N - I - S - F - D

NORDIC INITIATIVE FOR
SOLAR FUEL DEVELOPMENT

DESIGN OF A WONDER

Dinko Chakarov
(PROJECT COORDINATOR)

Department of Applied Physics
Chalmers University of Technology
GÖTEBORG, SWEDEN

Sustainable Energy Systems 2050
NORDIC ENERGY RESEARCH PROGRAMME

Final seminar for Sustainable Energy Systems 2050
21–22 October, Oslo

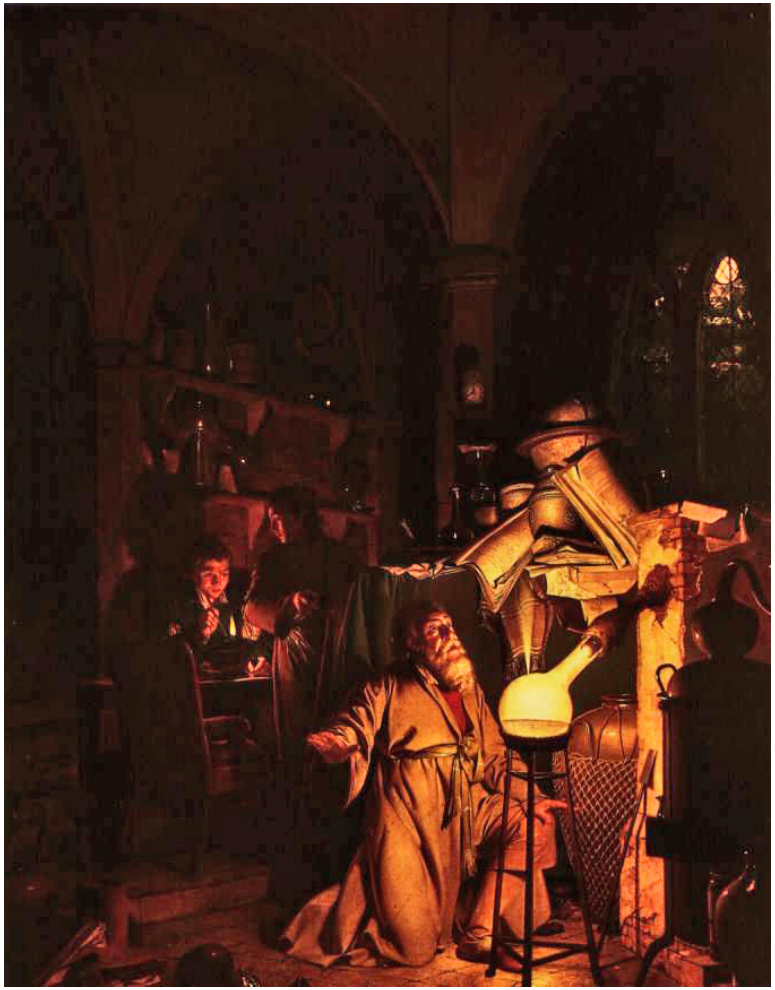
N - I - S - F - D

NORDIC INITIATIVE FOR SOLAR FUEL DEVELOPMENT

DESIGN OF A WONDER

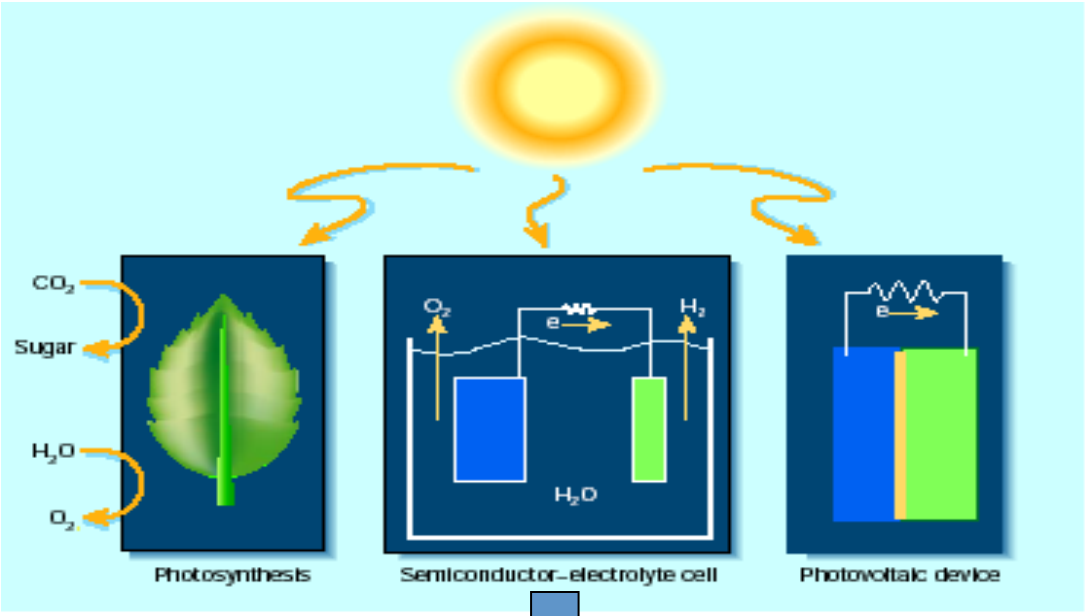
(Abstract of the project aims and selected results)

"One can convert with high efficiency and in a direct way CO_2 and water into renewable chemical fuels using only solar energy".



The Alchemist, in search of the philosopher's stone.
Painting by Joseph Wright of Derby, 1771.

SOLAR ENERGY *QUANTUM* CONVERSION SCHEMES AND THEIR EFFICIECY

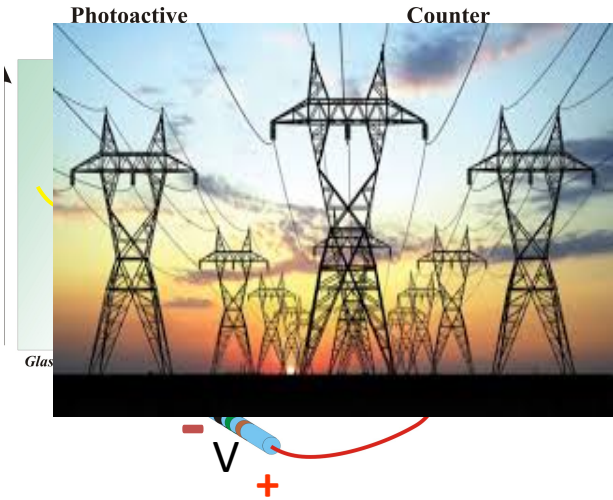


Efficiency = the ratio of the energy output (electrical or chemical) of a solar device to the incident energy in the form of sunlight

0.1 – 2 (6)%

4 – 12 (46)%

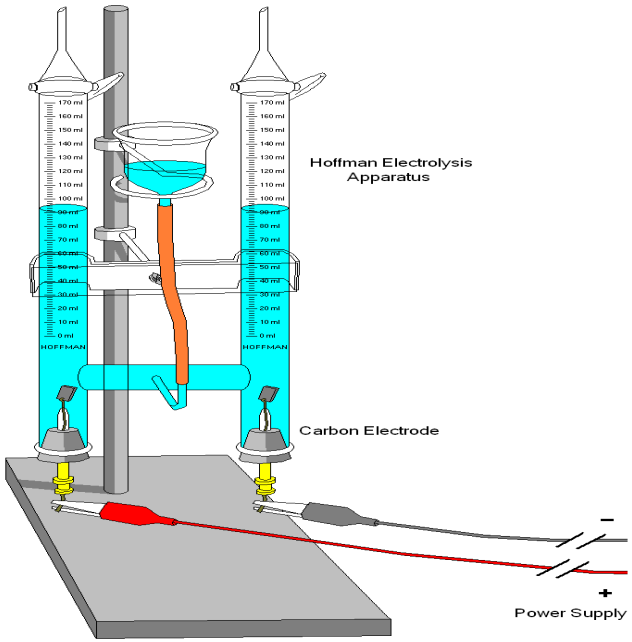
©N. S. Lewis, Nature **414** (2001) 589

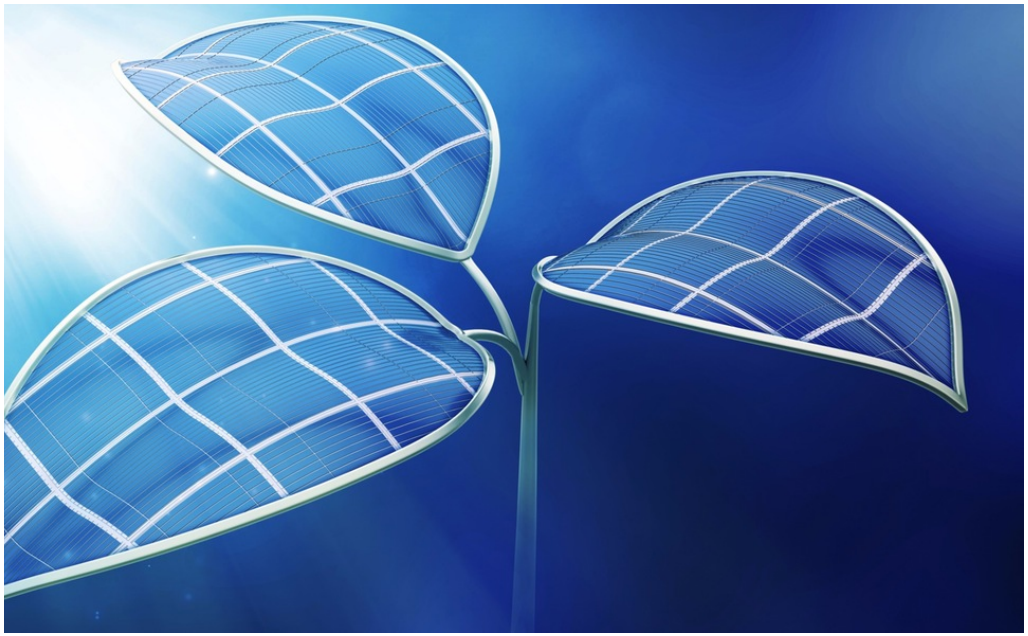


TEORETICALY SAME AS PV

COLIN JEFFREY

AUGUST 20, 2015





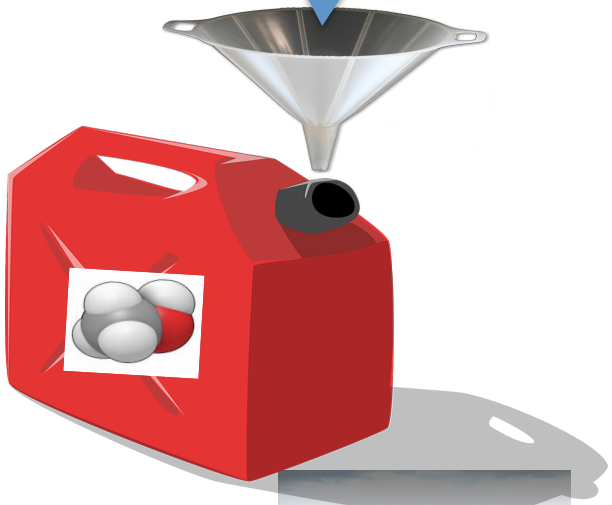
A new world-record → 22% conversion efficiency for solar-powered hydrogen production has been claimed by researchers from Australia's Monash University.
(Credit: Shutterstock)

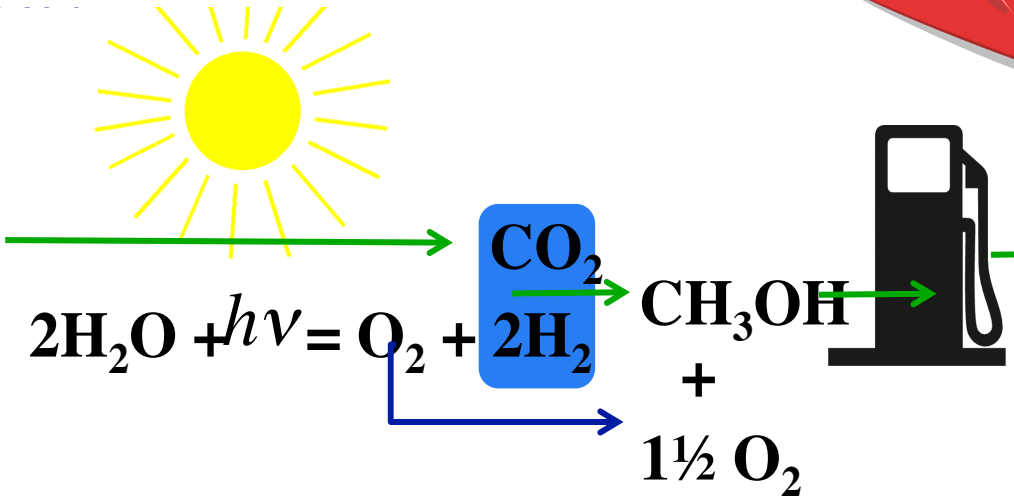
Reported working efficiencies of electrolyzers are in the range 60-75% for alkaline and 65–90% for PEM.
[E4tech Sàrl with Element Energy Ltd, Feb. 2014 - Development of water electrolysis in the European Union].

What we do and why it is a wonder?

Because it solves number of problems:

- Storage
- Efficiency
- Emissions
- Supply
- …





Main objectives → to design and develop a system that captures solar light and generates renewable chemical fuels from CO_2 and water.

The general reaction producing fuels* from sunlight, water and CO_2 follows:

$2H_2O + xhv \rightarrow O_2 + 4H^+ + 4\ e^-$
$CO_2 + 8H^+ + 8e^- \rightarrow CH_4 + 2H_2O$
$CO_2 + 6H^+ + 6e^- \rightarrow CH_3OH + H_2O$

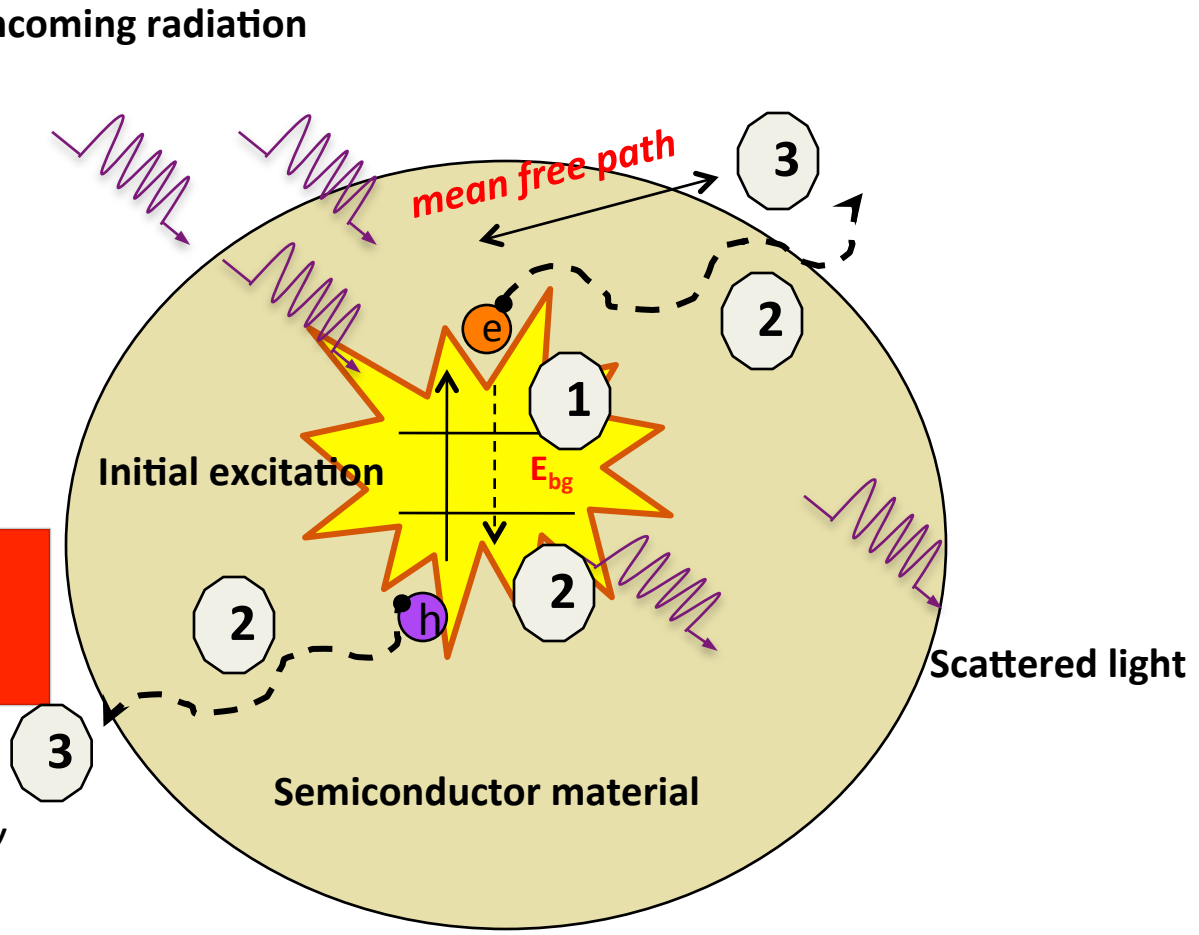
- the elements of these routes can be combined into ***ONE*** scheme for catalytic conversion of H_2O and CO_2 to fuels.
- significant advantage is the possibility to have all these complex transformations ***happening at the same photoelectrode*** (cathode).
- the three components of energy transformation: light harvesting, charge carrier separation and catalytic transformation ***can be optimized using nano-structured materials*.**

THE ELEMENTARY STEPS of photocatalysis

1. Light absorption and charge carriers generation
2. e-h pair separation, transport and recombination
3. Chemical work

$$\eta = \eta_A \times \eta_{CS} \times \eta_{CT} \times \eta_{CC}$$

η_A – *absorption efficiency*
η_{CS} – *charge separation efficiency*
η_{CT} – *charge transport efficiency*
η_{CC} – *charge collection efficiency*



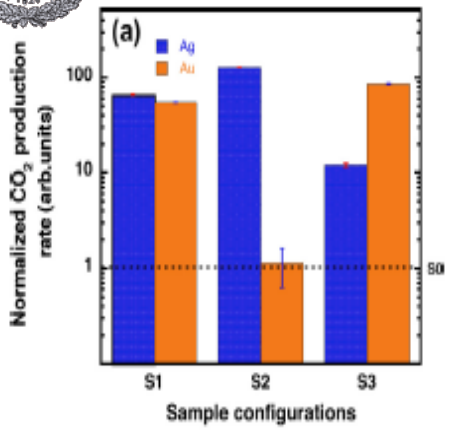
!!! The energy transfer is mediated* by charge carriers !!!

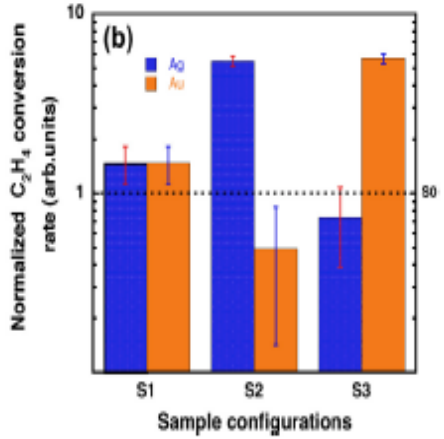
NISFD – Our MAIN SCIENTIFIC RESEARCH RESULTS:
(in several topics and areas → physics, chemistry, material-, nano- and engineering- science)

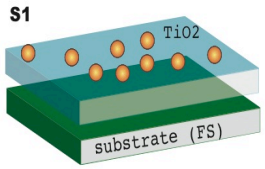
1. Band-gap engineering and sensitizing for optimal photon capture
2. Nanofab and nanostructures for promotion of photocat reaction(s)
3. Nanofab for optimal charge transport and suppressed recombination
4. Incorporation of metal co-catalysts for water splitting
5. Photo (electro) catalytic CO_2 conversion
6. Development of analytical and theoretical methods
7. Physical modeling and efficiency analysis

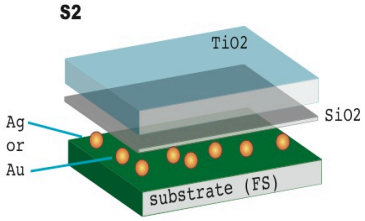
Specific RESULTS:

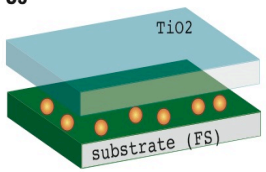
WP1 - Enhanced photon capture

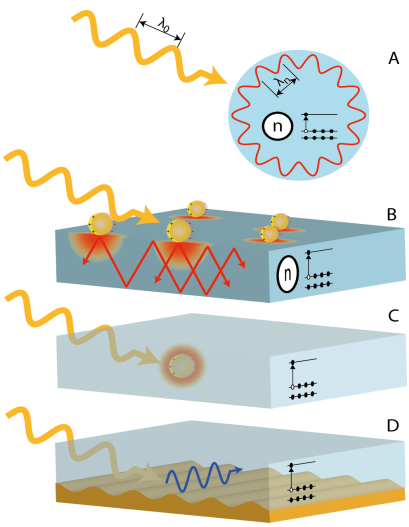




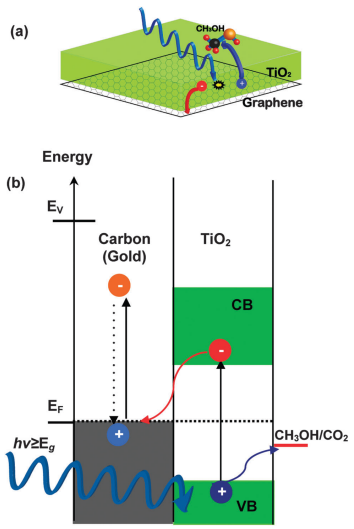




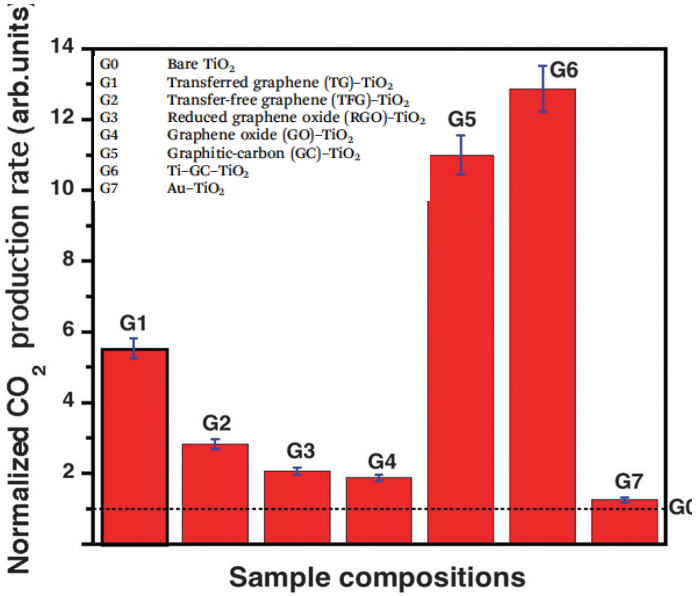




Plasmonic nanoparticles



Band-bending interfaces



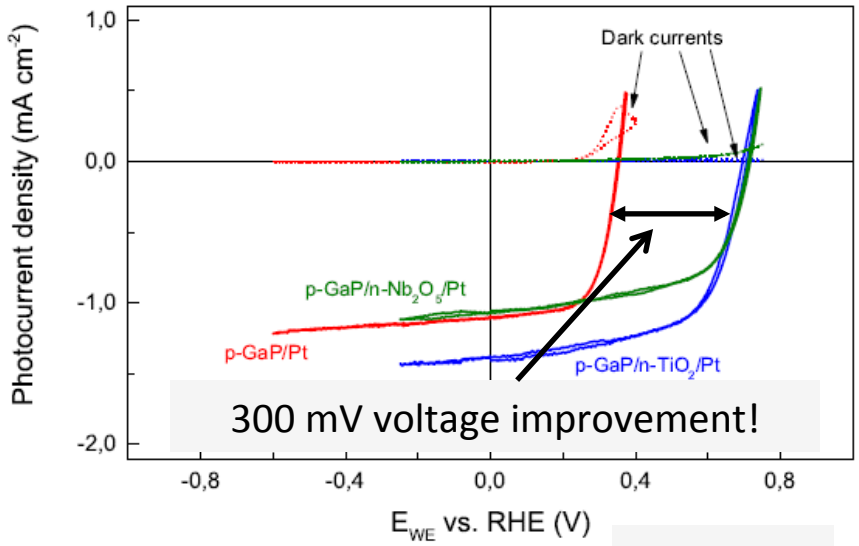
(a) Rate $CH_3OH \rightarrow CO_2$ production

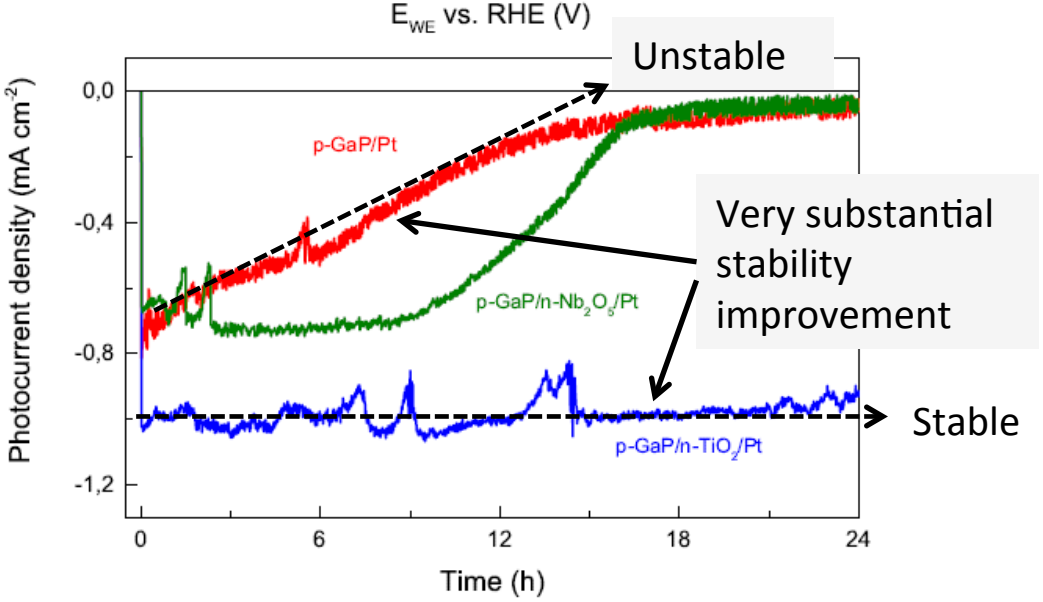
(b) Rate C_2H_4 conversion

Note: normalized to the activity of single TiO_2 films; logarithmic scale.

J. of Catalysis, **307**, 214 (2013)

Large bandgap photocathodes





- Main purpose
  - Identify cadidate materials for high-photovoltage photoelctrodes
  - High voltage are needed for ”difficult” reactions like CO_2 reduction and oxygen evolution
- Main results
  - GaP is a candidate (Eg = 2.25 eV)
  - GaP is unstable without protection
  - GaP gives lousy voltage on its own
  - GaP can be made very stable by protection with TiO2 overlayer
  - The photovoltage of GaP is much improved via a n-p heterojunction between the p-GaP and the protection layer
  - The protection layers found for GaP have general applicability for other materials

Main reference: Malizia, Seger, Chorkendorff & Vesborg, *Journal of Materials Chemistry A*, **2**, p. 6847-6853 (2014)

Specific RESULTS:

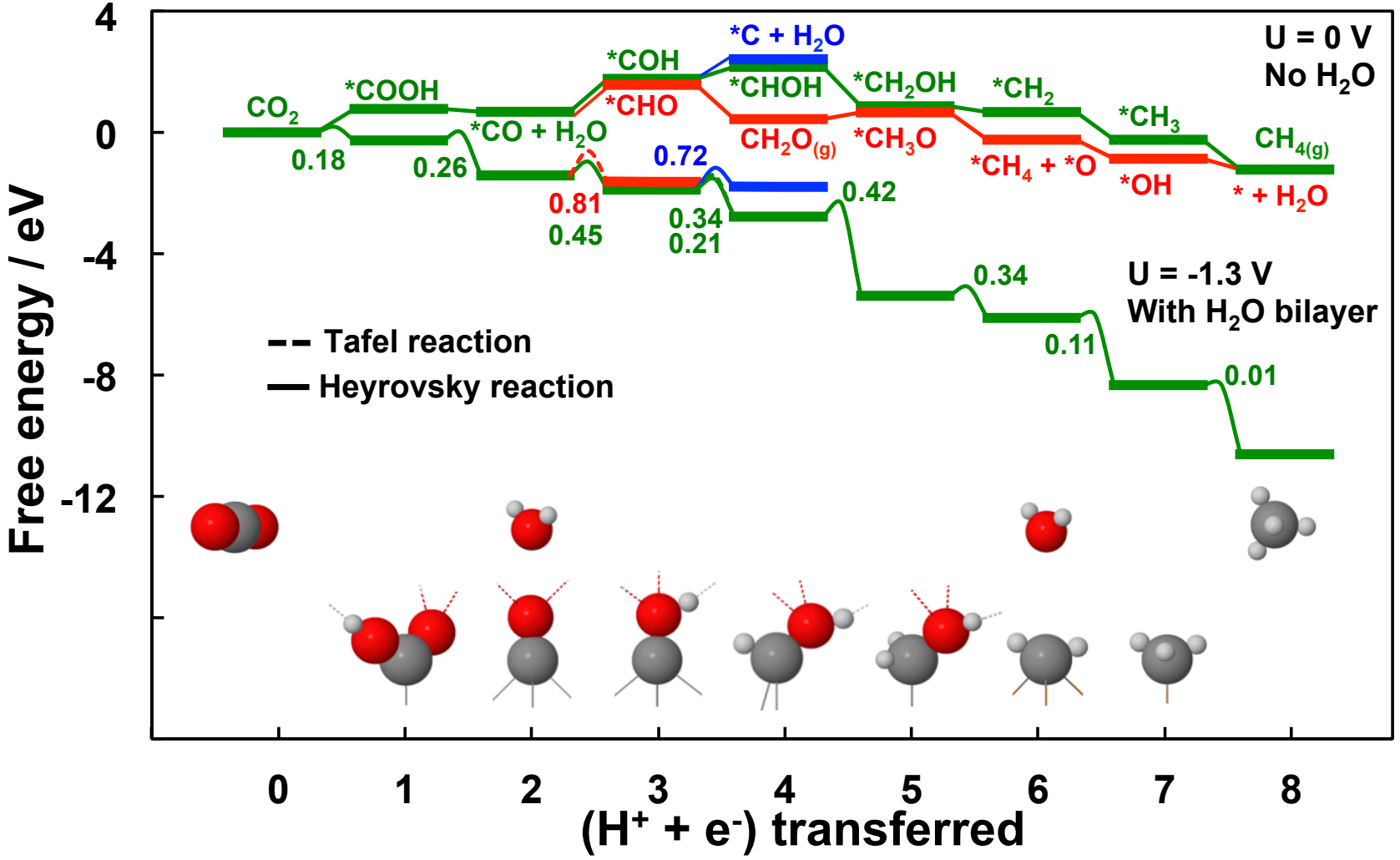
WP3 Cell for photoelectrochemical reduction of CO_2

Specific RESULTS:

WP4 Calculating of material properties and modeling of system efficiency and costs.

Optimal reaction mechanism

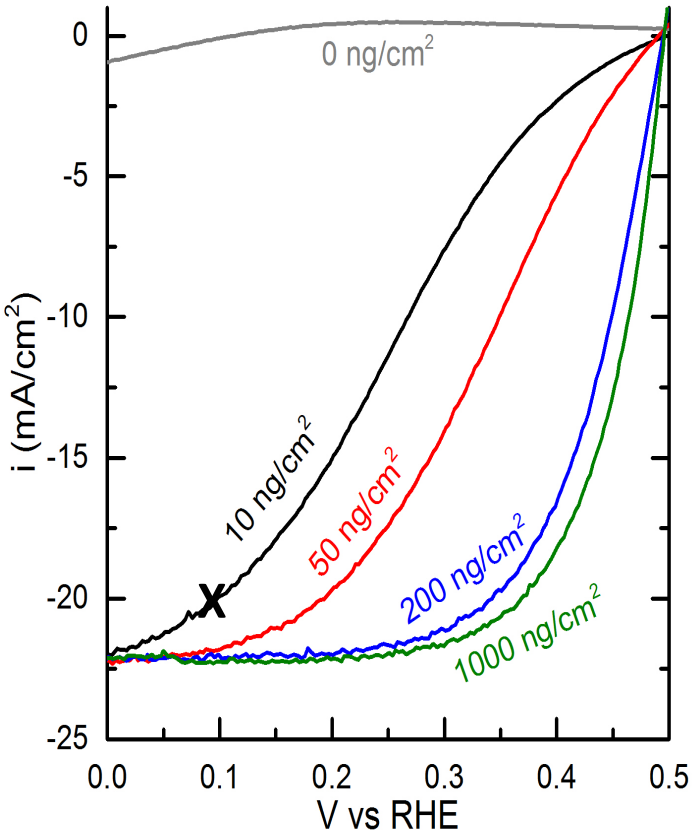
Calculated free energy for the optimal mechanism of CO_2 electroreduction at a Cu(111) surface and electron chemical potential corresponding to -1.3 V (lower green curve)



Hussain, J., Jónsson, H., Skúlason, E. "The Mechanism of CO_2 Electroreduction to Methane " (submitted)

Pt nanoparticles could be feasible as HER catalyst

- **1000 ng/cm^2 as good as much higher loadings, 200 ng/cm^2 almost as good.**
- **At 10 mA/cm^2 & 50 mV overpotential, only 100 ng/cm^2 needed ⇒ ~54 tons Pt/1 TW$_{avg}$ H_2 production capacity**
  - Less than e.g. the annual consumption of jewelry industry



Specific RESULTS:

Contacts with industry

- NorECs AS – Photoelectrodes and Solid-state photoelectrochemical H2 generation with gaseous reactants;
- Carbon Recycling International, is expanding its methanol production (and influence);
- Stena Line operates the first methanol driven ferryboat.

The Stena Germanica, which was inaugurated on the 27th March, is the first ferry to use methanol as its main fuel.

https://www.youtube.com/watch?v=oP4U0XDgJF4

N-I-S-F-D - *"Nordic Initiative for Solar Fuel Development"*

Göteborg København Oslo Reykjavík Helsinki

NORWAY

Prof. A Kuznetsov

Centre for Material Sci. and Nanotechnology, Oslo

Prof. T Norby

Department of Chemistry, U. of Oslo, also CEO for NorECs AS

ICELAND

Prof. H Jónsson

Icelandic Center of Computational Science, Sci. Institute of U. of Iceland

Prof. O Ingólfsson

Director of Research, Carbon Recycling Int.

SWEDEN

Prof. D Chakarov

Chalmers University of Technology, Dept. of Applied Physics

FINLAND

Prof. P Lund

Aalto U., Dept. of Applied Physics/Advanced Energy Systems

DENMARK

Prof. I Chorkendorff

Director, Center for Individual Nanoparticle Functionality (CINF), DTU

THE TEAM:

PhDs

* **Erno Kemppainen**, M.Sc., Aalto U., Finland ---
* **Raja Sellappan**, M., Sc. ,Chalmers, Sweden, 2013
* **Mauro Malizia**, M.Sc., DTU, Denmark, 2014
* **Marieke Trunk**, M.Sc., Oslo U., Norway, May 2013
* **Kingsley Iwu**, M.Sc., Oslo U., Norway, Nov. 2013
* **Hildur Gudmonsdottir**, M.Sc., Island U. Island, 2014
* **Javed Hussein**, M.Sc., Island U. Island, ---
* **Simon Kluepfel,** M.Sc. Reykjavik, 2012
* **Elias Bjarnason,** M.Sc. Reykjavik, ---

PostDocs

- **Egill Skulason,** PhD, University of Island, Island
- **Fernando Gonzales-Posada**, PhD, Chalmers, Sweden
- **Björn Wickman**, PhD, DTU, Denmark
- **Brian Seger,** PhD, DTU, Denmark
- **Kjartan Wikfeldt,** PhD, University of Island, Island

Others

* **Peter C. K. Vesborg,** Ass. Prof., DTU, Danmark
* **Janne Halme,** Docent, Aalto U., Finland
* **Augustinas Geleskas,** Senior scientist, Oslo U. Norway
* **Elina Nissilä,** M.Sc., Aalto, Finland
* **Bert Vanpoucke,** M. Sc., Chalmers, Sweden
* **Martin Bjerling,** M. Sc., Chalmers, Sweden