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Cobalt spin state and hyperfine interaction in ferromagnetic insulating $LaCoO_3$ thin films[1] RENATA WENTZCOVITCH, HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, CHRIS LEIGHTON, University of Minnesota — At low temperatures, bulk $LaCoO_3$ is a non-metallic diamagnet. In contrast, thin-film $LaCoO_3$ experiencing a tensile epitaxial strain is a ferromagnetic insulator in the same temperature range. It is difficult to properly describe this phenomenon with density functional theory (DFT) calculations, even with the Hubbard U correction. Previous calculations have found ferromagnetic conducting thin-film $LaCoO_3$ with all Co ions in the intermediate-spin (IS) state, incompatible with experimental data. In this work, using the DFT+U approach, we show that a strained $LaCoO_3$ thin film can be stabilized in a ferromagnetic insulating state. We also predict the electric field gradient (EFG) at the Co nucleus in the magnetic thin film, which can be helpful in identifying Co spin states via nuclear magnetic resonance (NMR) spectroscopy.

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Han Hsu
hsuhan@umn.edu
University of Minnesota

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