

Abstract Submitted
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Investigation of structural and magnetic properties of LaCo5 under pressure¹ MARKUS DAENE, JASON R. JEFFREYS, JON R.I. LEE, DANIEL ABERG, PATRICK HUANG, NICK P. BUTCH², SCOTT K. MCCALL, LORIN X. BENEDICT, BABAK SADIGH, Lawrence Livermore National Laboratory — We report a joint experimental and theoretical investigation of the crystal structure parameters and magnetic moments of LaCo5 under hydrostatic compression. Theoretical predictions were made using density-functional-based electronic structure methods; special attention was paid to the dependence of the results on the choice of exchange-correlation functional. We comment on the degree to which our predictions match those of our measurements and relate both to earlier studies of Koudela et al. [1]. [1] D. Koudela et al., Phys. Rev. B vol.77, 024411 (2008).

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