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Mode Analysis of the High Temperature Behaviour of some Ferroic Perovskites

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The advent of user-friendly on-line software (such as ISODISTORT [1] and AMPLIMODES [2]) to analyse crystal structures in terms of 'distortion modes' rather than the conventional approach of refining individual atomic coordinates, has opened up new possibilities in the understanding of structure-property relationships in functional materials. The perovskite family is ideally suited to this approach, with many different variants on the basic cubic structure-type being brought about by simple symmetry-lowering modes such as tilting or distortion of almost rigid metal-ligand octahedral groups. In this talk I will illustrate the use of distortion mode analysis in understanding the sometimes complex, unusual and surprising structural behavior of several functional perovskites, particularly ferroelectrics and multiferroics. Examples chosen will exploit the use of powder neutron diffraction as the primary experimental technique, and will include sodium niobate, NaNbO₃, which has the most complex high-temperature phase diagram of any simple perovskite, and derivatives of BiFeO₃ (such as La or Mn-doped) which display unusual magnetostrictive behaviour.

[1] B. J. Campbell et al., *Acta Crystallogr.*, 2006, 39, 607., [2] D. Orobengoa et al., *J. Appl. Crystallogr.*, 2009, 42, 820.

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