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Role of Entropy and Structural Parameters in the Spin State Transition of $LaCoO_3$ BISMAYAN CHAKRABARTI, TURAN BIROL, KRISTJAN HAULE, Rutgers, The State University of New Jersey — The spin state transition in $LaCoO_3$ has eluded description for decades despite concerted theoretical and experimental effort. In this study, we approach this problem using fully charge consistent Density Functional Theory + Dynamical Mean Field Theory (DFT+DMFT). We show, from first principles, that $LaCoO_3$ cannot be described by a single, pure spin state at any temperature, but instead shows a gradual change in the population of higher spin multiples as temperature is increased. We explicitly elucidate the critical role of the lattice expansion and oxygen octahedral rotations in the spin state transition. We also show that the spin state transition and the metal-insulator transition in the compound occur at different temperatures. In addition, our results shed light on the importance of electronic entropy, which has so far been ignored in all first principles studies of this material.

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