

Abstract Submitted
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LaCoO₃ (LCO) - Dramatic changes in Magnetic Moment in fields to 500T¹ Y. LEE, B. N. HARMON, Ames Laboratory, U.S. DOE and Dept. of Physics and Astronomy, Iowa State University — LCO has attracted great attention over the years (>2000 publications) because of its unusual magnetic properties; although in its ground state at low temperatures it is non-magnetic. A recent experiment^[1] in pulsed fields to 500T showed a moment of $\sim 1.3\mu_B$ above 140T, and above ~ 270 T the magnetization rises, reaching $\sim 3.8\mu_B$ by 500T. We have performed first principles DFT calculations for LCO in high fields. Our earlier calculations^[2] explained the importance of a small rhombohedral distortion in the ground state that leads to a suppression of the $1.3\mu_B$ moment for fields below ~ 140 T. By allowing fairly large atomic displacements in high fields, moments of $\sim 4\mu_B$ are predicted. [1] V. V. Platonov *et al.* Phys. Solid State **54**, 279 (2012) [2] Y. Lee and B. N. Harmon *et al.* J. Appl. Phys. **113**, 17E145 (2013)

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