Correlating crystalline structure of $LaCoO_3$ perovskites with the photocatalytic degradation of cefixime

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Lanthanum cobaltite ($LaCoO_3$ or LCO) is a rare-earth ABO_3 perovskite oxide that has attracted considerable attention in recent years due to its exceptional catalytic, oxygen-conducting, magnetic, and semiconducting properties [1–3]. Different synthesis routes lead to LCO variants that with different physical, chemical, and morphological properties that govern phase purity and performance. Achieving high phase purity is essential for reliable property evaluation and for elucidating structure-property relationships; however, the extensive links between synthesis pathways, crystallographic evolution, and functional properties remain insufficiently explored [4,5]. One important functionality of LCO is its superior photocatalytic activity in the photodegradation of organic water pollutants, which could potentially be used to eliminate antibiotic contamination in water sources. In this context, antibiotics, which are necessary for human, animal, and agricultural health, pose significant environmental concerns due to their widespread use, contaminating waterways worldwide. One example of this threat is cefixime (CFM), a widely used cephalosporin antibiotic.
We relate crystallographic characteristics, such as the oxygen positional parameter *x*(O) and the Co–O–Co bond angle, to the photodegradation efficiency of LCO. Morphology-tuned nanosized LCO powders were synthesised by systematically varying synthesis parameters, followed by post-treatment. These powders were then analyzed crystallographically through (micro)structural refinements against powder X-ray diffraction data. Finally, the LCO samples were tested for CFM photodegradation under xenon lamp irradiation. The degradation activity was complemented by morphological analysis using scanning electron microscopy and particle-induced X-ray emission analysis. We show that systematic tuning of synthesis parameters modulates key crystallographic features, such as *x*(O) and the Co–O–Co bond angle, thereby establishing the structural basis that governs LCO functionality.

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