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Solar-to-hydrogen efficiency limits for solar water splitting with tandem solar cells

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Hydrogen generated from solar-driven water-splitting has the potential to fill an important niche in the renewable energy landscape: it offers storage which could be used to mitigate the intermittency of solar and wind power; and could potentially be converted into liquid fuels to power heavy duty transportation. Recent advances in low cost, high efficiency tandem solar cells[1] - driven partly by the fact that silicon cells are approaching their theoretical limits – offer an economically viable option for bias free solar-driven water-splitting. In order to leverage these technological advances to their full potential, it is necessary to understand solar-to-hydrogen conversion efficiency (STH) limitations and how these depend on the system configuration, as well as the choice of semiconductors in the tandem pair.

There is a veritable zoo of different configurations for water splitting based on the photovoltaic (PV) effect. On one end of the spectrum, tandem solar cells can be used to drive a standard electrolysis setup; sometimes branded PV-electrolysis. On the opposite end, one or more semiconductors can be integrated directly with the catalysts to form photo-electrochemical cells (PEC) immersed in the electrolyte. Somewhere in the middle is the possibility of having one or more semiconductor-based photoelectrodes connected to a solar cell. While these approaches impose different restrictions on the material properties of the semiconductors and require different optimizations, the physical and chemical processes occurring are the same. The equivalence of the various configurations has recently been demonstrated by Jacobsson[2] – from grid connected PV-electrolysis, to the “artificial leaf” concept.

Here we show that while there may be physical and chemical equivalence, some configurations allow the photovoltaic action – transduction of optical energy to electrical energy – to be decoupled from the electrochemical action – transduction of electrical energy to chemical energy - by allowing us to integrate power conditioning. We extend standard solar-to-hydrogen efficiency models[3] to include different equivalent circuit models and compare a range of configurations for integrating PV for solar hydrogen generation. Our results clearly demonstrate that decoupling photovoltaic and electrochemical actions has significant consequences for efficiency limitations and the choice of semiconductor tandem pairs.

Coupled systems are defined by series connected components, as shown in Fig.1: where the PV cells are in series with each other and the catalysts. In this case, the photo-generated voltage and current generated by the series connected PV cells must be identical to the voltage and current that drives the electrochemical reaction. This circuit model holds whether the PV cells and catalysts are directly integrated (as in PEC or photoelectrodes) or are wired together (as in PV-electrolysis).

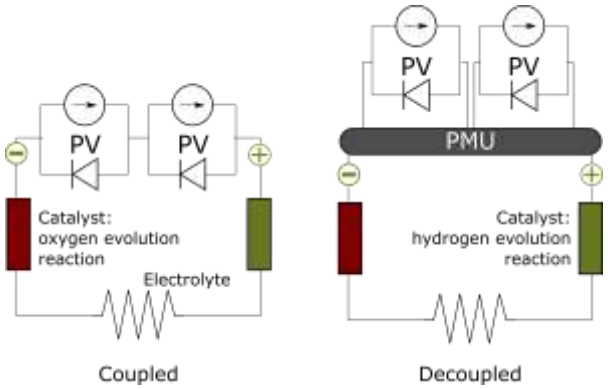

Figure 1: Equivalent circuit diagrams for coupled and decoupled tandem PV water splitting systems.

However, it is also possible to decouple photovoltaic and electrochemical actions, by introducing a power management unit (PMU) in the circuit. In this configuration, also shown in Fig.1, the solar cells can be connected separately to the PMU and operated at their maximum power points. The PMU can sum the power input from the cells and provide the optimized current and voltage output required to drive the water splitting reaction.

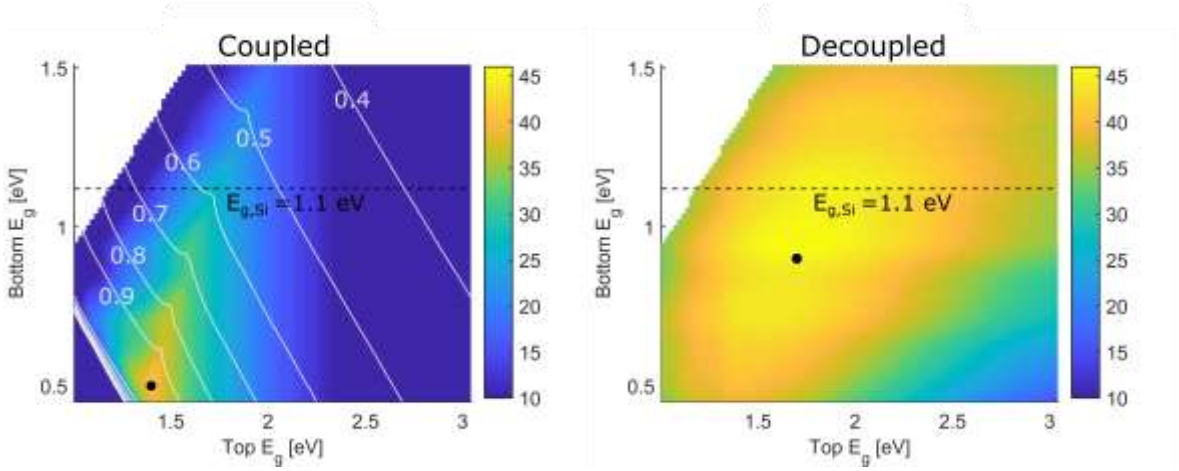

Figure.2 Ideal solar-to-hydrogen (STH) efficiency limits [%] for coupled and decoupled tandem PV water splitting systems, for different semiconductor bandgaps. The white contour lines indicate the ratio of the STH and PV efficiencies.

Fig. 2 shows thermodynamic limiting STH efficiencies, following the work of Fountaine[3] and employing standard Shockley- Quiesser formalism[4]. Our results clearly indicate that the STH efficiencies of coupled systems are significantly lower than decoupled systems for all bandgap combinations. Additionally, the maximum STH for the coupled system is lower than that for the decoupled system (40% compared to 46%) and is limited to a very narrow range of bandgaps and relatively low bottom cell bandgaps. Interestingly, coupled STH efficiencies can be significantly lower than those of the respective PV (2-terminal) tandems for a wide range of bandgap combinations (white contour lines), due to current matching requirements and the fact that water splitting requires a fixed voltage. In contrast, decoupled systems are not restricted by any current matching and have limiting efficiencies equal to those of their component PV tandem cells. Critically, there is no additional loss of efficiency due to the fixed voltage requirement.

For the technologically important case of an ideal Si bottom cell, coupled system efficiencies achieve a maximum of 27% for the optimal top band gap of 1.7 eV. In comparison, decoupled Si-based systems can achieve ~45% over a relatively range of top bandgaps 1.7-1.8 eV.

In conclusion, we present efficiency limits for solar-to-hydrogen generation for different photovoltaic based water splitting configurations. The results provide guidance on how to rationally design solar water-splitting systems to maximise efficiency.

References

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