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Heat Transport in Quantum Materials - The Intriguing Phonon Physics in Ever Surprising SrTiO3

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The model perovskite $SrTiO_3$ is well-known for its strongly anharmonic phonon properties underlying the intriguing physics of soft phonon modes. A plethora of unusual thermal transport properties derive from the interplay of ferroelectricity, phonon softening, quantum fluctuations and topological properties, including Poiseuille flow of phonons and the elusive coupling of phonons in $SrTiO_3$ to magnetic fields. We gain new insights by establishing a link between the macroscopic specific heat c_p of $SrTiO_3$ signalizing the displacive structural phase transition, and the soft-phonon behavior in the R-corner of the Brillouin zone. We devise a c_p model which is situated intermediate between the oversimplified Debye model, lacking the strongly temperature-dependent renormalization of phonon frequencies, on the one hand, and computationally expensive first-principles calculations based on self-consistent phonon theory, on the other hand. Most notably, our model replicates the temperature evolution of the specific-heat anomaly close to the cubic-to-tetragonal structural phase transition at T_C ~ 105 K. We demonstrate that the entropy-derived critical exponents are compatible with the Heisenberg universality class in the tetragonal phase, as is expected, and, interestingly, also mean-field Landau behavior in the cubic phase. Our analysis identifies the R-point soft phonons to be simultaneously responsible for both, the specific-heat anomaly close to T_C and a sizeable amount of specific heat in the temperature range below ~10 K. Consequently, the correlation between changes in the phase transition and the Debye temperature can be traced back to be microscopically rooted in the soft phonon physics. Quartic anharmonicity by itself is not sufficient to transform the discontinuous specific heat singularity of an idealized impurity-free compound into the experimentally observed specific-heat anomaly with its quasi-continuous shape. Instead, oxygen vacancies or impurity ions are identified to be responsible for changes of the temperature evolution of the R-corner phonon frequencies.

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