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Ferromagnetic insulating state in tensile-strained LaCoO₃ thin films¹ HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, RENATA WENTZCOVITCH, University of Minnesota — With local density approximation + Hubbard U (LDA+ U) calculations, we show that the ferromagnetic (FM) insulating state observed in tensile-strained LaCoO₃ epitaxial thin films is most likely a mixture of low-spin (LS) and high-spin (HS) Co, namely, a HS/LS mixture state. Compared with other FM states, including the intermediate-spin (IS) state (*metallic* within LDA+ U), which consists of IS Co only, and the insulating IS/LS mixture state, the HS/LS state is the most favorable one. The FM order in HS/LS state is stabilized via the superexchange interactions between adjacent LS and HS Co. We also show that Co spin state can be identified by measuring the electric field gradient (EFG) at Co nucleus via nuclear magnetic resonance (NMR) spectroscopy.

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Prefer Oral Session
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