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Magnetic coupling in CoCr_2O_4 and MnCr_2O_4 : an LSDA+ U study

CLAUDE EDERER, Trinity College Dublin, Ireland, MATEJ KOMELJ, Jožef Stefan Institute, Ljubljana, Slovenia — Competing magnetic interactions can lead to very interesting magnetic structures and pronounced effects due to spin-lattice coupling. Chromium spinels with additional magnetic A -site cations are prime examples for such systems, and have recently regained attention due to the discovery of a small electric polarization in CoCr_2O_4 [1]. The multiferroic character of CoCr_2O_4 is supposedly a result of its inversion symmetry-breaking magnetic structure, which has been classified as a “ferrimagnetic spiral” [2]. To achieve a better understanding of the complicated magnetic structure in CoCr_2O_4 and similar systems, an *ab initio* determination of the magnetic coupling constants is very desirable. Here, we present results of LSDA+ U calculations of the magnetic coupling constants in both CoCr_2O_4 and MnCr_2O_4 [3]. We carefully assess the predictive power of such calculations, and then give quantitative estimates for the strengths of the most prominent magnetic interactions. Our results highlight the possible importance of AA interactions in spinel systems with magnetic ions on both A and B sites, and provide an important link between previous theory and experimental observations.

[1] Y. Yamasaki *et al.*, Phys. Rev. Lett. 96, 207204 (2006). [2] D. H. Lyons *et al.*, Phys. Rev. 126, 540 (1962). [3] C. Ederer and M. Komelj, Phys. Rev. B 76, 064409 (2007).

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