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Phonon renormalization in LaCoO₃

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LaCoO3 features two broad crossovers observed around $T_1=100~\rm K$ and $T_2=200~\rm K$. These crossovers are typically associated with the temperature dependent population of excited spin states of the ${\rm Co}^{3+}$ ion, which evolves upon heating from the low-spin (LS), S=0, to high-spin (HS), S=2, configuration. Since the CoO6 octahedra expands around the larger HS sites, a static LS-HS order was proposed by Goodenough in the 1960's [1] but was never confirmed experimentally. More recent studies [2,3] propose a dynamic short-range order of alternating LS and HS Co sites. A corresponding dynamic distortion of the crystal lattice mimics closely the Co-O breathing mode. Here, we use inelastic neutron scattering to study the lattice dynamics of LaCoO3 over a wide temperature range, $5~\rm K \leq T \leq 700~\rm K$. We find strong phonon renormalization of low- as well as high-energy phonon modes with periodicities corresponding to the proposed superlattice.

- [1] P. M. Raccah and J. B. Goodenough, Physical Review 155, 932 (1967).
- [2] J. Kuneš and V. Křápek, Physical Review Letters 106, 256401 (2011).
- [3] V. Křápek et al., Physical Review B 86, 195104 (2012).

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