

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Early stage spin-state transition in LaCoO₃ investigated by first principles¹ HAN HSU, RENATA WENTZCOVITCH, MATTEO COCCIONI, CHRIS LEIGHTON, University of Minnesota — The existence of intermediate-spin (IS) state cobalt and its role in the thermally-induced spin-state transition in LaCoO₃ has been controversial. Using the local density approximation + Hubbard U (LDA+ U) method, we have successfully stabilized isolated single high-spin (HS) and IS excited cobalt ions in an array of low-spin (LS) cobalt in LaCoO₃. The Hubbard U is self-consistently determined from first principles. We show that at low temperatures, for isolated single ions, HS cobalt is the first excited state. Low concentrations of isolated IS cobalt produce a metallic state. This result supports the conclusions of quantum chemistry calculations on clusters, and contrasts with results from periodic calculations with 100% IS and HS cobalt population. It is also consistent with recent experiments at very low densities of excited states at low temperatures.

¹This work was supported primarily by the MRSEC Program of the NSF under Award Number DMR-0212302 and DMR-0819885. It was also partially supported by NSF grants ITR-0426757 (VLab). Calculations were performed at the Minnesota Supercomputing Institute (MSI)

Han Hsu
University of Minnesota

Date submitted: 18 Nov 2009

Electronic form version 1.4