Ultrathin Passivating HfO_2 as a Protection Layer to Silicon Photocathodes for Efficient Alkaline Water Splitting.

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Silicon (Si) photoelectrode is unstable in aqueous media for water splitting, particularly in alkaline electrolyte. Depositing a passivation layer that protects the surface of Si could form an effective strategy to alleviate the stability issues and improve the performance for solar water splitting. An appropriate passivation layer should possess high thermodynamic stability in aqueous solutions and good pH-independent stability in highly corrosive electrolytes. HfO_2 with high thermodynamic stability and high refractive index is a promising candidate as a passivation layer to protect the Si surface. In our work, we introduce HfO_2 as a surface passivating protection layer on c-Si photocathode with p^+nn^+ structure using atomic layer deposition (ALD) method. We investigated the optimisation of deposition temperature, thickness, annealing temperature to realise the best photocathode performance. Moreover, we evaluate the passivation effects, the photoelectrochemical (PEC) properties, and the underlying mechanisms leading to an enhanced PEC performance of HfO_2/Si photocathodes using current-potential, Mott-schottky (MS), and electrochemical impedance spectroscopy (EIS) measurements. Our results show that applied-bias photon-to-current conversion efficiency (ABPE) and stability of Si photocathodes greatly improved upon the addition of an ultrathin HfO_2 layer. [1-2]

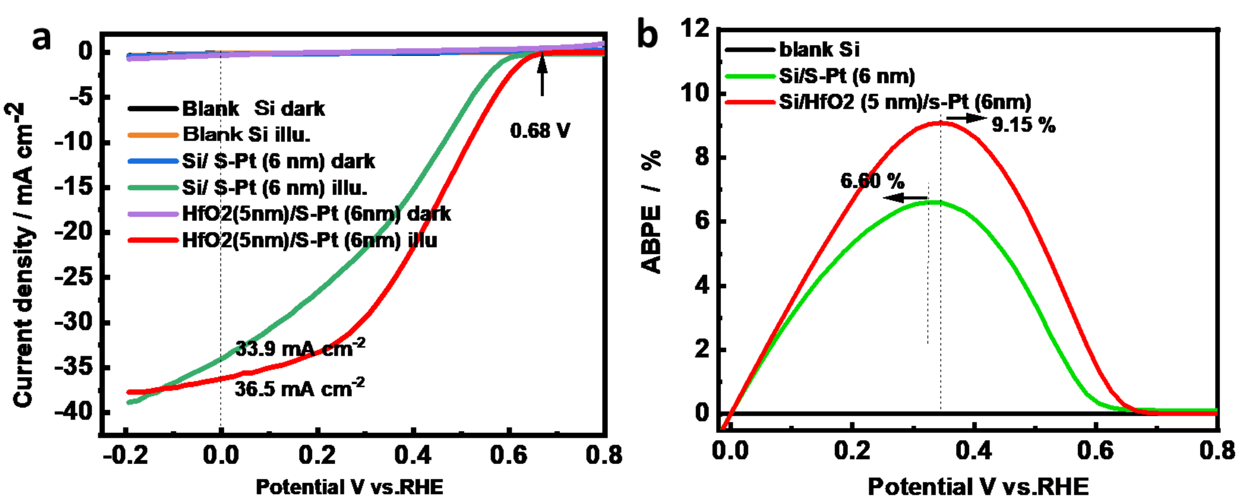

Figure 1. a) Current-potential curves of Si, Si/s-Pt, Si/HfO_2/s-Pt. b) ABPE curves Si/s-Pt, Si/HfO_2/s-Pt.

References

1. Gope J., Batra V. N., Panigrahi J., Singh R., Maurya K.K., Srivastava R., Singh P. K., 2015, 'Silicon surface passivation using thin HfO2 films by atomic layer deposition'. *Appl. Surf. Sci.* 357, p635-642.
2. Xing Z., Ren F., Wu H. Y., Wu L., Wang X. N., Wang J. L., Wan D., Zhang G. Z., Jiang C. Z., 2017, 'Enhanced PEC performance of nanoporous Si photoelectrodes by covering HfO2 and TiO_2 passivation layers', *Sci. Rep.* 7,p43901.