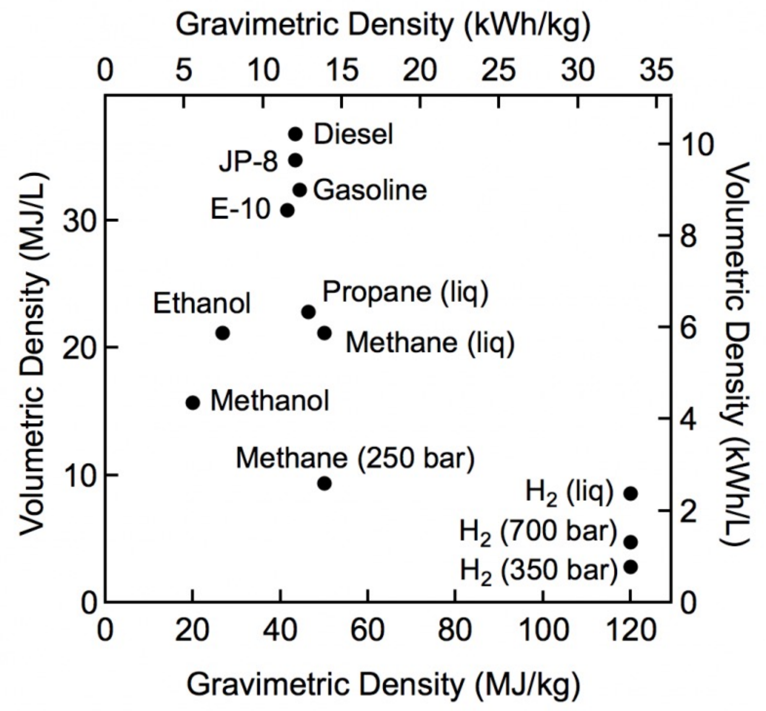
Innovation in Green Hydrogen (and related technologies)

Ludmilla Steier
Associate Professor, Inorganic Chemistry
ludmilla.steier@chem.ox.ac.uk



Oxford Energy Day
28 September 2023

HM Government

UK Hydrogen Strategy

This strategy sets out the approach to developing a thriving low carbon hydrogen sector in the UK to meet our increased ambition for 10GW of low carbon hydrogen production capacity by 2030. The page includes hydrogen strategy updates to the market.

https://www.gov.uk/government/publications/uk-hydrogen-strategy

Notice

Net Zero Hydrogen Fund strands 1 and 2: summaries of successful applicants round 1 (April 2022) competition

Published 30 March 2023

- Trecwn Green Energy Hub
- Ballymena Hydrogen
- Conrad Energy Hydrogen Lowestoft
- Didcot Green Hydrogen Electrolyser
- Green Hydrogen St Helens
- Green Hydrogen Winnington & Middlewich
- Inverness Green Hydrogen Hub
- Mannok Green Hydrogen Valley
- MCRU Integrated Hydrogen Delivery for a Fuel Cell Van Fleet Pilot
- Lanarkshire Green Hydrogen
- The Knockshinnoch Green Hydrogen Hub Project
- HyNet Hydrogen Production Plant HPP2
- Kintore Hydrogen
- H2NorthEast
- Port of Felixstowe Green Hydrogen Project

4 GW by 2030

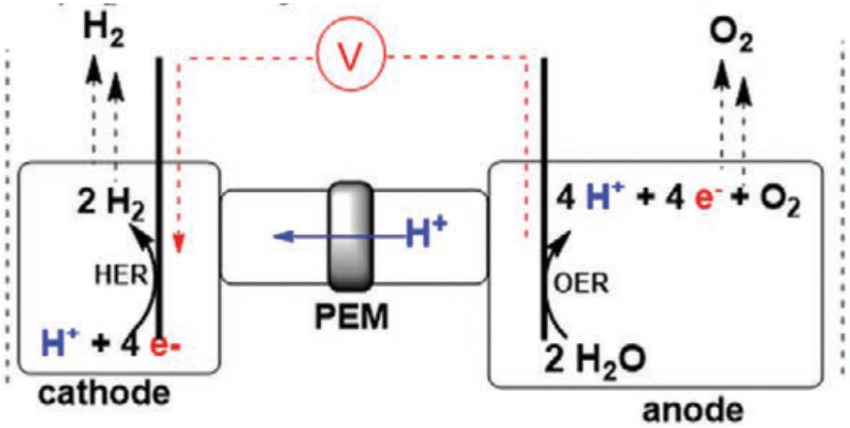
https://www.gov.uk/government/publications/net-zero-hydrogen-fund-strands-1-and-2-successful-applicants

Green Hydrogen via Electrolysis

with Electricity from Renewables

Catalyst: Pt/C

Requirements:
Low overpotential
High current density

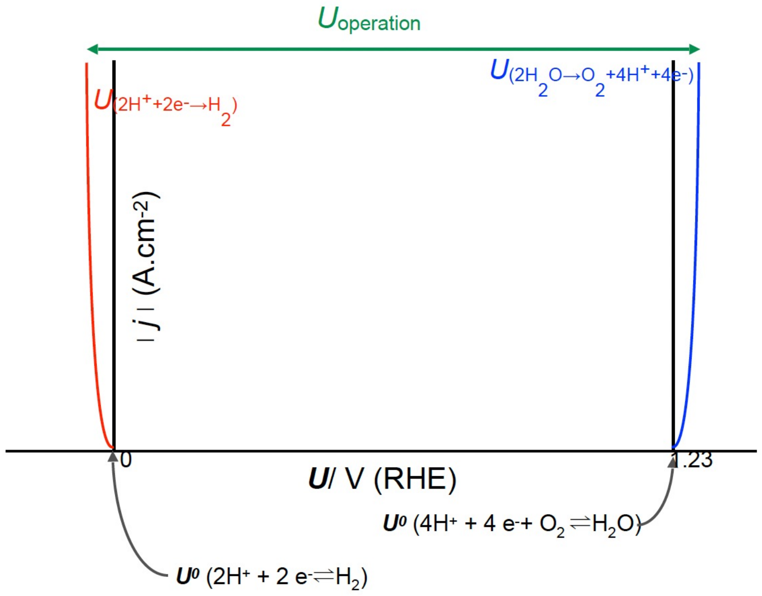


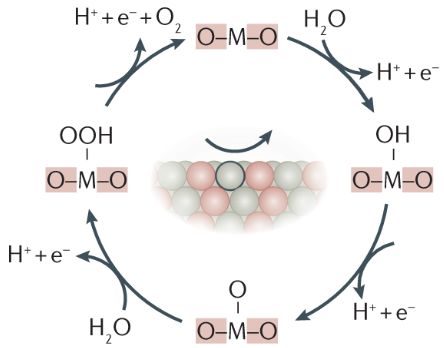
Catalyst: IrO_2

Requirements:
Low overpotential
High stability

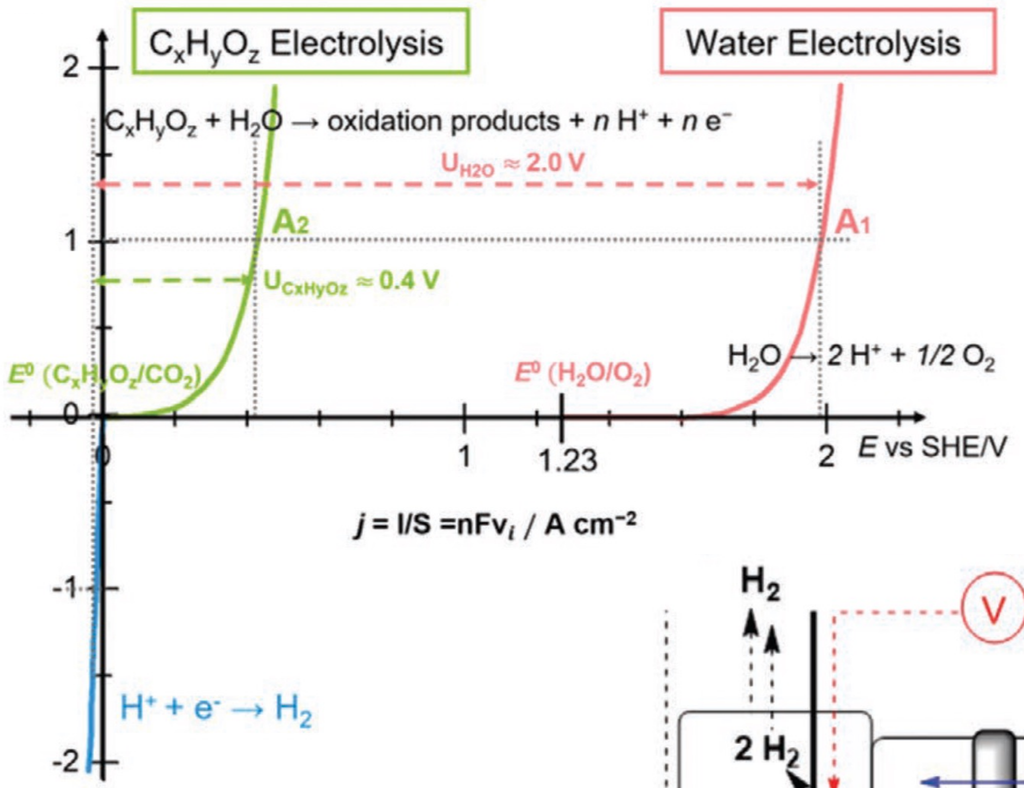
Challenge1: High overpotentials for OER (240 – 400 mV) → 1.7 – 2 V

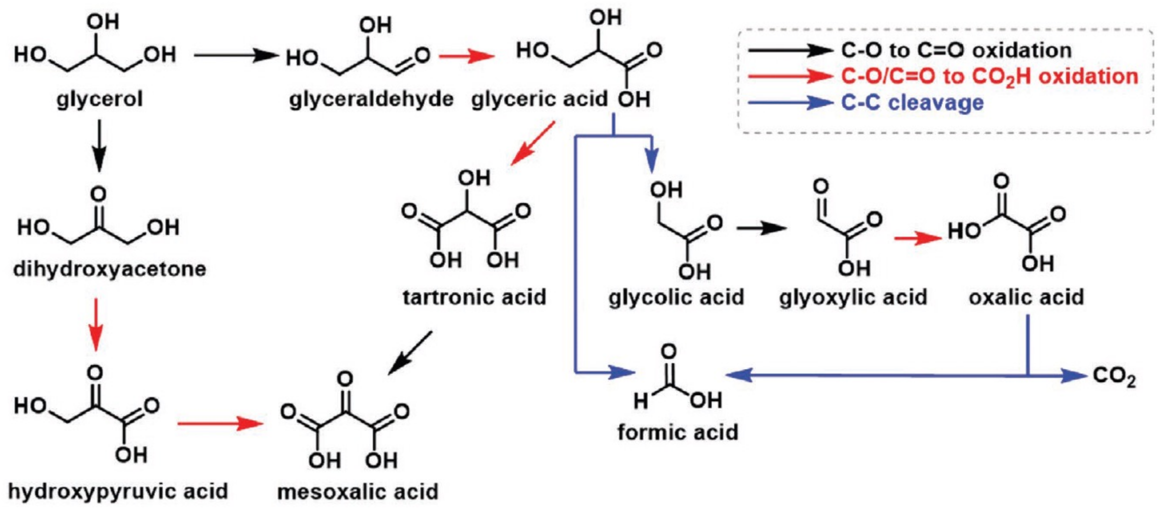
Challenge 2: IrO_2 is too precious and scarce

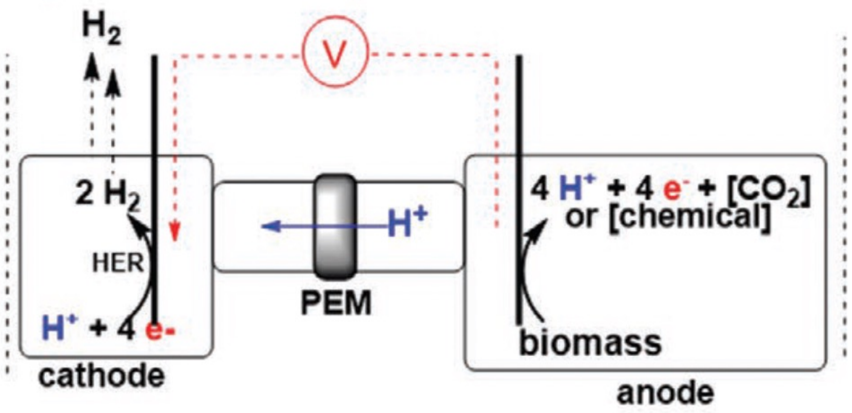




Green Hydrogen via Biomass Valorization





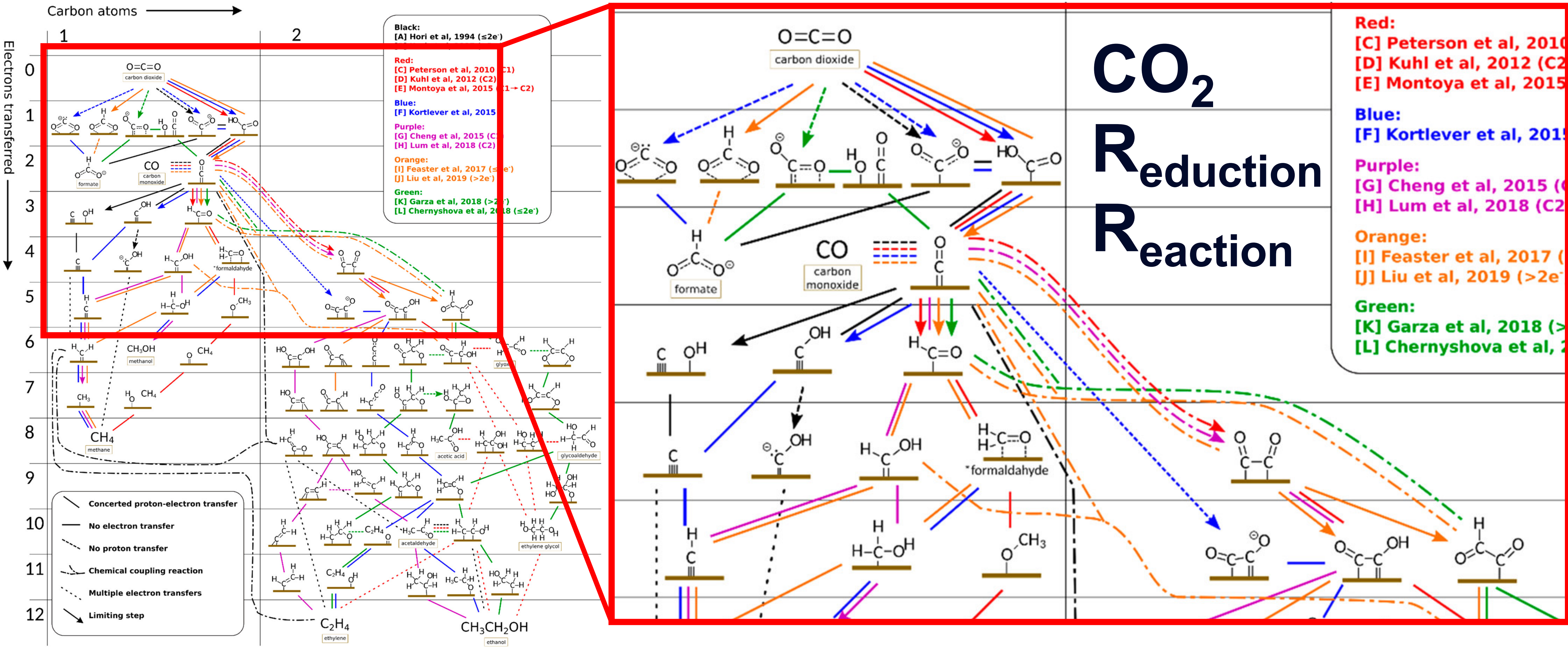


Advantage:
Much lower electricity demand (almost 50%)

Challenge: Catalyst selectivity towards partial oxidation products

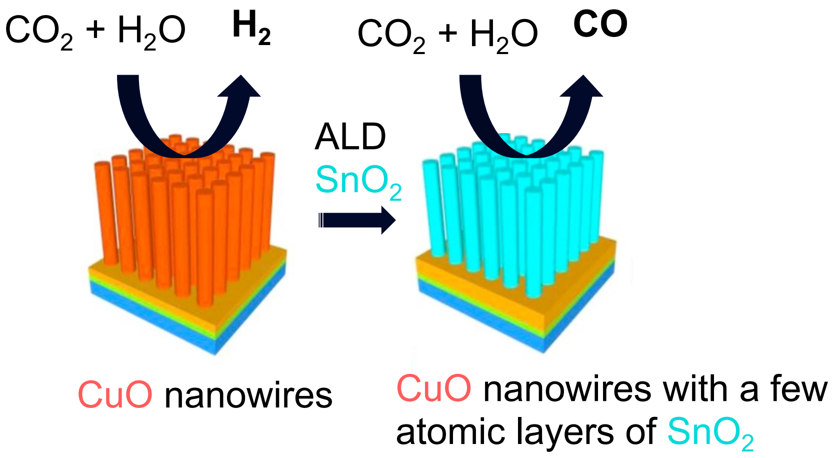
Luo, H. *et al.* Progress and Perspectives in Photo- and Electrochemical-Oxidation of Biomass for Sustainable Chemicals and Hydrogen Production. *Advanced Energy Materials* **11**, 2101180, doi:https://doi.org/10.1002/aenm.202101180 (2021).

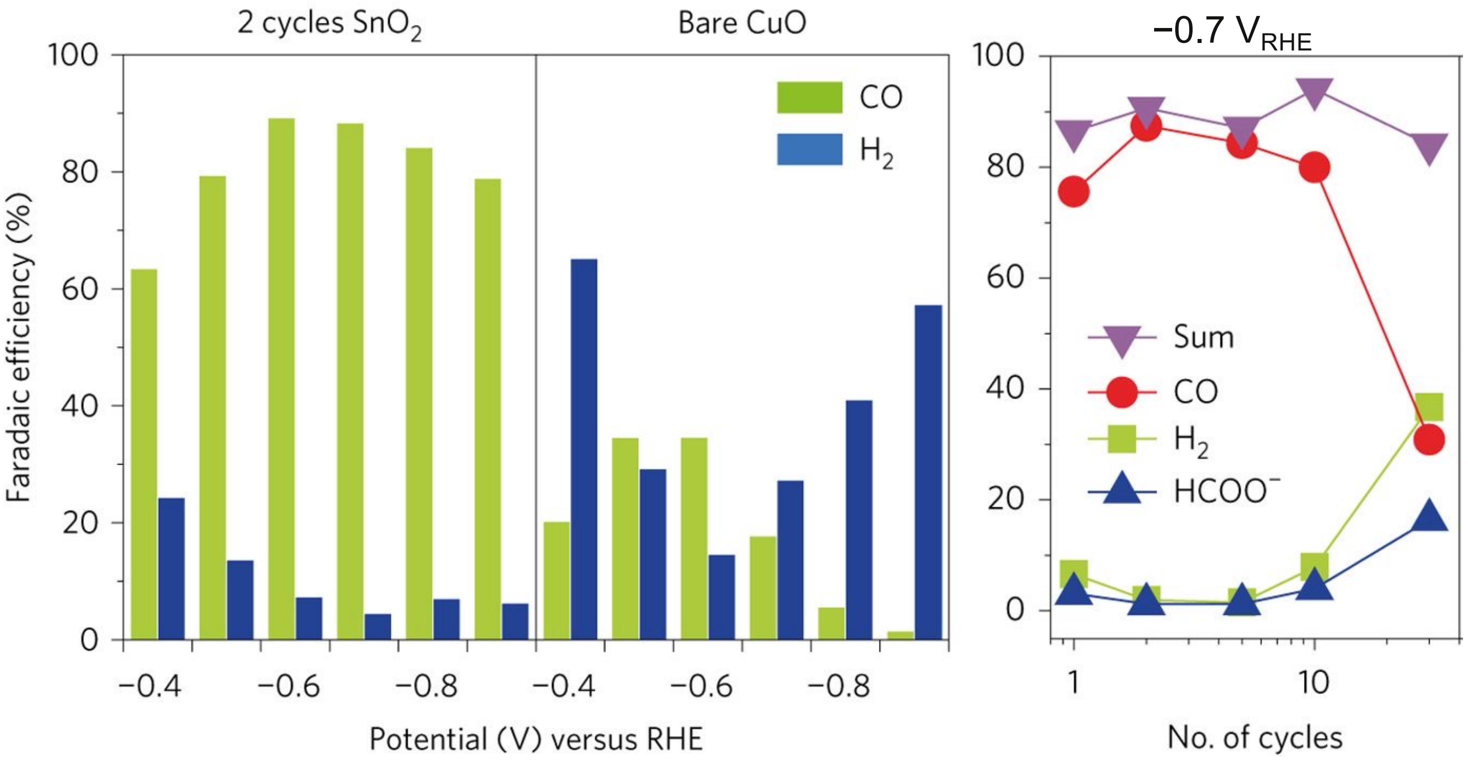
Green Hydrogen as a Co-product of CO_2RR



Nitopi, S. et al. Chem Rev, doi:10.1021/acs.chemrev.8b00705 (2019).

Importance of Single Atoms for Selectivity



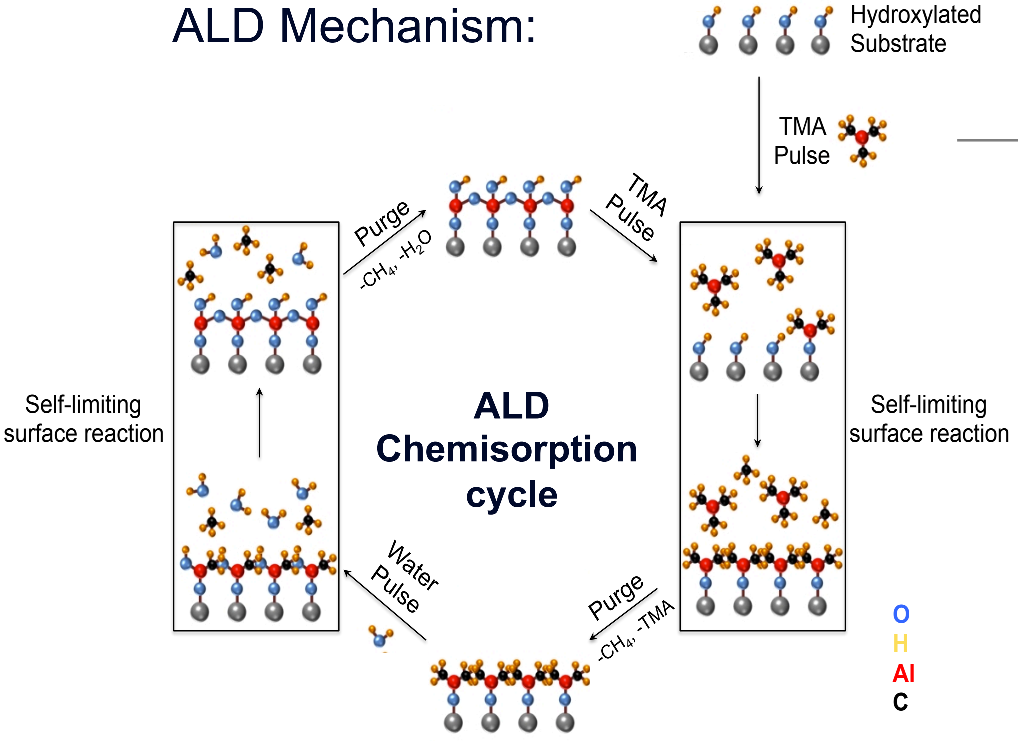


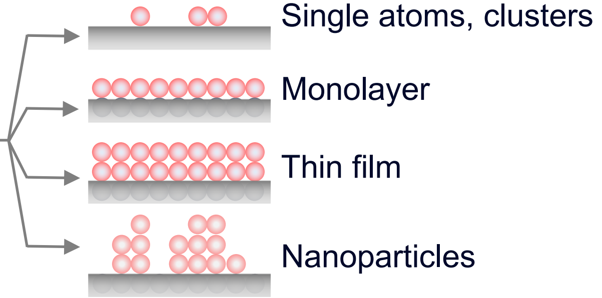
- Selectivity towards CO can switch from <20% to more than 70% with a single cycle of SnO_2 (less than a monolayer)
- Selectivity can be maintained between 80-85% for 2-10 cycles of SnO_2 (corresponding to <1.5 nm)
- When a dense pinhole-free film of SnO_2 begins to form (~30 cycles), selectivity towards CO drops sharply to 30% concomitant with increased production of formate and hydrogen

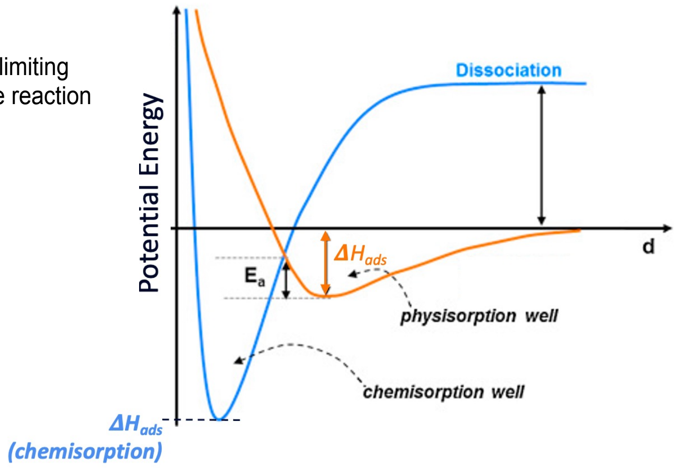
Nature Energy **2**, 17087 doi:10.1038/Nenergy.2017.87 (2017).

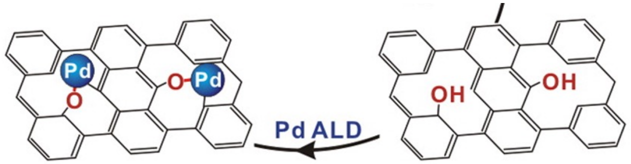
Nanoparticle and Single-atom catalysts with Atomic Layer Deposition

ALD Mechanism:

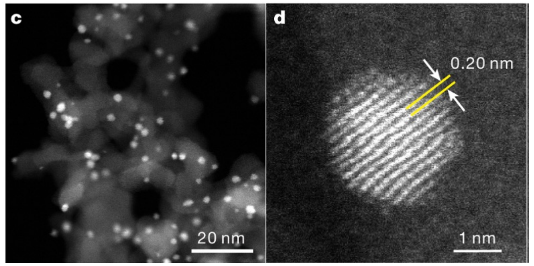




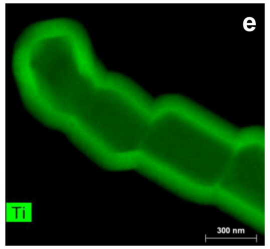




Yan, H. *et al.* J Am Chem Soc 137, 10484-10487 (2015).



Cao, L., Liu, W., Luo, Q. *et al.* *Nature* **565,** 631–635 (2019)



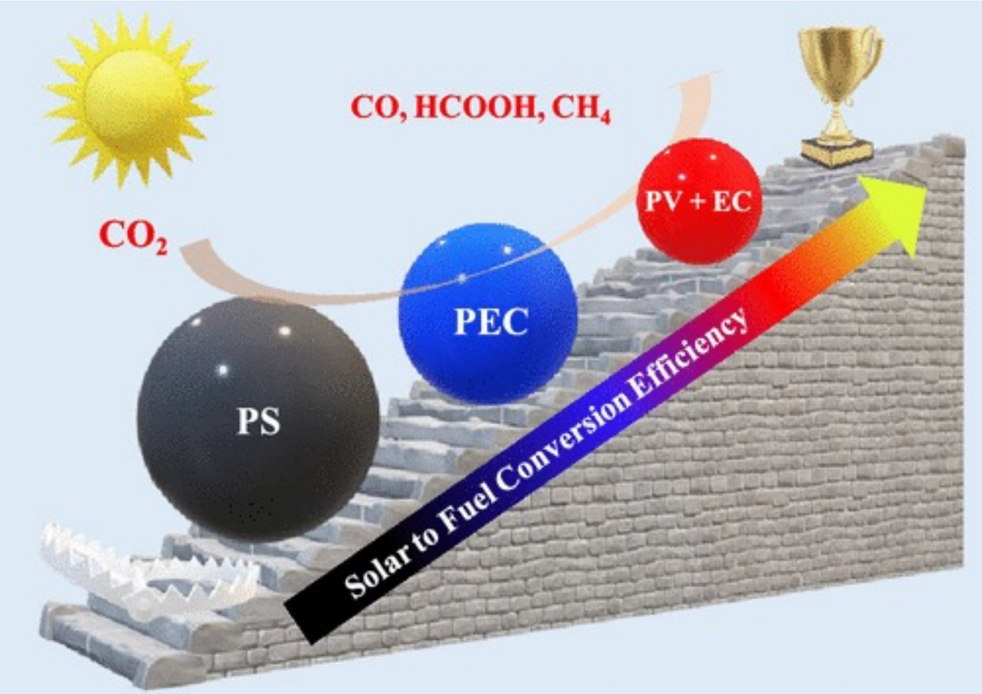
Luo, J., **Steier L.** *et al.* *Nano Lett* **16**, 1848-1857 (2016).

Coating of porous high surface area substrates

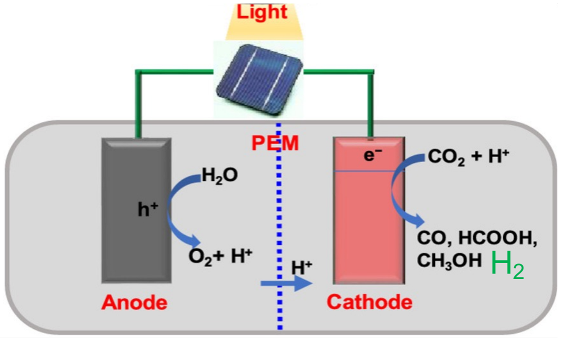
- Powerful tool to explore selectivity drivers and active site reactivity in catalysis
- Can help mitigating surface reconstruction of catalyst materials during operation

L. Steier, How to engineer surfaces to tailor selectivity?, in Stephens, I. E. L. et al. 2022 Roadmap on low temperature electrochemical CO2 reduction. *Journal of Physics: Energy* 4, doi:10.1088/2515-7655/ac7823 (2022).

Routes to Green Hydrogen and Solar Fuels



η_{CO_2RR}	<< 1%	≤ 10%	≤ 19%
η_{HER}	≤ 1%	≤ 19%	≤ 30%



Photovoltaic + electrochemical

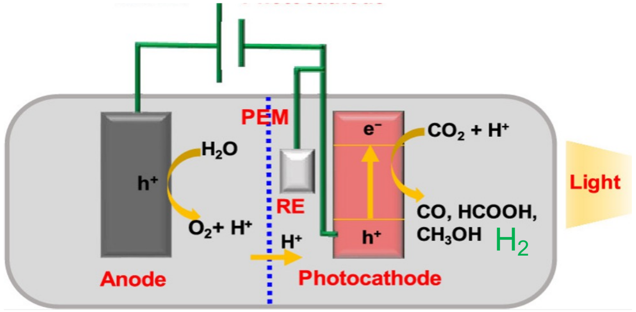
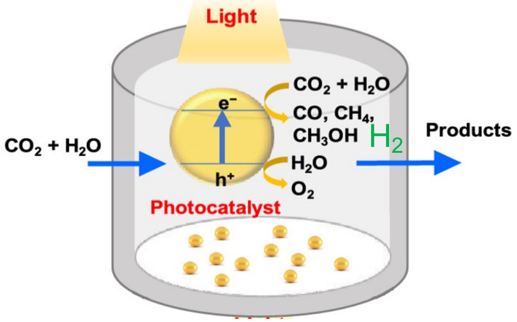


Photo-electrochemical

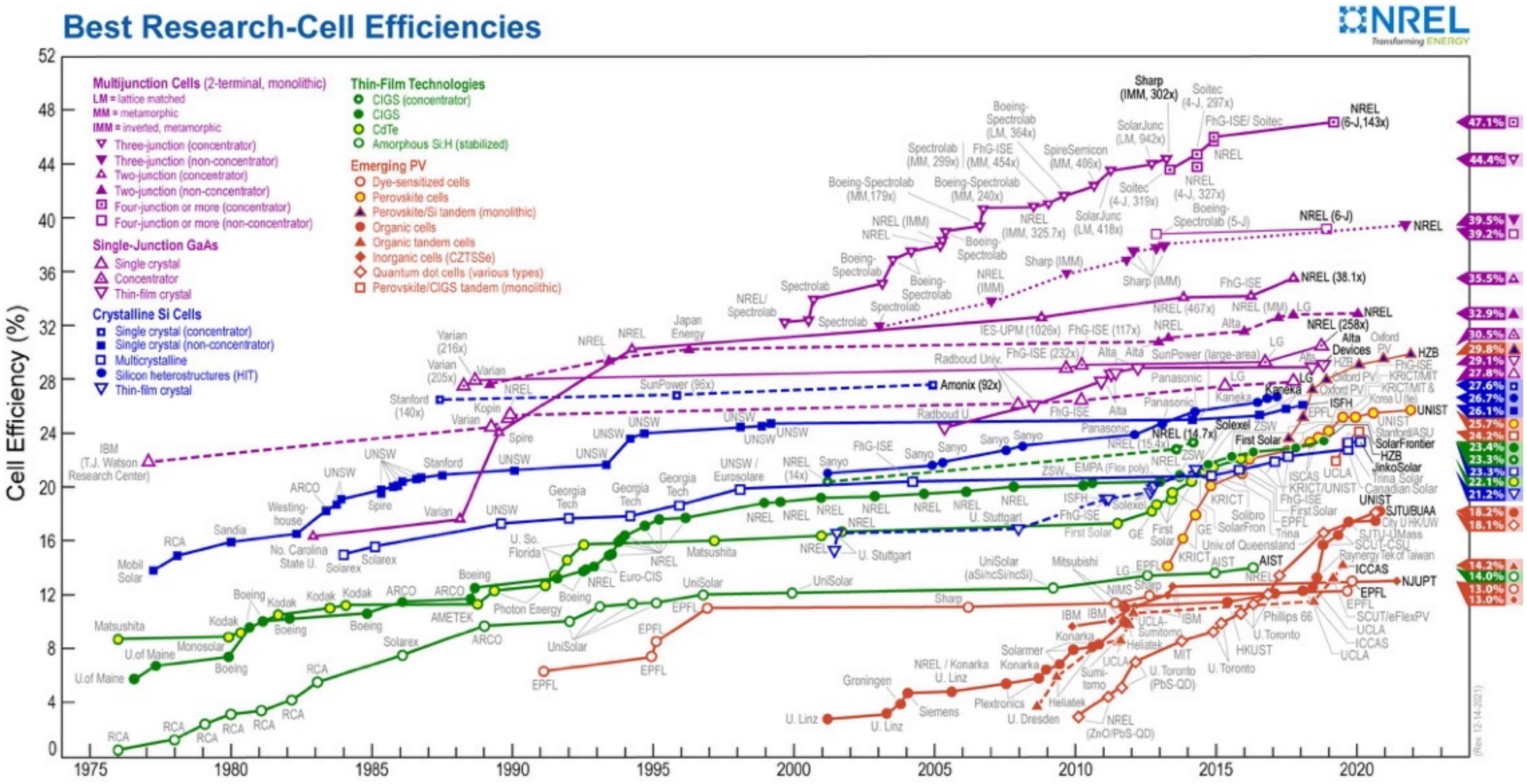


Photosynthetic/ photocatalytic

He, J. & Janaky, C. ACS Energy Lett 5, 1996-2014, doi:10.1021/acsenergylett.0c00645 (2020).

PV-Electrolysis

Overall efficiency = Efficiency of PV x Efficiency of Electrolyser



High carrier mobilities and long lifetimes in $Cu(In,Ga)Se_2$

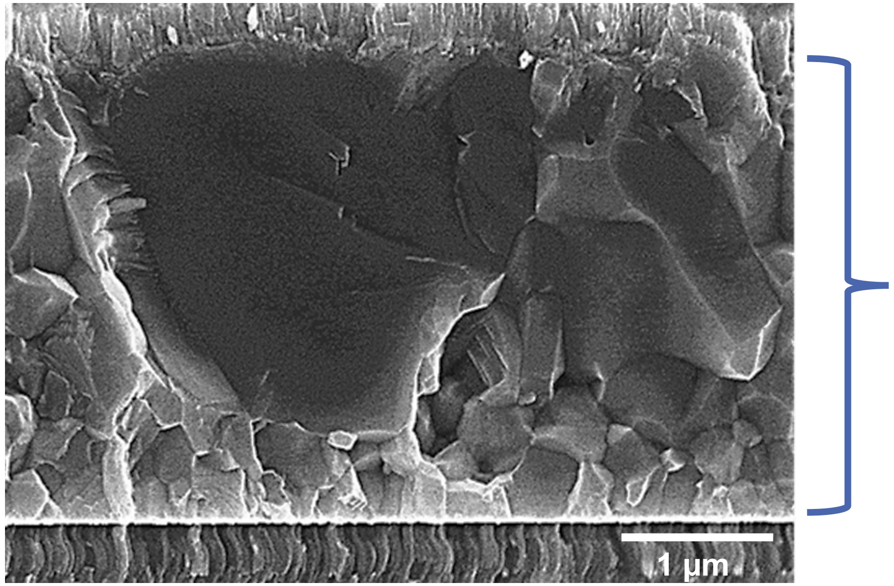
Dr Y. Chang

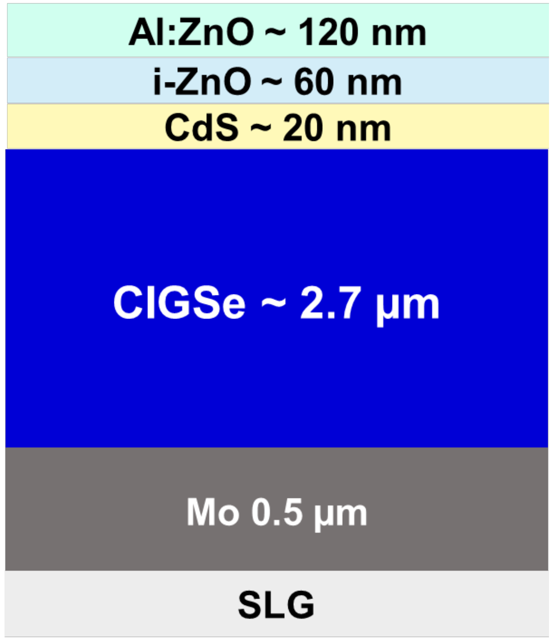
solar cells provided by the group of:

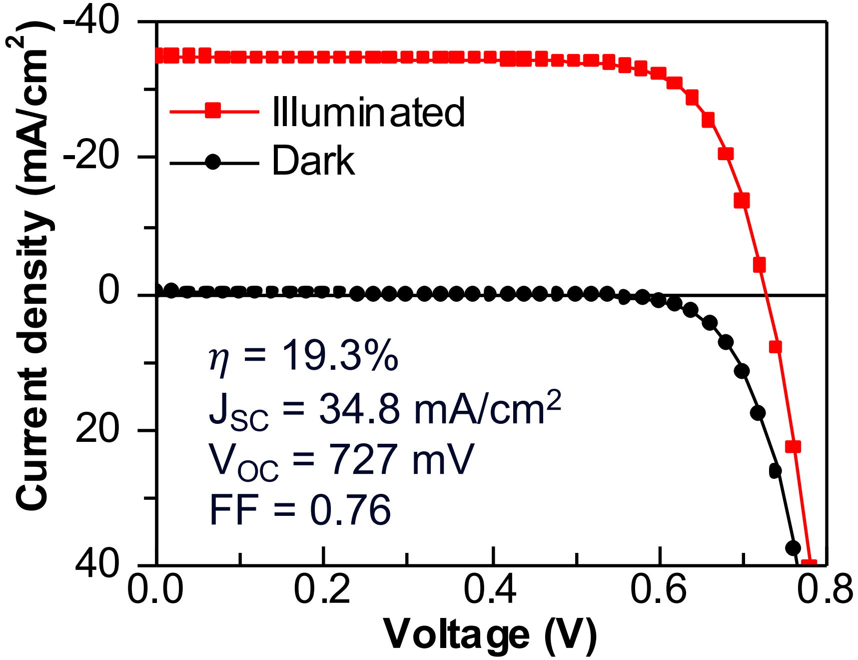
Empa
Materials Science and Technology

A. Tiwari

>19 ns carrier lifetimes in high-efficiency solar cells

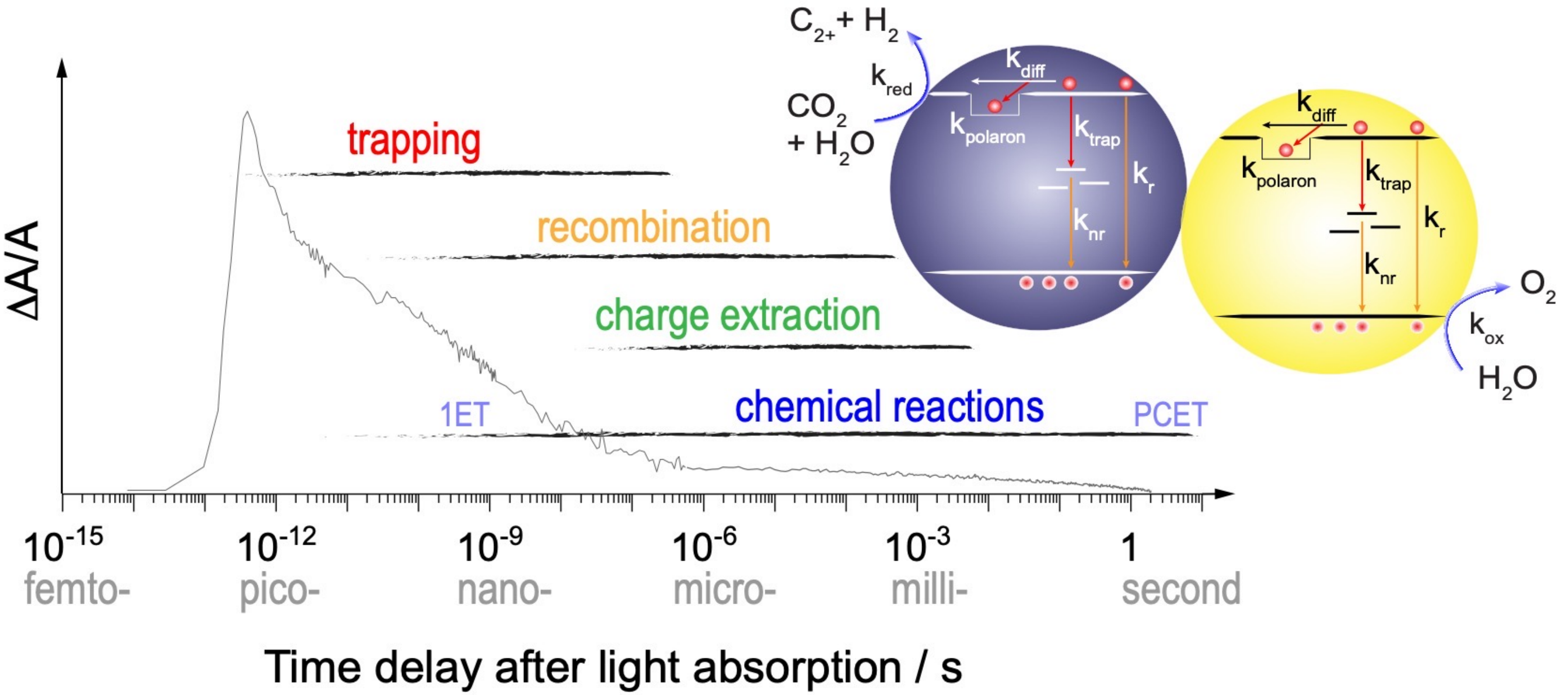






Y. Chang, R. Carron, … A. N. Tiwari, J. R. Durrant, L. Steier*, *Adv. Energy Mater.* 11, doi:10.1002/aenm.202003446 (2021)
Y. Chang, R. Carron, … A. N. Tiwari, J. R. Durrant, L. Steier*, *Adv. Funct. Mater.* 31, doi:10.1002/adfm.202103663 (2021)

Kinetic Dilemma in Oxide Photocatalysts

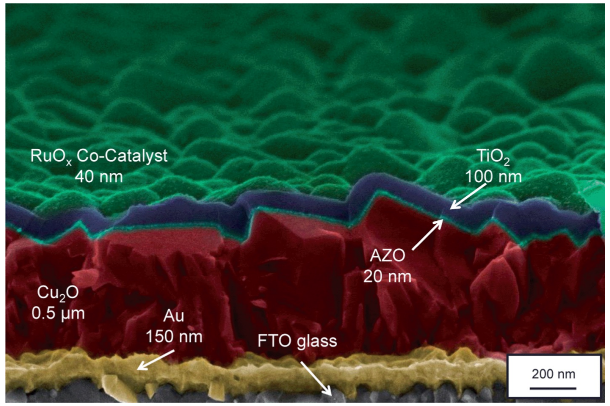


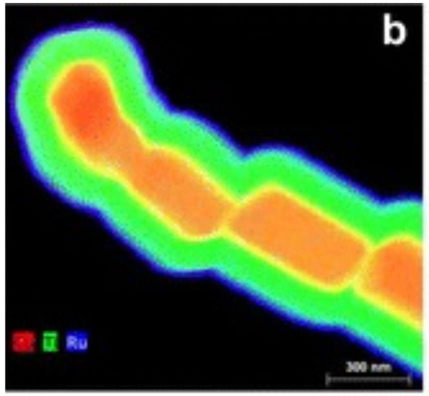
yield of photogenerated charge carriers on long timescales determines activity

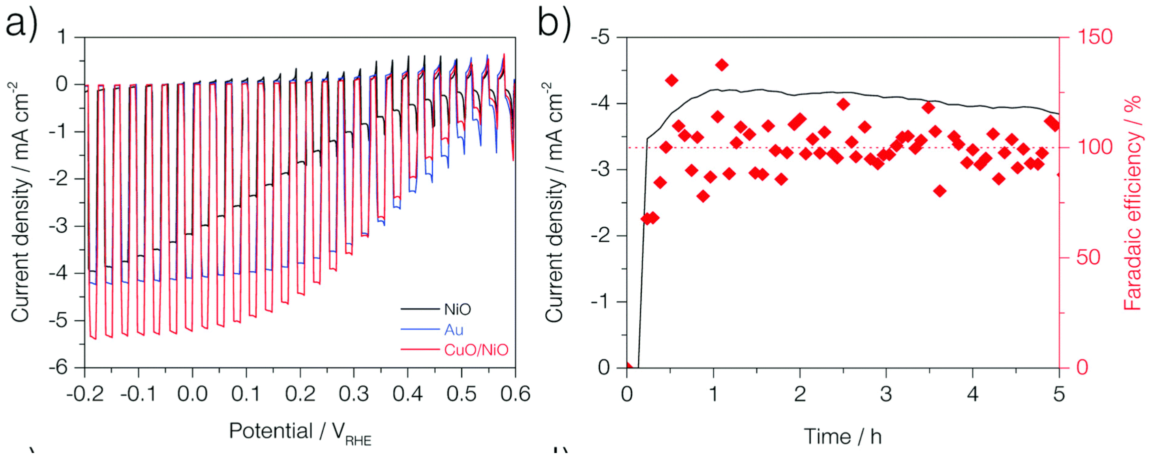
S. Corby, R. R. Rao, L. Steier, J. R. Durrant, *Nat. Mater. Rev*. doi:10.1038/s41578-021-00343-7 (2021)

Buried Junctions with TiO_2 overlayers

Cu_2O photocathodes

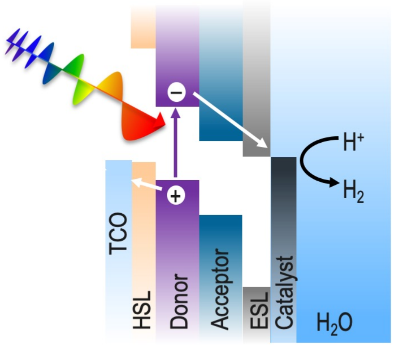


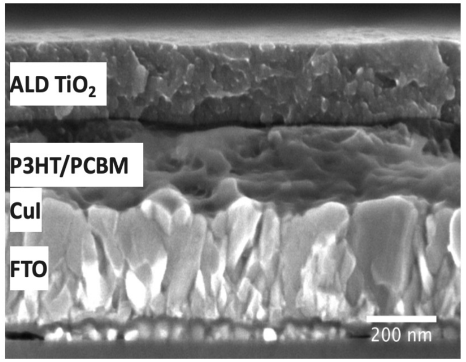


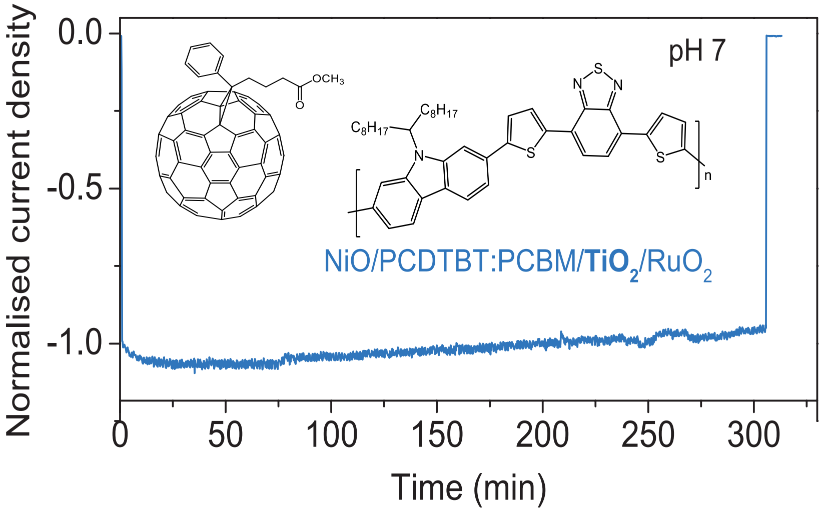


J. Azevedo, L. Steier *et al. Energy Environ. Sci.*, ***7***, 4044-4052 (2014)
J. Luo, L. Steier *et al. Nano Lett* **16**, 1848-1857 (2016)
M. K. Son, L. Steier* *et al. Energy & Environmental Science* **10**, 912-918 (2017).

Polymer bulkheterojunction photocathodes







L. Steier*, *et al. Sustainable Energy & Fuels* **2017**, 1, 1915-1920
L. Francàs, E. Burns, L. Steier *et al. Chemical Commun.* **2018**, *54*, 5732-5735
L. Steier*, S. Holliday, *J. Mater. Chem. A* **2018**, 6, 21809-2182

The Photocatalyst Sheet Device

nature materials
LETTERS
PUBLISHED ONLINE: 7 MARCH 2016 | DOI: 10.1038/NMAT4589

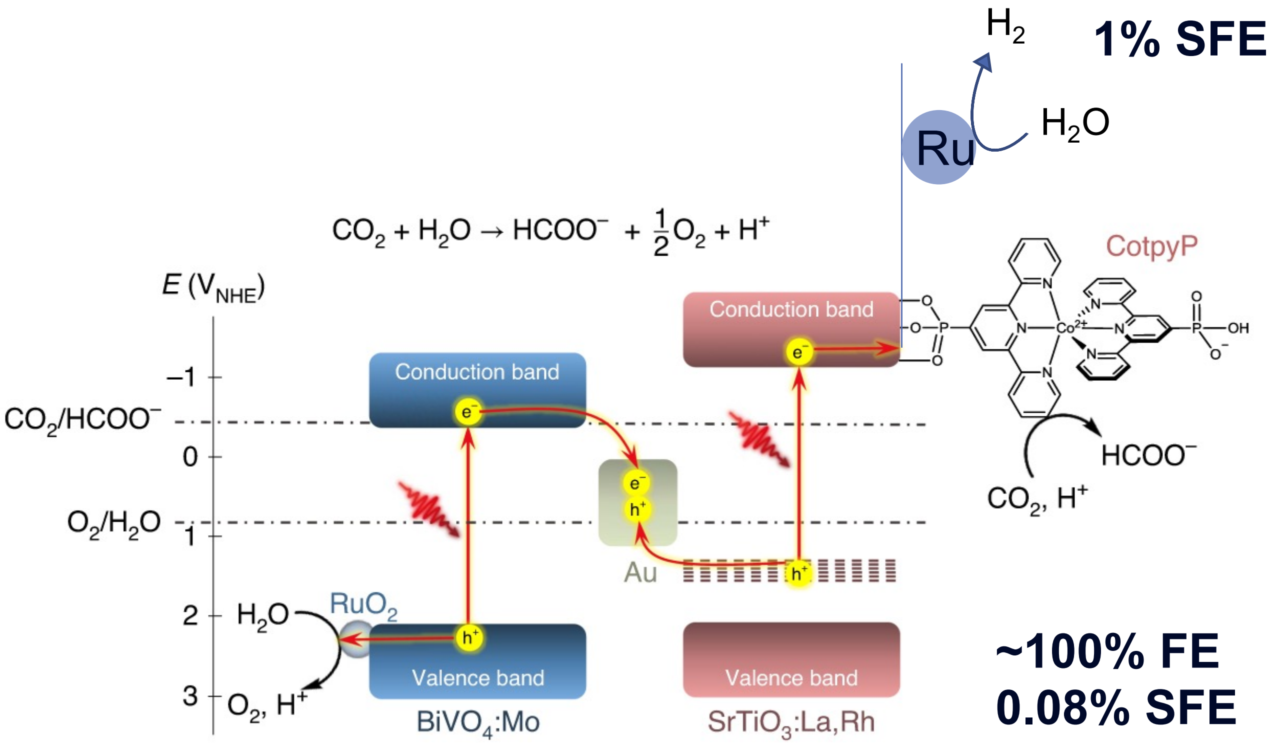
Scalable water splitting on particulate photocatalyst sheets with a solar-to-hydrogen energy conversion efficiency exceeding 1%

Qian Wang[1,2], Takashi Hisatomi[1,2], Qingxin Jia[1,2], Hiromasa Tokudome[2,3], Miao Zhong[1,2], Chizhong Wang[1], Zhenhua Pan[1], Tsuyoshi Takata[4], Mamiko Nakabayashi[5], Naoya Shibata[5], Yanbo Li[6], Ian D. Sharp[6], Akihiko Kudo[7], Taro Yamada[1,2] and Kazunari Domen[1,2]*

nature energy
ARTICLES
https://doi.org/10.1038/s41560-020-0678-6
Check for updates

Molecularly engineered photocatalyst sheet for scalable solar formate production from carbon dioxide and water

Qian Wang[1], Julien Warnan[1], Santiago Rodríguez-Jiménez[1], Jane J. Leung[1], Shafeer Kalathil[1], Virgil Andrei[1], Kazunari Domen[2,3] and Erwin Reisner[1]✉

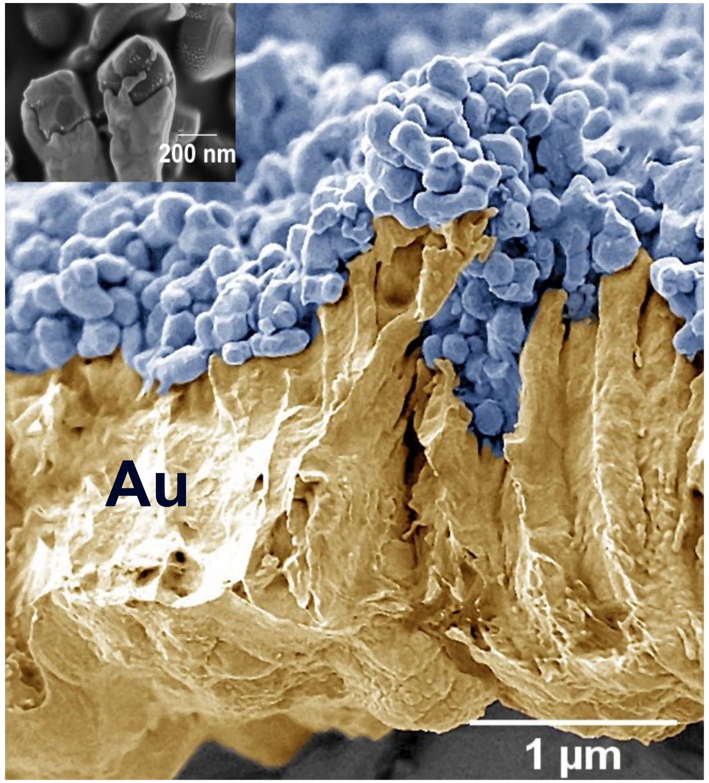


1% SFE

~100% FE
0.08% SFE

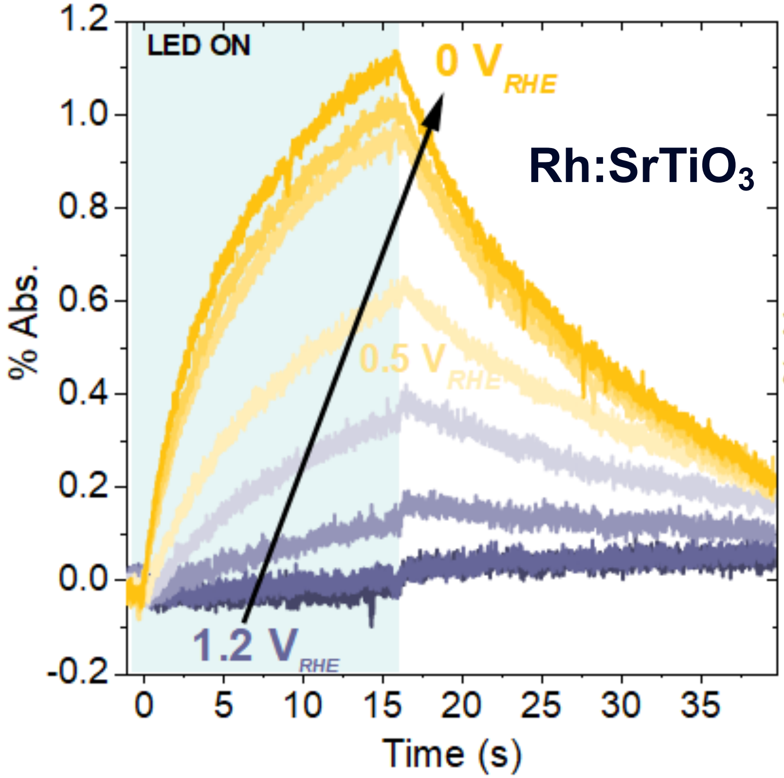
Wang, Q. *et al. Nature Energy*, **5**, 703–710 (2020). doi:10.1038/s41560-020-0678-6.
Wang, Q. *et al. Nature Materials* **15**, 611-+, (2016) doi:10.1038/nmat4589

Long electron lifetimes in La,Rh-doped $SrTiO_3$

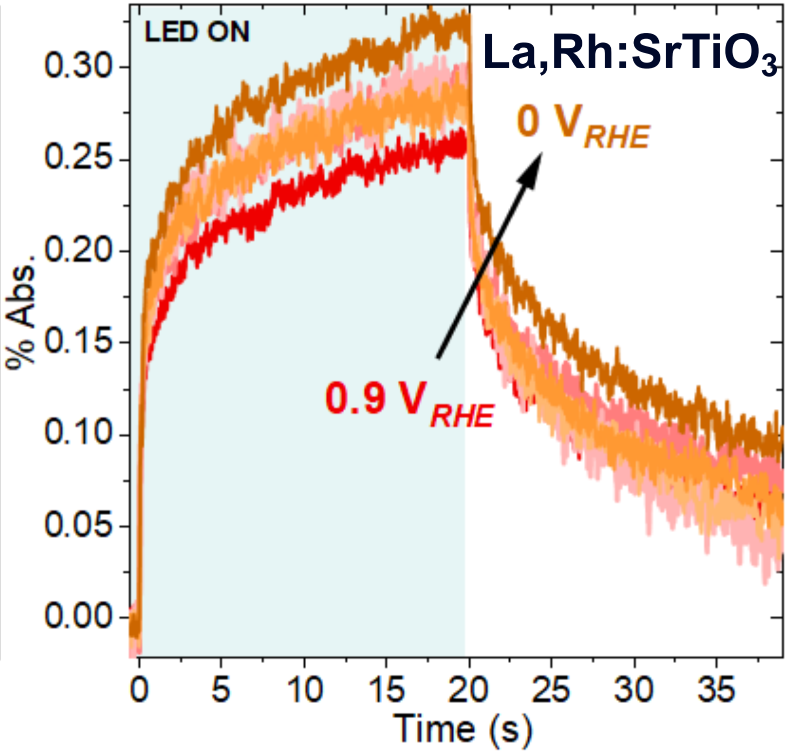


Photocatalyst sheet
half-electrode

Photoinduced absorption measurements
365 nm LED excitation, probe at 1100 nm (electrons)

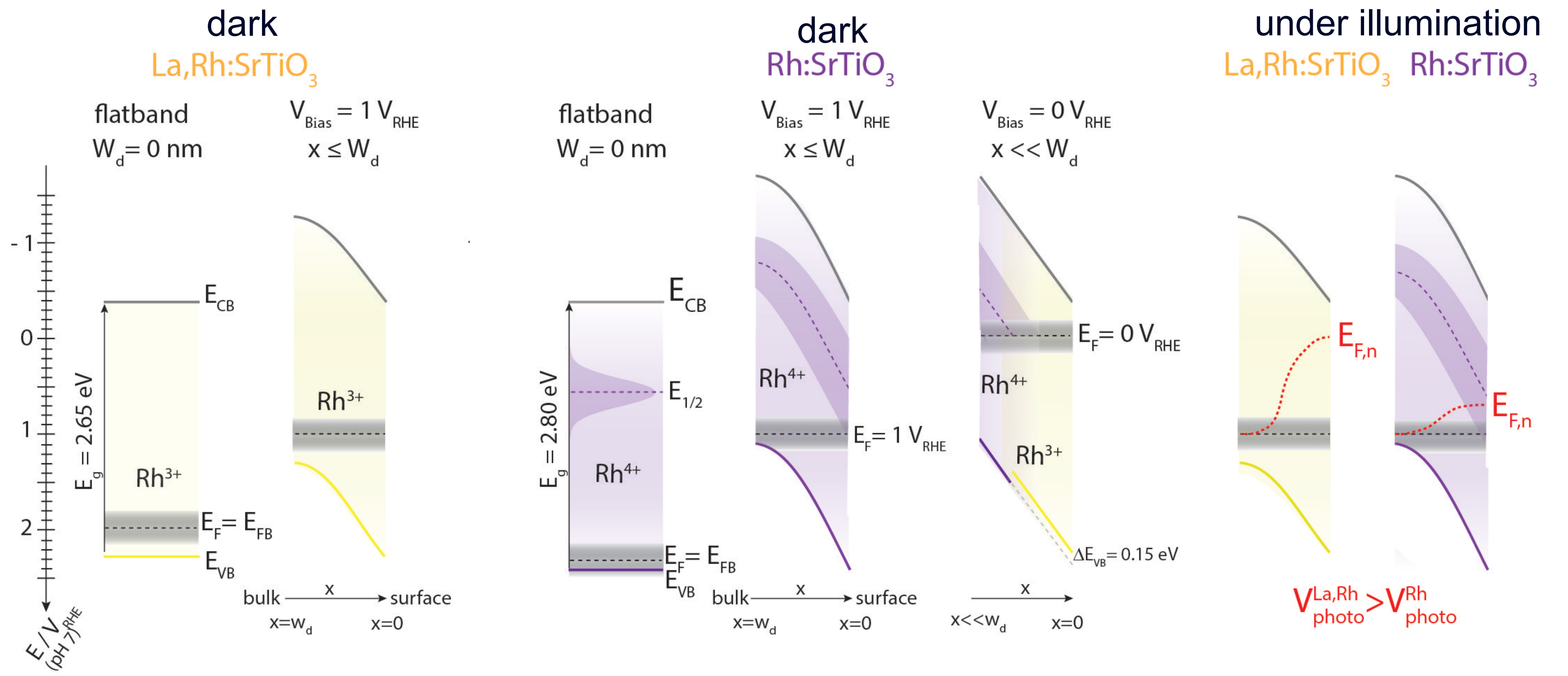


Rh^{4+}
strong potential dependence



Rh^{3+}
(almost) no potential dependence

Long electron lifetimes in La,Rh-doped $SrTiO_3$



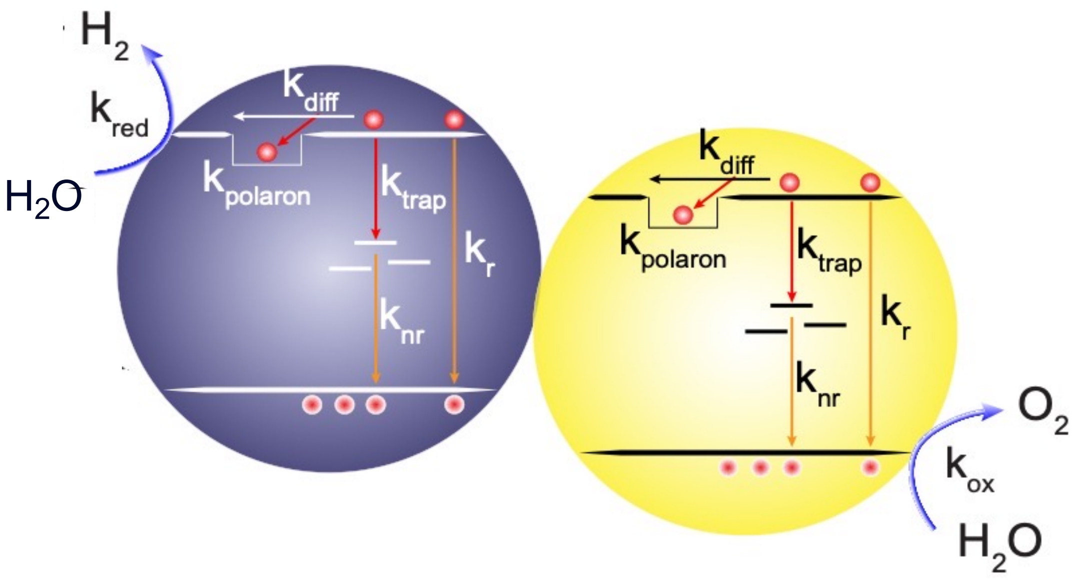
La co-doping reduces Rh^{4+} centres to Rh^{3+} - removing mid-bandgap Rh^{4+} recombination centres

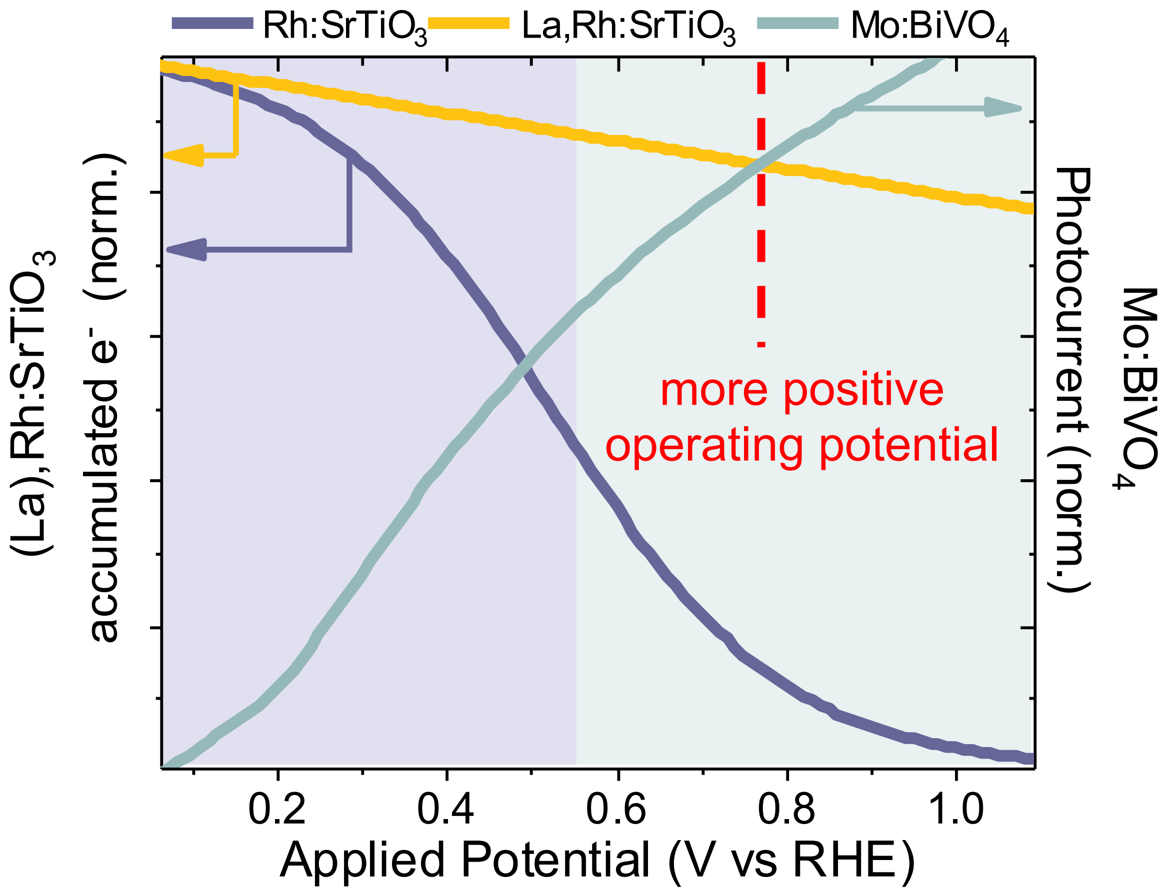
→ enables accumulation of persistent electrons even under positive applied potentials

→ enables larger quasi-Fermi level splitting (photovoltage generation)

B. Moss, Q. Wang,…K. Domen, L.Steier*, J. Durrant, *Nat. Mater.* **20**, 511–517 (2021).

Operation of Mo:$BiVO_4$-La,Rh:$SrTiO_3$ Photocatalyst Sheet Device





Defect engineering allows the full sheet to operate at remarkably positive potentials

UNIVERSITY OF OXFORD

Acknowledgements

Imperial:
Benjamin Moss
Yu-Han Chang

James Durrant
Ernest Pastor
Artem Bakulin
David J. Payne
Anna Ragoutz
Andreas Kafizas
Carlota Bozal-Ginesta

Harwell:
Keith Butler

Oxford:
Dermot O'Hare
Hao Zhang
Iain McCulloch

University of Tokyo:
Qian Wang
Takashi Hisatomi
Kazunari Domen

EMPA:
Mario Ochoa Gomez
Romain Carron
Ayodhya Tiwari

EPFL:
Marcel Schreier
Jingshan Luo
Matthew Mayer
Michael Grätzel

SEVENTH FRAMEWORK PROGRAMME
MARIE CURIE ACTIONS
Imperial College London
Research Fellowship