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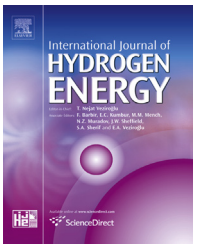

Architectures for scalable integrated photo driven catalytic devices-A concept study☆

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ABSTRACT

Architectures with various degrees of integration are investigated for water splitting devices using the energy of light for fuel production. The many approaches presented in literature for such 'photo driven catalytic (PDC) devices' are reviewed and discussed in perspective of their scalability to large area. Then, back-of-the-envelope type techno-economic considerations for such systems are presented. Compared to the benchmark, consisting of large electrolyzers coupled to the grid, it was found that PDC devices could be competetive in places with high irradiation, given the assumption that no compromises on system stability have to be made compared to stand-alone PV-systems for electricity generation. In agreement with literature, it was found that the cost of the PV part dominate the hydrogen generation costs, based on today's technology. Thus, device architectures that allow low cost PV (by e.g. avoiding use of costly materials or introducing further inherent loss mechanisms) are considered the most promising ones.

Introduction

The tremendous progress in photovoltaic (PV) installations worldwide in the past decade proves that this technology can provide a great share of clean and affordable electricity to the global energy demand [1]. In fact, studies about ultimate potentials of renewable energy sources reveal that solar conversion is the only source able to fulfill future demand for energy by itself, unlike e.g. wind [2]. However, PV has the inherent drawback that its supply is subject to the cycles of nature (day–night, summer–winter). Thus, affordable storage methods are needed to match the temporal differences to the demand for energy and hydrogen produced by electrolysis can be one of them [3]. The combination of PV with electrolysis to store the energy of light directly in the form of hydrogen is therefore an imperative field of study. Due to the comparatively high costs today, electrolysis is competitive only locally in places where electricity costs are exceptionally low. So far, only small scale systems have been demonstrated [4]. Due to

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the mentioned rapid and continuing decline in electricity cost from PV, sunny regions in the world could soon offer a great potential for clean and inexpensive hydrogen production – competitive with hydropower and wind. This study aims to contribute to the question if the cost of hydrogen production can be reduced by integrating the PV and electrolysis functionalities in a single monolithic device.

Direct solar-to-hydrogen (STH) conversion, coupling one or more photovoltaic cells (herein referred to as the PV-part) via catalysts to an electrolyte (herein referred to as the EC-part) to split water by using the oxygen- and hydrogen-evolving reactions (OER and HER), without need for further electronics, proved to work on lab scale with STH-efficiencies of up to 18%. The key-components and -processes of such 'photo driven catalytic (PDC) devices' are given in Table 1a.

Since the first observation of electrolysis on a semiconductor/electrolyte interface by Fujishima and Honda [5], numerous cell designs were presented in literature. In this study, we first review the fundamental processes, which allow converting and storing the energy of the sun's irradiation in hydrogen. Putting the focus on potentially scalable approaches, we highlight the parasitic influence of ohmic losses that occur both in the PV- as well as in the EC-part. The ohmic losses are in a fundamental trade-off with parasitic shading losses or losses of active area, which become relevant at large areas. Against this background, we discuss different approaches with varying levels of integration of PV- and EC-components as presented in literature. We concentrate on planar (as opposed to particle based) architectures, which potentially allow to generate hydrogen at low cost based on today's technology. Thereby, we only consider approaches, which are potentially wireless (monolithic), but do not limit ourselves to either alkaline or acidic electrolytes. Moreover, we consider both buried junction devices as well as devices that have one or more semiconductor/liquid junctions. The former can be classified as (integrated) PV-electrolysis devices, whereas the latter are called PEC or PEC-PV devices. The nomenclature used in this study is given in Table 1b. The term 'photo driven catalytic (PDC) device' was suggested by Jacobsson et al., describing any configuration of a PV-cell or -module in combination with an EC regardless of its level of integration [6]. We classify these PDC devices according to the possibility of scalability and identify inherent loss mechanisms related to optical shading, ohmic losses due to transport of charge carriers both in the PV- and in the EC-part and stability requirements. We highlight the advantages of the superstrate design (meaning light impinges through a transparent substrate), used in thin film device technology, such as the possibility of monolithic electrode connection and low optical losses due to limited catalyst transparency or bubble formation.

Then, we present back-of-the-envelope techno-economic calculations based on cost estimations for photovoltaic- (PV-) and electrolyzer (EC-) systems presented elsewhere. We conclude that, because the final cost of hydrogen from such systems is likely to be dominated by the cost of electricity (based on today's technology), very limited compromises on the cost of the PV-part can be made, compared to a stand-alone PV system. The largest cost saving potential is thus attributed to an efficient integration of the EC- into the PV-part, without introducing further cost increasing factors (such as the reduction of efficiency through the introduction of further loss mechanisms, the necessity for expensive/rare materials or a reduced system lifetime). For the same reason, we also neglect solar tracking- or concentration-systems, which are today not reducing the cost of PV electricity. Based on the classification and the techno-economic considerations, we propose a device architecture, which should minimize additional cost drivers. Certainly, the results of this study are based only upon a 'snapshot' of today's available technology. Future findings in material research might change the results and allow disruptive changes (e.g. emergence of novel, stable wide-bandgap light absorbers or efficient particle based systems).

Table 1

(A)

Key components		Key process
PV-part		$h\nu \rightarrow h^+ + e^-$
EC-part	OER (Anode)	Alkaline: $2OH^- \rightarrow \frac{1}{2}O_2 + 2e^-$ Acidic: $H_2O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^-$
	HER (Cathode)	Alkaline: $2H_2O + 2\,e^- \rightarrow H_2 + 2OH^-$ Acidic: $2H^+ + 2e^- \rightarrow H_2$
Total		$h\nu + H_2O \rightarrow H_2 + \frac{1}{2}O_2$

(B)

PEC	PV-EC
Photo driven catalytic (PDC) devices	
Monolithic (focus of this study)	Externally wired

Fundamentals

Direct hydrogen production by using solar radiation relies on two fundamental processes: First, like in any other electrolyzer, a potential difference larger than the thermodynamic potential of water (μ_{th} > 1.23 eV) has to be applied between cathode and anode. The amount of additional voltage ('overpotential') needed depends on the catalysts used as well as the resistive losses occurring in the system. Second, in a *photo driven* catalytic device, light induced splitting of the quasi-Fermi levels in one or more absorbers provides this potential difference. Besides these two processes, other secondary processes such as efficient light in-coupling, transport of charge carriers from absorber to the electrodes, transport of ions between electrodes as well as local separation and collection of reaction products (H_2 and O_2) have to be considered. The current density j_{op} flowing between anode and cathode under operation in such a device, can be used to calculate the solar-to-hydrogen conversion efficiency η_{STH} according to

$$\eta_{STH} = \left(\mu_{th} \cdot j_{op}\right) \Big/ P_{irr} \cdot \eta_F \quad (1)$$

with P_{irr} being the incident irradiance and η_F the Faraday efficiency, which describes the relation between mass of the reaction products and j_{op}. A PDC can be modeled using an

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