ARTICLE

Supporting Information

for

A GGA + U investigation into the effects of cations on the electromagnetic properties of transition metal spinels†

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Table S1. Hubbard U_{eff} (eV) values employed for metal ions.

M	Mn^T	Mn^O	Fe^T	Fe^O	Co^T	Co^O	Ni^T	Ni^O	Cr^O
U_{eff}	4.0	3.5	4.3	4.0	4.5	6.5	5.0	6.4	4.0

[T]the tetrahedral sites.

[O]the octahedral sites.

Table S2. The calculated energies (in eV) for spinels with different magnetic states

Spinel	AFM	FM	FM'
$MnCr_2O_4$	0.000	0.428	0.057
$FeCr_2O_4$	0.094	0.590	0.000
$CoCr_2O_4$	0.248	0.805	0.000
$NiCr_2O_4$	0.270	0.853	0.000
$ZnCr_2O_4$	0.000	0.182	
$ZnMn_2O_4$	0.000	0.889	
$ZnFe_2O_4$	0.000	0.381	
$ZnCo_2O_4$	0.000	1.070	
$ZnNi_2O_4$	0.278	0.000	
$LiCr_2O_4$	0.000	0.179	
$LiMn_2O_4$	0.000	0.167	
$LiFe_2O_4$	0.000	0.824	
$LiCo_2O_4$	0.000	1.031	
$LiNi_2O_4$	0.136	0.000	

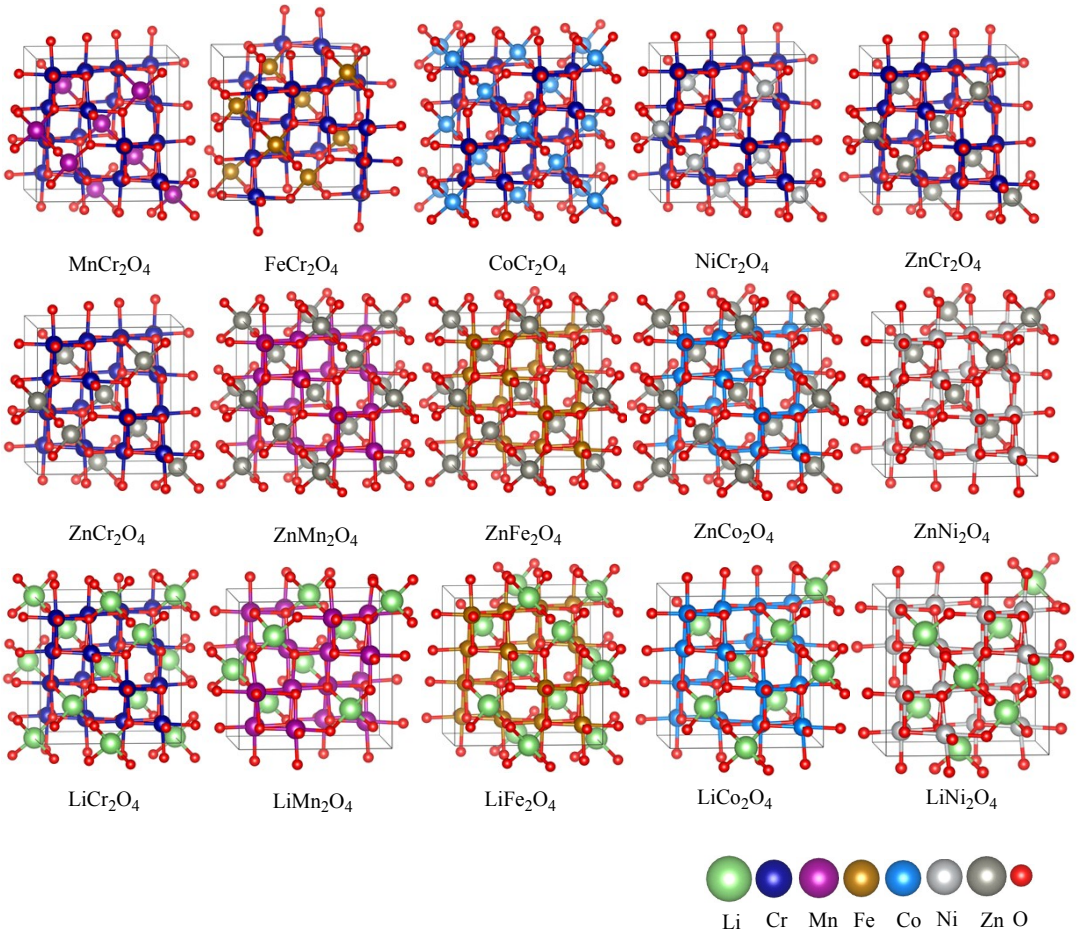

Figure S1. Optimized bulk structures for spinels.