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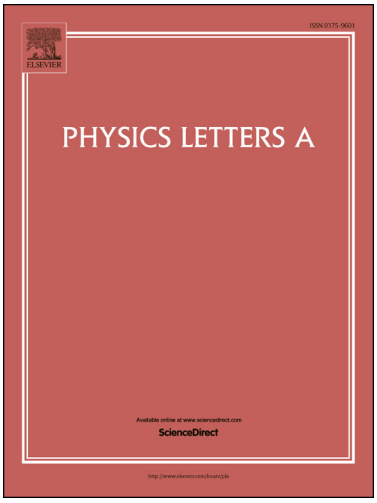

Constrained DFT+U approach for understanding the magnetic behaviour of ACr_2O_4 (A=Zn, Mg, Cd and Hg) compounds

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Highlights

- Inconsistency about the nearest neighbour exchange coupling constant (theoretically predicted by Yaresko) with increasing U is studied in chromium spinels.
- Unconstrained calculations give the inconsistent sign of nearest neighbour exchange coupling constant and variation of its magnitude with increasing U especially for $CdCr_2O_4$ and $HgCr_2O_4$ for $U > 3$ eV and U=2-6 eV, respectively.
- The sign of nearest neighbour exchange coupling constant and variation of its magnitude with increasing U observed in constrained calculations are consistent with experimental data and inverse relation of exchange coupling constant and U, respectively.
- The present study shows the importance of constrained calculations in understanding the magnetic behaviour of these spinels.