Semiconducting oxides for photoelectrochemical water splitting

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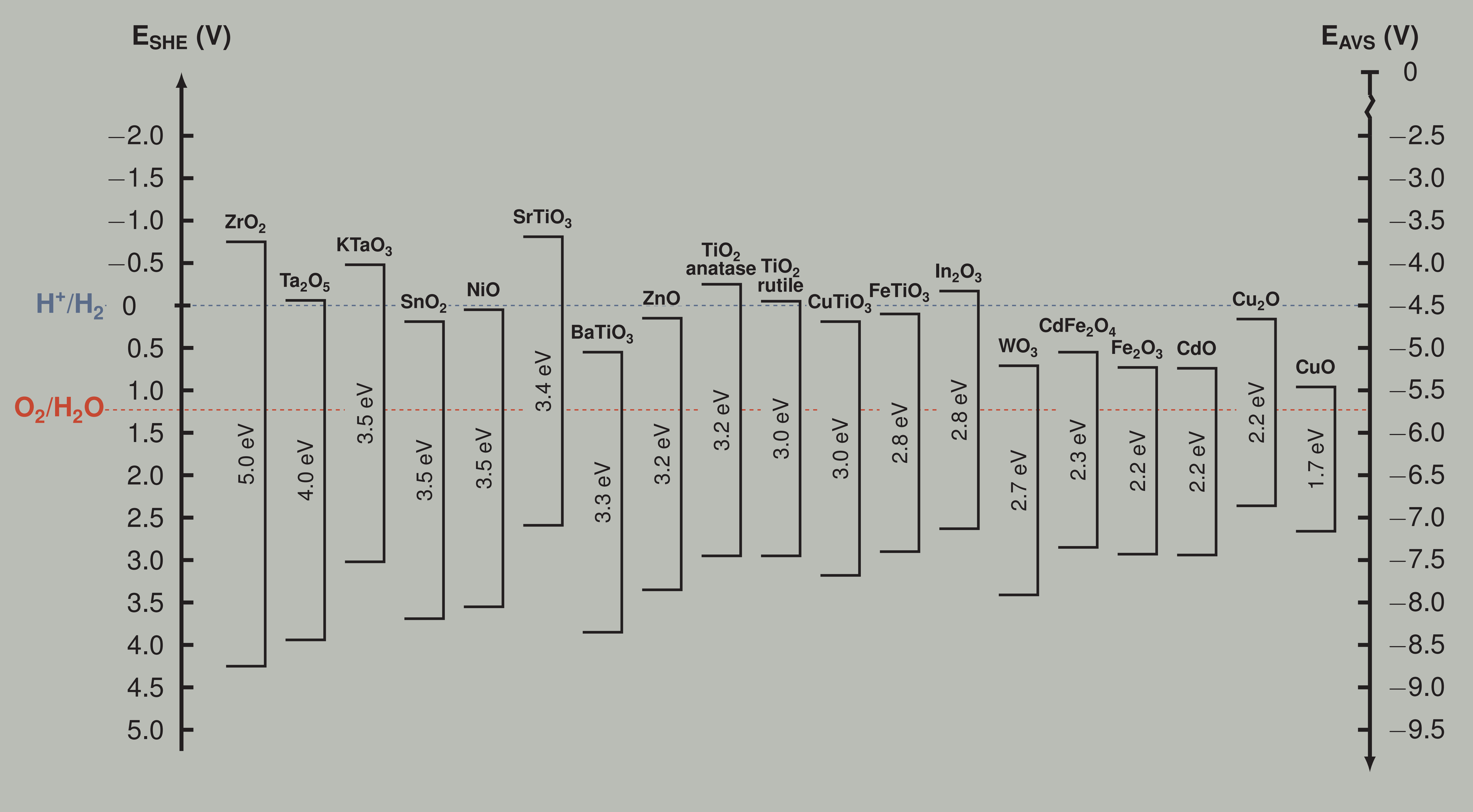
Photoelectrochemical water splitting

Net reaction:

$$H_2O \xrightarrow{h\nu} H_2 + \tfrac{1}{2}O_2, \quad (\Delta G^\circ = +237.2\,\mathrm{kJ\,mol^{-1}})$$

Absolute energy levels for some metal oxides



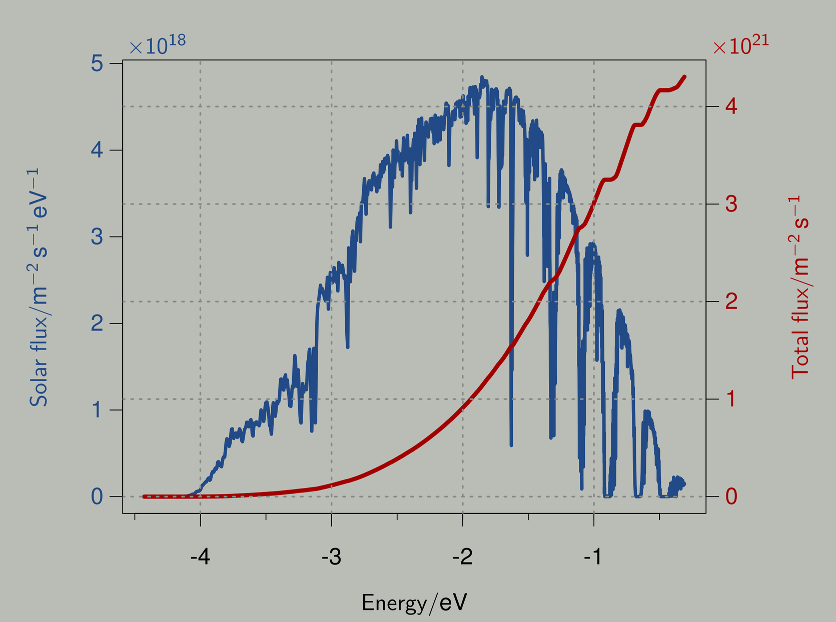
Calculated band gaps for oxides in contact with an aqueous electrolyte at pH 1.

What constitutes a good PEC anode material?

For direct photoelectrochemical decomposition of water, the following key criteria should be met:

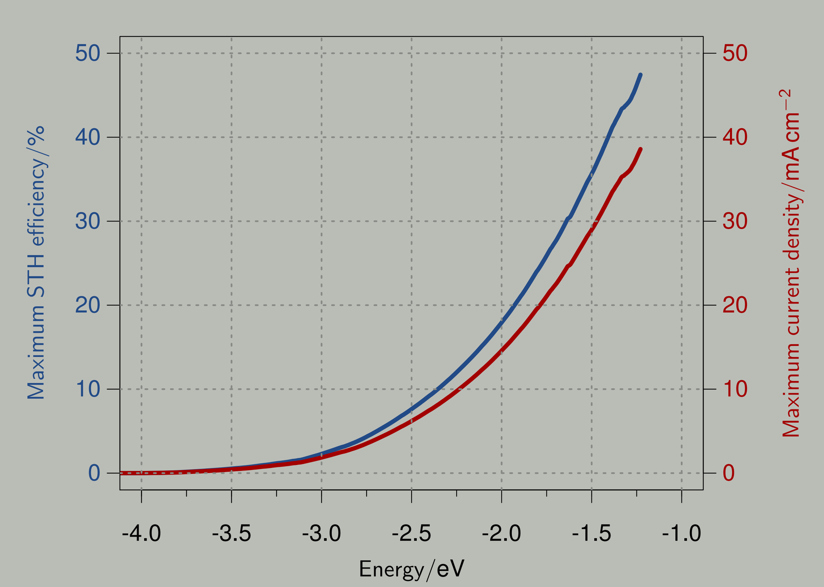
- the band gap must make efficient use of the solar spectrum,
- the band edge potentials must straddle the oxygen and hydrogen redox potentials,
- the material must possess long-term stability in aqueous electrolytes,
- the material's charge transfer kinetics must be favourable for water splitting.
- the material should preferably be non-toxic and low-cost.

Maximum STH efficiency obtainable under AM1.5G irradiation



Flux = photons per unit area

- Number of photons at the specified energy.
- Number of photons with energy more than or equal to the specified energy.



Maximum efficiencies

- Maximum solar-to-hydrogen efficiency.
- Maximum current density.
- Theoretical upper limit at -1.23 V.

- Assuming *all* incident photons (figure on the left) are absorbed and converted into electrons,
- we get the maximum efficiency plotted in the figure on the right.

Our project

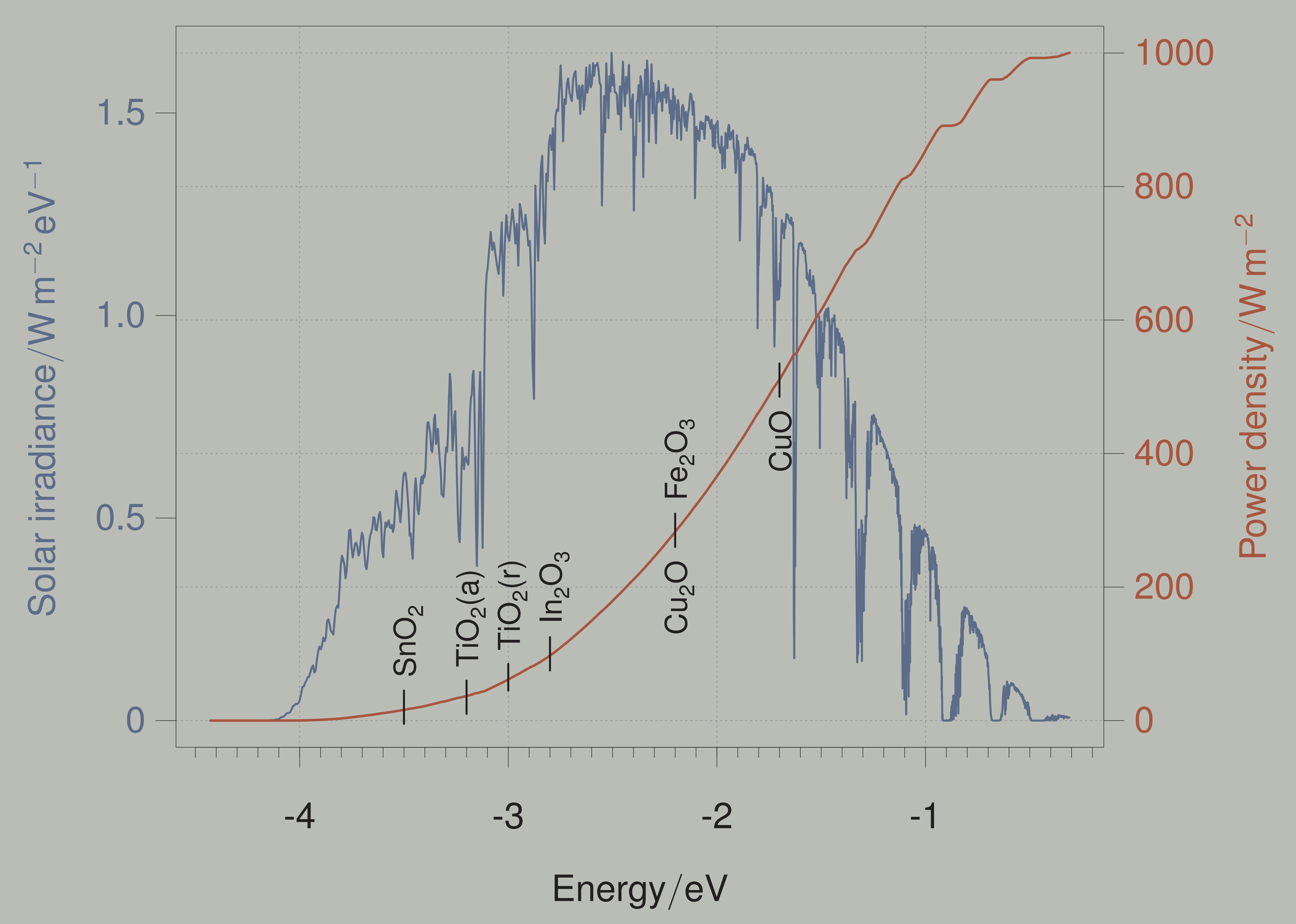
Our project will systematically study the electrodeposition of nanostructured and nanocomposite semiconducting oxides with regard to their photoelectrochemical performance.

Although most metal oxides show low efficiency, these cheap materials possess good corrosion resistance, and hence can exhibit stable performance for a long time.

The big picture

- The world's energy demand expected to double to 30 TW by 2050.
- The Earth is irradiated with 1×10^5 TW yearly of sunlight.
- To put things in scale, consider that natural photosynthesis uses 90 TW yearly.
- Producing 60 TW worth of electricity or fuel from sunlight is technically envisionable.
- Three major routes possible:
  - mimicking natural photosynthesis (cheap, but low efficiency),
  - using semiconductors to split water (average cost and efficiency),
  - using photovoltaics (expensive but efficient).
- This work falls under the second category.

The air mass 1.5 global tilt reference spectrum



Band gap engineering

In order to meet the design requirements of a good PEC material, the material's band gap must be controlled. This could be achieved by mixing two or more semiconductors in a controlled fashion, for example by coating nanorods of ZnO with CdS.

Controlling the structure of the semiconductor brings major advantages:

- a larger portion of the solar spectrum can be used for conversion,
- kinetics can be improved (by reducing unwanted recombination reactions),

which gives nanostructured semiconductors an overall performance gain with respect to bulk semiconductors.

Poster created with LaTeX and the beamerposter package. Poster template by Dreuw et al., RWTH Aachen University. Scatter plots created using R and pgfSweave. June 15, 2010.

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