

ORDER AND DISORDER IN LAYERED OXIDE PHOTOCATALYSTS VIA X-RAY AND NEUTRON POWDER DIFFRACTION

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Aurivillius phase oxides are members of the layered perovskite family of materials and consist of perovskite-like blocks interleaved with $[\text{Bi}_2\text{O}_2]^{2+}$ layers. Rietveld analysis of the three-layer Aurivillius phases $\text{Bi}_2\text{LnTi}_3\text{O}_{12}$ ($\text{Ln} = \text{La}_2, \text{Pr}_2, \text{Nd}_2, \text{LaPr}, \text{LaNd}$ and PrNd), $\text{Bi}_2\text{Sr}_{2-x}\text{A}_x\text{Nb}_2\text{TiO}_{12}$ ($\text{A} = \text{Ca}, \text{Ba}, x = 0, 0.5, 1$) and $\text{Bi}_2\text{Sr}_{2-x}\text{A}_x\text{Ta}_2\text{TiO}_{12}$ ($\text{A} = \text{Ca}, \text{Ba}, x = 0, 0.5, 1$) will be discussed with special emphasis on local bonding environments within the perovskite octahedra. Planar to non-planar distortions of the equatorial oxygens contained within perovskite-like blocks have been shown to vary with an inverse proportionality to the average A-site cation radius. Exfoliation of the layered phase, by removing the Bi_2O_2 layer, results in massive structural disorder that can be modeled using hkl-dependent line broadening.

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