Artificial Leafs Using Advanced Photoelectrosynthetic Cells – Physical boundary conditions and materials science challenges

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Surface Science

Introduction:

A long term transition to a completely renewable power mix employing wind and solar as power sources, requires efficient ways of storing the produced electrical energy, since their availability is extremely volatile. Therefore, one of the most promising alternatives is chemical energy storage. Here, surplus (renewable) energy is used to power the production of so called 'solar fuels', e.g. hydrogen and artificial methane.

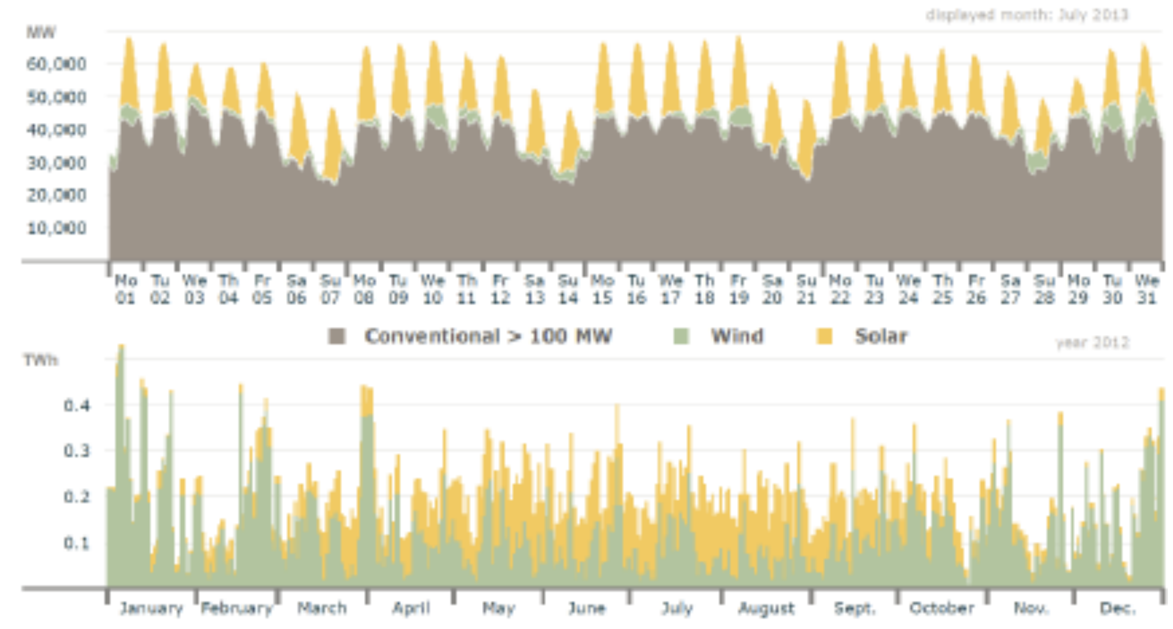
- New photoabsorbers, recyclability, self-healing
- New catalysts
- Layers with goos conductivity adaption to the electronic properties

Germany 2013

Annual Energy Consumption:	2670 TWh
2 week reserve:	103 TWh

For comparison, this equals:
164 billion car batteries
2050 car batteries per citizen

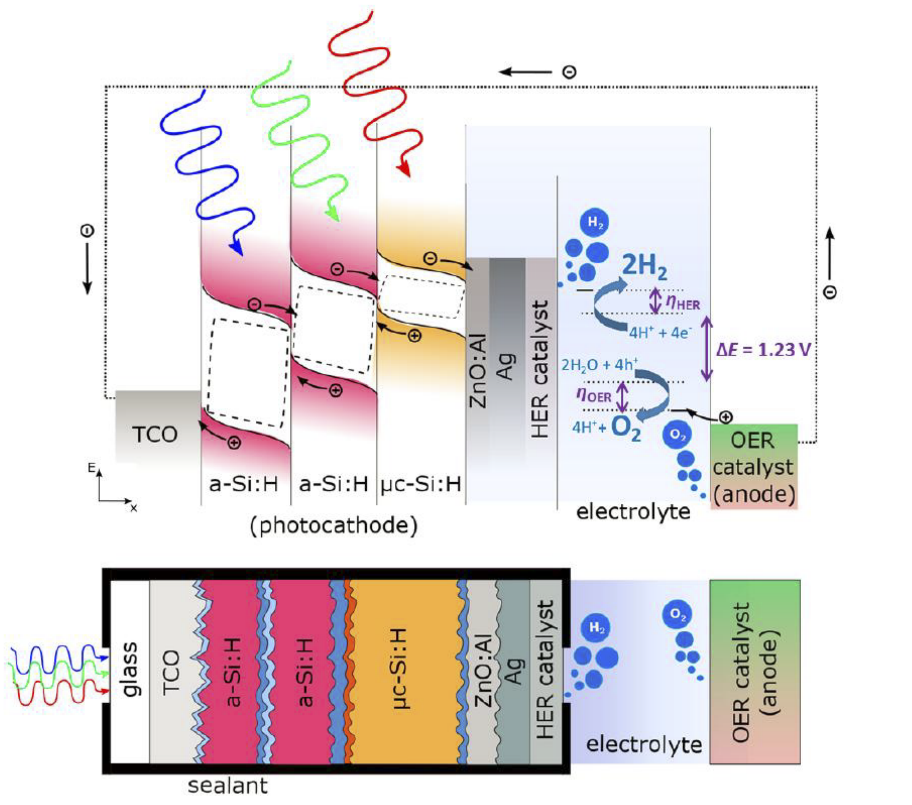
Daily electric energy production of wind and solar power plants



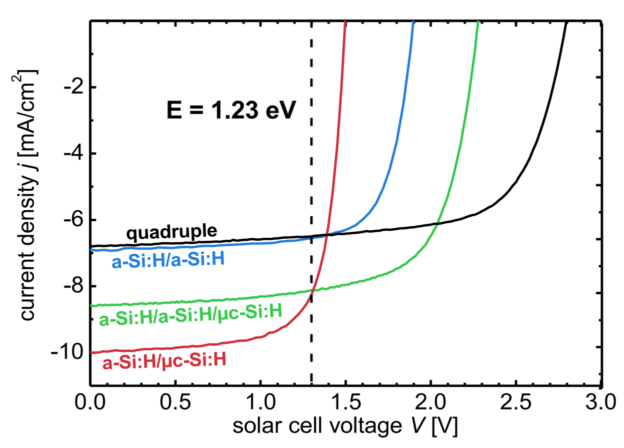
Bruno Burger, Electricity production from solar and wind in Germany in 2012, Fraunhofer Institute for Solar Energy Systems ISE

Photovoltaic Converter:

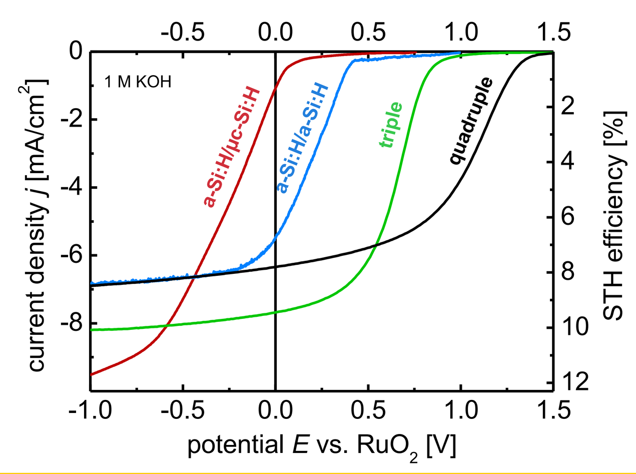
The basic idea of 'direct photoelectrochemical water splitting' is to combine photovoltaic energy conversion directly with electrolysis in one compact setup as shown below [1].



Solar cells: V_{OC} = 1.5 – 2.8 V

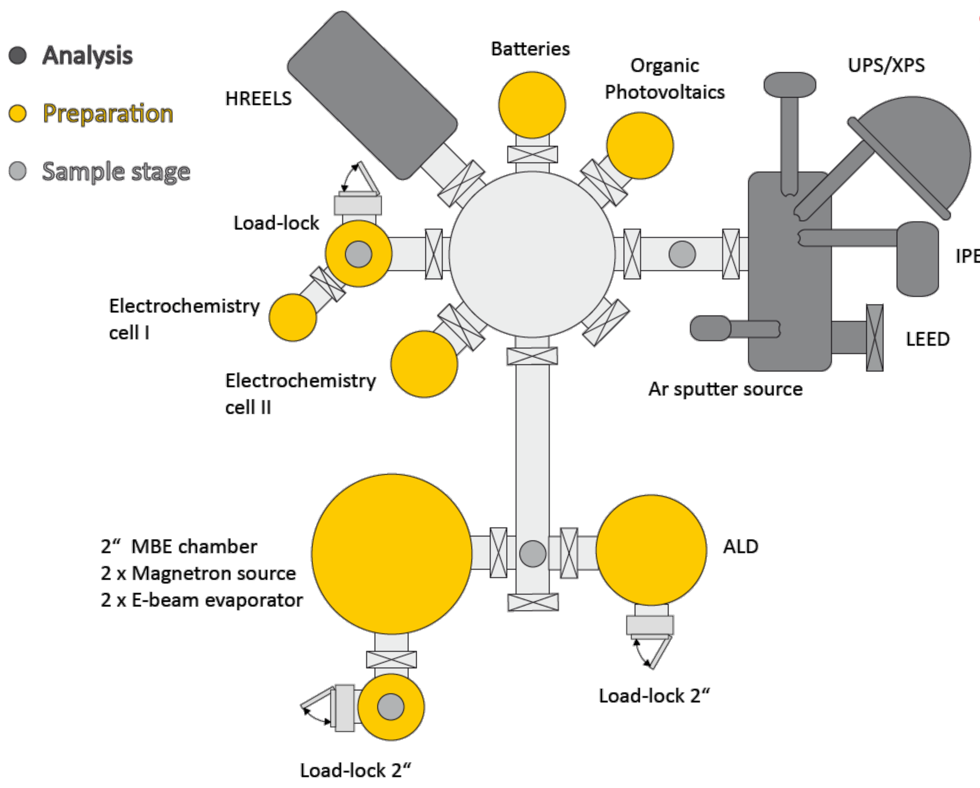


2-electrode integrated PV-EC device

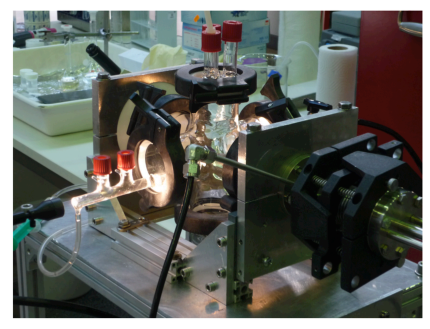


Preparation and characterization techniques:

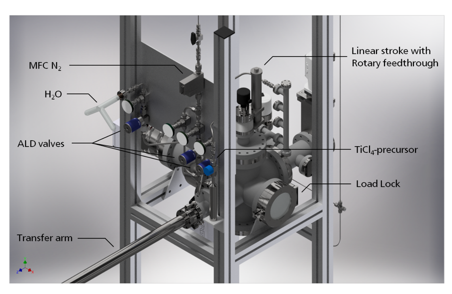
Daisy-Fun Lab in Darmstadt [2]:



(Photo)electrochemical characterization coupled with Surface Science methods



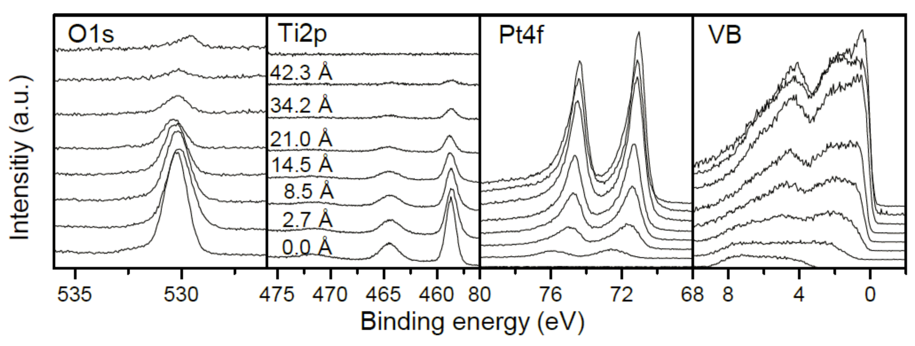
TiO_2 by atomic layer deposition

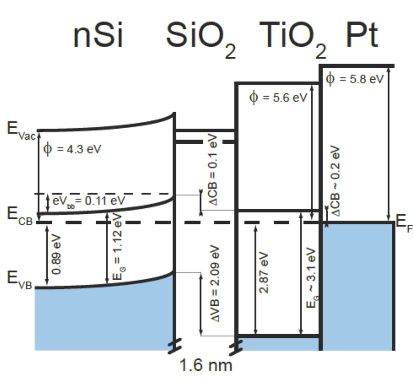


Vacuum based preparation by Sputtering, Atomic layer (ALD) and Chemical vapor deposition (CVD)
Analysis by Photoelectron Spectroscopy (XPS, UPS, IPES)and Electron Energy loss spectroscopy (EELS)

Interface optimization:

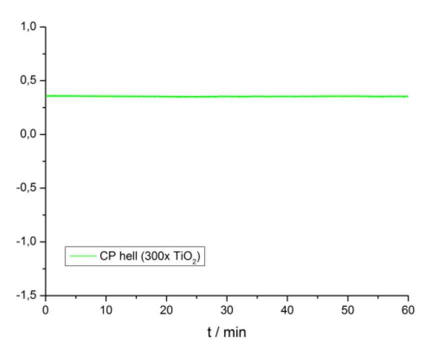
Solar cells are normally sealed in order to protect them from degradation. In order for them to survive prolonged contact with an electrolyte, good passivation layers, which do not impede the SC performance are needed. The passivation layers impact on cell performance is often determined by the interface properties[3].





In order to avoid efficiency losses during the charge transport, the layer structure has to be well adapted electronically.

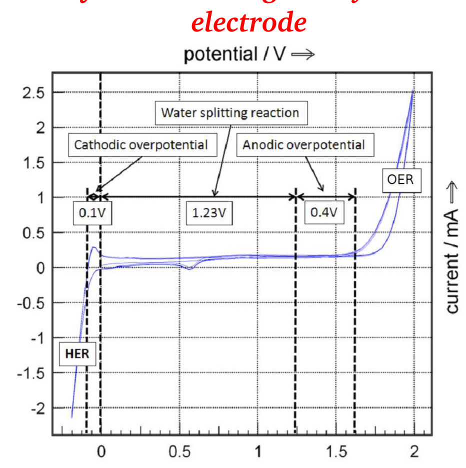
The interface layer has to stabilize the photoelectrode for prolonged periods of time in order to apply this technology in a competitive way [4].



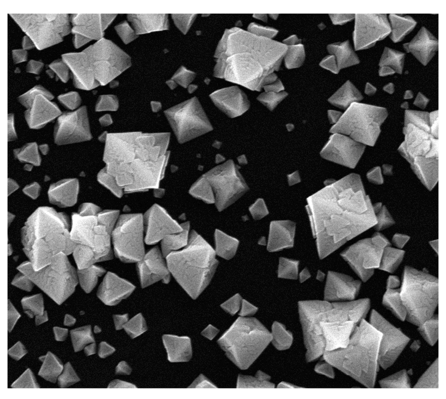
Catalysts for water splitting:

The current voltage behavior for electrolysis is defined by the 1.23 V thermodynamically necessary for the water splitting reaction, and the cathodic and anodic over-potentials, which are strongly dependent on the employed catalyst system[5,6|.

Cyclovoltammogram of a Pt-electrode

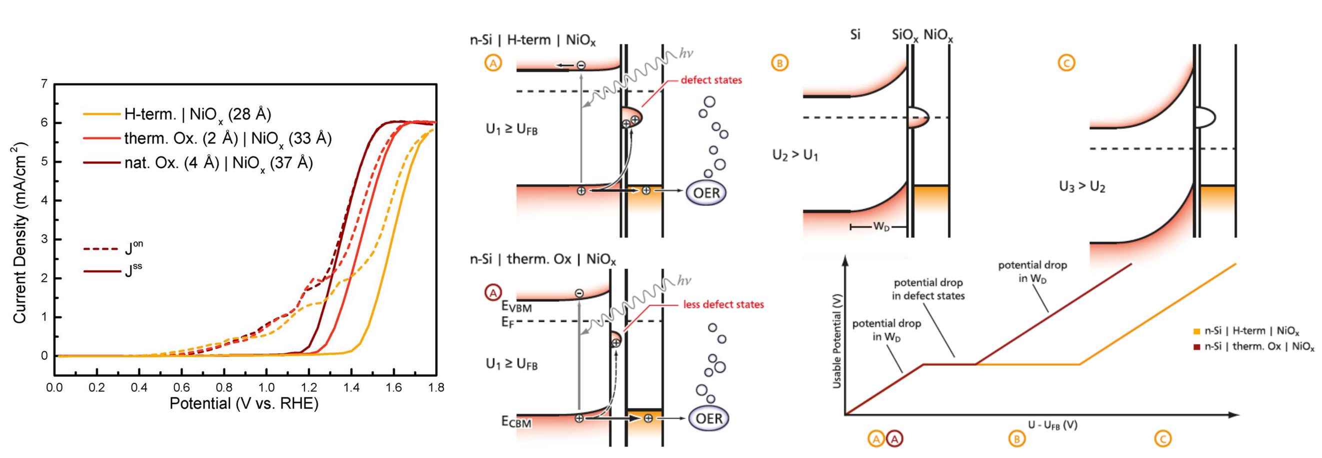


SEM of Pt nano-particles from CVD

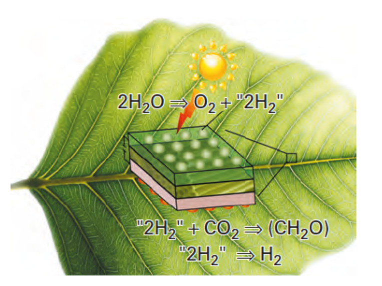


Nanoparticles: Larger surface area
Less material consumption

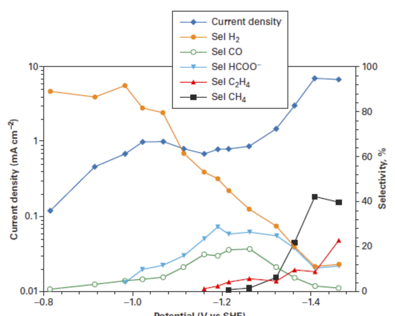
While Pt is clearly the best catalyst for the hydrogen evolution reaction (HER), research on cheap and abundant high performance hydrogen and oxygen evolution catalysts is still in progress. Nickel oxide composites for example are a very promising material system for the oxygen evolution reaction [7].

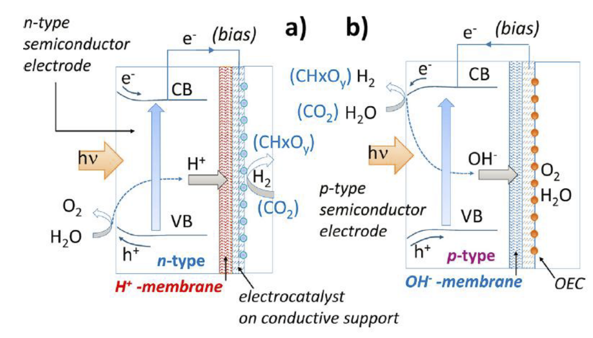


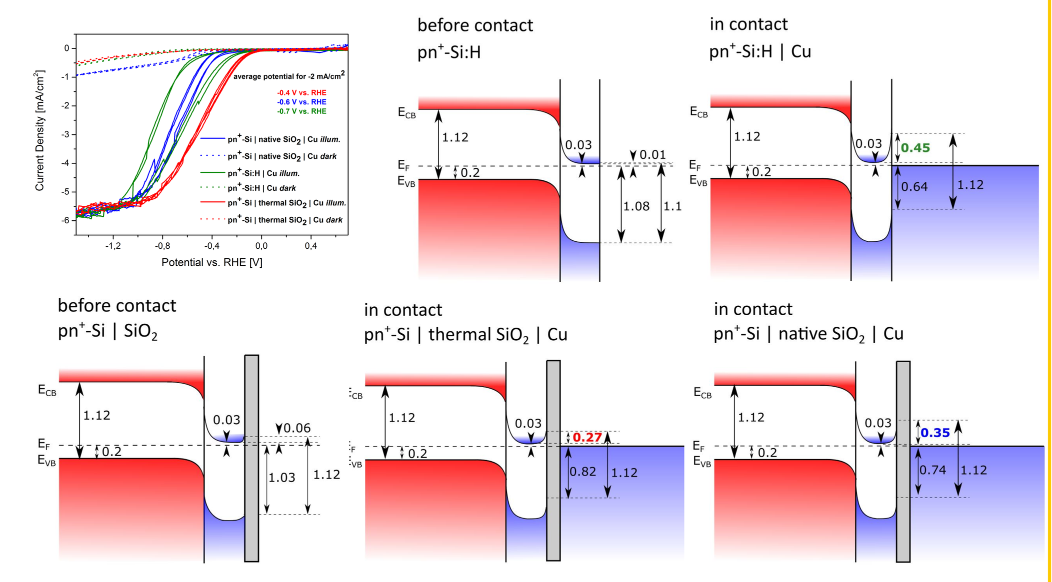
Catalysts for CO_2 reduction:



Hydrogen can be used and stored much like a fossil gas but has a very low volumetric energy density. For many applications it is desirable to have a higher volumetric energy density in the form of gases and/or liquids. Mimicking nature even closer in the form of an artificial leaf is the direct photoelectrochemical conversion of CO_2 to a carbohydrate compound [8, 9].







References:

[1] F. Urbain, V. Smirnov, J.-P. Becker, A. Lambertz, F. Yang, J. Ziegler, B. Kaiser, W. Jaegermann, U. Rau, and F. Finger, *Multijunction Si photocathodes with tunable photovoltages from 2.0 V to 2.8 V for light induced water splitting*, Energy & Environmental Science 9, 145 (2016).
[2] W. Jaegermann, B. Kaiser, J. Ziegler, and J. Klett, *Interface Engineering of Semiconductor Electrodes for Photoelectrochemical Water Splitting: Application of Surface Characterization with Photoelectron Spectroscopy* in *Photoelectrochemical Solar Fuel Production: From Basic Principles to Advanced Devices*, edited by S. Giménez and J. Bisquert (Springer International Publishing, Cham, 2016), p. 199.
[3] J. Klett, J. Ziegler, A. Radetinac, B. Kaiser, R. Schaefer, W. Jaegermann, F. Urbain, J.-P. Becker, V. Smirnov, and F. Finger, *Band engineering for efficient catalyst-substrate coupling for photoelectrochemical water splitting*, Physical Chemistry Chemical Physics 18, 10751 (2016).
[4] T. Cottre, *Präparation von Titandioxid-Schichten mittels Gasphasenabscheidung atomarer Lagen auf Tandem-Solarzellen*, Master thesis, TU Darmstadt (2016).
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