Electronic Supplementary Information

Physical and Photoelectrochemical Properties of Zr-doped Hematite Nanorod Arrays

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Fig. S1 Raman spectra of Zr-doped α-Fe₂O₃ nanorod arrays.
Fig. S2 XPS spectra of Zr-doped $\alpha$-Fe$_2$O$_3$ nanorod arrays. (A) Fe 2p spectra, (B) Sn 3d spectra, and (c) Zr 3d spectra.
Fig. S3 Molar ratio of Zr:Fe and Sn:Fe at the surface of Zr-doped α-Fe₂O₃ nanorod arrays as a function of amount of ZrO(NO₃)₂ in the precursor solution.

Fig. S4 XPS etching profile of the ZrFe-0.1 film showing the distribution of Zr and Sn as a function of depth.
Fig. S5 SEM-EDS mapping of the ZrFe-0.1 film showing the lateral distribution of Fe, O and Zr.
Based on the spectral transmittance of Zr-doped α-Fe₂O₃ nanorod arrays shown in Fig. S6A, the band gaps of these α-Fe₂O₃ films are quite similar and at ca. 2.1 eV (Fig. S6B), as estimated from Eq. 1 (Kubelka-Munk Equation) [1]:

\[ a \nu = C(h \nu - E_g)^m \]  

(1)

where \( \alpha \) is the absorption coefficient of the material, \( h \nu \) is the photon energy in eV, and \( E_g \) is the band gap in eV, \( C \) is a proportionality constant. \( m \) is also a constant, being 1/2 for a direct and 2 for an indirect band gap semiconductor. In this case, \( m \) is equal to 2 for α-Fe₂O₃ as an indirect band gap semiconductor [2, 3].

Fig. S6 (A) Spectral transmittance and (B) Tauc-Plots of Zr-doped α-Fe₂O₃ nanorod arrays.

References