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Communication

Insight into the influence of high temperature annealing on the onset potential of Ti-doped hematite photoanodes for solar water splitting

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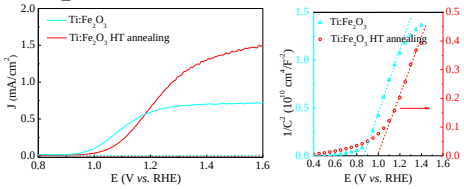
Graphical Abstract



The unfavorable onset potential shift of Ti:Fe_2O_3 photoanode induced by high temperature post-annealing was studied. The underlying mechanism is the surface Ti/Fe atomic ratio increase, leading to adsorption capacity change of surface hydroxide ions and the positive shift of flatband potential (*i.e.*, theoretical onset potential).

ABSTRACT

*For Ti-doped hematite photoanodes, high temperature annealing drastically increases the water oxidation plateau photocurrent, but also induces an anodic shift of onset potential by about 100 mV, thus hindering the performance under low applied bias. To the best of our knowledge, the effects of high temperature annealing on the onset potential have been rarely studied. Herein, both X-ray photoelectron spectroscopy (XPS) measurements and theoretical calculations indicated that the increase of surface Ti/Fe atomic ratio after high temperature annealing decreased the adsorption capacity of hydroxide ions on the hematite surface. Subsequently, the flatband potential (*i.e.*, the theoretical onset potential) of Ti doped hematite photoanodes positively shifted, which was supported by the Mott-Schottky measurements.*

Keywords:
Onset potential
Hematite
Ti doping
High temperature annealing
Flatband potential
DFT calculation

Photoelectrochemical (PEC) water splitting has been considered as a promising technology for storing solar energy [1]. Since the start-up work of Fujishima and Honda on a TiO_2 photoanodes, many visible-light responsive semiconductor materials, such as α-Fe_2O_3, Ta_3N_5, and $BiVO_4$, have attracted intensive attention from researchers [2-4]. Among these materials, α-Fe_2O_3 is one of the most promising photoanode materials due to its high theoretical efficiency (about 16%), excellent photochemical stability, non-toxicity and low cost [5]. However, the PEC performance of α-Fe_2O_3 is hindered by some intrinsic drawbacks, including short hole diffusion length, poor electrical conductivity, severe surface states recombination and so on.