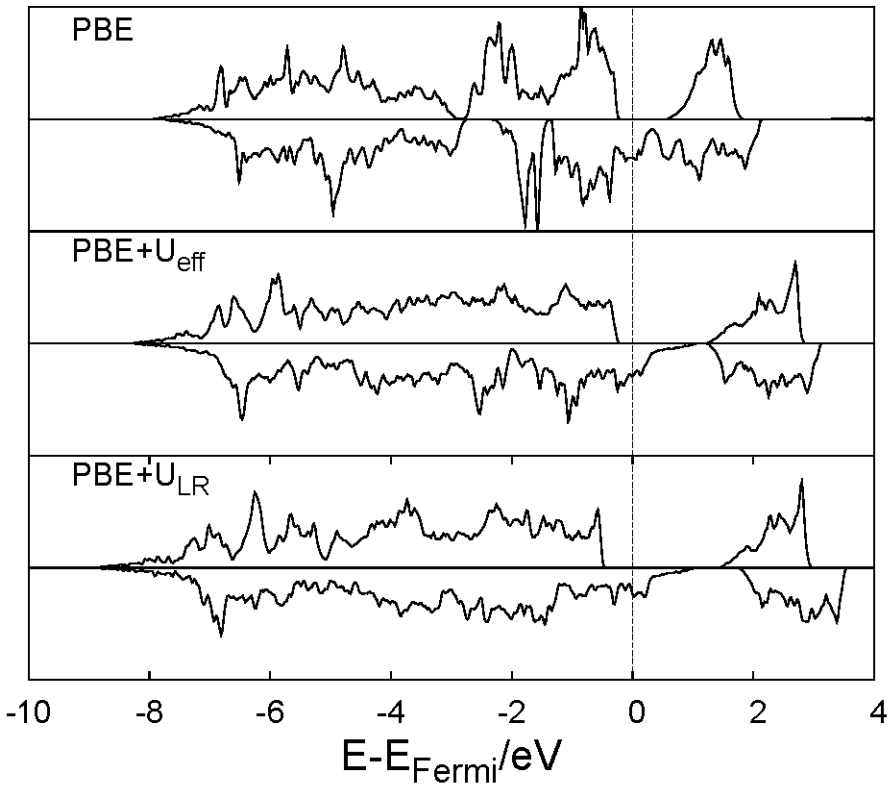

Figure S4 DOS of pristine NCO calculated using different U values, as indicated.

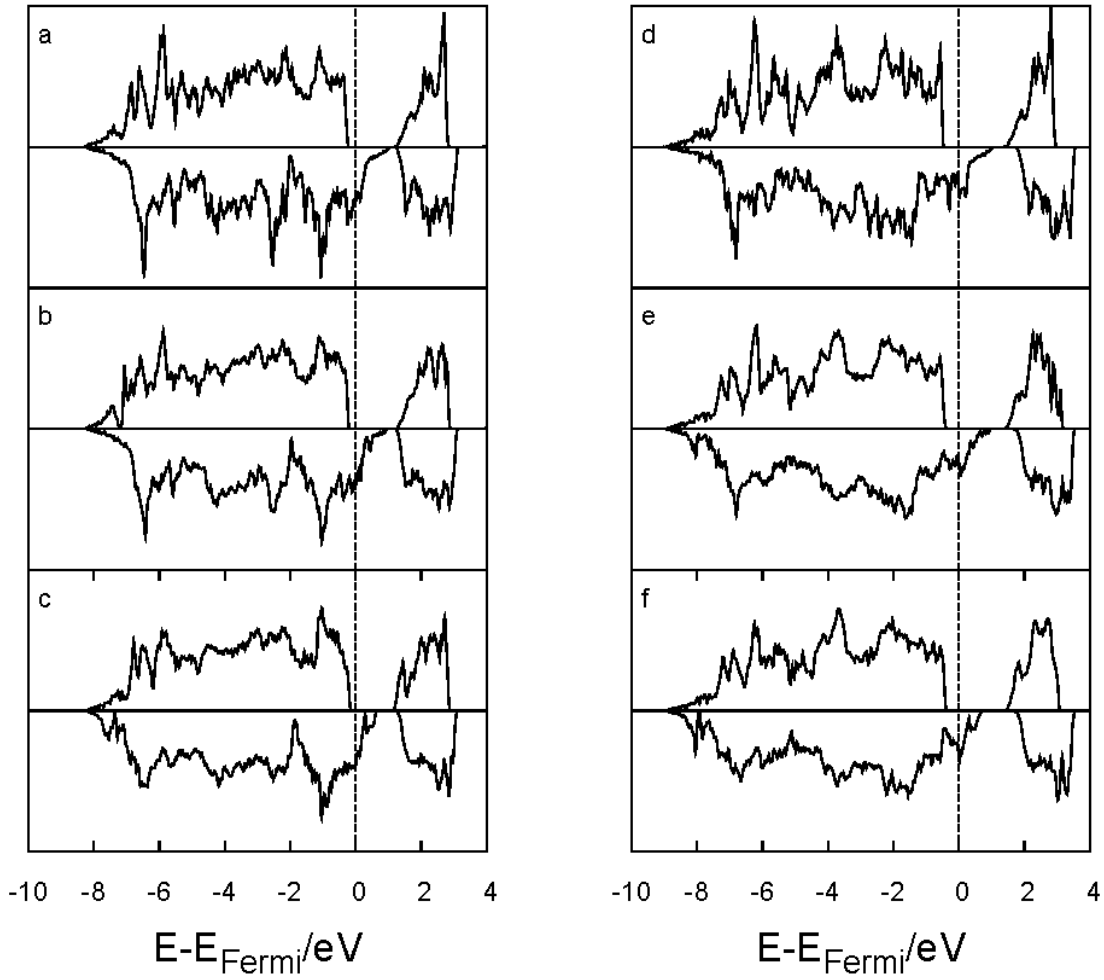

Figure S5 DOS calculated using U_{eff} (left) and U_{LR} (right) with: (a,d) no substitution, (b,e) 1/8 substitution and (c,f) 1/4 substitution.

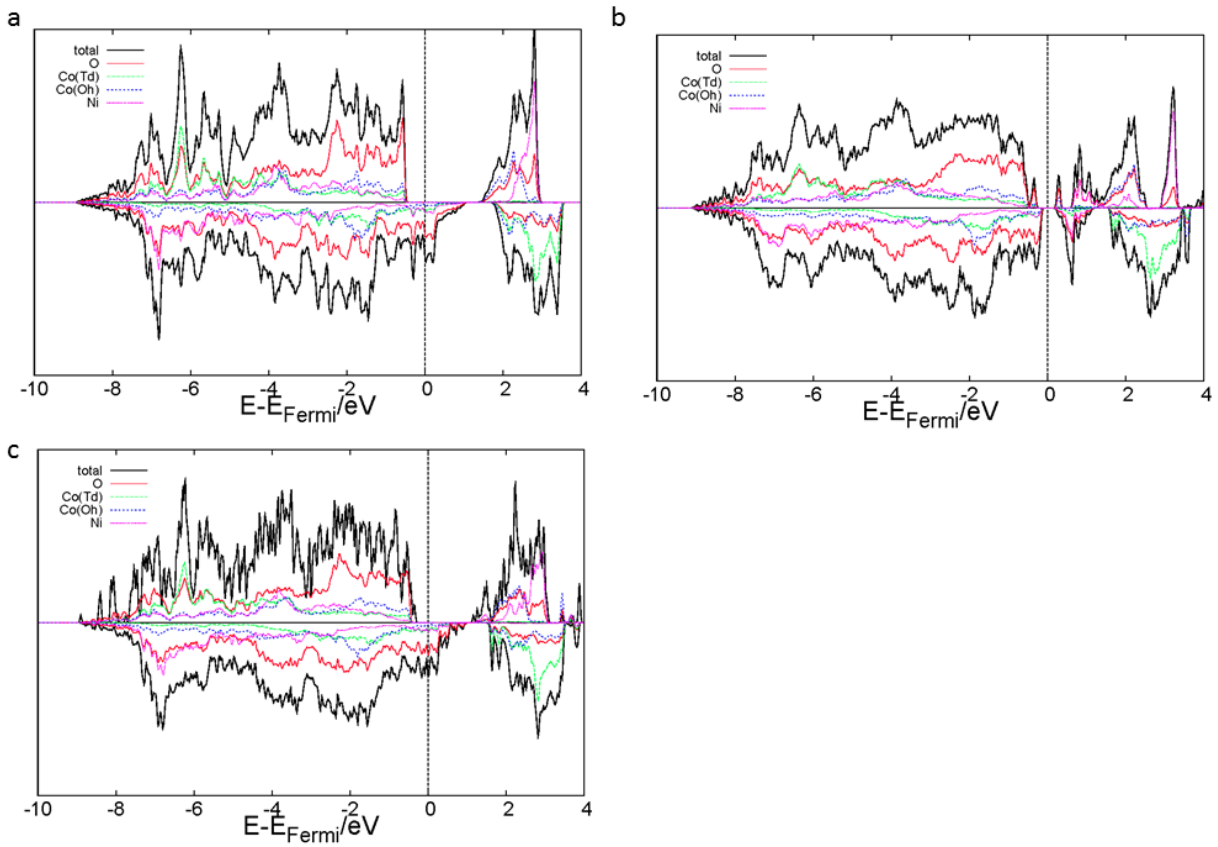

Figure S6 PDOS of defect free bulk (a), oxygen vacancy on Site A (b) and oxygen vacancy on Site B (c), calculated using DFT+U_{LR}.

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