Research Project #9

High-throughput material screening and device characterization for the production of green hydrogen using direct PV coupling (IET-1 & IMD-3)

"Green hydrogen" produced electrolytically using renewable resources is central to de-fossilize high carbon-emitting sectors like the transportation sector, but also heavy industries such as steel production and the chemical industry including ammonia synthesis. While electrolyzers have reached relative market maturity for several of the available technologies, many questions regarding their operational stability under dynamic power profiles still exist [1]. This is particularly relevant for the use with only intermittently available renewable energy sources such as photovoltaics (PV), which require long-term storage solutions to compensate for the significant seasonal variations in generation.

One especially attractive operational scenario is the direct coupling of the renewable energy device with the electrolyzer cell. In comparison to a typical grid connection of the electrolyzer cell, this can lead to significant cost reductions for balance-of-plant expenses such as transformers and rectifiers [2]. Additionally, direct coupling to PV enables capturing of excess PV generating capacity at the point of generation, which minimizes the need for grid extensions in future scenarios of massive PV capacity growth worldwide, and particularly in Germany. First studies in cooperation between IET-1 and IMD-3 have shown that an approach using virtual coupling with realistic simulated solar profiles is feasible for long-term operation of over 3000h in PEM electrolysis with comparatively low efficiency loss using commercial materials. There remains however a significant potential for optimization on the path towards highly efficient and stable directly coupled PV-electrolyzer devices [3].

This project aims to build upon these initial results by applying high-throughput approaches both on the fundamental material side as well as on the operational device side. First, a high-throughput characterization platform (HTCP) for rapid material screening is used to find the promising electrocatalysts as candidates for later use in the electrolyzer. The HTCP's parallel synthesis and rapid electrochemical evaluation are aggregated into three core stages: automated, robotized material library preparation; automated electrochemical characterization to determine the catalyst activity and short-term stability; and parallel, multichannel product selectivity analysis. This creates a unique opportunity to couple experimental data with predictive machine learning algorithms and explore an enormous landscape of material combinations of critical raw material (CRM) free electrocatalysts in an unprecedentedly short time, far surpassing traditional trial-and-error methods.

After suitable candidates are identified, they need to be applied in full electrolyzer cells for durability and performance tests using realistic solar profiles, as there are typically significant gaps between model systems and real cells using membrane electrode assemblies (MEAs) [4]. Furthermore, in real operation not only does the choice of catalyst play a role, but many other parameters (temperature, pressure, flow rate, type of membrane, diffusion/transport layers, etc.) influence the operation, necessitating again the use of rapid screening of different compositions. For this, the available high-throughput electrolysis unit at IET-1 can be used to screen up to 16 electrolyzer cells in parallel. This way relevant electrode parameters such as catalyst loading, in-plane resistance, ionomer content and porosity can be systematically tuned and rapidly tested.

For this project the focus is on PEM electrolysis as it is the most suitable and mature technology for dynamic electrolyzer operation. One of the biggest drawbacks of this technology is the use of noble metals, mainly Pt and Ir, as catalysts. In order to minimize the use of such CRMs the project will focus on the one hand on reducing the amount used through for example suitable support materials and on the other hand, on exploring catalyst combinations with reduced or even no noble metal content such as for example sulfide or phosphide materials for HER (e.g. CoP, FeS_2, MoS_2, etc.), (mixed) metal oxides (e.g. MnO_2, Co_3O_4, etc.) for OER as well as materials doped with low amounts of noble metal or alloy materials .

All in all, the project will aim to develop novel suitable catalyst materials for dynamically operated (PEM) electrolyzers, specifically for direct coupling with solar devices. Ideally this would provide the groundwork for the development of novel highly efficient directly coupled PV-electrolyzer devices that could overcome the significant challenge of seasonality in PV generation as PV capacity is set to exceed grid power capabilities.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Director: Prof. Dr. Rüdiger- A. Eichel https://www.fz-juelich.de/en/iet/iet-1
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Specific **requirements**	M.Sc. degree in Materials Science, Physics, Chemistry, Process Engineering or Mechanical Engineering; experience in electrolyzers or fuel cells preferable
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