Defect engineering to improve carrier transport in the LaFeO₃ photocathode for photoelectrochemical water splitting

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LaFeO $_3$ is a rare p-type metal oxide material which is stable against the photo-corrosion, which can be a significant benefit over Cu-containing oxide photocathode materials. Moreover, it has an extremely positive onset potential (> $1.3~\rm V$ vs. RHE) that can achieve high photovoltage for hydrogen evolution or $\rm CO_2$ reduction reaction. However, LaFeO $_3$ is required to modify its poor electronic properties to achieve high photoelectrochemical performance. In this study, LaFeO $_3$ thin film is fabricated via polymer assisted nitrate decomposition method. To improve the bulk carrier transport properties, intrinsic defect of LaFeO $_3$ was modified by post-annealing in various atmosphere such as oxygen, air, or hydrogen. Among them, oxygen-treated sample showed noticeable enhancement in photoelectrochemical performance, which is the highest photocurrent density reported on a pure LaFeO $_3$ photocathode. Through oxygen post-annealing, the intrinsic oxygen vacancy is effectively filled, and the majority carrier density is increased. Such an improvement can shorten the time required to realize the durable unbiased solar overall water splitting system.