

Ferromagnetism of LaCoO₃

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We theoretically study unconventional long-range ferromagnetic ordering in the film LaCoO₃ under tensile strain. According to the reported importance of the intermediate-spin (IS) excitations in LaCoO₃ with cubic structure [1,2], we argue that the experimentally-observed ferromagnetism in the strained compound [3,4] originates from the highly-fluctuative nature of high-spin (HS) states, which can be viewed as bi-excitons.

Employing *ab-initio* density-functional description followed by Wannier projection, strong-coupling, and exact-diagonalization approaches, we construct a series of approximations to account for crucial electron correlation effects responsible for HS fluctuations and magnetic exchange. The obtained amplitudes and spatial characteristics of magnetic couplings between the “dressed” HS states show a good agreement with experimental observations and provide important details to the physical picture of LaCoO₃.

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