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](image_url)

**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**