Final Report Summary - PECDEMO (Photoelectrochemical Demonstrator Device for Solar Hydrogen Generation)

Executive Summary:
PECDEMO’s main aim was to develop a photoelectrochemical (PEC) water splitting device based on low-cost and abundant materials that shows a solar-to-hydrogen (STH) efficiency of 10%, a stability of 1000 hours, and an active area of at least 50 cm².

PECDEMO has addressed these challenges by focusing its efforts on three metal oxide photoelectrode materials (Fe₂O₃, BiVO₄, and Cu₂O) and by combining them with a silicon- or perovskite-based photovoltaic (PV) cell in a tandem configuration. To improve the efficiency and stability of the metal oxides, modifications were made by doping, application of protection layers, nano-structuring, and surface functionalization with co-catalysts for hydrogen or oxygen evolution. Fe₂O₃ is the most stable material; lab tests showed negligible performance decrease after 1000 h operation. A new hydrogen treatment method significantly improved the performance of BiVO₄ photoanodes, resulting in a 9.2% STH efficiency for a small-area dual BiVO₄/Fe₂O₃ photoanode/Si PV tandem cell. PECDEMO’s highest efficiency achieved for
Small-area devices was 16.2%, obtained for a Ga2O3/Cu2O nanowire photocathode coupled to a silicon PV cell using a dichroic mirror for photon management. The highest large-area photocurrent densities were obtained for Cu2O, giving an unprecedented 3.5 mA/cm² for a 50 cm² photoelectrode. Various large-area cell designs were studied, resulting in an optimized design that features an open path for sunlight from the front to the back window, with counter electrodes placed at both sides of the central photoelectrode. CFD simulations were used to ensure an optimal flow path of the electrolyte, resulting in efficient removal of gas bubbles and good thermal management; the temperature of the cell did not increase above 55°C even under 17-suns concentrated light. Based on this design, a modular array of four PEC cells of 50 cm² each was constructed for field tests on the SoC Ratus facility at DLR in Cologne. The cell design showed limited cross-over of H₂, but the efficiencies for BiVO₄ and Fe₂O₃ were modest under concentrated sunlight – presumably due to poor carrier transport in these materials. Two conceptually new innovations were made to further improve the PEC concept. A power management scheme that allows co-generation of electricity and hydrogen; in combination with active light management, the PEC efficiencies can exceed those of PV-electrolyzer systems. The second one is the use of auxiliary NiOOH/Ni(OH)₂ electrodes, which avoids the need to separate H₂/O₂ reaction products within the same cell. This significantly reduces the overall complexity and costs of the concept. Plant design studies showed that cooling is a crucial issue, especially under concentrated sunlight. Life-cycle analyses revealed that the PEC-PV approach is potentially best in class in terms of global warming potential. Economic analysis showed that PEC-PV generation can compete with PV-driven electrolysis. However, STH efficiencies higher than 8%, solar concentration factors > 30, cell temperatures above 60°C, and active areas approaching 1 m² should be pursued. Finally, all PECDEMO targets (10% efficiency, 1000 h stability, 50 cm²) have been individually achieved, but meeting them simultaneously with a single system remains a major challenge to be addressed.

Project Context and Objectives:
1.2.1. Context
Sunlight is by far the largest sustainable source of energy, and there is little doubt that it will play a major role in any conceivable future energy scenario. One of the main challenges for the large-scale use of solar energy is its intermittent nature, which requires intermediate storage solutions. An attractive pathway to achieve this is by directly converting an abundant resource, such as water, into hydrogen using sunlight. The hydrogen can then be used directly as a fuel, or further processed into liquid hydrocarbons. These ‘solar fuels’ have up to 100 times higher energy and power densities than the best batteries and can be stored indefinitely. PECDEMO aimed at developing a Photo ElectroChemical DEMOnstrator that splits water into hydrogen and oxygen under solar irradiation. By integrating the light absorption and electrolysis functionalities into a single device, significantly lower balance-of-systems costs than coupled photovoltaic-electrolysis systems are, in principle, possible. Efficient and cost-effective solar hydrogen production would thus solve one of the major challenges for a solar-driven society, i.e. that of efficient large-scale storage of solar energy. However, before this dream becomes reality, some hard technological and economic targets have to be met. As outlined in the call that PECDEMO addressed, solar-to-hydrogen energy conversion efficiencies of 8-10% have to be achieved and lifetimes of more than 1000 h need to be demonstrated. Only then will there be a realistic chance to meet the FCH-JU’s cost target of 5 € per kg H₂ and can this technology have a significant impact on society.
1.2.2. Approach and main objectives
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Building on the breakthroughs achieved in the highly successful EU project “NanoPEC”, PECDEMO partners aimed to develop a module-sized hybrid tandem device for solar water splitting based on a stable metal oxide photoelectrode as a wide-bandgap top absorber and an efficient photovoltaic solar cell as a small-bandgap bottom absorber. Based on earlier work by the partners, three candidates were selected as promising metal oxide photoelectrode materials: Fe2O3, BiVO4, and Cu2O. The stability and durability of the photoelectrodes was planned to be enhanced through functionalization with efficient electrocatalysts, by applying selective transport layers and protective coatings, and selection of suitable electrolyte solutions and operating conditions. The photovoltaic cells were to be optimized for tandem operation with the metal oxide photoelectrodes. Here, silicon-based photovoltaic cells and the emerging class of perovskite PV cells have been selected as the most suitable candidates.

The second aim was to demonstrate the scalability of this technology by combining multiple devices into a larger water splitting module. Nearly all previous efforts in the field of photoelectrochemical water splitting have been done on < 1 cm2 cells, with only very few exceptions. At such small length scales, ion transport between the electrodes is sufficiently fast. At larger length scales, however, resistive losses due to mass transport limitations in the electrolyte quickly start to dominate the overall performance. Innovative cell designs are needed to minimize these losses and to manage the transport of photons, electrons, and ions in the water splitting system.

To achieve the project goals, five science and technology objectives were defined:

1. To demonstrate a chemically stable and highly efficient stand-alone hybrid water splitting cell based on a metal oxide photoelectrode in tandem with a photovoltaic solar cell
2. To develop deposition technologies that are suited for fabricating components for large-area hybrid PEC-PV devices
3. To design, construct, and test complete large-area hybrid PEC-PV devices for water splitting
4. To carry out extensive techno-economic and life-cycle analyses based on the devices’ demonstrated performance characteristics, and evaluate the potential for large-scale commercialization
5. To build a prototype module consisting of an array of large area devices and to test this prototype in the field

Project Results:
see attached pdf

Potential Impact:

1.4.1. Potential impact

By achieving its main project goals, PECDEMO has made an important step forward in the development of efficient, stable, and scalable water splitting concepts. The small-area solar-to-hydrogen efficiencies of up to 9.2% (BiVO4/Fe2O3/Si-HIT) and even 16.2% (Cu2O/3-HIT) are amongst the highest ever reported for this concept, and have put Europe at the forefront of efforts in this field. Moreover, PECDEMO has demonstrated the very first large-area (50 cm2) metal oxide-based PEC-PV water splitting systems that are based on a true tandem design, i.e. with a wide-bandgap absorber in front of a smaller-bandgap PV cell. These activities have attracted the interest of Toyota; as a direct result of the PECDEMO project, one of the project partners (HZB) has recently started a small seed project with (and funded by) Toyota to further explore photoelectrochemical water splitting devices.

Although the project represents a significant step forward, we are still far away from a viable PEC-based technology for solar water splitting. Specifically, the efficiencies for the large area devices are still modest.
technology for solar water splitting. Specifically, the efficiencies for the large-area devices are still modest. Moreover, fulfilling all three requirements (efficiency, stability, and scalability) within a single system remains a major challenge. Nevertheless, with our scaling work we pushed the limit for real application and performed important pioneering work to reveal (and overcome) limitation mechanisms and paved the way for solutions, which are of great importance for future work and coming projects towards commercial PEC-PV applicability.

On the systems level, cooling turned out to be an important aspect that has received little attention in the field. While all these technical issues can be addressed, the inherent complexity of the overall process tends to drive up the costs, and makes it challenging to compete with alternative approaches that make use of mature technologies, such as PV-driven electrolysis. While this can be partly remedied by developing more efficient materials, especially light absorbers, innovative new concepts may be needed in order to achieve the necessary breakthroughs.

PECDEMO has proposed several innovative solutions that may help achieve these breakthroughs. Examples are the PEC-PV power management strategy (i.e. co-generation of electricity and hydrogen) and the auxiliary electrode concept. These concepts have been published in high-ranking journals and are likely to have a significant impact on future efforts in the field. Continued efforts by multi-disciplinary teams consisting of materials scientists, chemical engineers, plant designers, and business developers are needed to further develop photoelectrochemical water splitting into a viable technology that has a substantial impact on society.

1.4.2. Dissemination activities

Dissemination activities concentrated on four tasks:
- To effectively communicate PECDEMO’s innovative research
- To establish and maintain a web database to foster communication within the consortium
- To organize two international workshops
- To conduct outreach activities

For Task 1 the following list compiles some relevant publications from PECDEMO:

- J. Luo et al. (2014), Water photolysis at 12.3% efficiency via perovskite photovoltaics and Earth-abundant catalysts, Science Vol. 345/Issue 6204, 26/09/2014 1593-1596
- J.H. Kim et al. (2016), Hetero-type dual photoanodes for unbiased solar water splitting with extended light harvesting, Nature Communications Vol. 7 Nature Publishing Group, 14/12/2016 13380
- Landman et al. (2017), Photoelectrochemical water splitting in separate oxygen and hydrogen cells, Nature Materials N/A Nature Publishing Group, 13/03/2017
- M-K Son et al. (2017), A copper nickel mixed oxide hole selective layer for Au-free transparent cuprous oxide photocathodes, Energy and Environmental Science Vol. 10/Issue 4, Royal Society of Chemistry, 01/01/2017 912-918
- Non oxide as stable protective layer for composite cuprous oxide water-splitting photocathodes
- Landman et al. (2017), Photoelectrochemical water splitting in separate oxygen and hydrogen cells, Nature Materials N/A Nature Publishing Group, 13/03/2017
In addition, PECDEMO was represented at conferences with oral and poster presentations as listed below (most important)

- HZB, Oral presentation to a scientific event, Direct current magnetron sputtering of photoactive BiVO₄: Role of stoichiometry on grain size, structure, carrier mobility and lifetime, 28/11/2016 MRS Fall 2016, Boston, USA
- HZB, Oral presentation to a scientific event, Photoelectrochemical Water Oxidation of BiVO₄ Photoanodes with 50 cm² Active Area 18/04/2017 MRS Spring 2017, Phoenix, USA
- HZB, Oral presentation to a scientific event, Surface and bulk recombination in spraydeposited BiVO₄
Regarding Task 2, the web domain www.pecdemo.eu was obtained and a comprehensive project website was built, hosted by EPFL. The site went live on July 15th, 2014. The website features many sections, including “About PECDEMO” (Project Details, Project Description, Consortium), “Partners”, “Activities” (Meetings, Deliverables, Demonstrations), and “Dissemination” (Publications, Presentations). The website was continuously updated with current news and publications from the project. Pictures of the demonstrator device were published on the website on November 30th 2016.

For Task 3, the first goal of organizing an international conference was successfully accomplished by realizing the IPS-20 meeting in Berlin in 2014. The meeting, titled “20th International Conference on Photochemical Conversion and Storage of Solar Energy” was organized by HZB and chaired by Prof. Roel van de Krol. The conference was a great success, attracting over 430 participants from 36 countries and featuring 14 plenary speakers, 19 keynote speakers, and hundreds of contributed talks and posters.

The second part of the task was to organize a symposium on solar fuels conversion at a large international conference. To this end, members of the PECDEMO consortium have co-organized the “Symposium EC4 – Materials, Devices and Systems for Sustainable Conversion of Solar Energy to Fuels” at the “2016 Materials Research Society Fall Meeting” in Boston. The five-day symposium took place November 28 – December 2, 2016, and featured 21 invited speakers, 73 contributed oral presentations, and 21 poster presentations. The four co-organizers were Roel van de Krol (HZB), Avner Rothschild (Technion), Matthew Mayer (EPFL), and Todd Deutsch (NREL), which were able to recruit symposium support by ACS Energy Letters, ACS Publications, Helmholtz-Zentrum Berlin für Materialien und Energie, Journal of Physics D: Applied Physics, IOP Publishing, Nature Energy, and Macmillan Publishers Ltd. The symposium was well-attended and during the presentation of Harry Atwater, the meeting room was even filled beyond capacity. Especially the PECDEMO project was well-represented within the symposium, with 16 oral presentations and 5 posters contributed by members of the project. For detailed information, see the links:
call for papers
program

Outreach activities were mainly undertaken in the form of teaching. PECDEMO’s main materials of interest (Fe2O3, BiVO4, and Cu2O) and overall approach were extensively discussed during the following courses.
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• MSc course on “Photo-Electrochemical Energy Conversion”, taught at the TU Berlin in the winter semester of 2014, 2015, and 2016
• Two-hour seminar on “Solar Fuels and Photocatalysis” as part of the MSc course on “Modern Developments in X-Ray and Neutron Methods for Science and Technology”, taught at the Free University of Berlin in 2015, 2016, and 2017
• Seminar (1/2 day) taught in August 2015 for students of the German Academy for Renewable Energy and Environmental Technology (http://www.germanacademy.net/)
• QuantSol Summer School, Hirschegg, Austria (September 2015)
• EPFL hosted a one-day research symposium “SwissPEC” on the topic of photoelectrochemical energy conversion, hosted by EPFL on 11 November 2016 in Lausanne

List of Websites:

www.pecdemo.eu

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