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Jahn-Teller coupling and magnetic ground state in vanadium spinels¹ GIA-WEI CHERN, OLEG TCHERNYSHYOV, Johns Hopkins University — The interplay of orbital, lattice, and spin degrees of freedom in vanadium spinels has attracted much interest among researchers. The V^{3+} ion has two electrons occupying three degenerate t_{2g} orbitals and is thus Jahn-Teller active. It also has a total spin $S = 1$ in accordance with Hund's rules. Moreover, the V^{3+} ions sitting on the B -site of spinel form a pyrochlore lattice, the interactions between these localized spin and orbital degrees of freedom are thus geometrically frustrated [1]. Here we present a theoretical model for the ground states of vanadium spinels. We view all of the vanadates (Cd, Zn, Mg on the one hand and Mn on the other) within the same model in which the influence of Mn is simulated by a magnetic field. In the case of MnV_2O_4 , our calculation yields a ground state with antiferro-orbital ordering accompanied by a tetragonal structural distortion with lattice constants $a = b > c$. In addition, the V spins develop an orthogonal antiferromagnetic order in the ab plane on top of a ferromagnetic moment along the c axis. The results are consistent with a recent experimental characterization of MnV_2O_4 [2]. In particular, we will discuss the important role played by cooperative Jahn-Teller interaction and spin-orbital coupling in stabilizing the orthogonal spin configuration. [1] O. Tchernyshyov, Phys. Rev. Lett., **93**, 157206 (2004). [2] V. O. Garlea *et al.*, cond-mat/0711.1844. ¹NSF Grant No. DMR-0348679

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