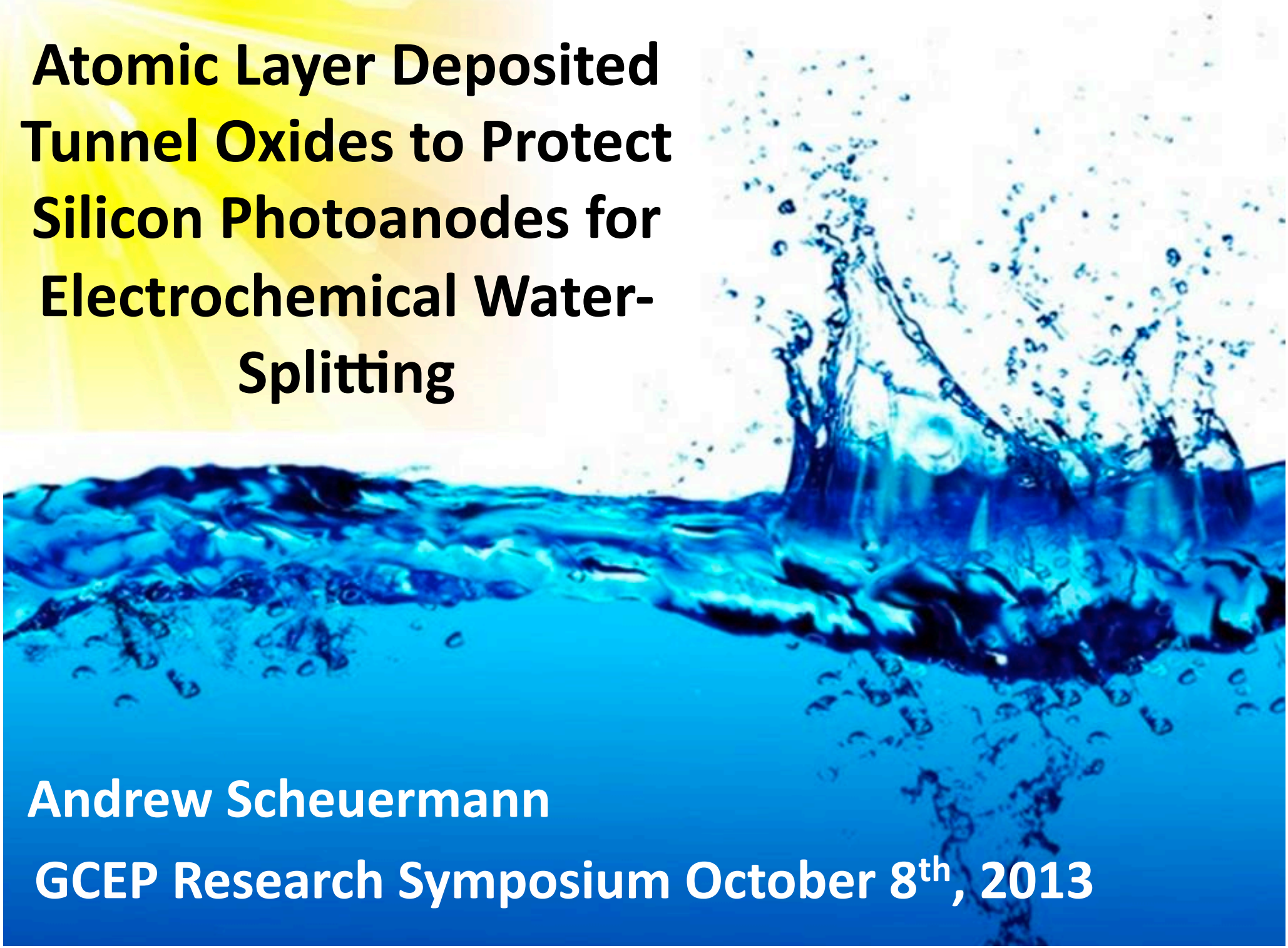
Atomic Layer Deposited Tunnel Oxides to Protect Silicon Photoanodes for Electrochemical Water-Splitting



Andrew Scheuermann

GCEP Research Symposium October 8th, 2013

How can we address GHG's?

Stop putting GHG's in the environment

Renewable sources

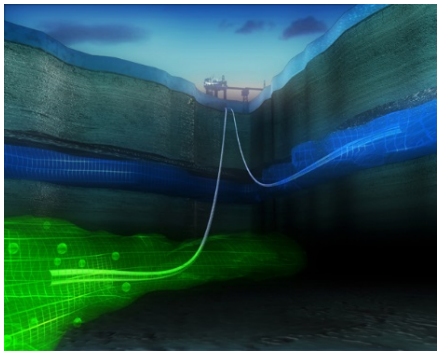
Efficiency, Demand Reduction

ENERGY STAR

Capture GHG's from the environment

Capture

and Store

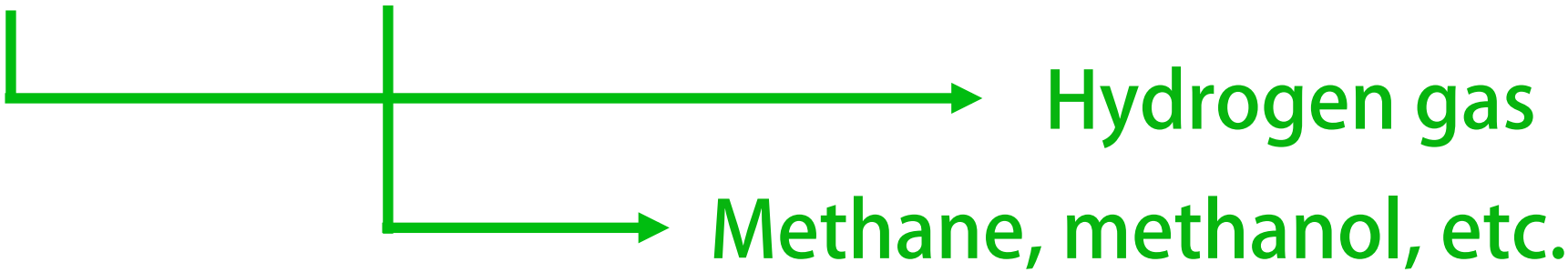


Renewable Fuel

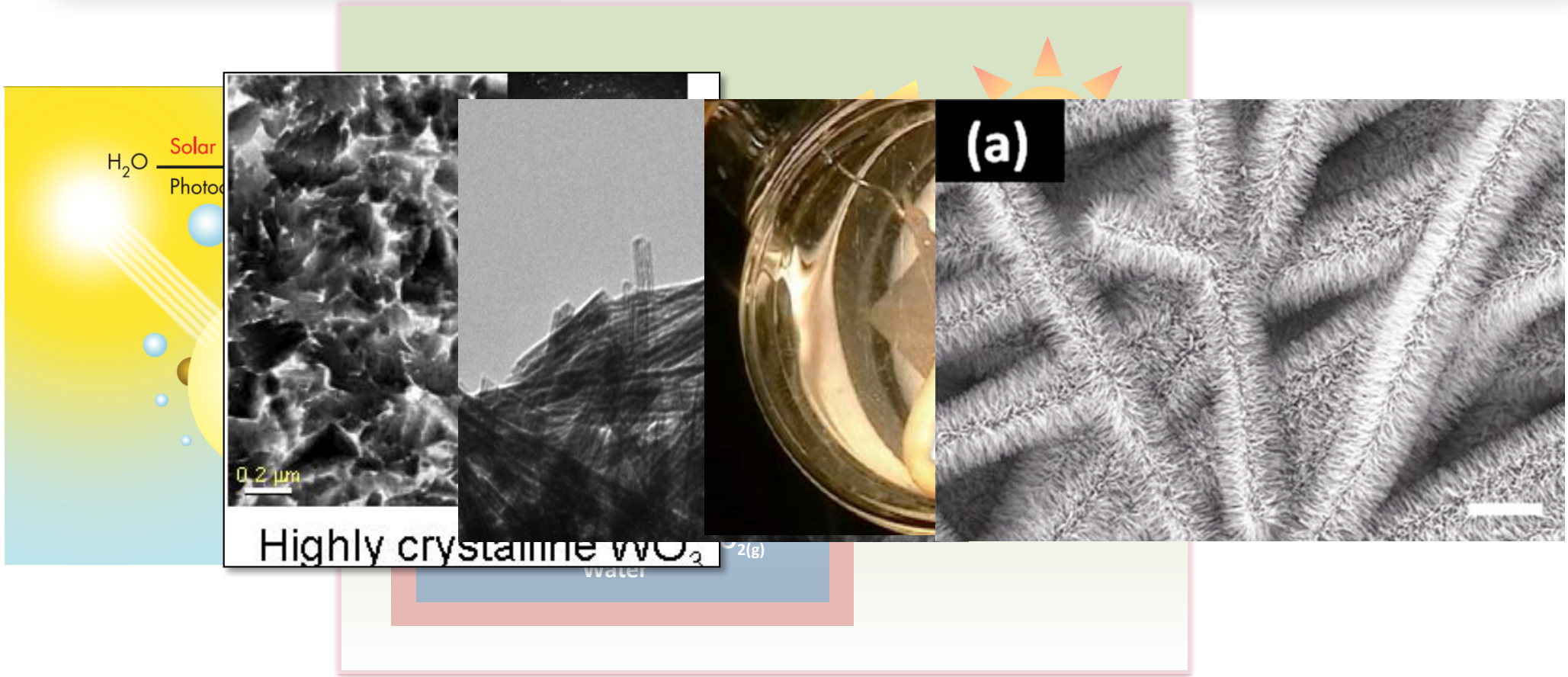
Use GHG's

Greenhouse Gases → Foods and Fuels

$$H_2O + CO_2 \rightarrow C_xH_yO_z + O_2$$



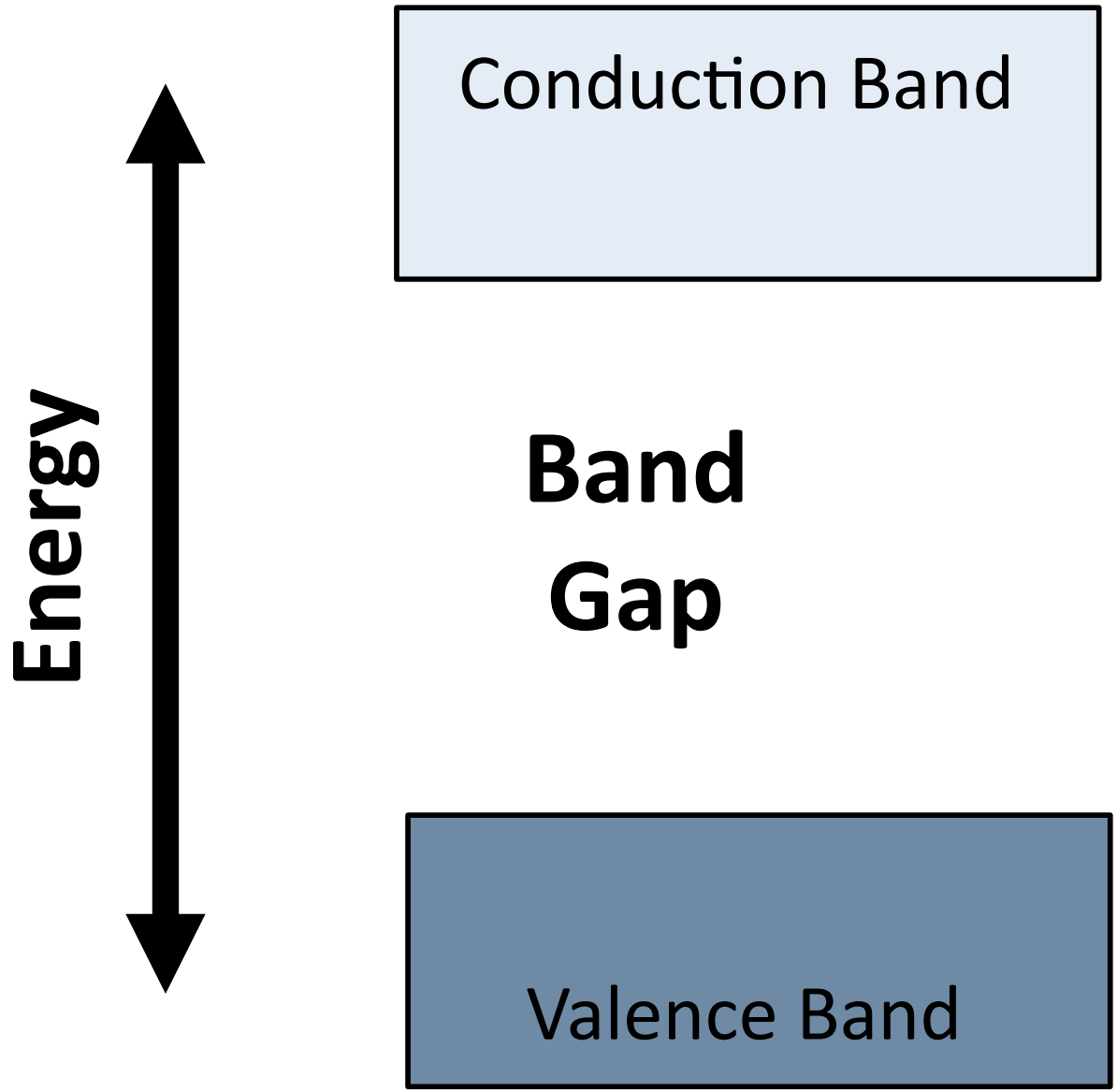
Photoelectrochemical Cells (PECs)

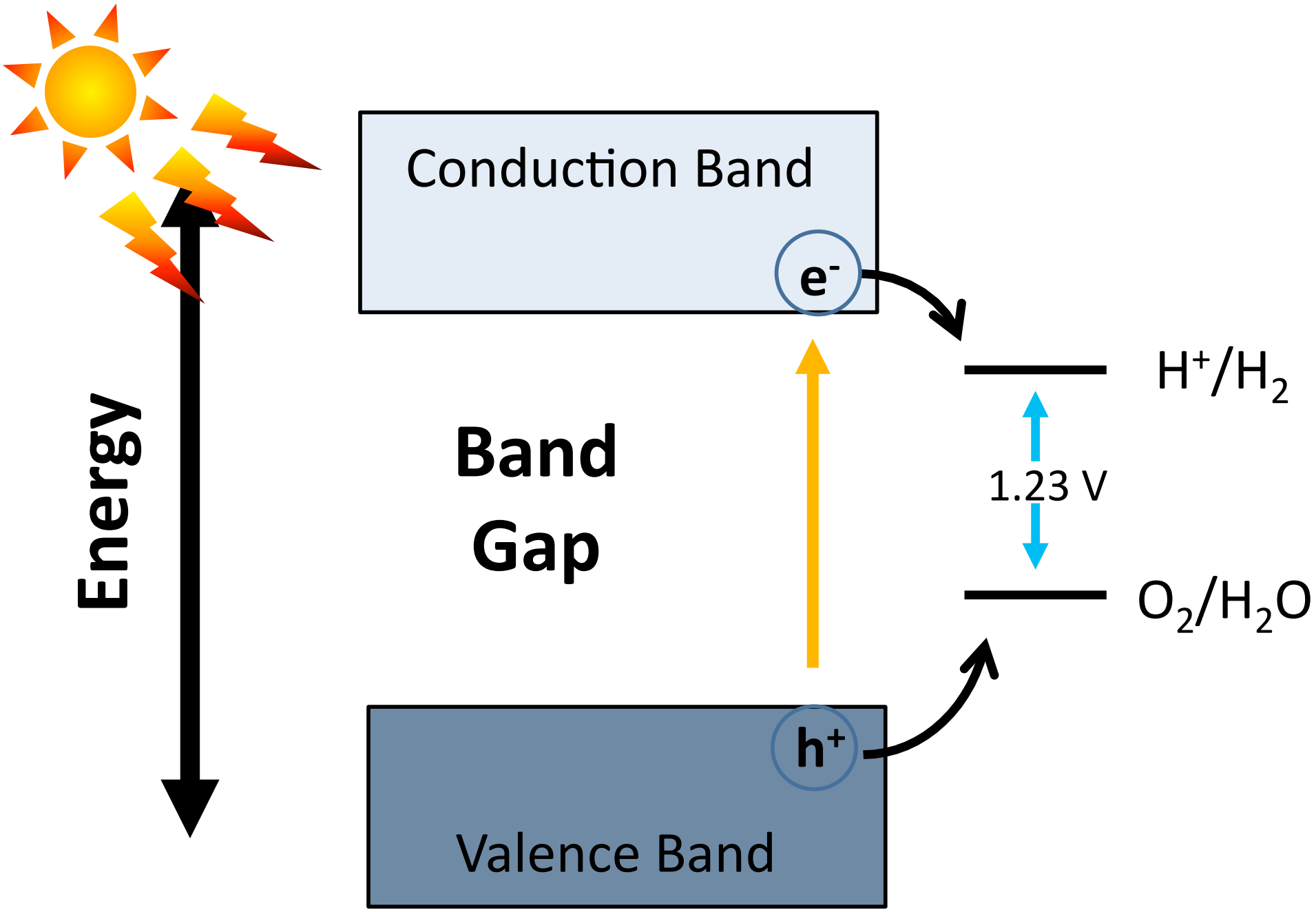


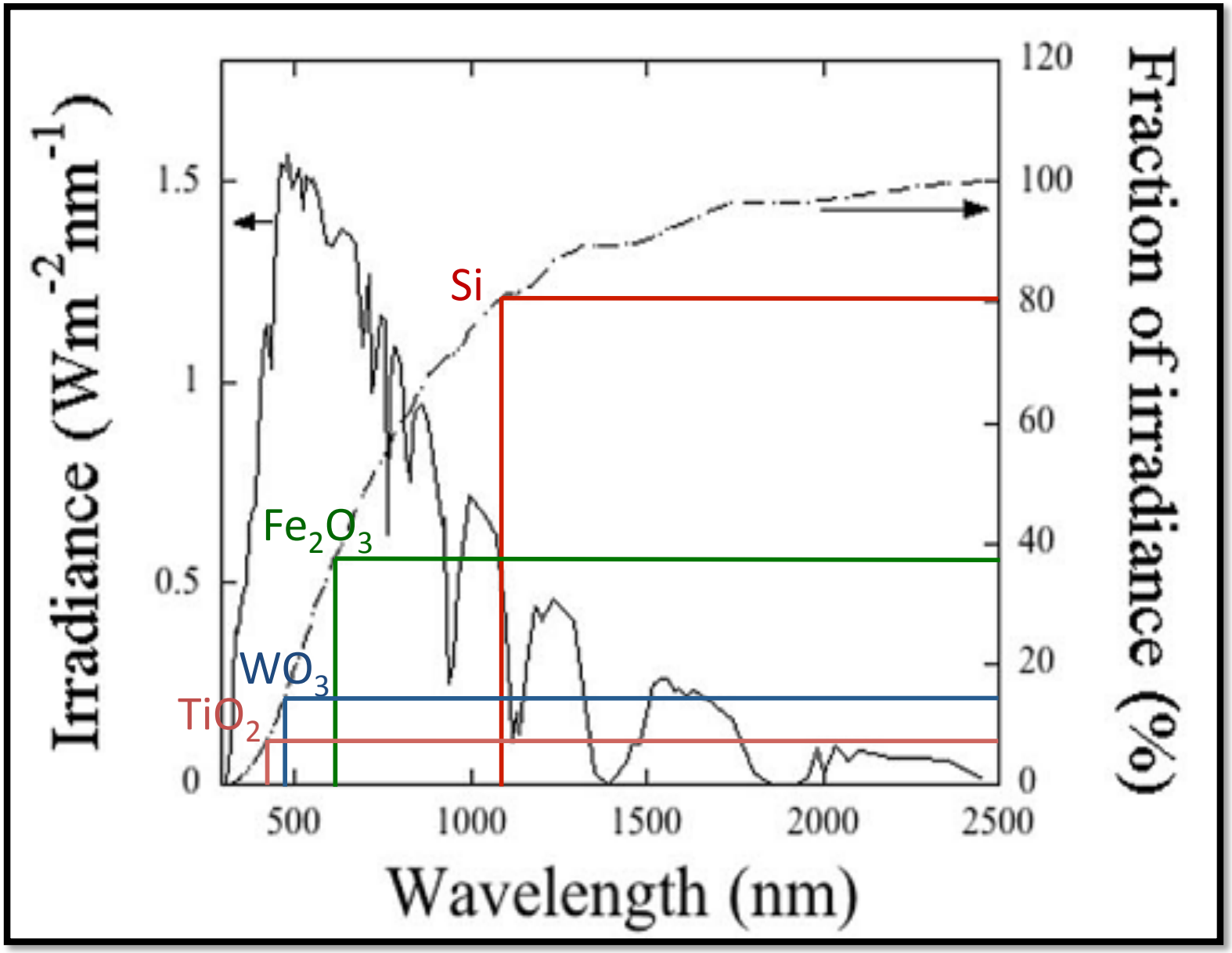
- TiO_2, $SrTiO_3$, WO_3, Fe_2O_3 III-V's and ZnO

Overall reaction: $2H_2O \rightarrow 2H_2 + O_2$ [1]

[1]A. Fujishima and K. Honda, *Nature* ***(1972)*** 238, 37-38.
M. Walter et. al. *Chem. Rev.* ***(2010)*** *110, 6446–6473.*

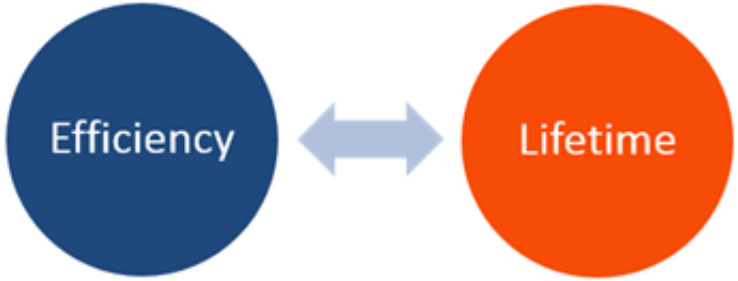

Conduction Band
Energy
Band
Gap
Valence Band


Conduction Band
e-
Energy
Band
Gap
H+/H2
1.23 V
O2/H2O
h+
Valence Band



Trade-off between efficient solar absorbers and chemically stable absorbers

The Scientific Challenge



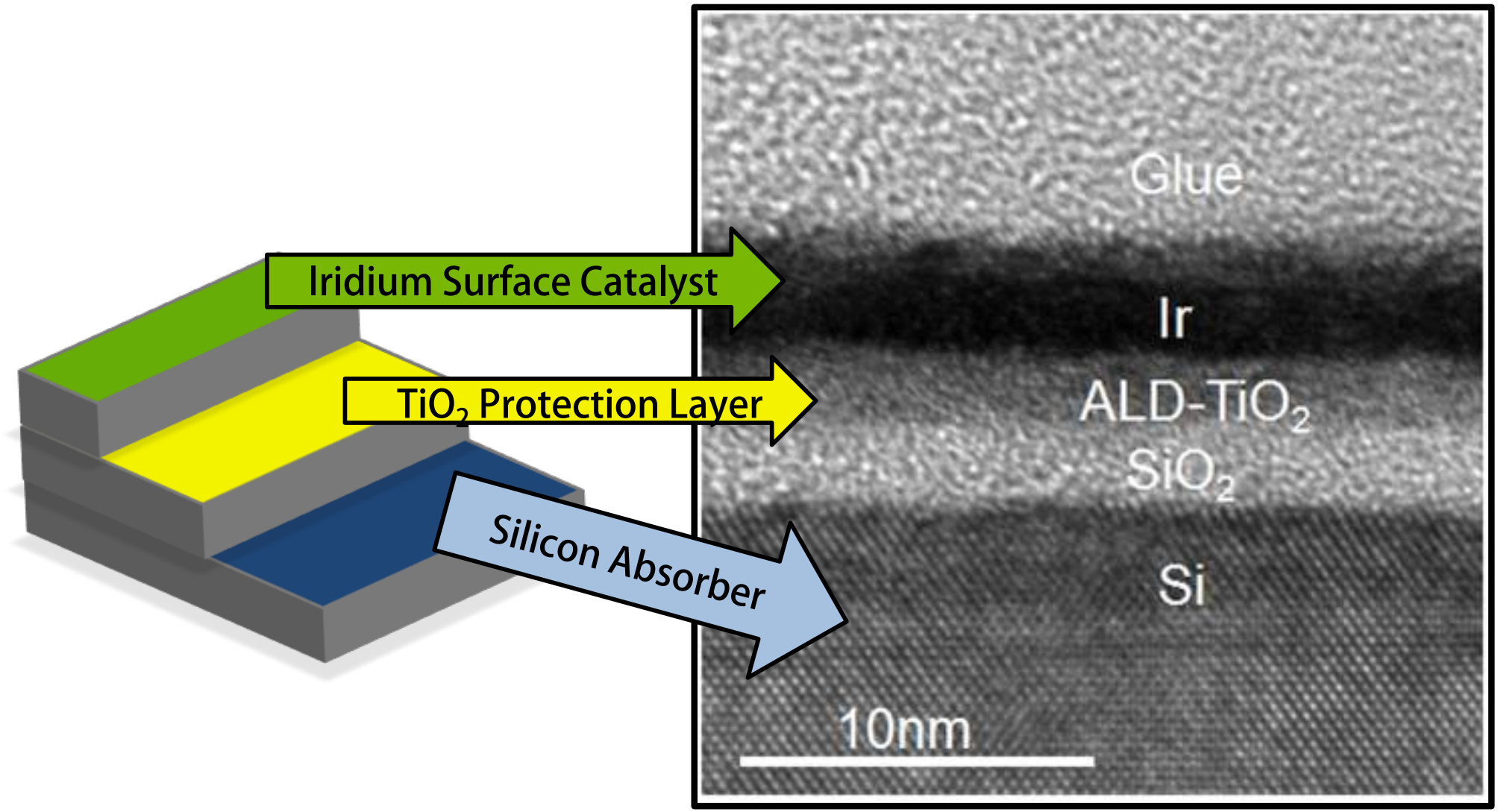
Si + TiO_2

<u>Barrier to oxidants</u>

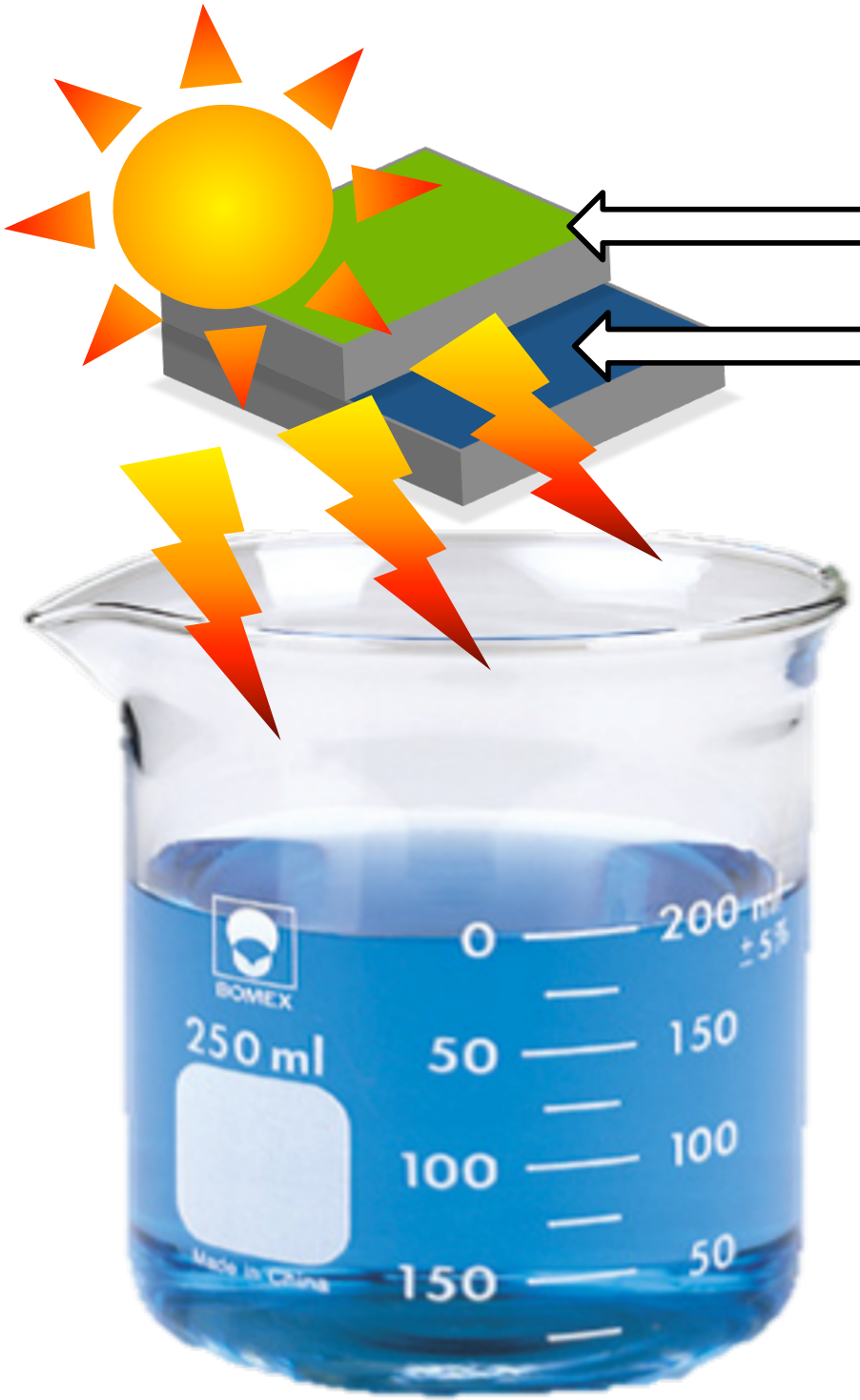
- Dense enough
- Pinhole-free

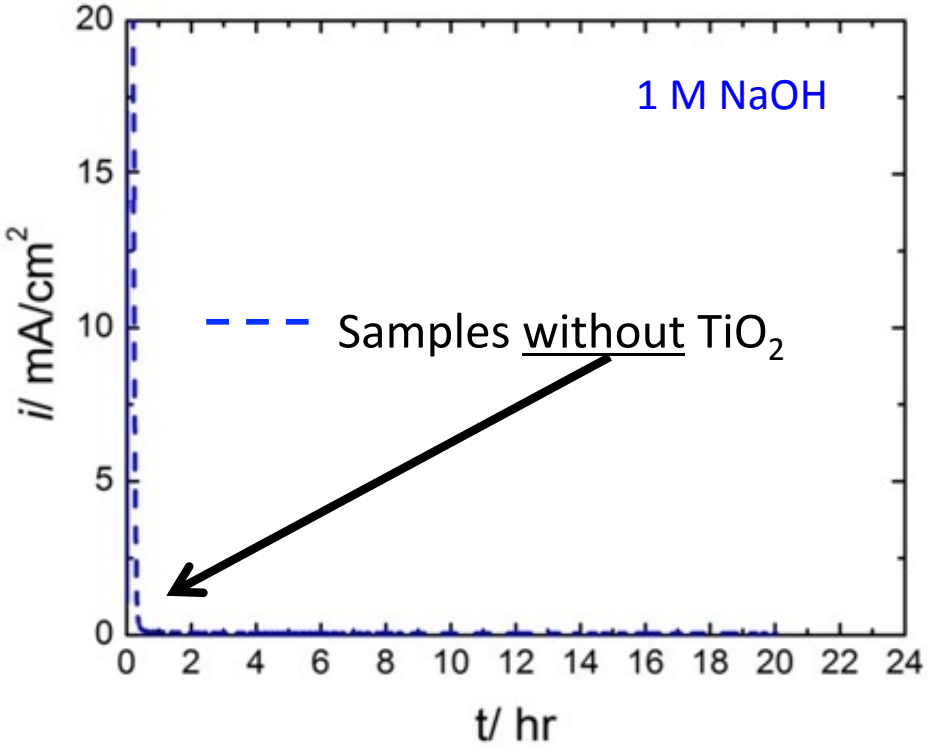
<u>No barrier to electrons</u>

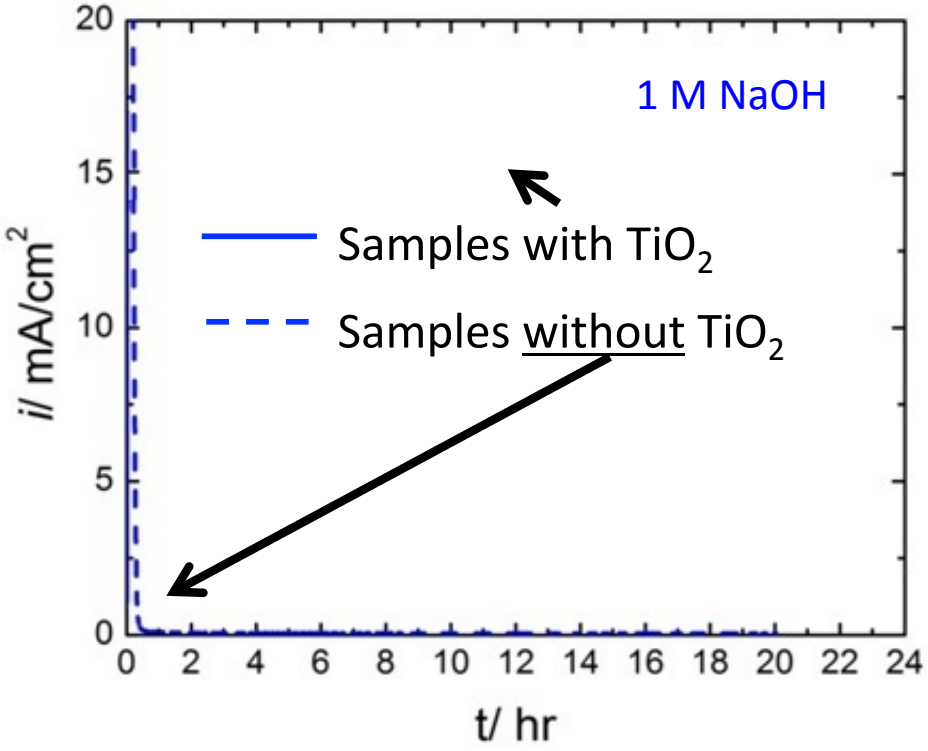
- Thin enough
- Uniform
- Not defective



ALD-TiO_2 Tunnel Oxide on Silicon Schottky Junction Solar Cell

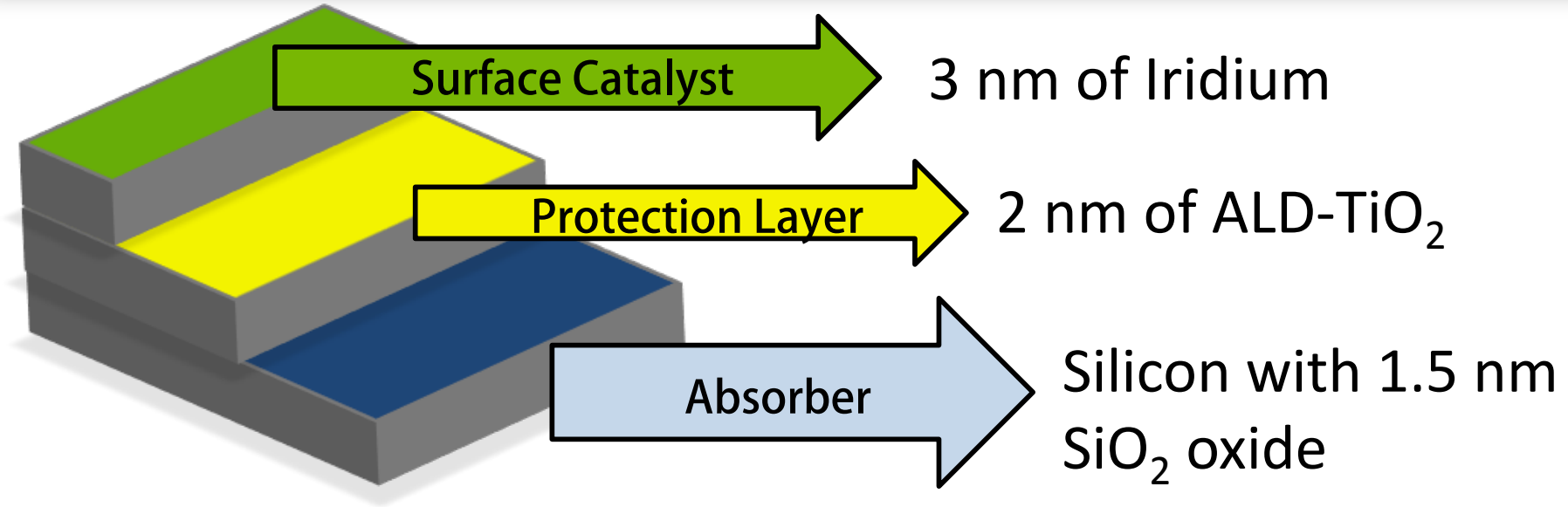

Iridium surface catalyst
Unprotected silicon absorber
250 ml
0
50
100
150
200 ml
150
100
50


1 M NaOH
Samples without TiO_2
i/ mA/cm^2
t/ hr
0
5
10
15
20
0
2
4
6
8
10
12
14
16
18
20
22
24



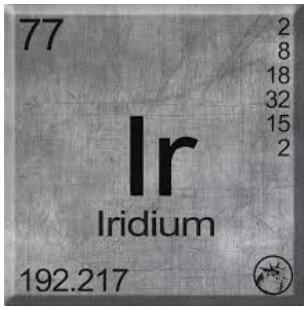
Lifetime	Minutes to days
Open circuit voltages	500-600 mV
Saturation current	28 mA/cm^2

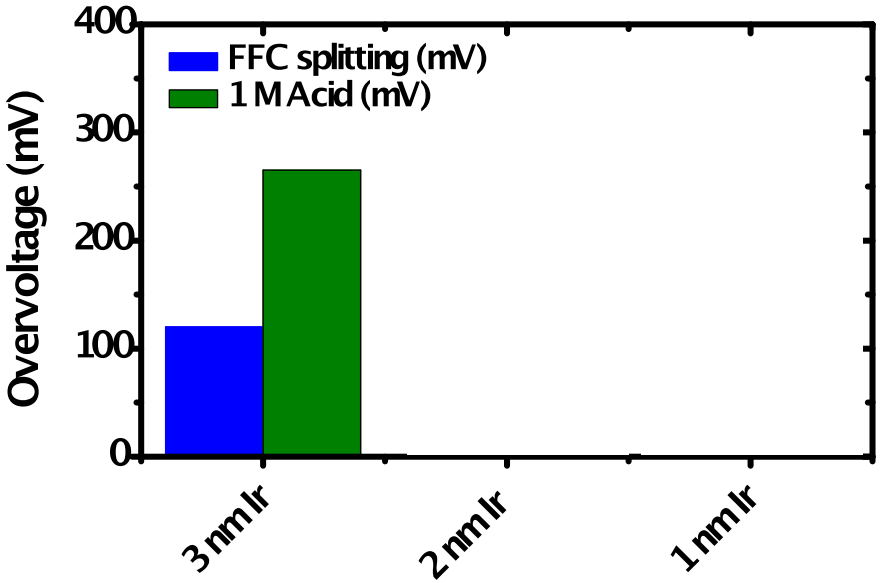
Investigating Further

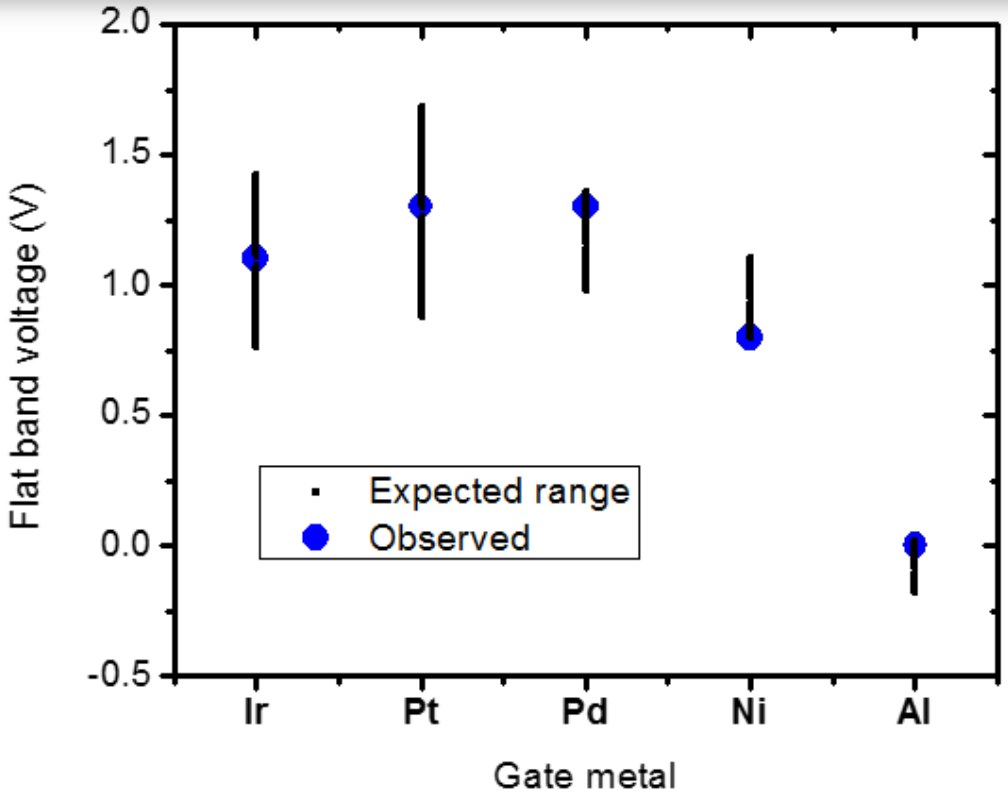


1. Do we need 3nm of iridium?
   - Do we have to use iridium?
2. What if the TiO_2 is thicker?

Less Iridium or Different Metals



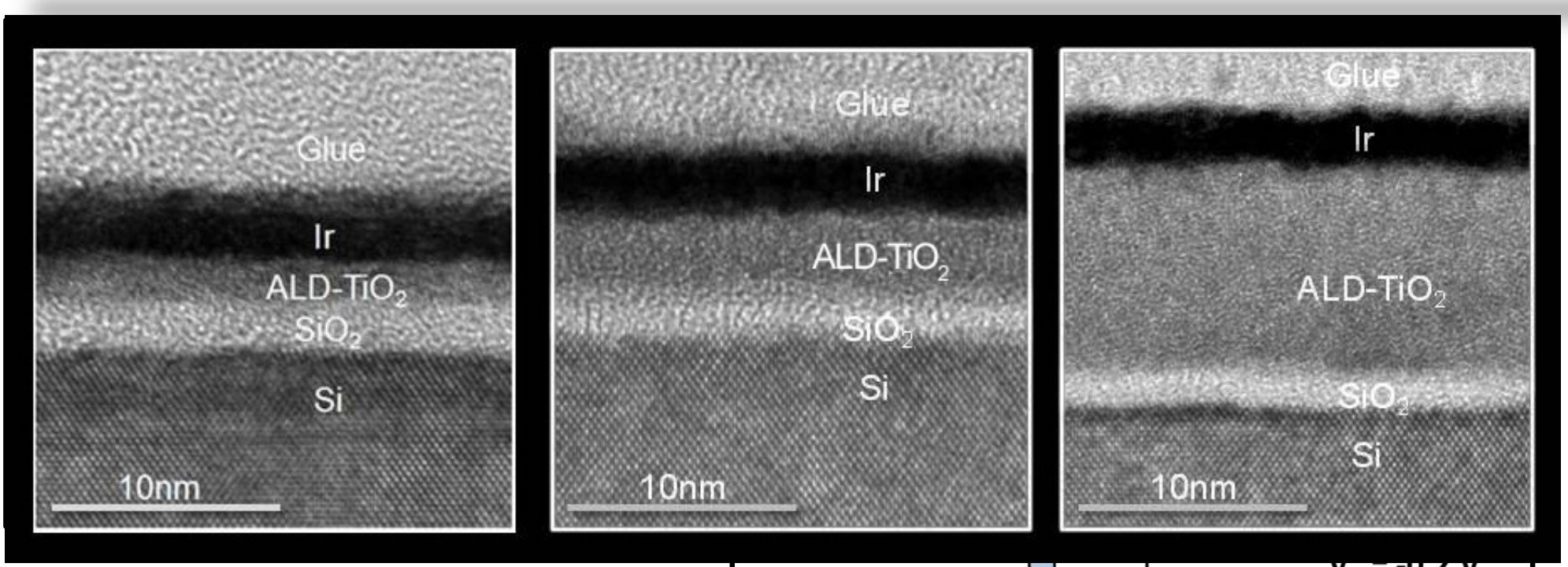




- Iridium usage can be reduced three fold with minimal impact on performance
- ALD-TiO_2 protection is viable for a range of catalysts

A.G. Scheuermann et al., *Energy Environ Sci.* **(2013)** 6, 2487.

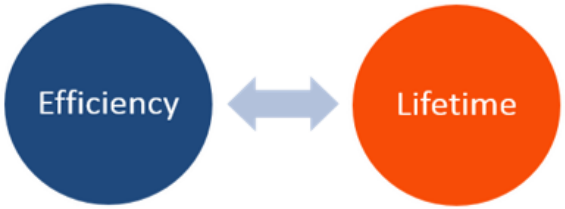
Thicker TiO_2 Films

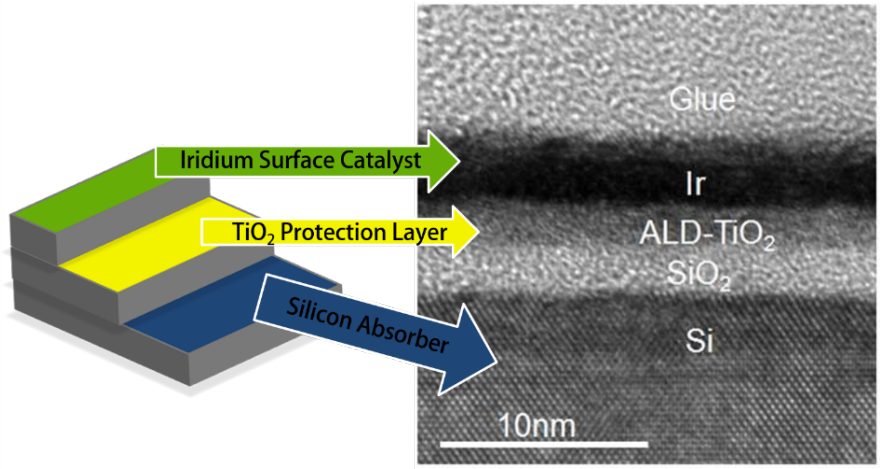


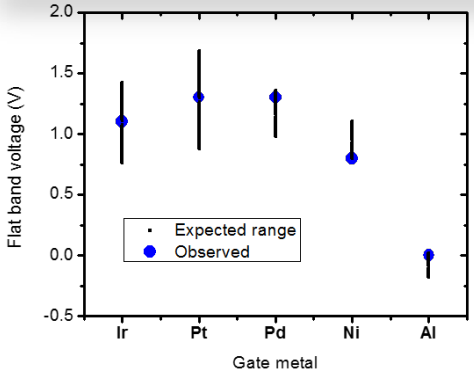
- Water oxidation overpotential increases linearly with TiO_2 thickness
- The penalty for increased protection is modest

$$V_G \approx -\left[\left(\frac{\varepsilon_{hk} t_{ox}}{\varepsilon_{ox}}\right) + t_{hk}\right] E_{hk} + V_{fb}$$

A.G. Scheuermann et al., *Energy Environ Sci.* **(2013)** 6, 2487.
A.G. Scheuermann et al., *ECS Transactions.* November, 2013.

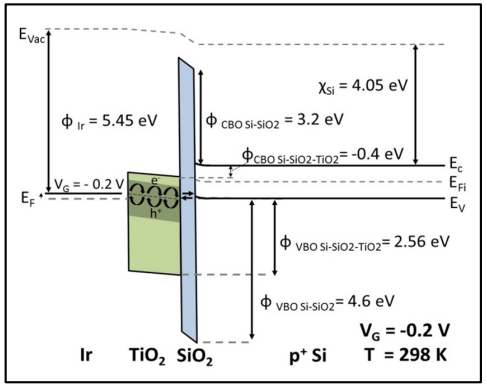


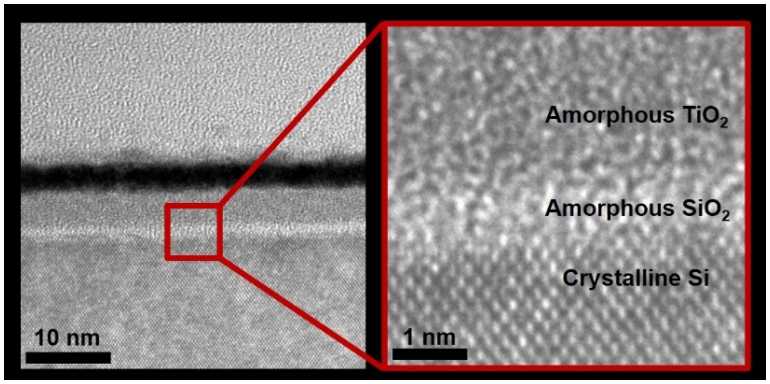




-Above 2nm of TiO_2, only modest penalty due to second conduction mechanism

-Thinner iridium catalyst
-Ability to use other catalysts





Electrical understanding
Chemical understanding
Implementable Devices

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Thank you for your attention!