# MS26-O2 Frustrated octahedral tilting distortion in the incommensurately modulated perovskites

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The 3D framework of corner-sharing octahedra in the perovskite $ABO_3$ structure is a very flexible construction. The ability of this framework to sustain distortions due to rotation/tilt of the octahedral units, or their deformations, or both together, without losing the corner-sharing connectivity, allows the perovskite structure to accommodate a very wide range of cations with diverse size, formal charge, and electronic properties. Crystallographic aspects of the distortions have been widely discussed in the literature and developed nowadays toward a rigorous group symmetry analysis for different types of distortions and their combinations. However, in some layered A-site ordered perovskites, such as $Li_{3x}Nd_{2/3-x}TiO_3$ and many others, substantially more complex pattern of the octahedral tilting distortion allegedly coupled to a compositional modulation at the A sublattice can be realized leading to incommensurability. Here we demonstrate a solution of the $Li_{0.15}Nd_{0.617}TiO_3$ incommensurate crystal structure using a combination of transmission electron microscopy, synchrotron X-ray and neutron powder diffraction [1, 2]. In contrast to earlier conjectures on the nanoscale compositional phase separation in the $Li_{3x}Nd_{2/3-x}TiO_3$ materials, all peculiarities of the incommensurate superstructure can be understood in terms of displacive modulations related to an intricate octahedral tilting pattern. It involves fragmenting the pattern of the out-of-phase tilted $TiO_6$ octahedra around the *a*- and *b*-axes into antiphase domains, superimposed on the pattern of domains with either pronounced or suppressed in-phase tilt component around the *c*-axis. The octahedral tilting competes with the second order Jahn–Teller distortion of the $TiO_6$ octahedra. This competition is considered as the primary driving force for the modulated structure. The A cations are suspected to play a role in this modulation affecting it mainly through the tolerance factor and the size variance. The reported crystal structure calls for a revision of the structure models proposed for the family of layered A-site ordered perovskites exhibiting a similar type of modulated structure.

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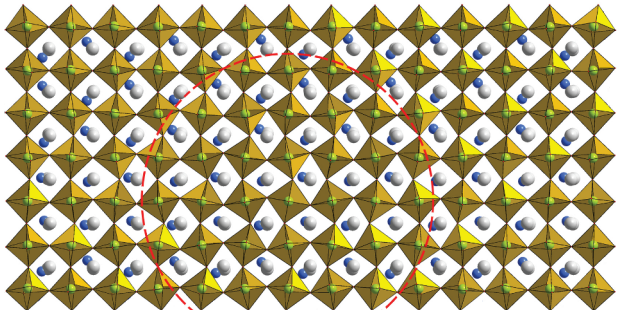

**Figure 1.** A part of the incommensurate $Li_{0.15}Nd_{0.617}TiO_3$ structure. The Ti atoms (green spheres) are in the oxygen octahedra. Nd and Li atoms are shown as gray and blue spheres, respectively. The dashed circle marks the region with a pronounced tilt of the $TiO_6$ octahedra around the *c*-axis.

**Keywords:** layered perovskite, incommensurately modulated structure, octahedral tilting, A-site ordering