Optimal band gap combinations of light absorbers for integrated photoelectrochemical water-splitting systems

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An integrated photoelectrochemical water-splitting system allows for direct production of fuels from sunlight, and thus provide a scalable, sustainable source of renewable chemical fuels for the transportation sector. To achieve the maximum solar-to-hydrogen (STH) efficiency at the system level, it is necessary to assess the operating conditions and required materials properties as a function of the band gaps of the light absorber component that serve to capture and convert sunlight into chemical fuels. Various combinations of band gaps in a tandem configuration have been evaluated. A current-voltage model was employed, with the light absorbers, electrocatalysts, solution electrolyte, and membranes coupled in series, and with the directions of optical absorption, carrier transport, electron transfer and ionic transport in parallel. The maximum STH efficiency for an integrated photoelectrochemical system was found to be 31.1% at 1 Sun (1 $kW{\cdot}m^{-2}$, air mass 1.5), fundamentally limited by a matching photocurrent density of 25.3 $mA{\cdot}cm^{-2}$ produced by the light absorber component. Practically, pairing 1.6–1.8 eV band gap semiconductors with Si in a tandem structure is promising for theoretical STH efficiency limits of >25%. We will further discuss the effects of operating parameters, including the overpotentials of earth-abundant catalysts for water oxidation and reduction reactions, the solution resistance and light absorber quality on the STH efficiency limits of an integrated water-splitting system.