Abstract Submitted
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First-principles study for low-spin $LaCoO_3$ with structurally consistent Hubbard U[1] HAN HSU, KOICHIRO UMEMOTO, MATTEO COCOCCIONI, RENATA WENTZCOVITCH, Chemical Engineering and Materials Science, University of Minnesota — We use the local density approximation + Hubbard U (LDA+U) method to calculate the structural and electronic properties of low-spin $LaCoO_3$. The Hubbard U is obtained by first principles and consistent with each fully-optimized atomic structure at different pressures. With structurally consistent U, the fully-optimized atomic structure agrees with experimental data better than the calculations with fixed or vanishing U. A discussion on how the Hubbard U affects the electronic and atomic structure of $LaCoO_3$ is also given.

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Han Hsu
Chemical Engineering and Materials Science, University of Minnesota

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