# Supplementary Information

# Elusive $Co_2O_3$: A combined experimental and theoretical study

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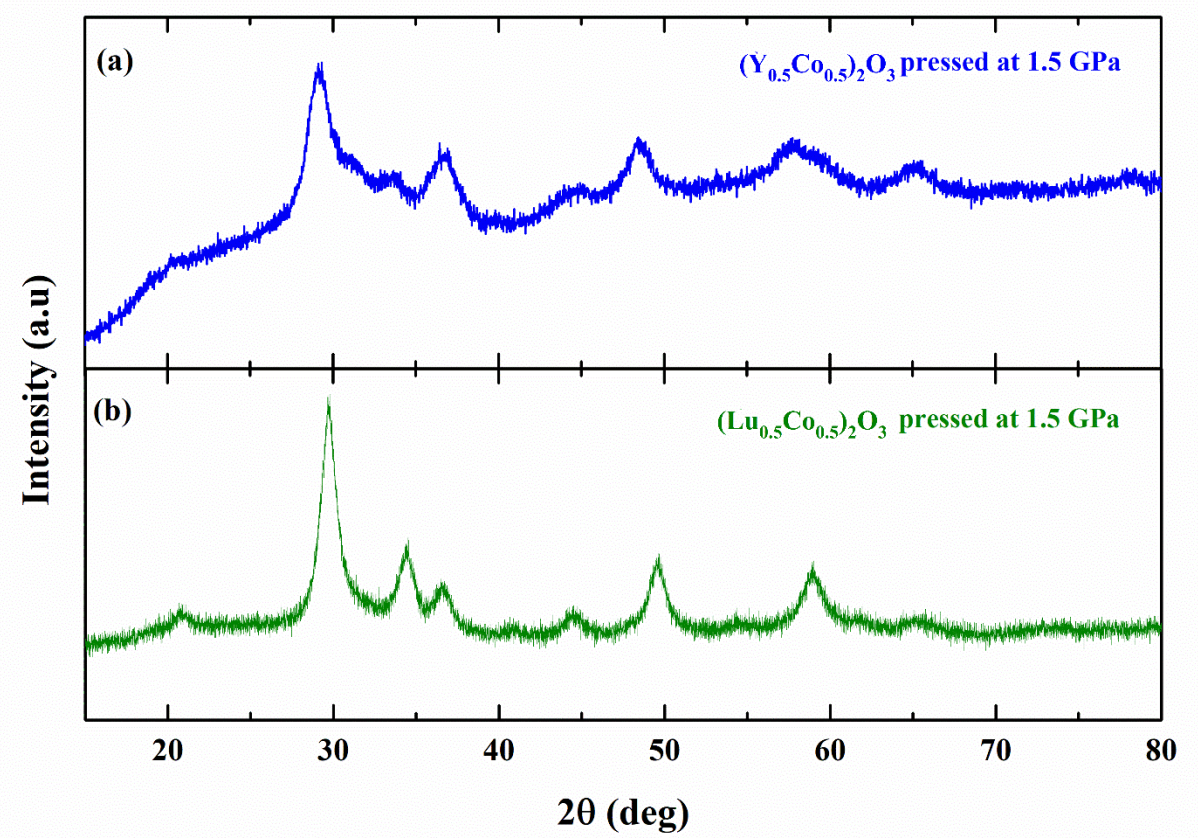


**Figure S1.** X-ray diffraction profiles of high pressure (1.5 GPa) treated (a) $(Y_{0.5}Co_{0.5})_2O_3$ and (b) $(Lu_{0.5}Co_{0.5})_2O_3$ solid solutions.

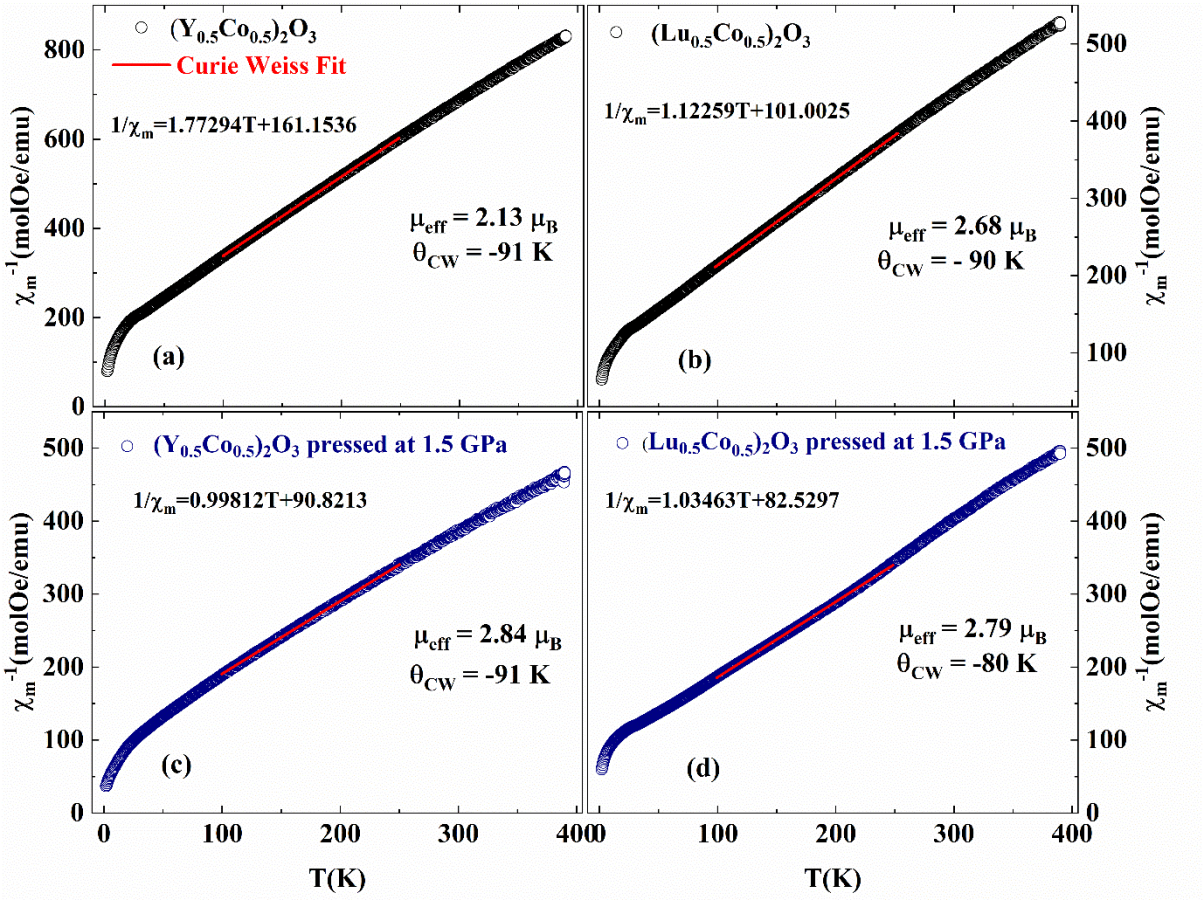


**Figure S2**. Temperature dependent inverse magnetic susceptibility curves of (a) $(Y_{0.5}Co_{0.5})_2O_3$ (b) $Lu_{0.5}Co_{0.5})_2O_3$ (c) $(Y_{0.5}Co_{0.5})_2O_3$ pressed at 1.5 GPa and (b) $Lu_{0.5}Co_{0.5})_2O_3$ pressed at 1.5 GPa, fitted using Curie Weiss Law in the temperature region 100-250 K

**Table S1:** Variation of phonon eigenvalues at Γ point as a function of Hubbard U:

| **Hubbard U** | U = 0.0 eV | U = 2.0 eV | U = 3.5 eV | U = 4.0 eV | U = 6.0 eV | U = 8.0 eV |
|---|---|---|---|---|---|---|
| **Phonon eigenvalues ($cm^{-1}$)** | -32 | -46 | -51 | -55 | -59 | -71 |

**Table S2:** Variation of Integrated COHP (ICOHP)[1-2] for Co-O bonding with the increasing values of Hubbard U:

| **Hubbard U** | U = 0.0 eV | U = 2.0 eV | U = 3.5 eV | U = 4.0 eV | U = 6.0 eV | U = 8.0 eV |
|---|---|---|---|---|---|---|
| **ICOHP (eV/cell)** | 0.447 | 1.208 | 1.216 | 1.221 | 1.234 | 1.272 |

ICOHP for different materials considered in the work are compared and shown in Table S3. Integrated COHP (ICOHP) signifies a measure of bond strength between the orbitals of distinct atoms. The negative/positive values of ICOHP suggest bonding characteristics between two atoms are bonding/antibonding in nature. Here, we observe that bonding strength between Al-O in $Al_2O_3$ is higher than Y-O bonds in $Y_2O_3$. The bonding strength describes the structural stability of the crystal.

**Table S3:** Integrated COHP (ICOHP) in eV/atoms for different materials

| **Materials** | **ICOHP (eV/atoms)** |
|---|---|
| Al-O bonds in $Al_2O_3$ | -0.026 |
| Co-O bonds in $Co_2O_3$ | 0.08 |
| Y-O bonds in $Y_2O_3$ | -0.013 |
| Co-O bonds in 50% Co doped $Y_2O_3$ | -0.001 |
| Co-O bonds in 100% Co doped $Y_2O_3$ | 0.0012 |

## References:


1. Maintz, S.; Deringer, V. L.; Tchougréeff, A. L.; Dronskowski, R., Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. *Journal of Computational Chemistry* **2013,** *34* (29), 2557-2567.

2. Lücke, A.; Gerstmann, U.; Kühne, T. D.; Schmidt, W. G., Efficient PAW-based bond strength analysis for understanding the In/Si (111)(8× 2)–(4× 1) phase transition. *Journal of Computational Chemistry* **2017,** *38* (26), 2276-2282.