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Low temperature lattice dynamics of KTaO3

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Many emergent properties of great interest occur near a quantum critical point were a second-order transition is suppressed to zero temperature. Hence, a significant focus of current condensed matter is the study of susceptibilities and order parameters in materials that are influenced by quantum fluctuations. Structural phase transitions close to zero temperature provide ideal platforms for such studies, and the ferroelectric transition, in which cations and anions within a unit cell coherently displace to generate a net, switchable electric dipole moment, is particularly valuable since ferroelectrics have clearly defined susceptibilities (electric permittivity) and order parameters (net dipole moment) that can be investigated in conjunction with the structural phase transition. In this vein, quantum paraelectrics are of significant interest because they are thought to have ferroelectric order suppressed by quantum fluctuations. KTaO3 is considered a prototypical paraelectric, lying very close to a quantum critical point such that slight compositional substitutions induce ferroelectricity or even superconductivity to emerge as ground-states.

We applied cold neutron triple-axis and thermal neutron time-of-flight spectroscopy techniques combined with x-ray diffraction and DFPT calculations to provide a complete picture of the lattice dynamics in KTaO3 and answer the question concerning its alleged quantum paraelectric low-temperature properties.

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