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Phononic signature of spin-state crossovers in $LaCOO_3$

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$LaCoO_3$ has been the subject of an intense investigation due to its intriguing transformation from a non-magnetic insulator at low temperatures to a paramagnetic semiconductor, followed by an insulator-to-metal crossover. The nature of these transitions is the topic of long-standing and ongoing discussions. Generally, these crossovers are associated with the population of Cobalt low-spin (S = 0), medium-spin (S=1) and high-spin state (S = 2). An originally proposed order of low- and high-spin states should be visible via a concomitant structural distortion of $LaCoO_3$.
We have studied the lattice dynamical behavior of LaCoO3 with inelastic neutron and x-ray scattering over a large temperature range T = 2 K −650 K combined with ab-initio lattice dynamical calculations based on density-functional-perturbation theory (DFPT). Our results reveal a pronounced anomalous softening of a low-lying phonon mode at $q_{pseudo-cubic}$ = (½,½,½) present over the range of the two crossover temperatures. The temperature range of the anomalous softening coincides with that in which magnetic fluctuations are observed in polarized neutron scattering. Thus, our results demonstrate a coupling of the magnetic to the lattice degrees of freedom and indicate the presence of dynamic spin-state order in $LaCoO_3$.

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