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Behaviour of the Jahn-Teller effect in NaNiO2 with changing temperature and pressure

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The structural chemistry of NaNiO2 is driven by the Jahn-Teller distortion. NaNiO2 consists of alternating layers of edge-sharing NiO6 and NaO6 octahedra. The high-temperature phase has a rhombohedral symmetry, but with cooling there is a monoclinic distortion, as a result of a cooperative Jahn-Teller-driven elongation of the NiO6 octahedra, with the axis of elongation parallel for all octahedra. This JT effect is common in battery materials such as LiNiO2 and its Co-, Mn-, and Al-doped solid solutions, however, these exhibits non-cooperative behaviour, with no JT effect seen by diffraction, although the JT distortion can be observed with local probes such as PDF. The resulting ambiguity has led to various differing interpretations of the experimental data for these lithium nickelates.
We present a study of NaNiO2 using neutron total scattering and EXAFS as a function of temperature, along with neutron diffraction at elevated pressures, with the hope that a better understanding of NaNiO2 may aid the understanding of the LiNiO2-based cathode materials. Additionally, we show advanced statistical analysis of the total scattering data using Rietveld analysis of a supercell.
Our results differ from prior works on LaMnO3, with differences in part attributed to the reduced degrees of freedom in NaNiO2 due to the edge-sharing octahedra. We contextualise our findings in terms of theoretical and computational works, and make predictions for the lithium nickelates based on our results.

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