European Twinning for research in Solar energy to (2) water (H2O) production and treatment technologies
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Sol2H2O

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Fast Track School #2

Beyond State of the Art in Solar-driven Water production & Treatment technologies and brine treatment processes

POZO IZQUIERDO, GRAN CANARIA, 25.26.09.2024

Sol2H2O

ULPGC
Universidad de Las Palmas de Gran Canaria

Ciemat P.S.A.

Raul Quesada-Cabrera

New photocatalysts for H_2 production and water treatment

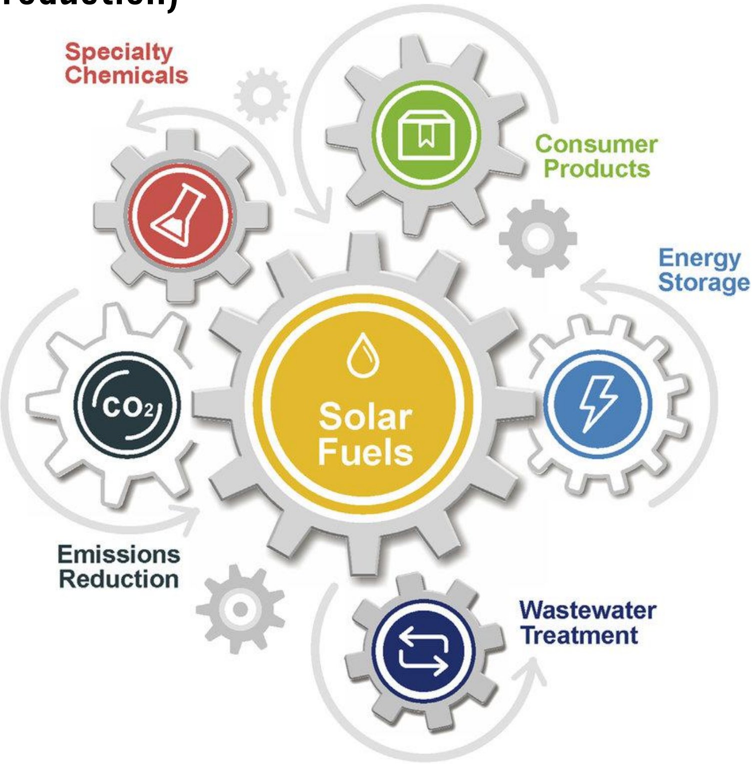
POZO IZQUIERDO, GRAN CANARIA, 25.26.09.2024

Photocatalytic materials

Photocatalysts are semiconductor materials that use light to promote chemical processes such as:

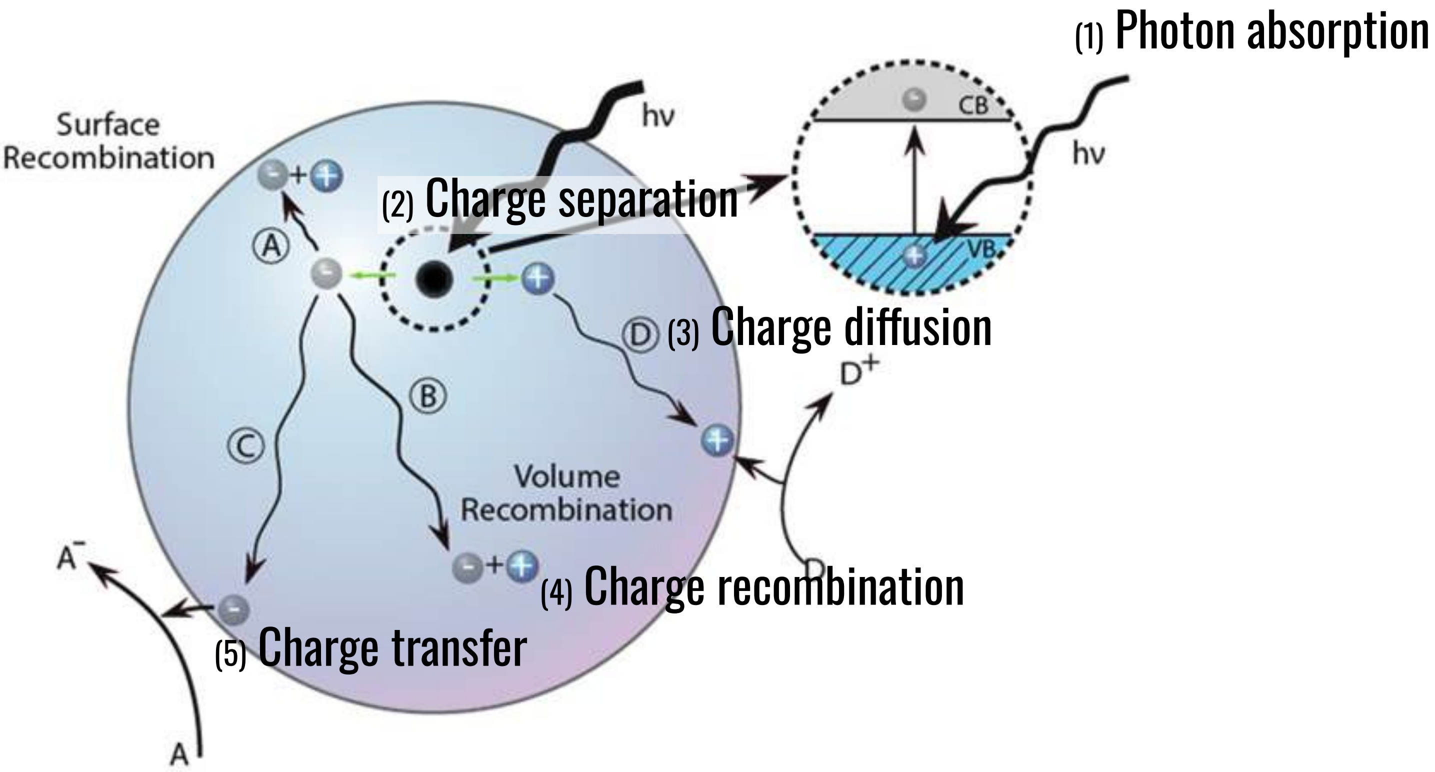
- Solar-to-chemical energy conversion systems (H_2 production)
- Air/water treatment
- Toxic metal extraction
- Waste reuse

Challenge: Efficiency



Photocatalysis: mechanism

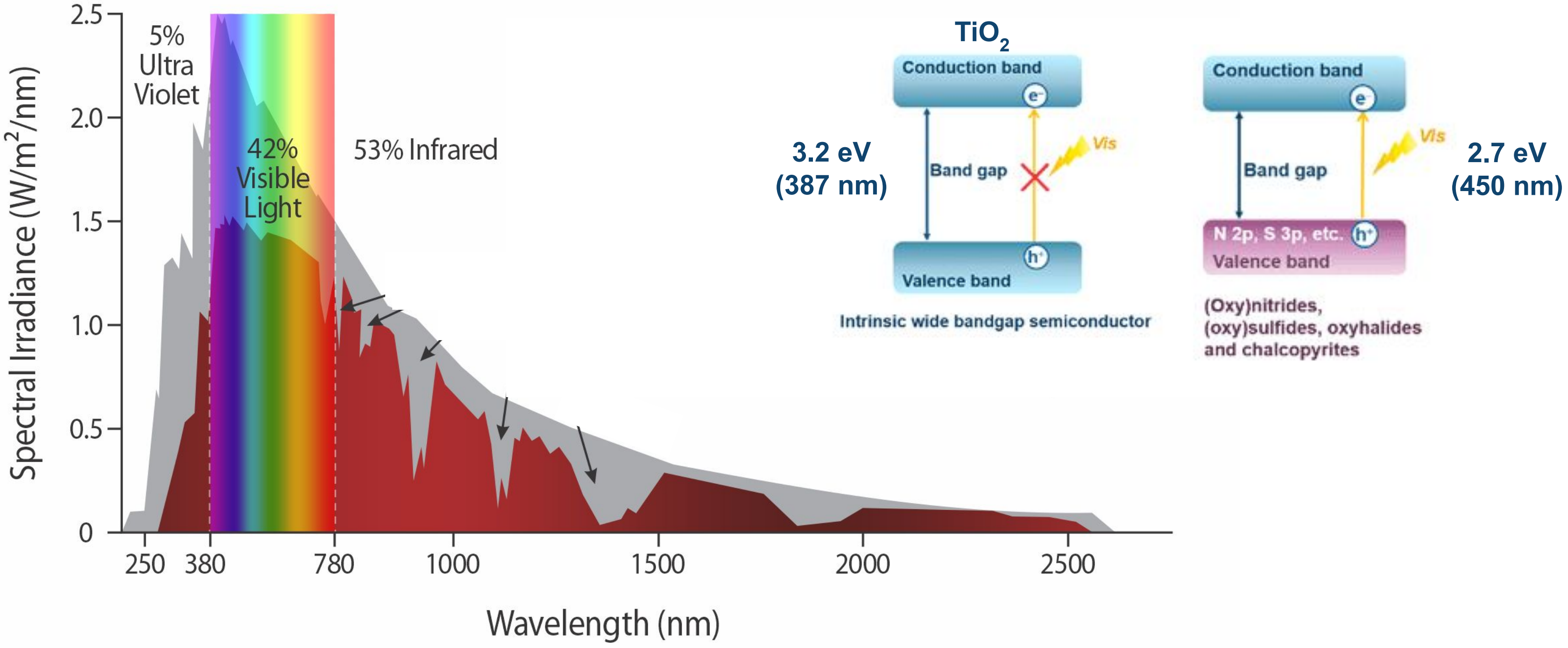
The absorption of photons can promote reduction/oxidation reactions on the photocatalyst surface



Solar photocatalysis

Efficiency Challenge: TiO_2 is a standard photocatalyst but it shows limited photon absorption (UV range).

Solar Radiation Spectrum



Band engineering

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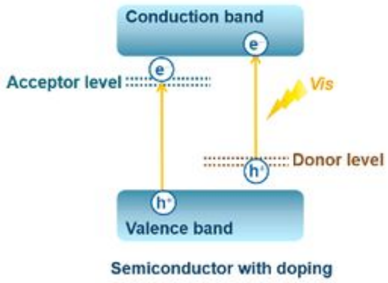
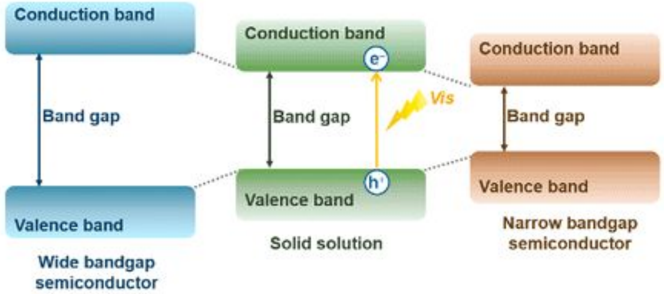
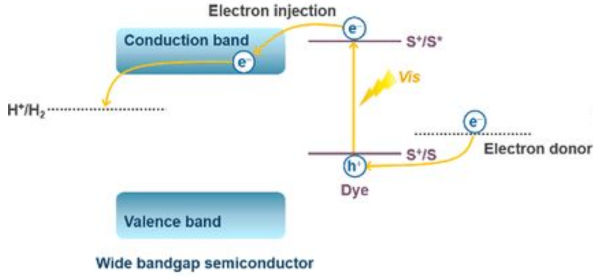
Photon absorption and key charge processes can be promoted via band engineering and other strategies



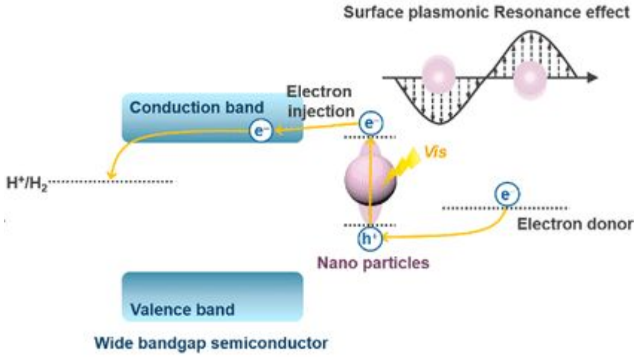
Doping



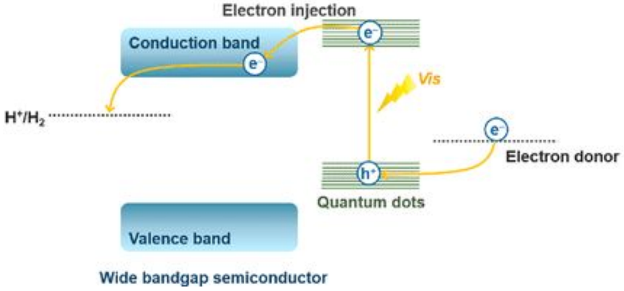
Solid Solutions



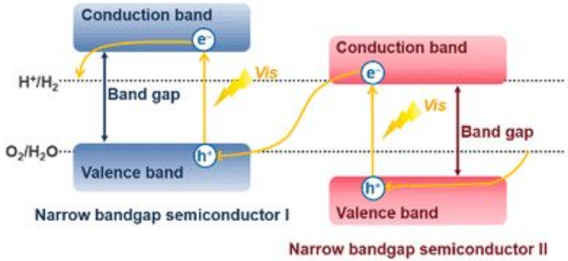
Dye-sensitised



Plasmonics



Quantum dots



Heterojunctions

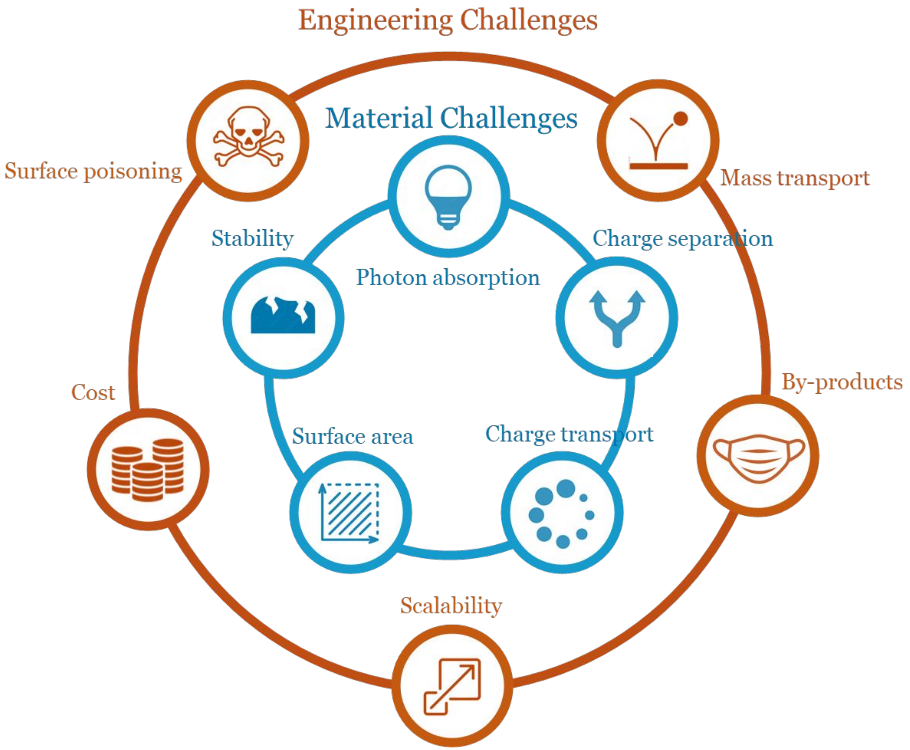
Domen *et al.* Chem. Rev. (2020), 120, 2, 919

Other key challenges

Effective photon absorption and charge transport is a good start...

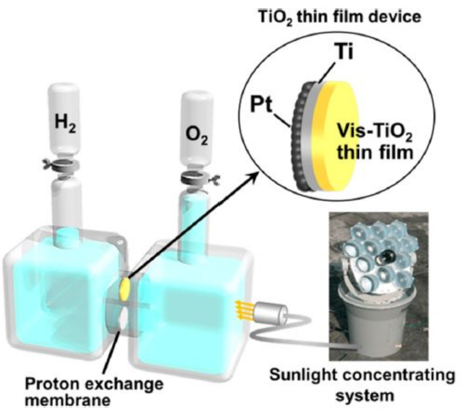
Practical applications depend on many factors:

- Material stability
- Reaction selectivity (competition)
- Poisoning
- Scalability
- Cost efficiency
- ...



Photocatalysts for H_2 evolution

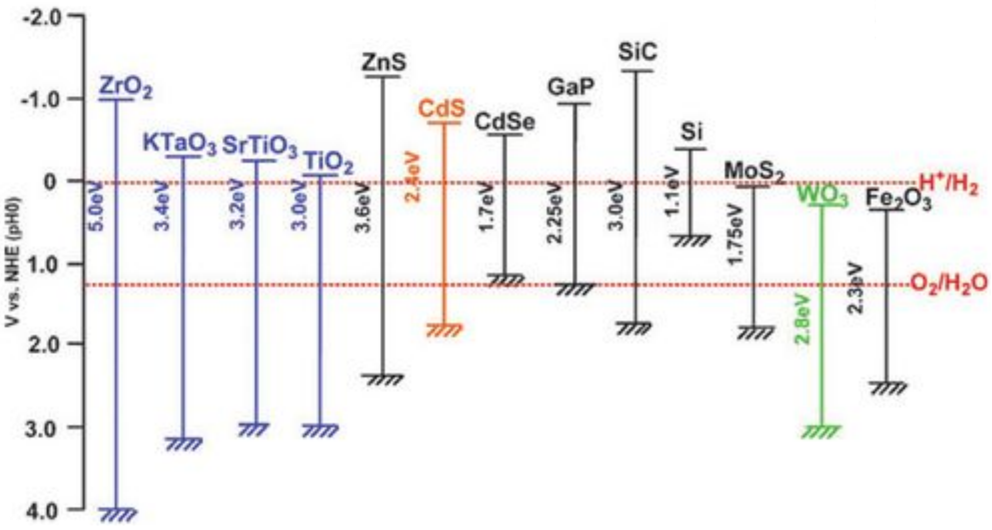
Photogenerated charges need enough energy (overpotential) to produce H_2 and O_2



Artificial Photosynthesis: Water splitting into H_2 and O_2

Reduction: $2H^+ + 2e^-$ □ H_2 $E^0 = 0$ V

Oxidation: $2H_2O$ □ $4H^+ + 4e^- + O_2$ $E^0 = 1.23$ V



Gunawan *et al.* Adv. Mater. (2024) 2404618

Solar-to-Hydrogen (STH) Efficiency

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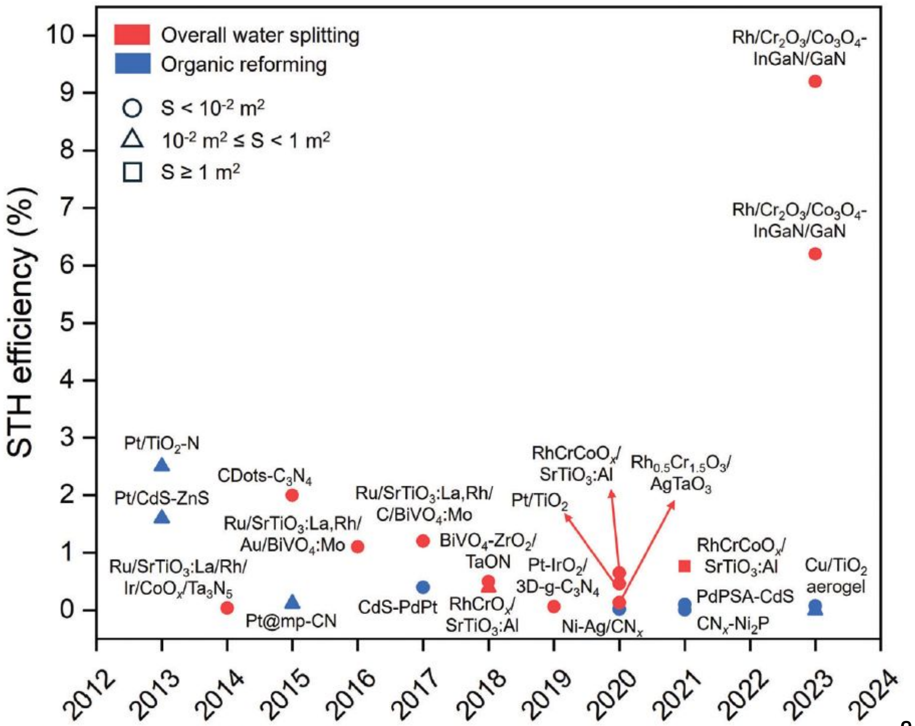
It ranks photoelectrochemical devices and sets a benchmark for solar water-splitting efficiency.

$$STH = \frac{\text{Hydrogen rate (mmol/s}^{-1}) \times \text{Change in Gibbs free energy } (\Delta G = 237 \text{ kJ/mol}_{H2})}{\text{Irradiance (mW/cm}^2) \times \text{Illuminated area (cm}^2)} \times 100$$

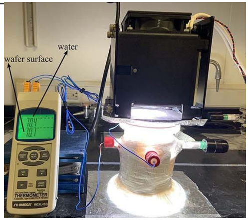


Current STH efficiencies at <2% with one study reaching 9.2% (lab) and 6.2% (concentrated solar conditions).

Gunawan *et al.* Adv. Mater. (2024) 2404618

Article

Solar-to-hydrogen efficiency of more than 9% in photocatalytic water splitting



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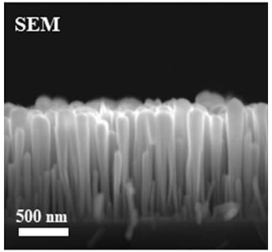
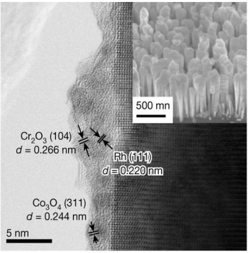
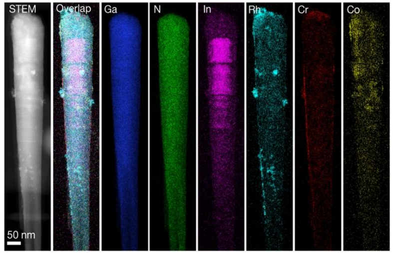
$Rh/CrO_3/Co_3O_4$-loaded InGaN/GaN nanowires.

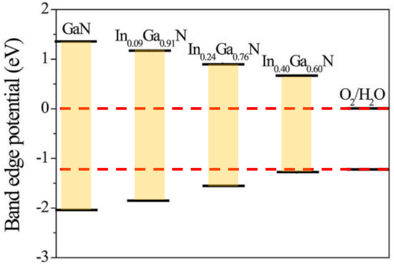
https://doi.org/10.1038/s41586-022-05399-1
Received: 19 January 2021
Accepted: 29 September 2022
Published online: 4 January 2023

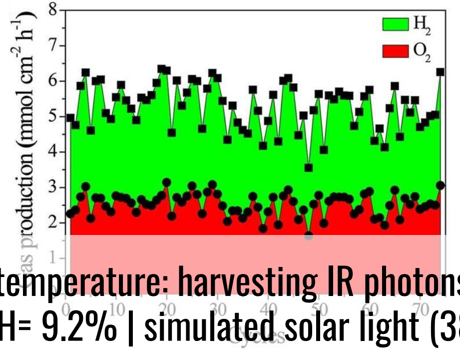
Peng Zhou[1], Ishtiaque Ahmed Navid[1], Yongjin Ma[1], Yixin Xiao[1], Ping Wang[1], Zhengwei Ye[1], Baowen Zhou[1], Kai Sun[2] & Zetian Mi[1]✉









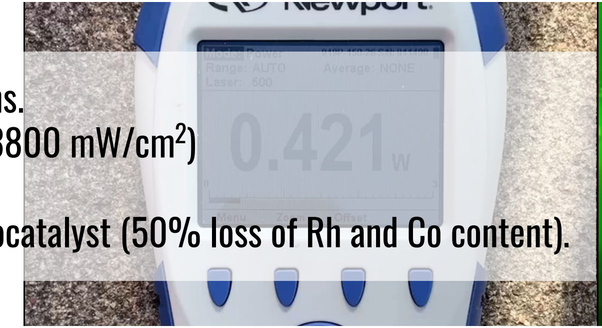


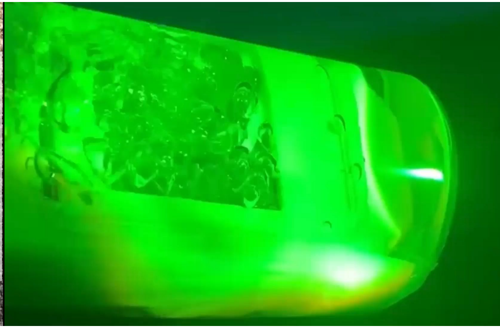
InGaN/GaN photocatalysts show visible-light-response (400–700 nm) and suitable band-edge potentials for water splitting.

Cocatalysts: Rh/CrO_3 (H_2 evolution) and Co_3O_4 (O_2 evolution).

Strong dependence of temperature: harvesting IR photons.
74-h test: T= 70°C | STH= 9.2% | simulated solar light (3800 mW/cm^2)

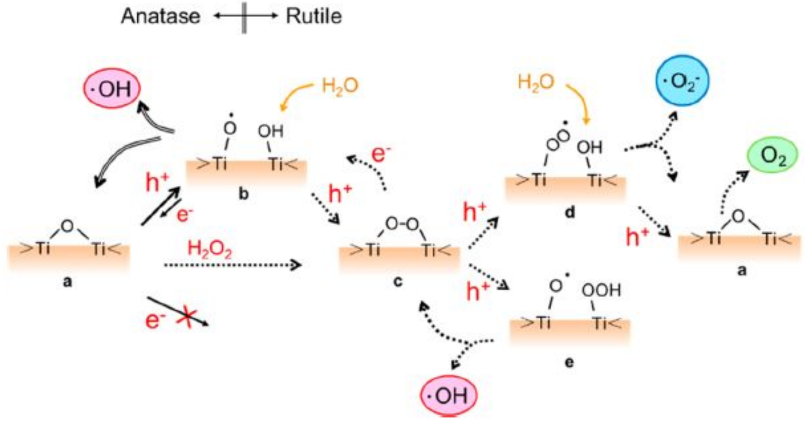
Further irradiation (+6 h) led to deactivation of the photocatalyst (50% loss of Rh and Co content).

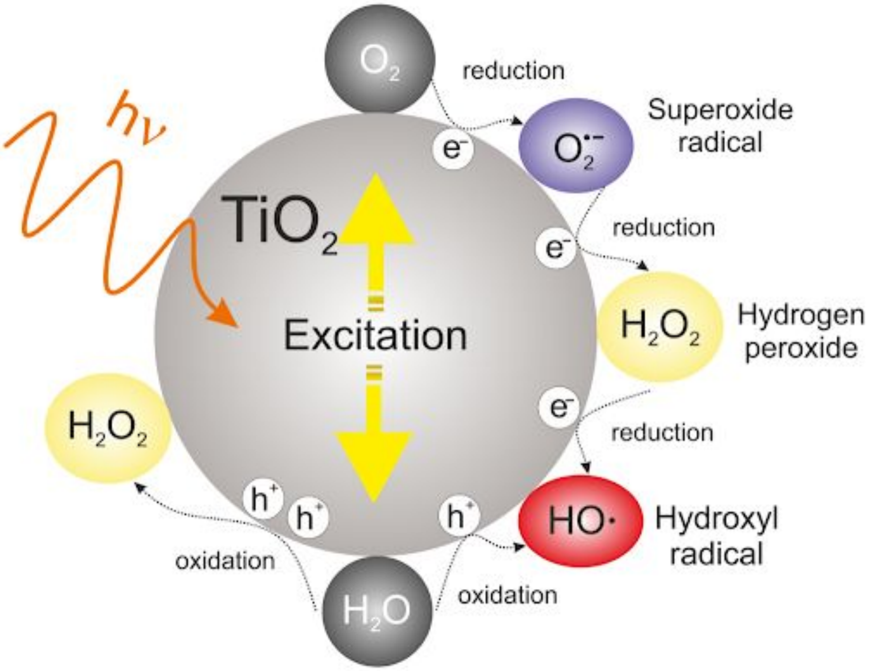




Photocatalysts for water treatment

Titanium dioxide (TiO_2): key formation of reactive oxygen species (ROS)





Lab-scale success is far from real applications

Kim *et al.* Angew. Chem. Int. Ed. (2014) 53, 14036; Nosaka *et al.* ACS Energy Lett. (2016), 1, 356.

Titanium dioxide (TiO_2)

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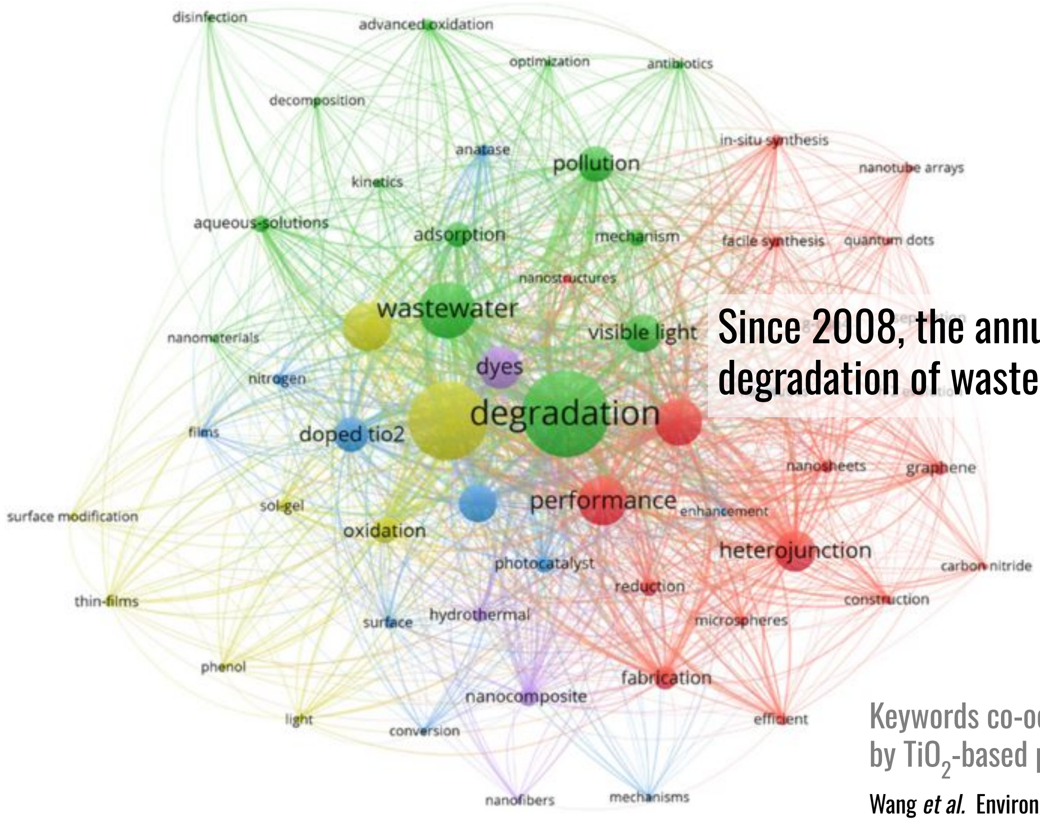
Anatase TiO_2 is still the standard commercial photocatalyst (after >50 years of active research)



Since 2008, the annual number of papers on TiO_2-based photocatalytic degradation of wastewater has increased from 9 to 114.

Keywords co-occurrence analysis of wastewater treatment by TiO_2-based photocatalytic materials after 2017

Wang *et al.* Environ. Sci. Poll. Res. (2023) 30,125417

Reconfigurable self-assembly of photocatalytic magnetic microrobots for water purification

Mario Urso, Martina Ussia, Xia Peng, Cagatay M. Oral & Martin Pumera

Nature Communications **14**, Article number: 6969 (2023) | Cite this article

Reconfigurable, reversible, and active self-assembly of microrobots at 60 s on/off switching of UV light irradiation in 1% hydrogen peroxide

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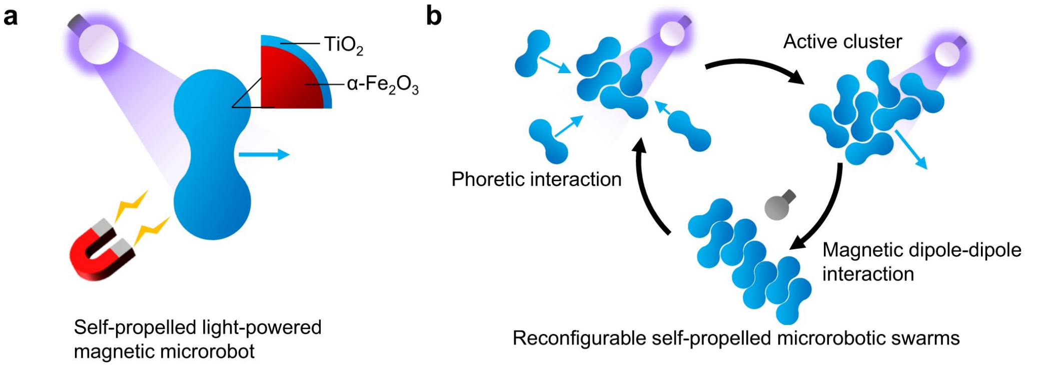
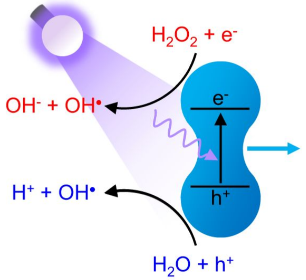
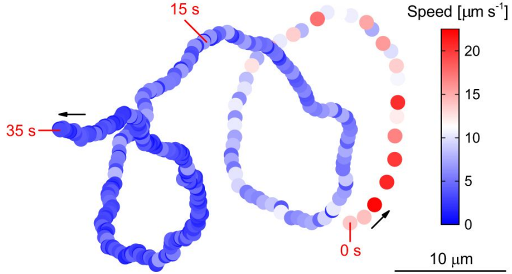
Light-active self-assembly of $TiO_2/\alpha\text{-}Fe_2O_3$ microrobots



Due to their photocatalytic and ferromagnetic properties, microrobots autonomously move in water under irradiation, while a magnetic field precisely controls their direction.





Urso *et al.* Nature Commun. (2023) 14, 6969

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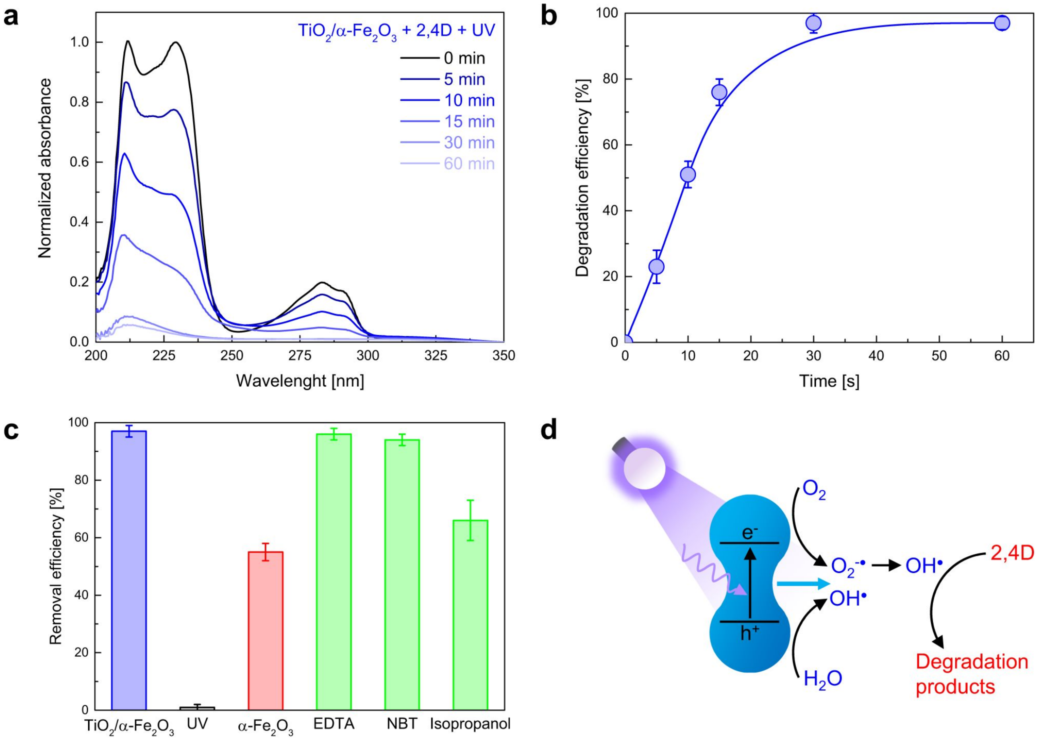

Urso *et al.* Nature Commun. (2023) 14, 6969

a Absorbance spectra of herbicide 2,4Dichlorophenoxyacetic acid (2,4D) after treatment with $TiO_2/\alpha Fe_2O_3$ microrobots under UV light irradiation in pure water.

b Degradation efficiency as a function of time.

c Comparison of efficiencies after different treatments and in the presence of scavengers.

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