Towards the sustainable synthesis of fuels and chemicals

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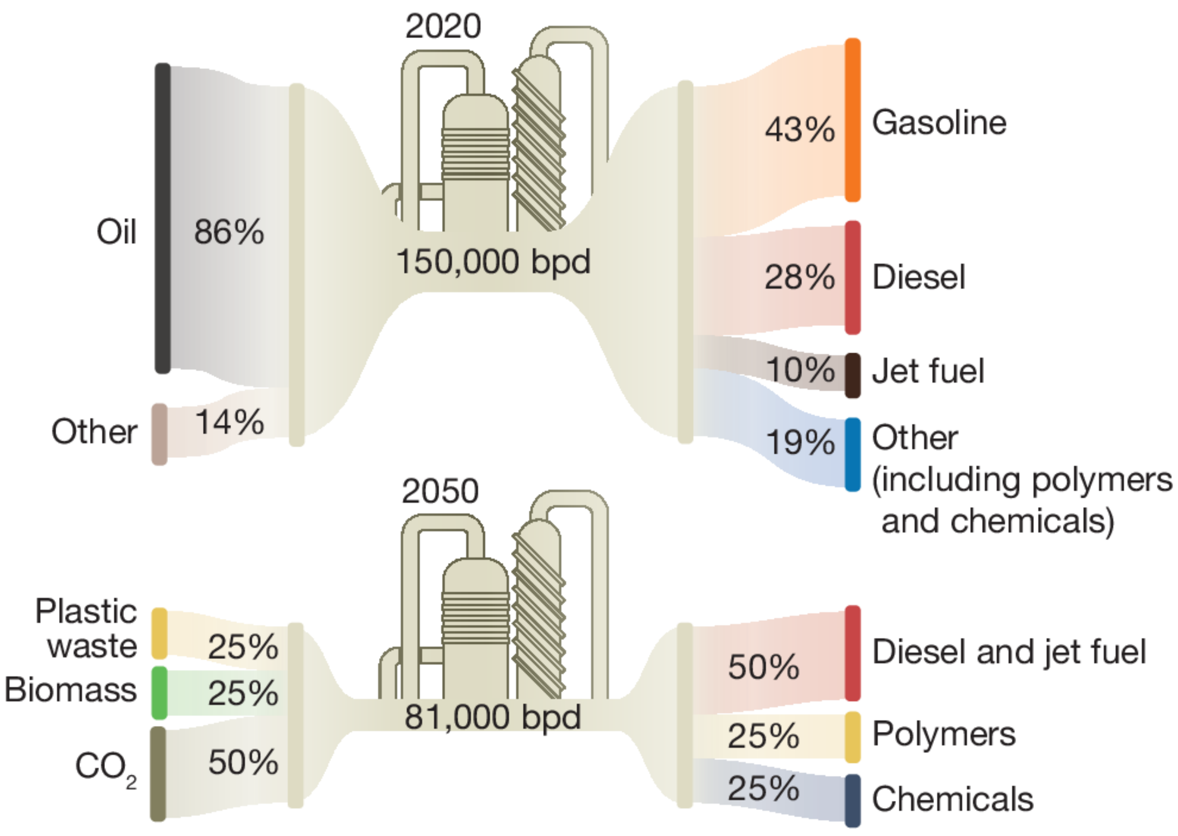
The Sustainable Chemical Refinery of the Future



Vogt & Weckhuysen, Nature 2024

Today's Refineries:

- Chemical refineries based on fossil fuels for both starting chemicals and energy requirements
- Chemical industry directly responsible for 5-6% of global CO_2 emissions, with a further 21% from transportation fuels use.

Net Zero Future Refineries:

- Sustainable starting chemicals – waste, biomass, atmospheric CO_2, N_2…..
- Chemical transformations driven by sustainable energy inputs – renewable power, green H_2 etc.

Sustainable Fuels and Chemicals

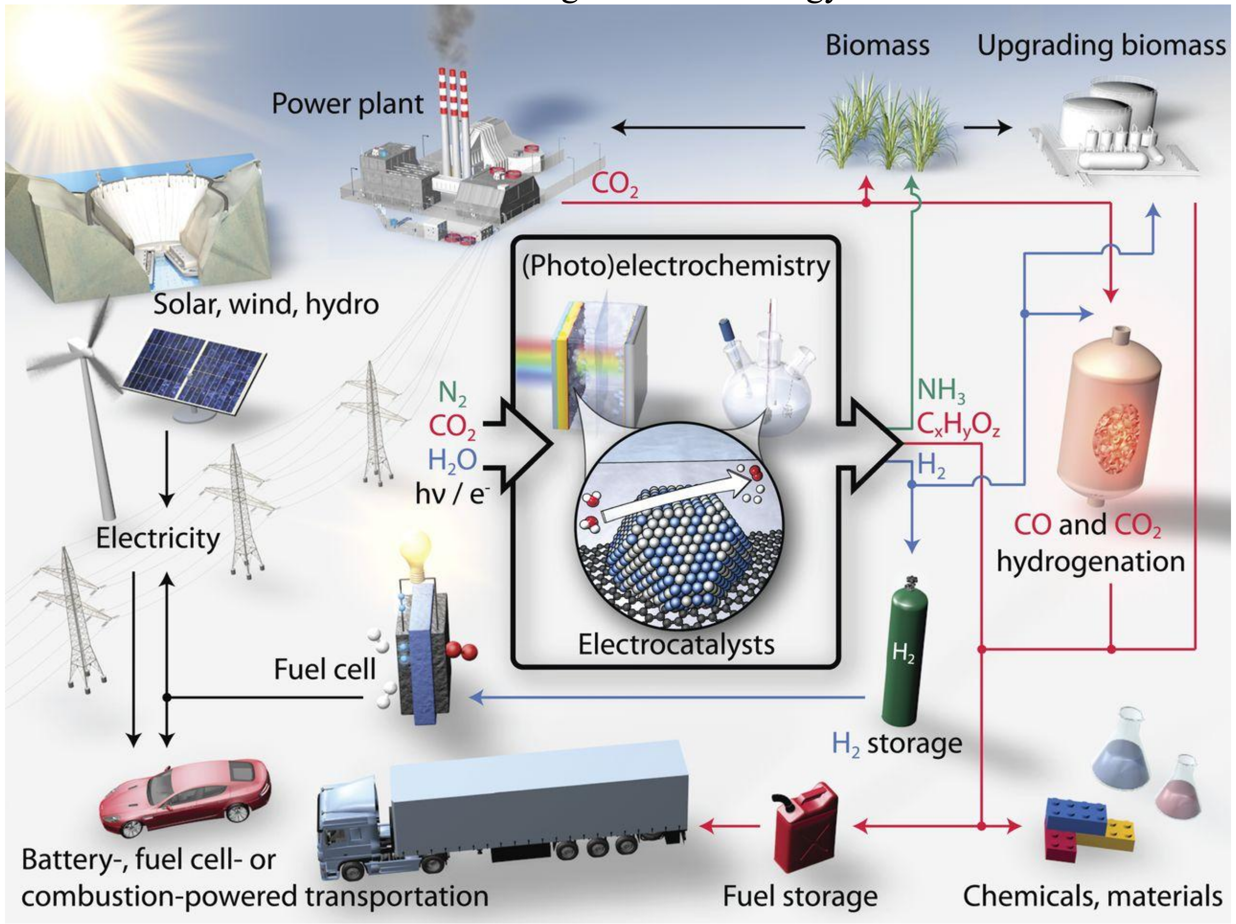
Drivers:

- Fossil-fuel-free fuels and chemicals
- Storage of intermittent renewable energy
- Transportation of renewable energy around globe
- CO_2 utilisation

Key challenges:

- Scale
- Cost competiveness

A sustainable energy system based on fuels and chemicals synthesised using renewable energy



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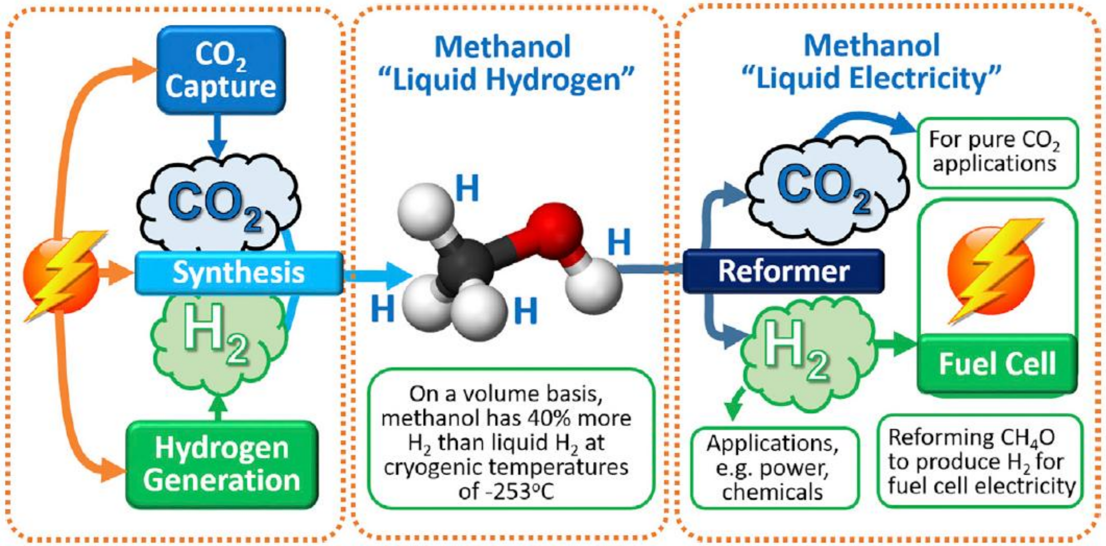


'Liquid Sunshine'

Shih et al. Joule 2018

Chemistry for Sustainable Fuels and Chemicals

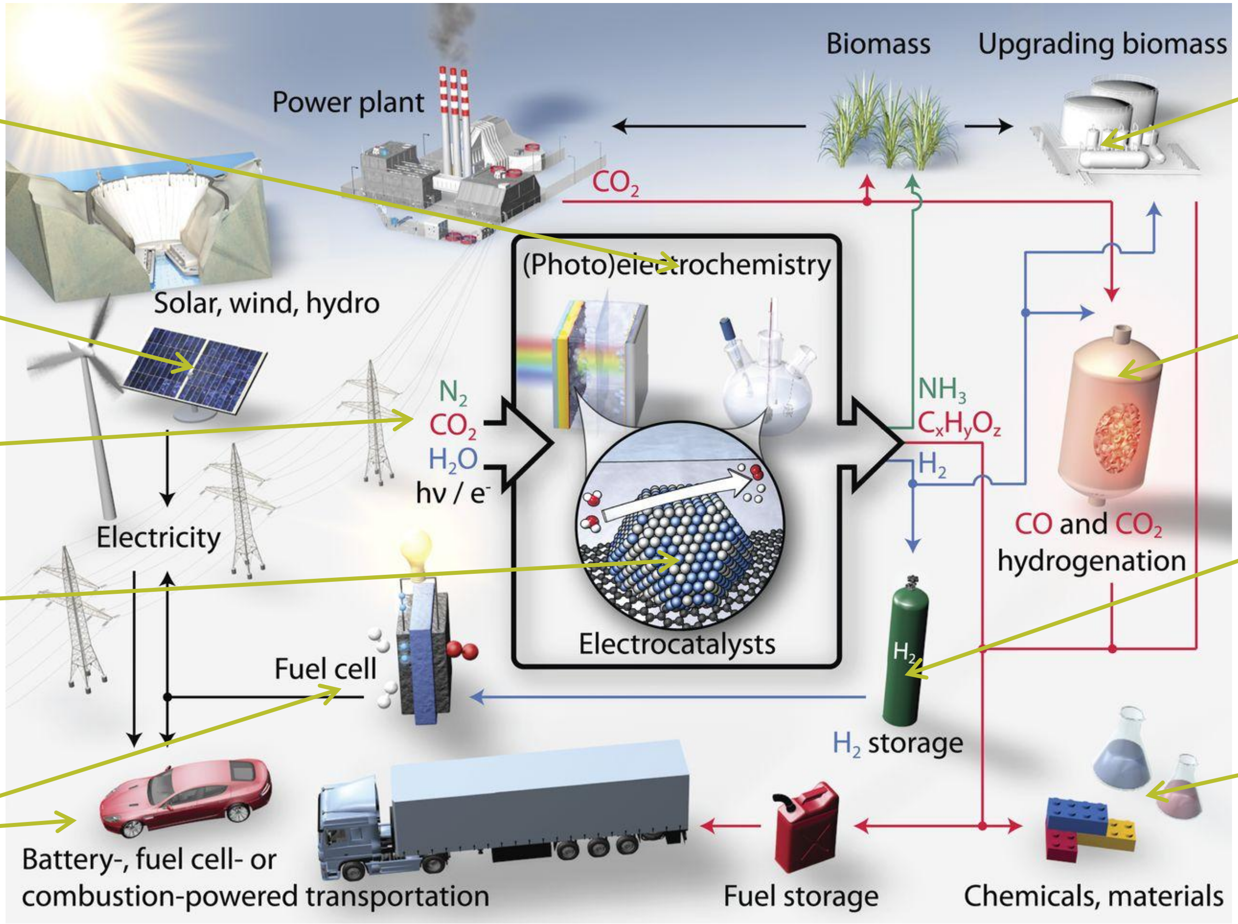
Photoelectrochemistry

Solar cell materials

Chemicals for direct air capture of CO_2

Electrocatalysis

Battery and fuel cell materials



Biomass and waste upgrading

Chemistry with CO_2 (CO_2 utilisation)

H_2 storage materials

Downstream chemistry: Sustainable synthesis of chemicals polymers, aviation fuels,

Chemistry for Net Zero & Sustainability in Oxford

- **Catalysis**
  - Kylie Vincent, Edman Tsang, Charlotte Williams OBE FRS, Luet Wong, Véronique Gouverneur FRS, Ed Anderson, Darren Dixon
- **Chemicals and energy**
  - Claudia Tate, Iain McCulloch FRS, Robert Hoye, Ludmilla Steier, Harry Anderson, James Durrant CBE FRS, Ji Seon Kim, Filip Podjaski, Dan Congrave, Anna Ragoutz
- **Computation and digital**
  - Volker Deringer, Fernanda Duarte, Michail Stamatakis
- **Materials and electrolytes for batteries**
  - Simon Clarke, Andrew Goodwin, Michael Hayward, Georgina Gregory, Susan Perkin
- **Environmental chemistry and resources**
  - Michael Cotterell, Claire Vallance, Grant Ritchie, Dermot O'Hare, Michael Neidig

In partnership with the wider Oxford sustainable research ecosystem:

Catalysis for Net Zero & Sustainability in Oxford

CatalysisHub

www.ukcatalysishub.co.uk

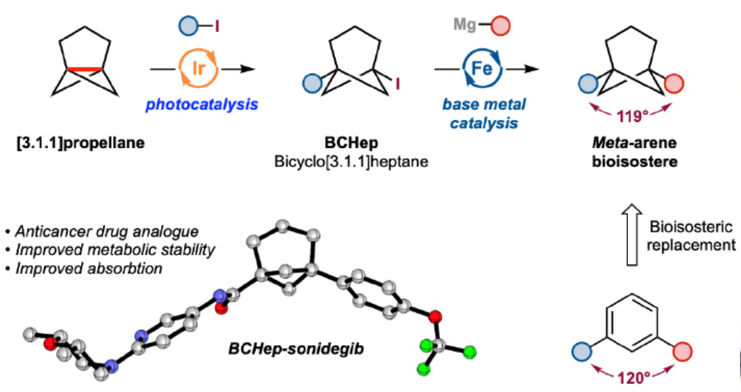
- £28M, EPSRC Investment supporting postdocs, early career researchers, students, strategic infrastructure (2014-current)
- 46 Universities and >50 companies across the UK
- UK Catalysis Hub Phase III – Charlotte Williams (Director) Focus on Net Zero Chemicals Industry and Digital Catalysis
- Kylie Vincent, Charlotte Williams, Simon Aldridge & Michail Stamatakis

Sustainable Chemicals & Materials Manufacturing Hub

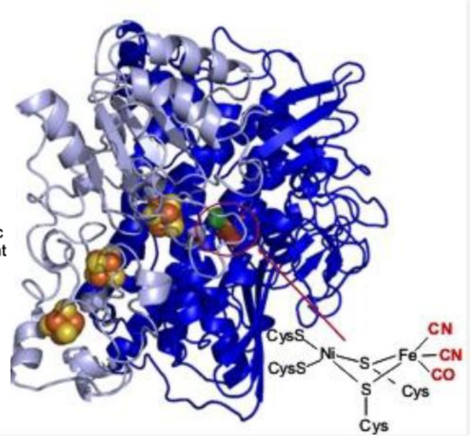
https://schemahub.ac.uk/

- Flagship EPSRC Investment for Future Chemical Industry and Manufacturing (£13.5 M EPSRC, £22M Industry and partners)
- Charlotte Williams (Director) , Georgina Gregory, Kylie Vincent

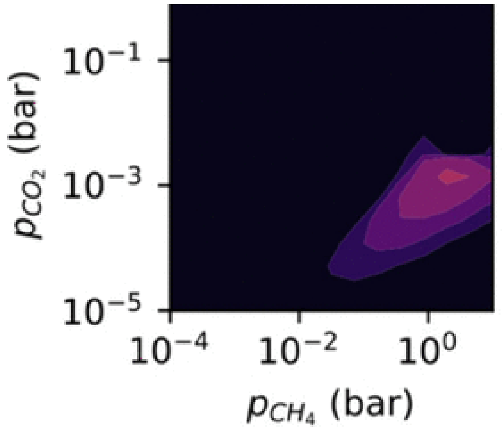
Charlotte Williams



Ed Anderson



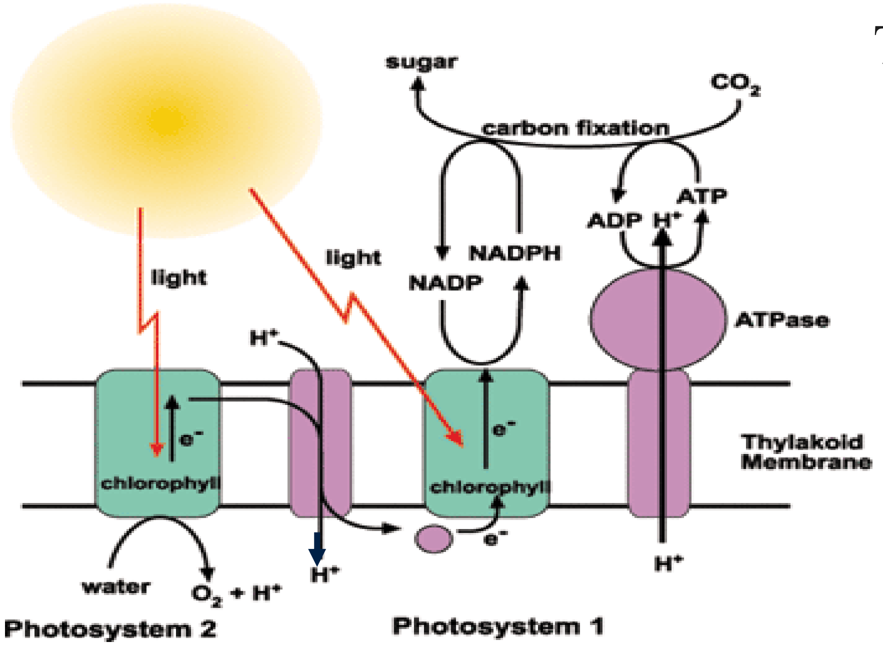
Kylie Vincent



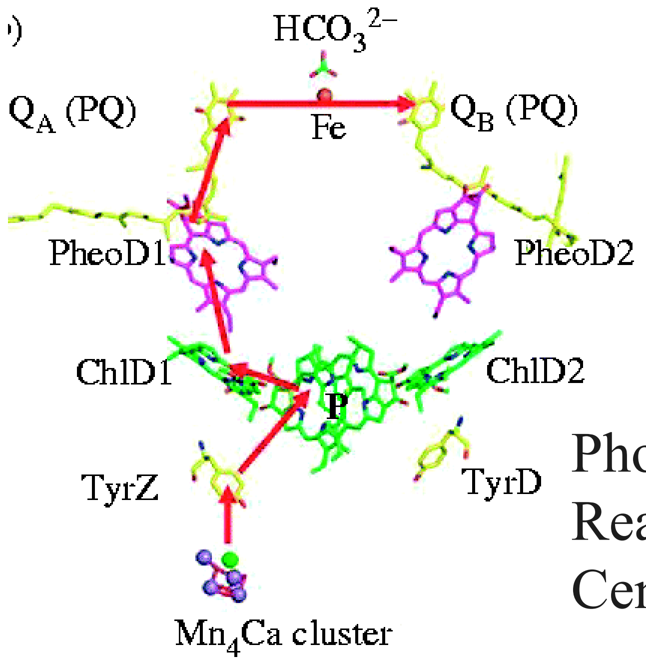
Michael Stamatakis

Inspiration from biological photosynthesis

Leaf



Thylakoid Membrane

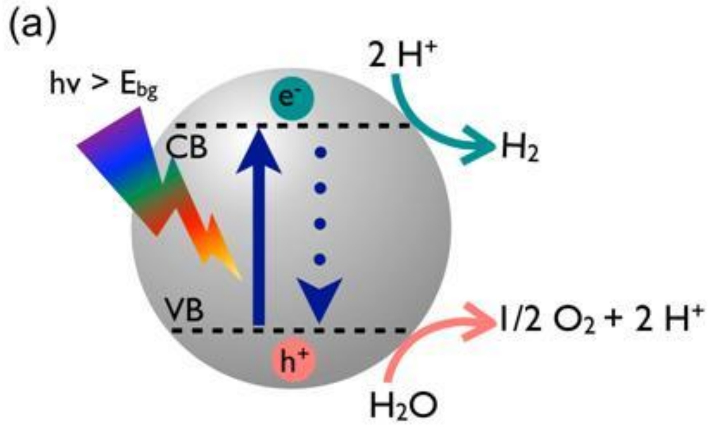


Photosystem Reaction Centre

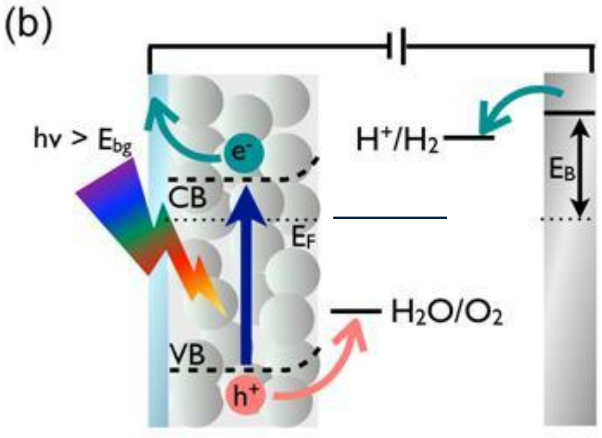
Biological solar to chemical efficiency:

to NADPH, O_2 and ΔpH:	upto 20%
to glucose and O_2:	upto 7 %
to biomass:	typically < 1 %
c.f.: silicon cell:	18-25%

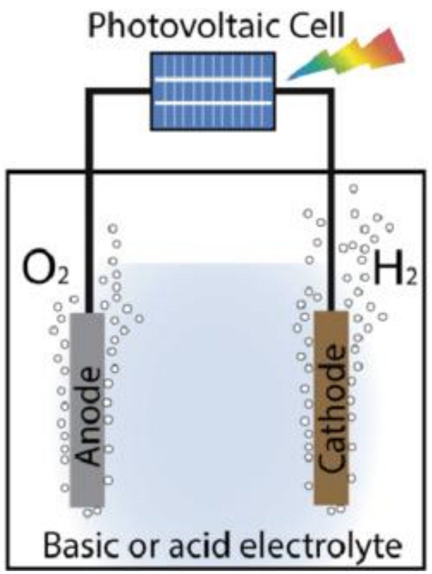
Harnessing the Sun: Artificial Photosynthetic Devices



Photocatalyst particles



Photoelectrodes



PV + electrocatalysis

Technology readiness level

Potentially lowest cost if efficiency could be improved

~ Green H_2 from PV + electrocat circa 3 x more expensive than H_2 from methane

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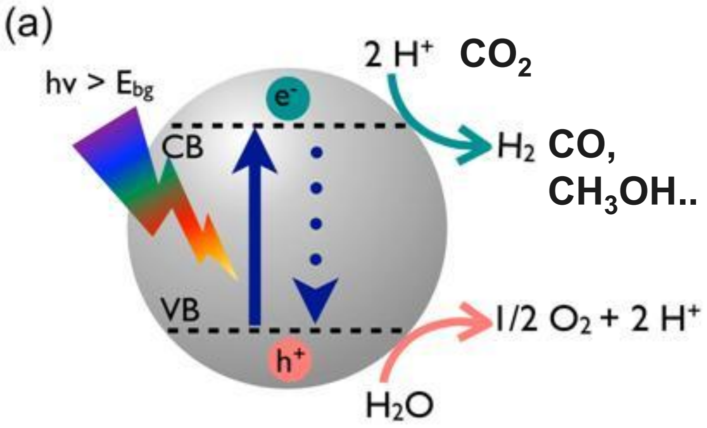
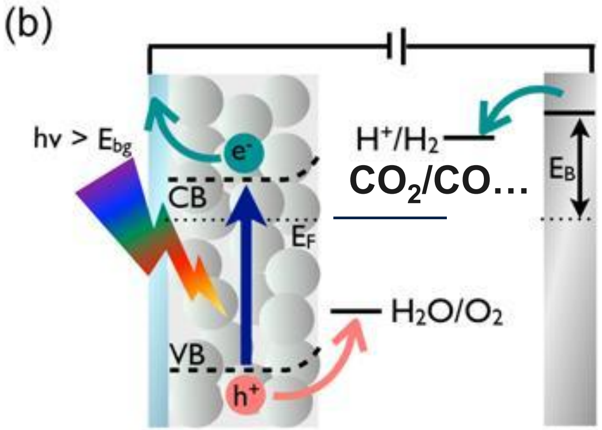
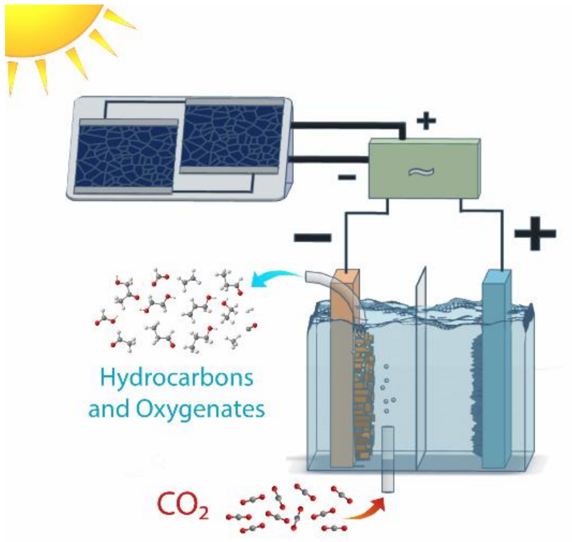


Photocatalyst particles



Photoelectrodes



PV + electrocatalysis

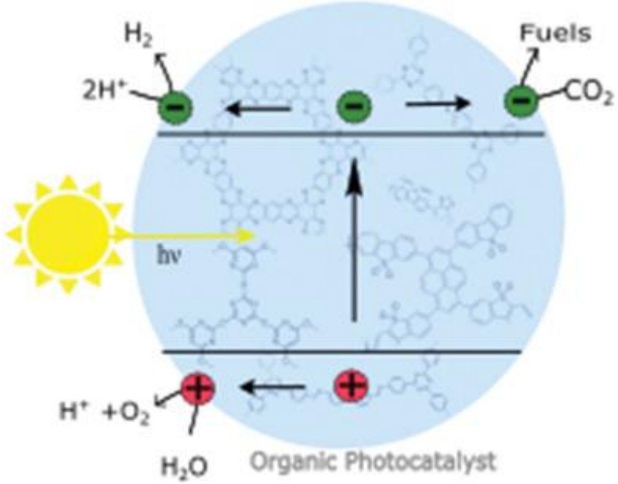
Potentially lowest cost if efficiency could be improved

100m^2 $SrTiO_3$ ‘photocatalyst sheet’ demonstration plant

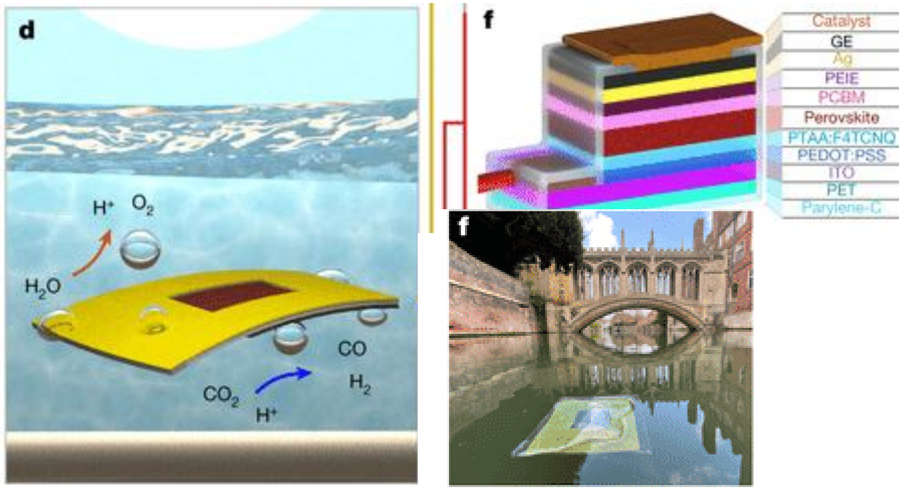
Domen et al. Nature 2020 & 2021

~ Green H_2 from PV + electrocat circa 3 x more expensive than H_2 from methane

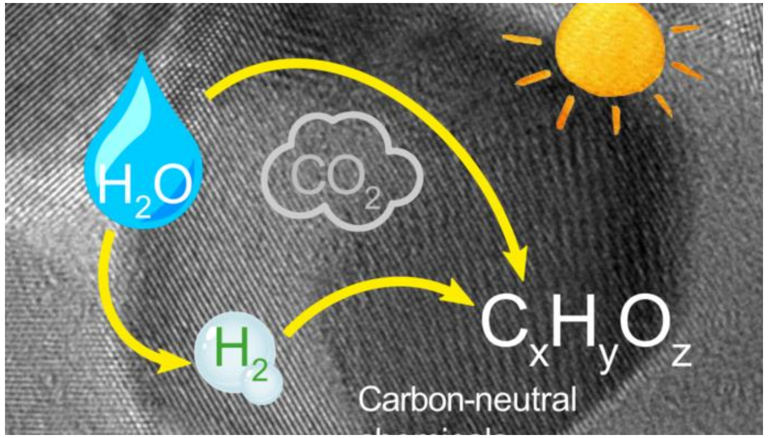
Artificial Photosynthesis @ Oxford Chemistry



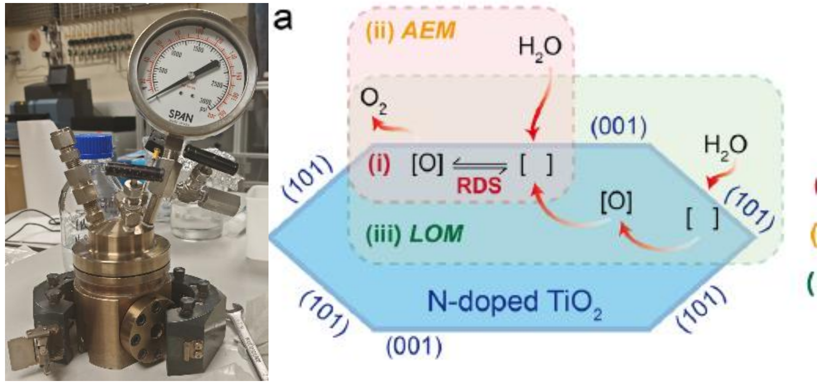
Iain McCulloch:
Organic photocatalysts



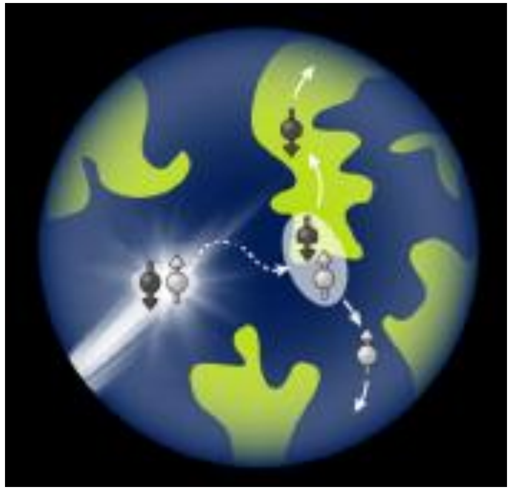
Robert Hoye:
Inorganic materials for artificial leaves



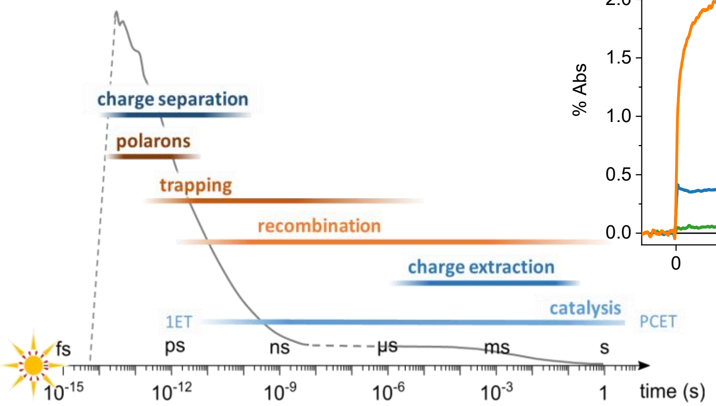
Ludmilla Steier
Inorganic photocatalysts

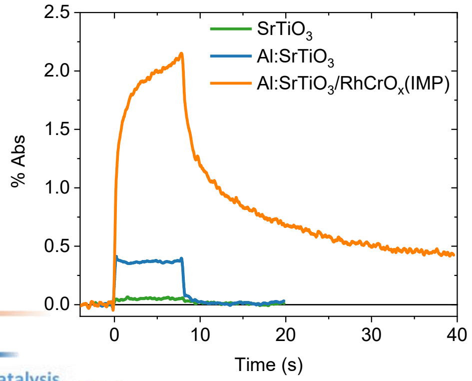


Edman Tsang:
High Temp and pressure photocatalysis



Claudia Tate:
Photoinduced EPR





James Durrant:
Photochemistry & dynamics