The future of PGM-rich photocatalysts - Challenges from a Circular Economy point of view

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Introduction

The direct production of hydrogen from solar energy via photocatalysis is seen as one option to cope with the increasing supply of intermittent renewable energy sources such as wind or solar power which destabilize the electricity grid. There is a race for synthesizing ever better photocatalysts with higher conversion efficiencies and larger turnover numbers (TON) (TON = number of hydrogen molecules produced by one photocatalyst molecule before it decomposes). As the photocatalyst typically contains the platinum-group metals (PGMs) platinum (Pt) and ruthenium (Ru) in the photocatalytically active centres (Fig. 1), the question arises which strategy is best: Continue the race with photocatalysts containing PGMs or start a new race from the beginning by substituting PGMs with less scarce metal cations such as iron and accept loosing the progress made.

Approach and Methods

Strategies analysed are:

I. Continue with both PGMs Pt and Ru but without recycling ("PGM strategy")

II. Continue with both Pt and Ru but assuming an end-of-life recycling rate (EOL-RR) of 99% and 76% for Pt and Ru ("PGM recycling strategy")

III. Replace Ru by Pt avoiding Pt-Ru-separation in recycling and increasing EOL-RR for Pt to 100% ("Monometallic strategy 100% Pt-Recycling")

IV. Substitute PGMs with Fe, same photochemical assumptions.

A life cycle assessment (LCA) and life cycle costing (LCC) analysis are performed using OpenLCA software and ecoinvent 3.3. ReCiPe (H/A) endpoint method was used for impact assessment as it results in a single point number allowing direct comparison.

The functional unit is 1 kg of hydrogen produced. As photocatalysis is still on a lab scale, assumptions had to be made for upscaling and PGM recycling (see above). Hydrogen production via electrolysis using electricity from wind turbines serves as a benchmark photocatalysis will have to meet to be competitive on an economical and ecological level.

Results

- Substituting PGMs by Fe is advantageous:
  - It results in lower costs and lower environmental impacts (Fig. 2).
  - The minimum TON necessary for economic competitiveness is lower (Fig. 3).
  - Widespread application of photocatalysis is not hindered by PGM supply constraints.
- Environmental impacts in PGM recycling mainly arise from electricity demand for thermal separation of Pt and Ru.
- The monometallic strategy results in lower recycling costs but the chemically complicated synthesis route remains a economic and ecologic cost driver.
- Photocatalysis is inferior to current hydrogen production techniques, even with highly ambitious assumptions like an EOL-RR of 100% for Pt.
- Substitution highlights the need for further process optimisation.

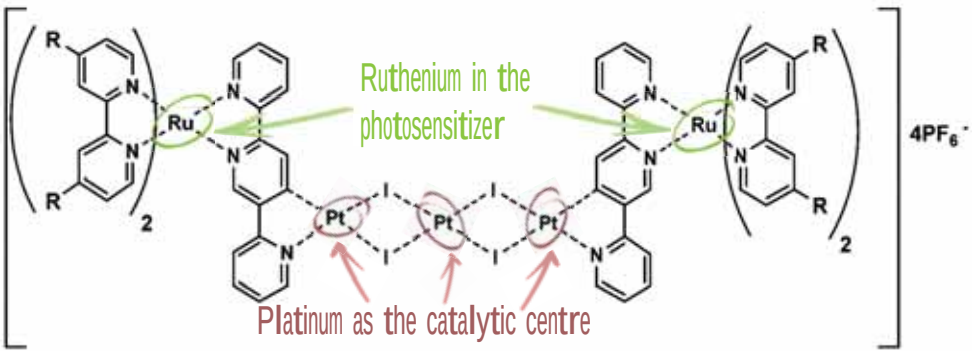
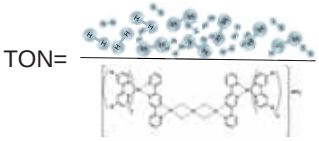


Fig. 1: Studied photocatalyst for hydrogen generation[1]



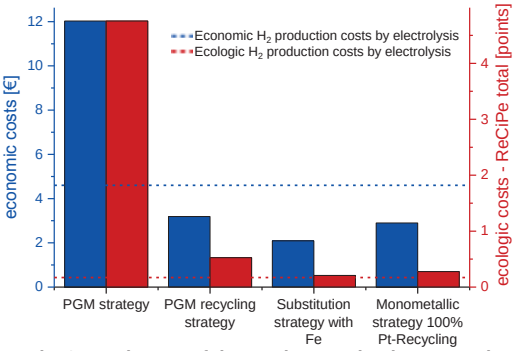


Fig. 2: Total costs of the catalyst production strategies for 1 kg of H_2 and a TON of 1M

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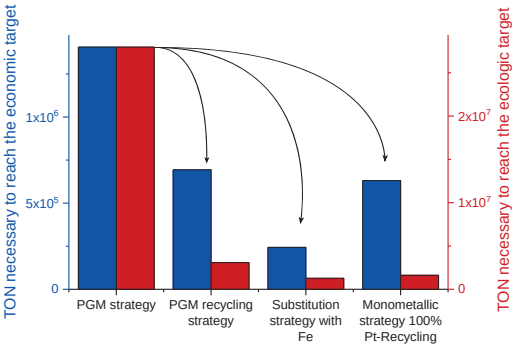

Fig. 3: How the different strategies impact the research targets exemplified by the TON

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Conclusion

- For photocatalysis research, the substitution of scarce PGMs is apparently the most promising.
- PGM substitution is inevitable for large scale applications.
- The new race should be extended to a biathlon: First, identify a promising photocatalyst with abundant as well as environmentally and economically cheap metal cations and optimize it. Then, foster recycling at the level of the photocatalyst and the contained metal cations.
- Synthesis optimisation is necessary to reduce production costs.
- A chemical catalyst reactivation process could be highly beneficial for further cost reductions.

Limitations and outlook

- Photocatalysis is in the early stages of research and a number of significant assumptions had to be made.
- So far ruthenium is a by product in PGM production. If its demand increases, its allocation will change.
- Little can be said about how the TONs will evolve in the future.

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1. Derived from Kowacs et al. *Inorg. Chem.* **2017**, 6, 2685.
2. Mengele et al. *ChemCatChem* **2017**, 9, 4369.
3. Photo taken at the Institute of Inorganic Chemistry I, University of Ulm.