

Emerging Rare earth perovskite nanostructures for energy conversion

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This study focuses on synthesizing nanoparticles of the rare-earth perovskite LaFeO₃ (LFO) with varying Ytterbium (Yb) doping levels using the co-precipitation method. All samples crystallized in the orthorhombic perovskite phase, with crystallite sizes ranging between 36.3 and 37.5 nm. The nanoparticles exhibited a relatively uniform distribution across the sample surface, and their chemical composition aligned precisely with the stoichiometric composition of LaFeO₃, as confirmed quantitatively. A comparative investigation of the structural and electronic properties of La_{1-x}Yb_xFeO₃ nanoparticles ($x = 0.00$ to 0.04) is also performed in this manuscript. Optical bandgap energies, determined via computational investigation, were 2.30 eV and 2.06 eV following [100] and [001] directions, respectively. Afterward, this parameter was reduced to 2.14 eV and 2.06 eV (along [100] and [001] directions, respectively) by adding 4 % of Yb at La sites. LFO compound exhibits indirect bandgap energies with p-type semiconductor behavior. The unique properties of the synthesized LFO nanoparticles suggest their potential application in photoelectrochemical water splitting, catalysis, gas sensing, and energy conversion devices

Keywords: Rare-earth perovskites; LaFeO₃ nanoparticles; Co-precipitation technique; Computational Investigation; Energy conversion devices.