

Structure And Dynamics in BaTiS₃ Hexagonal Perovskite as Seen by Neutron Scattering

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BaNiO₃-type "hexagonal perovskite" materials are known to exhibit complex phase diagram, and BaTiS₃ is no exception. This structure is comprised of columns of sulphur coordinated Ti that are linked by barium. We have carried out a systematic study of the global and local structure, as well as of the lattice dynamics, by means of neutron diffraction and inelastic scattering. Notably, Ti atomic displacement parameters increase with decreasing temperature which suggests ferroelectric-type fluctuations. However, inelastic x-ray scattering phonon spectroscopy and high-resolution inelastic neutron scattering reveals instead a dynamic disorder scenario that involves atomic tunneling, i.e. quantum paraelectric behavior [1]. Structural variability complicates this picture, as different synthesis methods lead to significant changes in lattice parameters, and, consequently suppress the tunneling dynamics.

[1] Sun, B., Niu, S., Hermann, R.P. et al. High frequency atomic tunneling yields ultralow and glass-like thermal conductivity in chalcogenide single crystals. *Nat Commun* 11, 6039 (2020). <https://doi.org/10.1038/s41467-020-19872-w>

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