Project Summary

H_2 is a particularly valuable product given its high demand for agricultural, pharmaceutical, chemical, and renewable energy applications. However, to-date, > 95% of H_2 is produced via fossil fuel sources and thus, alternative and more sustainable options will be key in ensuring the adoption of H_2 as a green energy vector in the very near future.[1] My previous lab, the Reisner Lab, has been working on a solar-driven photoreforming (PR) system, which uses sunlight and a suitable photocatalyst to generate H_2 fuel from waste (primarily poly(ethylene terephthalate) (PET), municipal solid waste, and biomass) at ambient temperature and pressure.[2–4]

The reported waste-PR system features a nontoxic and inexpensive polymeric photocatalyst, carbon nitride (CN_x),[5] coupled with a noble-metal-free nickel phosphide (Ni_2P) H_2 evolution cocatalyst (Figure 1). CN_x has a band gap of 2.7 eV that allows for visible light absorption, and band edges suitable for the PR reactions. The majority (86%) of plastic packaging accumulates in landfills or escapes into the environment,[6] and hence there is a sense of urgency and importance of having to deal with this global form of pollution.

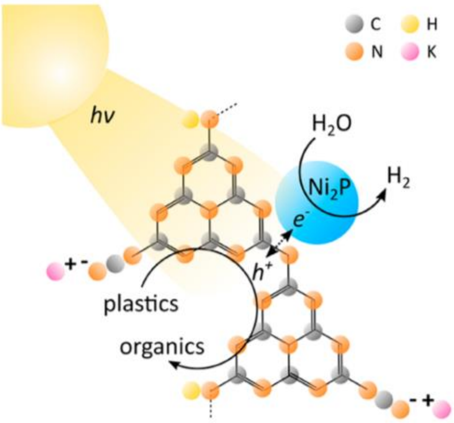

Figure 1: Schematic diagram of the polymer photoreforming process using a $CN_x|Ni_2P$ photocatalyst. In the PR process, sunlight and a photocatalyst generate H_2 from an organic substrate and water.[2] The substrate acts as an electron donor and is oxidised by the excited photocatalyst to other organic molecules. The photogenerated electrons are then transferred from the photocatalyst to a cocatalyst and reduce water to H_2 (reprinted from reference [2]).

The latest work stemming from the lab was focused on the immobilisation process of the catalytic system onto textured glass sheets, which facilitates reusability and improved light absorption of the photocatalyst.[3] The 1 cm^2 panels photoreform plastic, biomass, food and mixed waste into H_2 and organic molecules with rates comparable to those of photocatalyst slurries. 25 cm^2 panels were also prepared for use in a custom-designed flow reactor to generate H_2 under "up-scaled" conditions. When PET was used as the substrate, the areal efficiency of the latter setup was found to be equal to 52 μmol H_2 m^{-2} h^{-1}. Other photocatalytic systems described in the literature comprised of a similar carbon nitride photocatalyst have efficiencies that are two orders of magnitude higher.[7] However, such systems require the expensive and precious cocatalyst platinum, and also utilise a sacrificial electron donors (e.g. Na_2SO_3) to source the electrons for proton reduction (rather than making use of a waste source such as in the case of Reisner and co-workers). These costly approaches are unsustainable and uneconomical when considering the scaling options of PR-based technologies. Further studies are thus needed to improve the durability and efficiency of the $CN_x|Ni_2P$ waste-PR system, to investigate further scaling options to design panels that have a surface area of ~ 1 m^2, and to assess deployment of such a system in a Southern European locality where irradiance is high.

The approximate budget to initiate this scaling study would be of the order of EUR100k. A list of standard lab equipment and potential consumables are listed below.

Required equipment

i. Catalyst preparation:
- Access to wet lab w/ fume hood
- Muffle oven (under air)
- Tube Furnace (under Ar)
- Ultrasonicator

ii. Material characterisation (non-essential for scalability experiments, but useful to have access to such equipment):
- FTIR
- UV-Vis
- XRD
- XPS
- SEM
- TEM

iii. Reactor assembly:
- Access to mechanical workshop (mostly working with PEEK material)
- Pumps
- Tubing and connectors

iv. Analytics:
- Gas chromatography
- HPLC
- NMR

v. Up-scaling/manufacturing of 1 m^2 panels:
- Spray coater
- Slot-die coater

References

[1] "The Future of Hydrogen," can be found under https://www.iea.org/reports/the-future-of-hydrogen, **2019**.

[2] T. Uekert, H. Kasap, E. Reisner, *J. Am. Chem. Soc.* **2019**, *141*, 15201–15210.

[3] T. Uekert, M. A. Bajada, T. Schubert, C. M. Pichler, E. Reisner, *ChemSusChem* **2020**,

cssc.202002580.

[4] T. Uekert, C. M. Pichler, T. Schubert, E. Reisner, *Nat. Sustain.* **2020**.

[5] X. Wang, K. Maeda, A. Thomas, K. Takanabe, G. Xin, J. M. Carlsson, K. Domen, M. Antonietti, *Nat. Mater.* **2009**, *8*, 76–80.

[6] R. Geyer, J. R. Jambeck, K. L. Law, *Sci. Adv.* **2017**, *3*, 25–29.

[7] M. Schröder, K. Kailasam, J. Borgmeyer, M. Neumann, A. Thomas, R. Schomäcker, M. Schwarze, *Energy Technol.* **2015**, *3*, 1014–1017.